



Dr.BGR
Publications

International Conference on Advanced Materials and Modern Technologies (ICAMMT)



Guest Editors

D.Sheeba
Rev.Sr.Dr.P. Arockia Michael Mercy
S.Jeswil

2026



Dr.BGR
Publications

International Conference on Advanced Materials and Modern Technologies (ICAMMT)

Guest Editors

D.Sheeba

Head & Assistant Professor

Department of Physics

Madonna Arts and Science College for Women

Virahanur | Madurai

Rev.Sr.Dr.P. Arockia Michael Mercy

Vice Principal and Assistant Professor

Department of Physics

Madonna Arts and Science College for Women

Virahanur | Madurai

S.Jeswil

Assistant Professor

Department of Physics

Madonna Arts and Science College for Women

Virahanur | Madurai

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Dr. Kuppan Gokulan
The Division of Microbiology at NCTR
USA

It gives me immense pleasure and a profound sense of privilege to present the Preface to the **International Conference on “ADVANCED MATERIALS AND MODERN TECHNOLOGIES–2026” (ICAMMT–2026)**. This international academic gathering is conceived as a vibrant platform for bringing together distinguished academicians, scientists, researchers, industry professionals, research scholars and students to share knowledge, exchange innovative ideas and explore emerging frontiers in materials science and modern technological development. It provides a meaningful forum for discussing these emerging frontiers. The conference encourages participants to move beyond conventional approaches and to explore innovative solutions that combine scientific excellence with societal relevance. Particular emphasis is placed on research that contributes to sustainability, energy efficiency, environmental protection, technological advancement, and the development of affordable and accessible solutions for the future.

This Proceedings Volume is particularly significant because it brings together **both the abstracts of research contributions and selected research papers presented at the conference**. The abstracts provide a concise overview of the research objectives, methodologies, major findings, and potential applications, while the presented research papers offer deeper scientific insights into the investigations undertaken by the contributors. Together, they provide a broader picture of current research activities and emerging directions in advanced materials and modern technologies.

We gratefully acknowledge the valuable contributions of all **authors, researchers, resource persons, invited speakers, reviewers, session chairs, organizing committee members, faculty members, research scholars, students, and supporting staff** whose collective efforts have made this conference and its proceedings possible. Our sincere appreciation is extended to the experts and academicians who have generously shared their knowledge and experience with the participants.

We also place on record our heartfelt gratitude to the institutional leadership and management for providing encouragement, academic support, and the necessary facilities for conducting this international academic event. Their commitment to promoting higher education, research, innovation, and knowledge dissemination has been a significant source of inspiration. The proceedings before you are therefore more than a compilation of scientific papers and abstracts. They represent a **collective expression of curiosity, creativity, collaboration, and commitment to scientific advancement**. Each paper contributes a small but meaningful step towards understanding the possibilities of advanced materials and modern technologies. We hope that these contributions will encourage researchers to develop new ideas, establish interdisciplinary collaborations, and transform promising concepts into practical and sustainable solutions.

With warm Regards

KUPPAN GOKULAN -5
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Date: 2025.08.27 10:07:01 -0700

Dr. Kuppan Gokulan
The Division of Microbiology at NCTR
USA

Rev. Dr. M.ANBARASU, S.J.
M.A., Ph.D.,
Principal



ARUL ANANDAR COLLEGE
(AUTONOMOUS)
Karumathur - 625 514.
Madurai Dt. Tamil Nadu.



Rev. Dr. Anbarasu M. S.J.
Principal
Arul Anandar College

It is my great pleasure to share the proceedings of the International Conference on 'Advanced Materials and Modern Technology'. This conference brings together researchers, academicians, scientists, engineers, industry experts, and students to share their latest research findings, innovative ideas, and technological developments in the fields of advanced materials and modern technology. The rapid advancement of materials science and emerging technologies has created new opportunities for innovation and sustainable development. Advanced materials, nanotechnology, artificial intelligence, smart manufacturing, robotics, energy technologies, and digital transformation are contributing significantly to progress in diverse areas such as healthcare, energy, electronics, aerospace, manufacturing, and environmental protection.

The conference aims to encourage interdisciplinary interaction and foster meaningful collaborations between academia, research institutions, and industry. It provides an opportunity to discuss recent developments, explore innovative solutions, identify emerging research directions, and translate scientific discoveries into practical applications. The exchange of ideas among participants from diverse disciplines is expected to contribute significantly to the advancement of knowledge and the development of technologies that are efficient, sustainable, and socially beneficial.

I sincerely appreciate the valuable contributions of all authors, reviewers, keynote speakers, invited speakers, session chairs, organizing committee members, and participants who have made this conference possible. Their dedication and support have contributed greatly to the success of this event. I am confident that the ideas, discussions, and collaborations emerging from this conference will inspire further research and innovation. I hope this conference will be an enriching experience for all participants and contribute to the advancement of knowledge and technology for a sustainable future.

With Best Wishes for a Successful and Memorable International Conference!

With warm Regards

Rev. Dr. Anbarasu M. S.J.

**Mobile: 78451 15901, Website: www.aactni.edu.in
Email: manbusj@gmail.com, manbusj@aactni.edu.in, principal@aactni.edu.in**



ST. XAVIER'S COLLEGE

(Autonomous)

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Website : www.stxavierstn.edu.in

Rev. Fr. Dr. GODWIN RUFUS, S.J., M.A., M.Phil., Ph.D.

Principal



PREFACE

We live in an age of extraordinary scientific and technological transformation. Advanced materials, nanotechnology, quantum science, renewable energy, artificial intelligence and smart technologies are reshaping the frontiers of knowledge and redefining the possibilities of human development. In this rapidly changing context, higher education must move beyond the transmission of knowledge towards the formation of reflective, responsible and lifelong learners.

It is in this spirit that **ICAMMT-2026: International Conference on Advanced Materials and Modern Technologies**, organised by the Department of Physics, Madonna Arts & Science College for Women, brings together academicians, researchers, scientists, students and industry professionals to exchange ideas, foster interdisciplinary collaboration and explore innovative pathways towards a sustainable future.

The conference is particularly meaningful when viewed through the complementary lenses of **Ignatian Pedagogy, Andragogy and Heutagogy**. Ignatian Pedagogy, through **Context-Experience-Reflection-Action-Evaluation**, reminds us that knowledge must be connected with reality, ethical discernment and service to humanity. **Andragogy** recognises the value of experience, relevance and active participation in adult learning, while **Heutagogy** promotes **self-determined, autonomous and lifelong learning**. Together, these approaches encourage learners not merely to acquire knowledge, but to question, create, reflect, adapt and take responsibility for its application.

The theme of advanced materials and modern technologies therefore invites us to consider not only **what technology can achieve**, but also **what it ought to achieve for humanity and the planet**. Scientific innovation must be guided by wisdom, ethical responsibility and a commitment to the common good.

The four guiding words of this conference—**Innovate, Collaborate, Inspire and Transform**—capture this vision. We innovate by imagining new possibilities; collaborate by crossing disciplinary boundaries; inspire by turning knowledge into hope; and transform when research becomes meaningful action for society.

May **ICAMMT-2026** become a space where knowledge leads to reflection, reflection to responsible action, and action to transformation. May it inspire us to *read the signs of the times*, discern the needs of our world and place science and technology at the service of humanity and creation.

Innovate. Collaborate. Inspire. Transform.

"Finding God in all things and all things in God" - St. Ignatius of Loyola


PRINCIPAL
ST. XAVIER'S COLLEGE
(Autonomous)
PALAYAMKOTTAI - 627 002

Tel: (Off) 0462 - 2560744 **Mobile:** (Off) 9361898870 **E-mail:** sxcprincipal@stxavierstn.edu.in / sxcprin@gmail.com



முனைவர் செ. பூமிநாதசெல்லராஜன்., Ph.D.,

Dr. S. Boominathasellarajan, M.Sc., M.Phil., M.Tech., Ph.D.,

Principal Project Scientist,

HPHT Diamond Factory,
India Centre for Lab Grown Diamond (InCent-LGD),
Indian Institute of Technology Madras (IITM),
Chennai - 600036
Tamil Nadu, India.



Director,

Munnarivan Technologies Private
Limited CIN: U62099TN2023PTC165176
Email: munnarivan.tech@gmail.com
Chennai - 600042
Tamil Nadu, India.

The International Conference on Advanced Materials and Modern Technologies (ICAMMT-2026) organized by the Department of Physics at Madonna Arts & Science College for Women on September 3, 2026. I am happy to share a few words in this occasion.

There is intense competition when comparing degrees in science and engineering. Students that enroll in science programs have the good fortune to get a deeper understanding of science and cultivate an appreciation for life. Attending or organizing an international conference is one of the best methods for students to engage with technology and research. In this context, this conference upholds the fundamental scientific disciplines while covering transdisciplinary themes in every aspect of modern engineering fields. Without an understanding of science, technological innovation and breakthroughs are impossible to achieve.

The publication of this proceedings volume marks a significant milestone in the contemporary discourse surrounding material sciences and engineering. The critical intersection of fundamental laboratory physics and scalable technological applications is emphasized by this collection. The editorial matrix of these proceedings successfully categorizes diverse technical inquiries into distinct, impactful trajectories:

- Fundamental Materials & Synthesis: Critical assessments of nanomaterials, thin films, functional ceramics, and semiconductor quantum dots.
- Green Technology & Infrastructure: Cutting-edge research targeting photovoltaics, eco-friendly manufacturing, and sustainable waste management matrices.
- Digital Integration & Automation: Insights into how Artificial Intelligence, Machine Learning, and the Internet of Things (IoT) are reshaping advanced processing systems.

There is no doubt that many students who benefit from this conference may use it as a springboard to pursue further education in order to broaden and enhance their knowledge.

From an external viewpoint, the execution of ICAMMT-2026 deserves high praise. Under the visionary stewardship of Chief Patron Rev. Dr. Mary Delphine, Patron Rev. Dr. Thiraviya Regina Rajam, and the tireless coordination of the Conveners, Prof. D. Sheeba and Rev. Dr. Arockia Michael Mercy, the institution has provided a vital global stage. By bringing together prominent international voices from the United States and Italy alongside distinguished national scholars, the organizers have fostered an environment of high-level intellectual exchange.

I hope this event is a huge success and goes on forever to inspire more young people to pursue science and technology through enrichment activities and information sharing.

(S. Boominathasellarajan)



Dr.Nimma Elizabeth R
Vice Principal
Head and Associate Professor
Department of Physics
Lady Doak College
Madurai

I am delighted to share a few words on the occasion of the International Conference on Advanced Materials and Modern Technologies (ICAMMT-2026), organized by the Department of Physics, Madonna Arts & Science College for Women, Virahanur, Madurai. The conference brings together research and technological developments across disciplines, with a particular focus on areas that are shaping the future of science and its applications. Scientific progress today rarely happens within the boundaries of a single discipline. Some of the most interesting developments emerge when ideas from physics, materials science, engineering, computing and related fields come together. ICAMMT-2026 provides such an opportunity, bringing scientists, academicians, researchers, industry professionals, research scholars and students onto a common platform to share their work, exchange perspectives and learn from one another.

The conference covers a wide range of contemporary research, broadly spanning **advanced and functional materials; nanoscale and semiconductor technologies; energy, environmental and sustainable materials; smart, biomedical, polymer and composite systems; materials processing and characterization; and emerging computational, digital and intelligent technologies**. This wider scope is particularly relevant at a time when advances in materials research are increasingly connected with developments in artificial intelligence, automation, advanced manufacturing and digital technologies.

The papers presented in this conference reflect this interdisciplinary character. They also remind us that research becomes more meaningful when fundamental scientific understanding is connected with real-world needs and applications. Conferences such as ICAMMT-2026 are valuable not only for presenting completed research, but also for the conversations they begin, the questions they raise and the possibilities for future collaborative work.

I hope these proceedings of the conference will be useful to students, research scholars, teachers, scientists and professionals, and that some of the ideas presented here will lead to further enquiry and meaningful research.

I sincerely appreciate the invited speakers, authors and reviewers for their academic contributions. I also congratulate the organizing committee, faculty members, research scholars, students and supporting staff whose time and effort have gone into organizing the conference and bringing out these proceedings.

I wish ICAMMT-2026 every success and hope that the discussions and research shared through this conference will encourage new ideas, stronger academic connections and research that contributes meaningfully to science and society.

With Regards

Nimma Elizabeth R

Nimma Elizabeth R



MADONNA

ARTS AND SCIENCE COLLEGE FOR WOMEN

Affiliated to Madurai Kamaraj University
Rameswaram High Road, Virahanur, Madurai – 625 009.



Rev.Dr.S.Thiraviya Regina Rajam CIC
M.C.A., Ph.D.
PRINCIPAL

Phone : 9363769975
E.Mail : madonnacollegemdu@gmail.com
Website : <http://madonnacollege.org>



Principal's Message

“Somewhere, something incredible is waiting to be known.” — Carl Sagan

It gives me immense pleasure to extend my warm greetings to all scientists, academicians, researchers, industry experts, faculty members, scholars, and students participating in this International Conference on “Advanced Materials and Modern Technologies.”

We are living in an era of remarkable scientific progress, where advanced materials, nanotechnology, smart materials, semiconductors, energy storage, and sustainable technologies are transforming science and society. This conference provides a valuable platform to share knowledge, present innovative research, and build meaningful academic collaborations. At Madonna Arts and Science College for Women, we believe that education should inspire curiosity, scientific thinking, creativity, and innovation. I am delighted that our students and faculty have this opportunity to interact with eminent researchers and explore the latest developments in advanced materials and modern technologies.

I sincerely appreciate the Department of Physics and the organizing committee for their dedicated efforts. May this conference inspire young researchers, promote collaboration, and contribute to scientific advancement and a sustainable future. I wish the conference great success and all participants a fruitful and enriching experience.

“The future of technology begins with the materials we create today”.

Rev.Dr.S.Thiraviya Regina Rajam

Principal



Rev.Sr.Dr.P.Arockia Michael Mercy CIC

M.Sc., PGTRB., Ph.D

Vice Principal

Madonna Arts & Science College for Women,

Virahanur, Madurai-625009

It is with profound gratitude to God Almighty, whose divine wisdom, grace, and providence inspire every pursuit of knowledge, that I am deeply honored to present this Proceedings Volume of the International Conference on “**ADVANCED MATERIALS AND MODERN TECHNOLOGIES–2026**” (**ICAMMT–2026**). This publication is a scholarly compilation of research abstracts and presented research papers, representing the intellectual contributions, scientific efforts, innovative ideas, and research aspirations of academicians, scientists, research scholars, faculty members, and students. Science is a precious gift through which humanity seeks to understand the wonders of creation and transform knowledge into meaningful solutions for the betterment of society. Every scientific discovery, technological advancement, and innovative material is, in its own way, an expression of the human capacity to explore, question, create, and serve. In this spirit, **ICAMMT–2026** has been conceived as a platform where scientific excellence is harmoniously connected with social responsibility, ethical values, sustainability, and the service of humanity.

This Proceedings Volume carries special significance as it brings together both the abstracts and the research papers presented during the conference. The **Abstracts** offer concise glimpses into the objectives, methodologies, findings, and applications of the research, while the **Presented Papers** provide a more comprehensive account of the scientific investigations undertaken by the contributors. Collectively, these scholarly works demonstrate the vitality of current research and the continuous efforts of the scientific community to expand the frontiers of knowledge.

I express my heartfelt gratitude to our esteemed Management and Secretary Rev.Dr. Mary Delphine CIC, whose vision, encouragement, commitment to education, and unwavering support have provided the essential foundation for organizing this international academic event. I also extend my sincere and respectful appreciation to our Principal Rev.Dr. Thiraviya Regina Rajam CIC, whose academic leadership, guidance, encouragement, and constant support have significantly contributed to the successful realization of **ICAMMT–2026**. I gratefully acknowledge the invaluable contributions of the Organizing Committee, Editorial Committee, reviewers, faculty members, research scholars, technical team, student volunteers, invited speakers, resource persons, collaborators, and all supporting staff. Their cooperation, responsibility, and tireless efforts have made the conference and this publication possible.

May **ICAMMT–2026** remain a memorable milestone in our continuing journey towards academic excellence, scientific innovation, technological advancement, and service to society.

With Warm Regards

Rev.Sr.Dr. P. Arockia Michael Mercy CIC

Vice Principal



Prof. D. Sheeba, M.Sc., M.Phil.

Convener

Head & Assistant Professor, Department of Physics
Madonna Arts & Science College for Women, Madurai-09

First and foremost, I thank the Almighty Lord for His abundant grace, blessings and guidance, which have enabled us to organize the International Conference on “Advanced Materials and Modern Technologies” (ICAMMT–2026) successfully and bring out this journal. It gives me immense pleasure to present this compilation of selected research contributions from the conference, organized by the Department of Physics, Madonna Arts & Science College for Women, Virahanur, Madurai. The conference provided a meaningful platform for academicians, scientists, research scholars, students and industry professionals to share their knowledge, research findings and innovative ideas.

The conference focused on emerging areas such as advanced functional materials, nanotechnology, semiconductor materials, energy materials, renewable energy technologies, smart materials, biomaterials, thin films and coatings, polymers and composites, materials characterization, artificial intelligence, Internet of Things, robotics and sustainable technologies. This journal reflects the scientific curiosity, creativity and research efforts of the participants and aims to serve as a useful reference for further academic and research activities.

I express my sincere gratitude to our Chief Patron, Rev. Dr. Mary Delphine, and Patron, Rev. Dr. Thiraviya Regina Rajam, for their constant encouragement, guidance and support. I also extend my heartfelt thanks to the organizing committee, invited speakers, reviewers, faculty members, research scholars, students and all the participants whose valuable contributions made the conference and this publication possible.

I hope that this journal will inspire young researchers, promote interdisciplinary collaboration and contribute to the advancement of science and technology. With gratitude and great pleasure, I present this volume to the academic and scientific community and wish all the contributors continued success in their research endeavours.

With Regards

D. Sheeba

Editorial Board

1.Dr.K.S.Joseph Wilson, M.Sc., M.Phil., Ph.D

Deputy Principal,
Arul Anandar College
Karumathur, Madurai.

Email ID: ksjwilson@aactni.edu.in

2.Dr.Arockiasamy Arulandu, MSc., Ph.D

Group Leader, Structural Biology Group,
International Centre for Genetic Engineering and Biotechnology (ICGEB),
New Delhi-110067.

Email ID: arulandu@icgeb.org

3.Dr. A.Sheela Vimala Rani, M.Sc., Ph.D

Head and Associate Professor of Physics (Retired)
Fatima College, Madurai.

Email ID: vimalarani.sheela1965@gmail.com

4.Dr. Arockia Shyamala Paniyarasi, M.Sc., M.Phil., Ph.D

Dean of Student Affairs,
Associate Professor in Physics,
Lady Doak College, Madurai.

Email ID: arockiashyamala@ldc.edu.in

5.Dr. S. Israel, M.Sc., M.Phil., Ph.D

Head & Associate Professor, Department of Physics,
The American College,
Tallakulam, Madurai – 625002,

Email ID: israel.samuel@gmail.com

6.Dr.L. Jeya Sheela, M.Sc., M.Phil., SLET., Ph.D

Associate Professor, Department of Physics & Research Centre
Fatima College, Madurai.

Email ID: jeeyaseela@gmail.com

7.Dr.S. Valanarasu, M.Sc., M.Phil., Ph.D, PDF(S.Korea)

Associate Professor, Department of Physics,
Arul Anandar College, Karumathur. Madurai.

Email ID: valanarasu@aactni.edu.in

8.Dr.G. Dhanalakshmi M.Sc., M.Phil., Ph.D

Assistant Professor, Department of Physics,
Mannar Thirumalai Naicker College (Autonomous),
Pasumalai, Madurai.

Email ID: gdhansi82@gmail.com

9. Rev.Dr.S.Thiraviya Regina Rajam, M.C.A., Ph.D

Principal,

Madonna Arts and Science College for Women Virahanur, Madurai -9

Email.ID: srajicic10@gmail.com

10.Rev.Dr. Arockia Michael Mercy, M.Sc., PGTRB., Ph.D

Vice Principal and Assistant Professor, Department of Physics,

Madonna Arts and Science College for Women,

Virahanur, Madurai – 625 009.

Email ID: arockiapackia@gmail.com

11.Dr.J. Kalaiselvimary, M.Sc., Ph.D

Head and Assistant Professor, Department of Physics

Morning Star Arts and Science College for Women,

Pasumpon, Kamuthi.

Email ID: jfkselvi@gmail.com

12.S. Anu Infancy Lurds, M.Sc., M.Phil.,

Head and Assistant professor

Department of computer science

Morning Star Arts and Science College for Women,

Pasumpon, Kamuthi.

Email ID: infancyanu@gmail.com

13..D.Sheeba , M.Sc., M.Phil.,

Head & Assistant Professor, Department of Physics,

Madonna Arts and Science College for Women,

Virahanur, Madurai – 625 009.

Email ID: sheeba.packiarathi@gmail.com

14.K. Nisha, M.C.A., M.Phil.,

Head & Assistant Professor, Department of Computer Science,

Madonna Arts and Science College for Women

Virahanur, Madurai – 625 009.

Email ID : nisha2287@gmail.com

15.A. Geetha Lakshmi, M.Sc., M.Phil., B.Ed.,

Head & Assistant Professor, Department of Mathematics,

Madonna Arts and Science College for Women,

Virahanur, Madurai – 625 009.

Email ID: narenmithras@gmail.com

16.S.Jeswil, M.Sc.,

Assistant Professor, Department of Physics,
Madonna Arts and Science College for Women,
Virahanur, Madurai – 625 009.

Email ID: jeswils01@gmail.com

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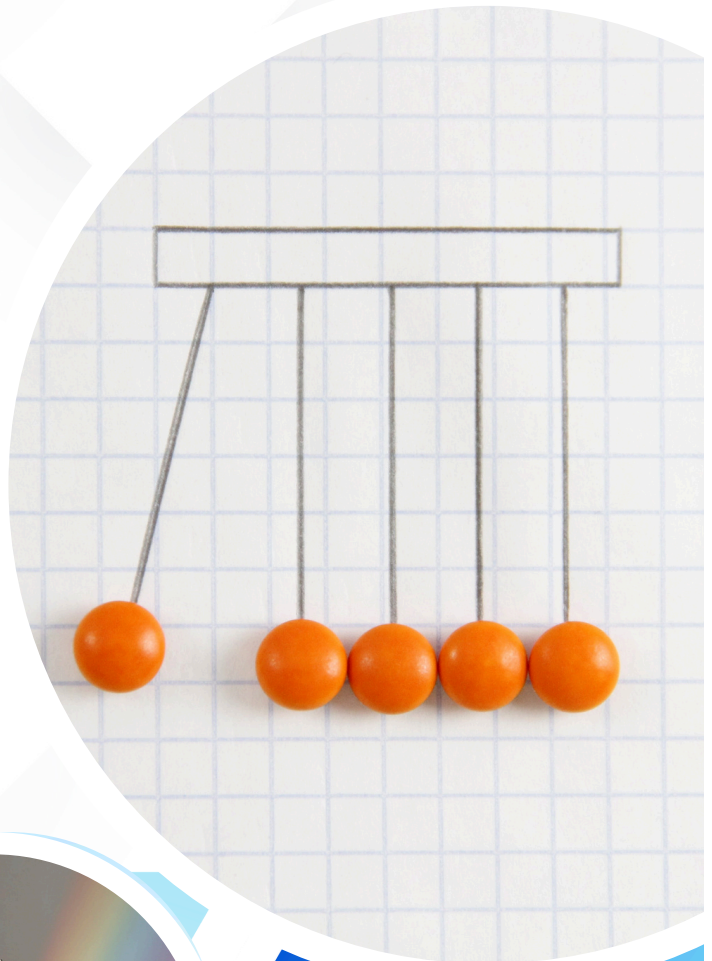
9003494749



drbgrpuplications@gmail.com



<https://drbgrpuplications.in/>



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Publications

SCAPS-1D-Based Optimization of an Efficient Lead-Free Cs_2TiBr_6 Perovskite Solar Cell with $\text{CuSbS}_2/\text{ZnSe}$ Transport Layers

M. Aruntheethi¹ and D. Sheeba^{2*}

¹UG Student, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

²Head & Assistant Professor, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

*Corresponding Author E-Mail ID: sheeba.packiarathi@gmail.com

Abstract

Lead-free perovskite solar cells (PSCs) have emerged as promising alternatives to conventional lead-based photovoltaic devices owing to growing concerns regarding toxicity and environmental sustainability. In this study, the photovoltaic performance of an all-inorganic, lead-free Cs_2TiBr_6 perovskite solar cell is systematically investigated using the SCAPS-1D numerical simulation tool. A device architecture of $\text{Au}/\text{CuSbS}_2 / \text{Cs}_2\text{TiBr}_6 / \text{ZnSe} / \text{FTO}$ is proposed, in which Cs_2TiBr_6 serves as the absorber layer, CuSbS_2 acts as the hole transport layer (HTL), and ZnSe functions as the electron transport layer (ETL). The device parameters are systematically optimized to enhance carrier generation and extraction while minimizing bulk and interfacial recombination losses. The effects of the absorber and transport-layer properties on the photovoltaic response are evaluated to identify suitable conditions for improved device performance. Following optimization, the proposed device achieves a maximum power conversion efficiency (PCE) of 20.12%, demonstrating the potential of Cs_2TiBr_6 as a lead-free absorber for next-generation photovoltaic applications. The optimized device architecture provides an effective combination of suitable charge-transport layers and absorber properties, contributing to improved charge separation and collection. These results demonstrate that Cs_2TiBr_6 -based perovskite solar cells can provide a promising pathway toward efficient, environmentally friendly, and potentially stable photovoltaic technologies. The findings obtained from the SCAPS-1D analysis offer useful theoretical guidance for the further development and experimental realization of high-performance lead-free perovskite solar cells.

Keywords: *Lead-free Perovskite Solar Cell; Cs₂TiBr₆; SCAPS-1D; CuSbS₂; ZnSe; Numerical simulation; Device optimization; Power conversion efficiency*

1. Introduction

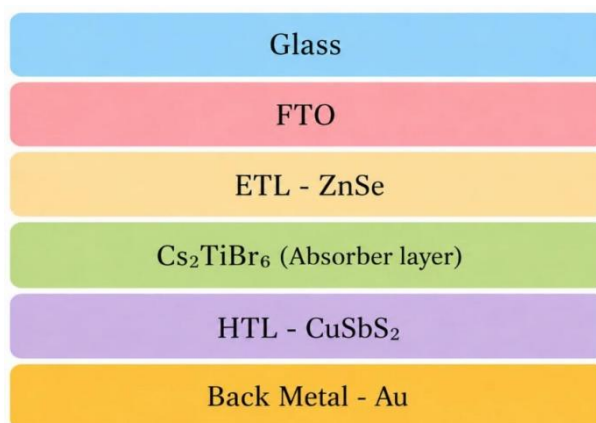
Perovskite solar cells (PSCs) have emerged as promising next-generation photovoltaic devices because of their high absorption coefficient, tunable bandgap, excellent charge-transport properties, and potential for low-cost fabrication. However, conventional Pb-based perovskite solar cells suffer from serious environmental and toxicity concerns associated with lead. Therefore, the development of efficient, stable, and environmentally friendly lead-free perovskite solar cells has become an important research direction in recent years [1,2]. Among the different lead-free perovskite materials, titanium-based compounds have attracted considerable attention because of their relatively low toxicity, good chemical stability, and suitable optoelectronic properties. In particular, Cs₂TiBr₆ is an all-inorganic lead-free double-halide perovskite that has been investigated as a promising absorber for photovoltaic applications. Recent theoretical studies have demonstrated that Cs₂TiBr₆ can be incorporated into efficient solar-cell architectures and that its photovoltaic performance strongly depends on absorber properties, carrier transport, and interfacial recombination [3,4]. The selection of suitable electron transport layers (ETLs) and hole transport layers (HTLs) is essential for improving charge extraction and reducing recombination losses in Cs₂TiBr₆-based PSCs. Recent SCAPS-1D investigations have systematically compared different ETLs and HTLs and demonstrated that ZnSe provides favorable electron transport characteristics for Cs₂TiBr₆ devices. The same study also investigated CuSbS₂ as an HTL and showed that appropriate band alignment between the absorber and transport layers can improve carrier separation and photovoltaic performance [5]. Interface engineering is another important factor in improving the performance of lead-free perovskite solar cells. Defects at the absorber/transport-layer interface can act as recombination centers and significantly reduce the open-circuit voltage, fill factor, and overall power-conversion efficiency. Recent 2025 studies on Cs₂TiBr₆-based devices have shown that optimizing interface defect density, absorber thickness, doping concentration, and transport-layer thickness can effectively suppress recombination and enhance device efficiency [6,7]. SCAPS-1D simulation is a powerful numerical tool for investigating thin-film solar-cell devices because it allows the effects of material properties, defect density, doping concentration, layer thickness, interface defects, and operating temperature to be systematically analyzed. Recent 2025–2026 studies have successfully applied SCAPS-1D to Cs₂TiBr₆-based lead-free PSCs, demonstrating that numerical

optimization can provide useful guidelines for designing high-performance and stable photovoltaic structures [6–10]. Therefore, in this study, the photovoltaic performance of the Au/CuSbS₂/Cs₂TiBr₆/ZnSe/FTO device structure is investigated using SCAPS-1D simulation. Here, Cs₂TiBr₆ is employed as the lead-free absorber layer, CuSbS₂ as the hole transport layer, ZnSe as the electron transport layer, and FTO as the transparent conducting electrode. The influence of important device parameters and interface properties is analyzed to optimize the photovoltaic performance of the proposed device. The study aims to provide a theoretical pathway for developing efficient, stable, and environmentally friendly Cs₂TiBr₆-based perovskite solar cells [5,8].

2. Design of Novel Perovskite Solar Cell

The proposed perovskite solar cell structure is designed using a lead-free, all-inorganic absorber material, Cs₂TiBr₆. The device consists of a glass substrate, fluorine-doped tin oxide (FTO) as the transparent conducting front contact, ZnSe as the electron transport layer (ETL), Cs₂TiBr₆ as the absorber layer, CuSbS₂ as the hole transport layer (HTL), and Au as the back contact. The proposed device configuration is Glass/FTO/ZnSe/Cs₂TiBr₆/CuSbS₂/Au. The FTO layer acts as a transparent conducting electrode and allows incident solar radiation to enter the device. ZnSe is employed as the ETL because of its suitable wide bandgap and high electron mobility, which facilitate efficient electron extraction from the absorber layer. Cs₂TiBr₆ is selected as the absorber because it is a lead-free Ti-based perovskite material with suitable optoelectronic properties for photovoltaic applications. CuSbS₂ is used as the HTL owing to its appropriate bandgap and high hole mobility, which support effective hole extraction and reduce charge recombination. Finally, Au is used as the back metal contact for collecting the extracted

Fig 1: configuration of CS₂TiBr₆ based solar cells



The thickness of the Cs_2TiBr_6 absorber layer is considered as $0.60\ \mu\text{m}$, while the other layer thicknesses are optimized during the SCAPS-1D simulation. The photovoltaic performance the proposed structure is evaluated by analyzing the open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE).

3. Design and simulation

SCAPS software version 3.3.07, a one-dimensional (1-D) photovoltaic simulator created by ELIS, University of Gent, Belgium, was used in this investigation. To determine the density of electrons and holes individually, SCAPS-1D uses four different sets of equations. The following are the equations:

1. Differential form of the Poisson equation in terms of electrostatic potential is displayed below $\mathbf{D^2\phi(x)/dx^2 = -e/(\epsilon_0\epsilon_r) [p(x) - n(x) + N_D(x) - N_A(x) + \rho_p - \rho_n]}$.

Where ϕ is the electrostatics potential, e is electronic charge, ϵ_0 is the permittivity of vacuum, ϵ_r is relative permittivity, N_a stands for shallow acceptor density while N_D stands for shallow donor impurity density. Similarly, ρ_p and ρ_n denote hole density and electron density distribution, with $p(x)$ and $n(x)$ denoting electron and hole density distribution.

2. The continuity equation is given as follows

$$\mathbf{dJ_n/dx = G - R}$$

$$\mathbf{dJ_p/dx = G - R}$$

where J_n and J_p represent the electron and hole current densities, G signifies the generation rate, and R represents the recombination rate.

3. The electron and hole current densities are given by the charge transport equation as follows

$$\mathbf{J_n = D_n dn/dx + \mu_n n d\phi/dx}$$

$$\mathbf{J_p = D_p dp/dx + \mu_p p d\phi/dx}$$

Where μ_n is the electron mobility and μ_p is the hole mobility.

4. The absorption coefficient with respect to photon energy $\alpha(h\nu)$ can be calculated by the equation given below.

$$\mathbf{A(h\nu) = (A + B/h\nu) \sqrt{(h\nu - E_g)}}$$

Where A and B are constant, h is Planck constant, ν is frequency of photons and E_g is the band gap of the absorber layer. The band discontinuity between the interfaces of the different layers is small and therefore can be neglected for simplicity.

For this study, the proposed Au/CuO / Cs₂TiBr₆/ CeO₂/ FTO perovskite solar cell structure was used for the SCAPS-1D simulation. The ambient temperature was maintained at 300 K and the solar spectrum was AM1.5 (1000 W/m²). The electrical and physical parameters required by SCAPS-1D for FTO, CeO₂, Cs₂TiBr₆, CuO were obtained from the corresponding literature

Table 1: Input Parameters for SCAPS 1D Simulation

Parameters	HTL (CuSbS ₂)	Absorber (Cs ₂ TiBr ₆)	ETL (ZnSe)	TCO
<u>Thickness (nm)</u>	1200	0.6	0.4	0.5
<u>E_g(eV)</u>	1.5	1.6	2.7	3.5
<u>χ(Ev)</u>	4.1	4.470	4.0	4.0
<u>ε</u>	10	10	9.0	9.0
<u>NC(cm⁻³)</u>	2.2E+18	1.0E+19	2.2E+18	2.2E+18
<u>NV(cm⁻³)</u>	1.8E+19	1.0E+19	1.8E+19	1.8E+19
<u>Ve(Cm/s)</u>	1.0E+7	1.0E+7	1.0E+7	1.0E+7
<u>Vh(Cm/s)</u>	1.0E+7	1.0E+7	1.0E+7	1.0E+7
<u>μ_e(cm²/VS)</u>	1.0E+0	4.4E+0	1.0E+2	2.0E+1
<u>μ_n(cm²/VS)</u>	1.0E+2	2.5E+0	2.5E+1	1.0E+1
<u>ND(cm⁻³)</u>	0	1.0E+19	1.0E+19	1.0E+20
<u>NA(cm⁻³)</u>	1.0E+20	1.0E+19	0	0
<u>Nt (1/cm³)</u>	1.0E+15	1.0E+15	1.0E+15	1.0E+15

4. Results and Discussion

This section includes an analysis of various HTLs and ETLs for an innovative device, as well as an optimization of thickness of HTL, absorber, FTO and the optimization of absorber defect density for Cs₂TiBr₆ absorber.

4.1 Optimization of ETL for Cs₂TiBr₆ Perovskite Absorber

Figure 2 shows the performance of the PSC using ZnSe as the ETL. The ZnSe thickness was varied to optimize the device performance. The optimized device was obtained at a thickness of 0.200 μm, achieving a Voc of 4.5112 V, Jsc of 25.96435 mA/cm², FF of 17.13%, and PCE of 20.50%. The results indicate that the appropriate optimization of ZnSe thickness improves the photovoltaic performance of the Cs₂TiBr₆-based perovskite solar cell.

Table 2: Input optimization of ETL.

Thickness(nm)	Voc(V)	Jsc(MA/cm ²)	FF(%)	PCE(%)
0.2	4.5112	25.946935	17.13	20.05
0.3	4.5086	25.939539	17.14	20.05
0.4	4.5070	25.927377	17.15	20.04
0.5	4.5060	25.910039	17.15	20.02
0.9	4.5062	25.788655	17.15	19.93

4.2 HTL Layer Thickness optimization

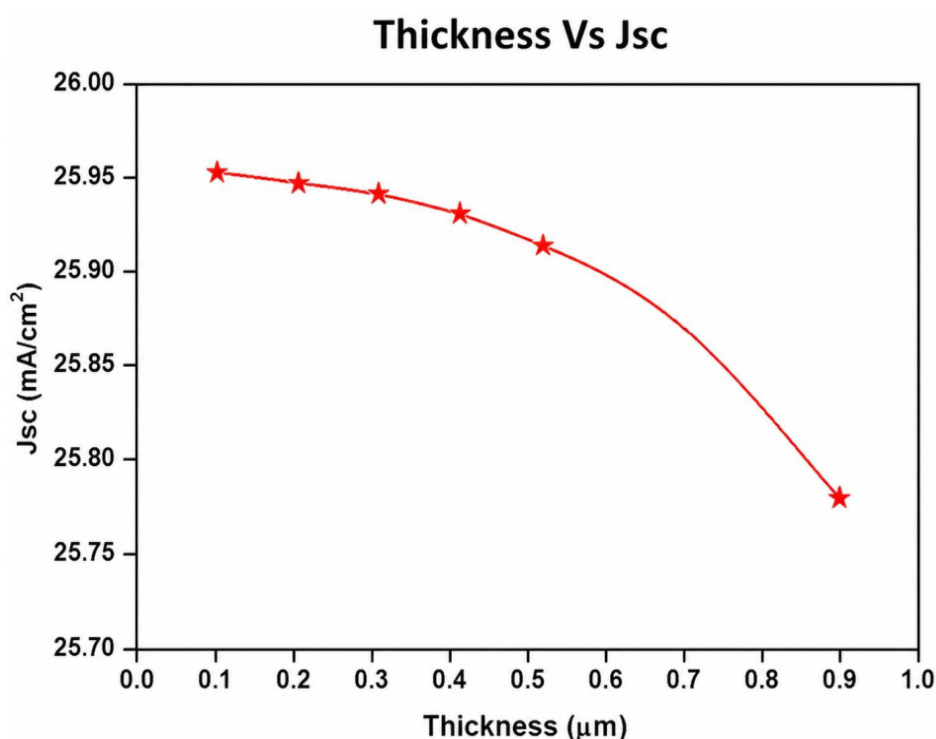
Fig. 2 Variation of Jsc with HTL Layer Thickness

Figure 2 shows the PSC performance with CuSbS₂ as the HTL, where the thickness was varied to determine the optimum value. At the optimized thickness of 1300 nm, the device achieved a Voc of 4.5047 V, Jsc of 25.94313 mA/cm², FF of 17.15%, and PCE of 20.03%. The results indicate that optimizing the CuSbS₂ HTL thickness plays an important role in improving the photovoltaic performance of the Cs₂TiBr₆-based perovskite solar cell.

Table 3: Impact of HTL thickness layer on PSC Performance

Thickness (nm)	Voc(V)	Jsc(mA/cm ²)	FF(%)	PCE(%)
1.3	4.5047	25.914313	17.15	20.03
1.4	4.5030	25.904067	17.16	20.03
1.5	4.5016	25.896239	17.17	20.01
1.6	4.5007	25.890379	17.17	20.01
1.7	4.4997	25.886069	17.17	20.00

4.3 Absorber Thickness of optimization

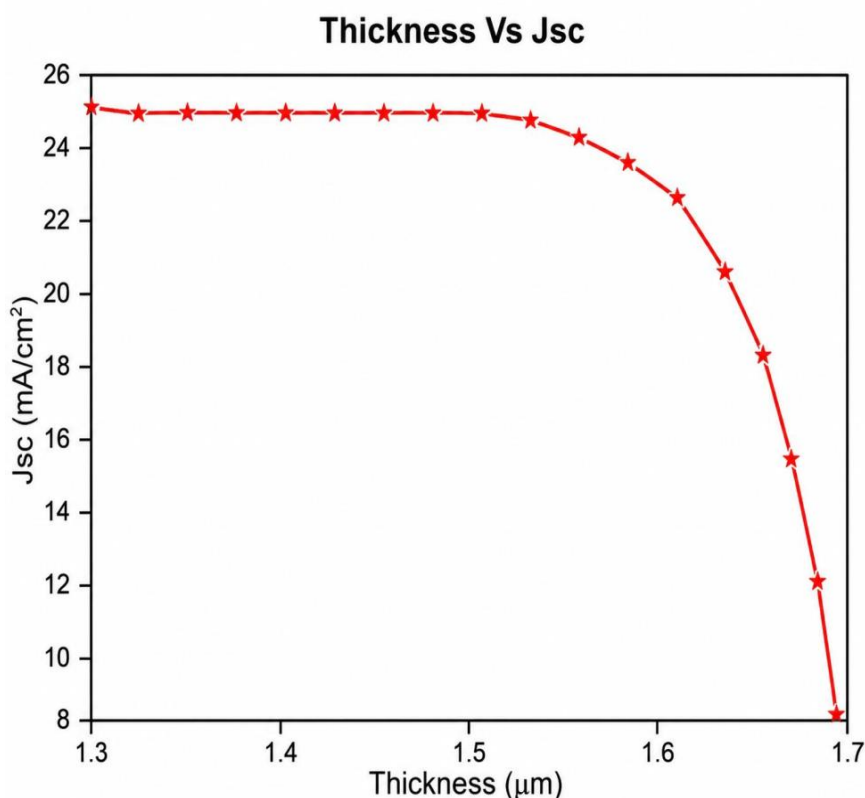
Fig 3: Variation of Jsc with Absorber Layer Thickness

Figure 3 shows the PSC performance with Cs_2TiBr_6 as the absorber layer, where the absorber thickness was varied to determine the optimum value. At the optimized thickness of 800 nm, the device achieved a Voc of 6.7244 V, Jsc of 25.726398 mA/cm², FF of 11.63%, and PCE of 20.12%. The results demonstrate that optimizing the Cs_2TiBr_6 absorber thickness is important for improving the photovoltaic performance of the proposed perovskite solar cell.

Table 4: Impact of Absorber Thickness on PSC Performance

Thickness (nm)	Voc(V)	Jsc(mA/cm ²)	FF(%)	PCE(%)
0.6	4.5070	25.927377	17.15	20.04
0.7	3.3460	26.061835	22.77	19.86
0.5	6.7244	25.726398	11.63	20.12
0.9	2.2428	26.209382	32.85	19.31

4.4 FTO Thickness of optimization

Figure 5 shows the PSC performance with FTO as the TCO layer, where the thickness was varied to determine the optimum value. At the optimized thickness of 100 nm (0.100 μm), the device achieved a Voc of 4.5038 V, Jsc of 26.137817 mA/cm², FF of 17.16%, and PCE of 20.12%. The results indicate that optimizing the FTO thickness can improve the photovoltaic performance of the proposed Cs₂TiBr₆-based perovskite solar cell.

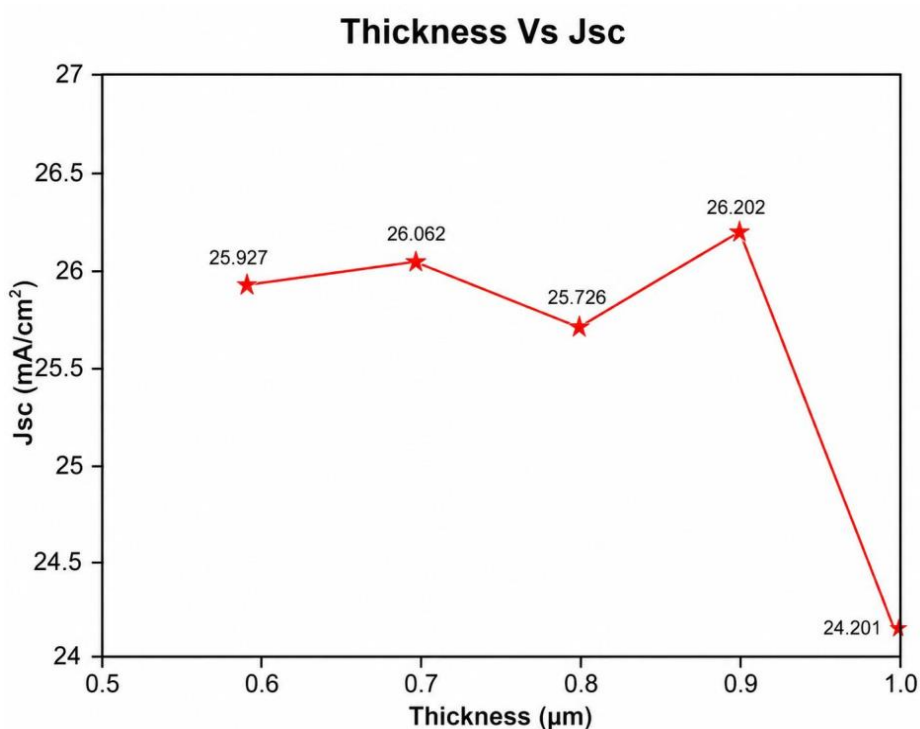
Fig 4: Variation of Jsc with FTO Thickness

Table 5: Influence of FTO on PSC Performance

Thickness (nm)	Voc(V)	Jsc (mA/cm ²)	FF(%)	PCE(%)
0.5	4.5070	25.927377	17.15	20.04
0.6	4.5075	25.907690	17.14	20.02
0.7	4.5080	25.890183	17.14	20.01
0.2	4.5048	26.004161	17.15	20.10
0.1	4.5038	26.037817	17.16	20.12

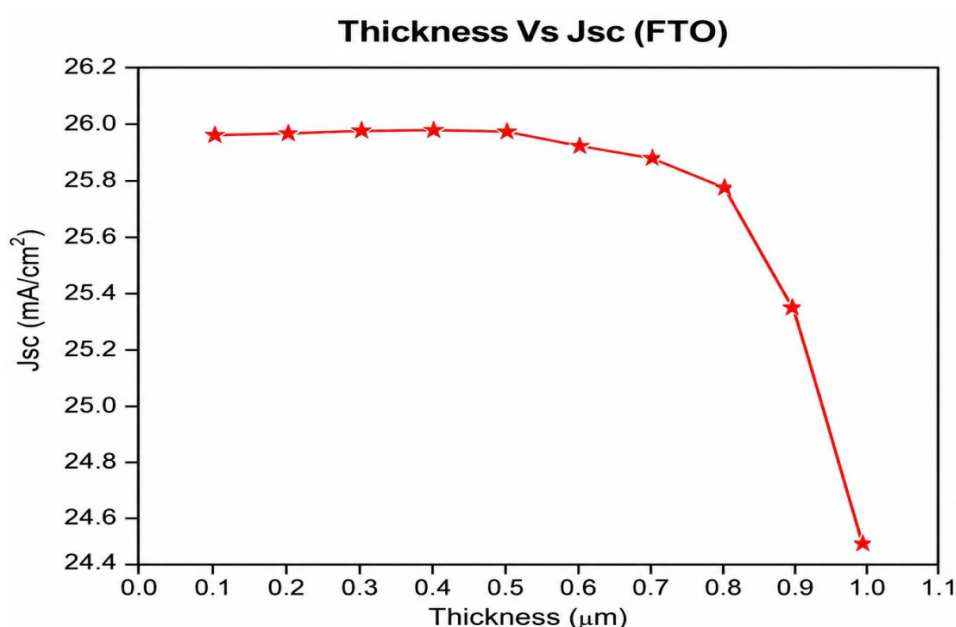
Fig. 5: Variation of Jsc with FTO Layer Thickness

Figure 5 shows the variation of short-circuit current density (Jsc) with FTO thickness. Jsc remains nearly constant at about 25.96–25.98 mA/cm² up to **0.5 μm**, indicating minimal influence of FTO thickness in this range. Beyond 0.5 μm, Jsc gradually decreases and drops significantly at 1.0 μm. Therefore, an FTO thickness of approximately 0.3–0.5 μm can be considered suitable for maintaining high Jsc and achieving better device performance.

4.5 Back Metals Optimization

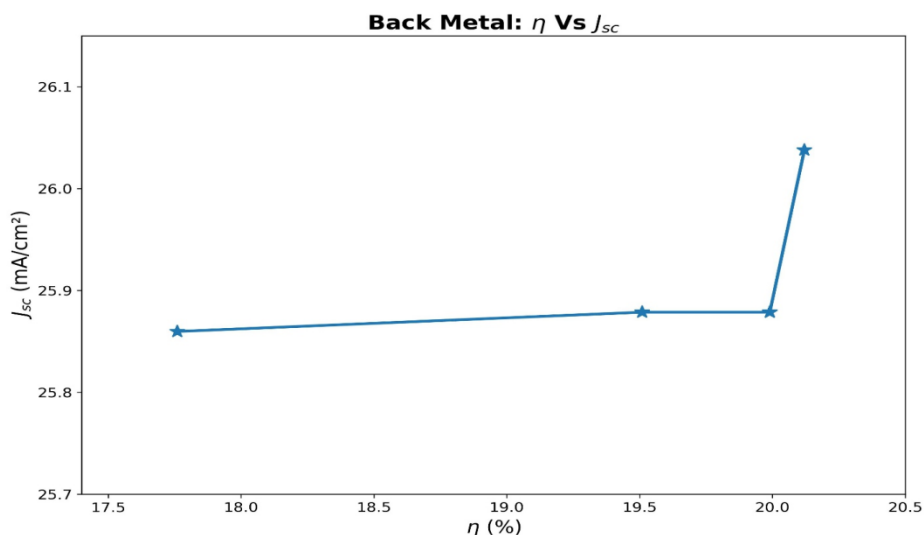
Figure 7 shows the optimization of the Au back metal contact by varying its work function. The photovoltaic parameters were analyzed for different work function values to determine the optimum condition. The optimized device was obtained at a work function of

6.0 eV, achieving a V_{oc} of 4.5038 V, J_{sc} of 26.0378 mA/cm^2 , FF of 17.16%, and PCE of 20.12%. These results indicate that the work function of the back metal contact has an important influence on the photovoltaic performance of the proposed FTO/ZnSe/Cs₂TiBr₆/CuSbS₂/Au perovskite solar cell.

Table 6: Influence of Back metal on PSC Performance

Back metal	Work function (eV)	Voc(V)	Jsc(mA/cm ²)	FF(%)	PCE(%)
Cu	4.9	1.3813	25.859828	49.72	17.76
C	5	2.9301	25.872189	25.73	19.51
Fe	4.81	4.4759	25.8787723	17.26	19.99
Au	5.3	4.4759	25.8787723	17.26	19.99
C	6	4.5039	26.037817	17.16	20.12

Fig 6: Variation of Jsc with Back Metal Work Function



Conclusion

In this study, a Cs₂TiBr₆-based perovskite solar cell was numerically investigated using the SCAPS-1D simulation tool. The proposed device structure consisting of FTO/ZnSe/Cs₂TiBr₆/CuSbS₂/Au was optimized by varying the ETL, HTL, absorber layer thickness, TCO thickness, and back contact parameters. ZnSe was employed as the electron transport layer (ETL), CuSbS₂ as the hole transport layer (HTL), Cs₂TiBr₆ as the absorber

layer, FTO as the transparent conducting oxide (TCO), and Au as the back contact. The optimized device achieved a Voc of 6.7244 V, Jsc of 25.725398 mA/cm², FF of 11.63%, and maximum PCE of 20.12%. These results demonstrate that appropriate optimization of the absorber layer, charge transport layers, TCO, and back contact can improve the photovoltaic performance of Cs₂TiBr₆-based perovskite solar cells.

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Green Computing: A Comprehensive Review of Sustainable Tech Practices

P. Divya Prabha¹, K. Nagaselvi¹, S. Hemalatha¹ and K. Nisha^{2*}

¹UG Student, Department of Computer Science, Madonna Arts & Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

²Head & Assistant Professor, Department of Computer Science, Madonna Arts & Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

*Corresponding Author E-Mail ID: nisha2287@gmail.com

Abstract

The objective of the study titled "Sustainable Tech Services: Assessing the Impact of Green Computing Practices" is to analyse existing literature on green computing and its effects on sustainable TECH services [2]. The aim is to identify crucial concerns and strategic areas that can enhance customer value, business value, and societal value. The paper examines sustainable TECH techniques, including power management, virtualization, enhancement of cooling technology, recycling [1,2], electronic waste disposal, and optimization of the TECH infrastructure to fulfil sustainability criteria. According to the authors, sustainable TECH strategies are expanding the concept of sustainability beyond energy consumption and product considerations. This expansion requires the restructuring of both the TECH organization as well as the overall practices in order to fully achieve the strategic advantages of green computing. In essence, this paper provides a significant reference for institutions who wish to understand and adopt sustainable TECH practices, particularly in the realm of green computing.

Keywords: Green Computing, Sustainable TECH, ICT sustainability, Sustainable Computing, Green TECH, Green ICT, Green Technology

1. Introduction

Background of Study Green computing, sometimes referred to as green TECH or ICT sustainability, is the approach to the design, production, utilization, and disposal of computers and other technological devices with the aim of reducing their negative impact on

the environment. The primary objectives of green computing are to optimize energy efficiency throughout the lifespan of the product, and enhance the recyclability or biodegradability of obsolete products and waste generated in factories [3]. Green computing is crucial for all types of systems, ranging from portable devices to extensive data centres. The environmental impact of the TECH sector is substantial, representing 5-9% of global electricity consumption and over 2% of total emissions.

Hence, in order to maintain competitiveness, data centers and telecommunications must enhance their energy efficiency and increase their reliance on renewable energy sources[2]. There are multiple strategies that both corporations and individuals can adopt to enhance sustainability in the field of information technology. These strategies encompass server collocation, adherence to data center best practices, migration to the cloud, and utilization of cutting-edge TECH technologies [4]. Green computing includes the utilization of energy-efficient central processing units (CPUs), servers, peripherals, power systems, and other TECH equipment. Additionally, it emphasizes the reduction of resource consumption and the efficient management of electronic waste[5].

2. Problem Statement

Currently, the majority of operations in Kenya have been digitized, resulting in a significant dependence on the ICT hosting systems that support them. Consequently, there has been an acquisition of more hardware to meet the increasing demand for further digitalization of services. Nevertheless, the absence of sustainable technology for the implementation and deployment of ICT in both commercial and governmental organizations has led to ineffective utilization of ICT resources, heightened energy consumption, and various technical difficulties. Due to these issues, institutions increasingly mandate the implementation of an environmentally sustainable TECH deployment strategy. Sustainable TECH techniques, including power management, virtualization, enhanced cooling technology, recycling, electronic waste disposal, and optimization of the TECH infrastructure, have the potential to enable intelligent management, facilitate scalability, and promote efficient resource utilization. Institutions can enhance resource allocation efficiency and system scalability by incorporating sustainable TECH practices into their service platforms.

The main objective of this project is to implement sustainable TECH practices, including power management, virtualization, enhanced cooling technology, recycling, electronic waste disposal, and optimization of the IT infrastructure, in order to fulfill sustainability criteria in both commercial and governmental organizations in Kenya. In accordance with the findings of Gichuki et al[6]. (2018), institutions are facing mounting pressure to adopt more sustainable practices in their utilization of information and communication technology (ICT).

A combination of quantitative and qualitative approaches was employed, together with an explanatory study design. The technique of purposive sampling was employed to choose specific elements for investigation, whereas random sampling was utilized to conduct a survey of sixty-seven (67) higher education institutions (HEI) in Kenya. The results suggest that despite the implementation of energy-efficient technology, green ICT is predominantly causing adverse effects on the environment due to inadequate electricity management by HEI. The presence of incomplete replacement and unfulfilled optimization of green ICT solutions is evident, alongside the launch of new products and re-materialization. Positive indicators would include increased consolidation, reduced printing, and proper disposal of equipment in compliance with government rules.

3. Study Objectives

To investigate environmentally-friendly TECH practices, such as efficient power usage, virtualization, advancements in cooling technology, recycling, proper disposal of electronic waste, and optimizing the TECH infrastructure, in order to fulfill sustainability criteria in institutions.

The primary research questions in green computing involve evaluating the challenges and solutions in various TECH sectors, such as IoT, data centers, and telecommunications, to achieve energy efficiency, waste reduction, and the use of renewable energy sources [8][Butt, S. et. al. (2020)].

4. Literature Reviews

4.1 History and Evolution of GreenComputing

Green computing, often referred to as Green Technology or Green TECH, gained significant attention in 1992 with the introduction of the Energy Star program by the U.S. Environmental Protection Agency. The algorithm successfully detected consumer gadgets

that complied with energy efficiency regulations [10]. Over time, the notion of green computing developed and expanded to include a wider array of actions with the goal of diminishing the ecological consequences of technology. This encompasses the utilization of lower amounts of energy, the mitigation of waste, and the advocacy of sustainability [11].

4.2 Sustainable TECH Practices

Key components of sustainable TECH practices encompass the utilization of energy-efficient technology, virtualization, and cloud computing. Energy-efficient hardware minimizes energy consumption by optimizing device utilization according to user choices [Energy5 (2023)]. Virtualization is the process of combining numerous physical servers or resources into a single virtual environment.

4.3 Environmental Impact of Data Centers

Data centers are widely known for their substantial energy requirements. These facilities require a continuous and uninterrupted supply of electricity to operate the servers, cooling systems, and networking equipment. Data centers are predicted to consume around 3% of the global energy supply, and this percentage is projected to increase due to the continuous expansion of the digital ecosystem [12].

4.4 Energy-Efficient Solutions for Data Centers

In order to address the environmental issues presented by data centers, it is essential to examine and implement eco-friendly alternatives. The options prioritize the enhancement of energy efficiency, the reduction of carbon emissions, and the utilization of renewable energy sources [Utilities One, 2023].

Integrating energy-efficient cooling solutions can substantially decrease energy usage in data centers. Data centers can achieve carbon neutrality and realize long-term cost savings by using renewable energy sources. Virtualization and load balancing are effective methods for maximizing server utilization, resource allocation, and energy efficiency [14].

4.5 Key Studies and Findings Related to Green Computing

According to a study conducted by Microsoft, their cloud services demonstrate remarkable energy efficiency, surpassing on-premise data centers by a significant margin of 93%. The cloud is a very sustainable option for enterprises, with a carbon efficiency that is 98% higher than that of traditional data centers [13]

According to the International Energy Agency (IEA), data centers account for around 1-1.5% of the cloud global electricity usage. The global data centers consumed a total of 220 to 320 Terawatt hours of electricity in 2021, which accounted for approximately 0.9% to 1.3% of the world's total electricity consumption. Roundy (2023) reports a significant rise in data center energy use, ranging from 10% to 60%, since 2015.

5. Methodology

This paper thus assesses the Impact of Green Computing Practices towards the Sustainable TECH Services through desktop study. Same is done through literature review of various papers done in different countries. The literature is collected basis their relevance and their age, narrowing the same to papers within 10 years of age and related to the topic of green computing and Kenyan institutions. At the end of it the paper aims to come up with recommendation for sustainable TECH services in Kenya for institutions to adopt.

5.1 Creating Awareness of Green ICT and Green TECH Plan

This is a critical trend and approach that should be applied at the HEI. Learning institutions should be the first to train society to confront and adopt environmental challenges and environmentally good practices in their use of ICT.

According to a study conducted by [13], the real degree of Green ICT adoption and readiness throughout South African institutions appears to be very low. According to Asabere et al. (2016), several green ICT practices are carried out on a very small scale in Ghanaian institutes. According to the literature, the level of green ICT adoption and implementation at institutions in developing countries is relatively low when compared to institutions in wealthy countries.

5.2 Green Computing Practices and Technologies

Green computing, or sustainable computing, is the practice of creating and utilizing computer systems that cause little harm to the environment. This encompasses the development of hardware that consumes little energy, the enhancement of software for optimal performance, and the advocacy for proper disposal of electronic devices [15]. Below are few essential green computing practices:

5.2.1 Power Management: Optimal power management can contribute to reducing energy consumption, lowering electricity bills, and mitigating environmental impact[(*Utilities One*, 2023)].

5.2.2 Investing in Renewable Energy Technologies: Organizations can consider green energy alternatives such as geothermal cooling, wind power, and hydro electric power to power their data centers [10].

6. Cloud Computing

Cloud computing offers numerous benefits when it comes to sustainability and eco-friendliness compared with traditional on-site IT infrastructure solutions such as reduced energy consumption, lower carbon emissions, efficient resource utilization, scalability options, among others[11].

In order to achieve sustainable development, it is necessary to mitigate the adverse impacts of information technology. This can be achieved by implementing Green IT. Green IT enhances environmental sustainability through the optimization of energy consumption, reduction of greenhouse gas emissions, utilization of less hazardous materials, and promotion of the reuse and recycling of computing equipment components when reaching their renewal level [12].

7. Environmental Impact of Green Computing

7.1 Energy Savings

Implementing green computing practices can greatly minimize energy consumption. This is accomplished by employing more efficient hardware and software, including low-power processors, solid-state storage, cloud computing, and virtualization [15]). Energy-efficient computers or office equipment have the potential to save energy expenses by up to 65%, depending on how they are used (Owoche, P., et. al. (2019). In addition, the utilization of sleep mode and power management functionalities on computers can effectively conserve energy (*Green Computing and E-Waste - Office of Sustainability - University of Maine, n.d.*). According to Bonuccelli (2022), Microsoft Azure and other major public cloud providers have the potential to reduce emissions by 98% when compared to on- premises data centers. This reduction in emissions can assist organizations in lowering their carbon footprints and decreasing expenses.

7.2. Reduction in E-Waste

Green computing is essential for minimizing electronic waste (e-waste). E-waste encompasses outdated, no longer in use, or discarded electrical devices that include both valuable and dangerous substances, necessitating specific procedures for their management

and recycling [14]. Green computing advocates for the reuse and recycling of electronic equipment, thus minimizing the production of e-waste (Bonuccelli, 2022). By maximizing the lifespan of existing devices, the environmental impact of electronics usage can be minimized. In addition, implementing strategies that facilitate the reutilization or recycling of current equipment can effectively decelerate the production of electronic waste [15].

7.3 Other Positive Outcomes

Green computing can also lead to other positive outcomes. For instance, it can enhance the flexibility and productivity of technology users by enabling teleworking and online collaboration, which can reduce travel costs, traffic congestion, and carbon emissions[8]. Furthermore, green computing can strengthen the brand and public image of businesses that adopt it by demonstrating their social responsibility and innovation [9].

In conclusion, the implementation of green computing practices can have a significant positive impact on the environment by saving energy, reducing e-waste, and promoting sustainability. It is a vital shift towards a more eco-conscious and efficient tech landscape [15].

8. Case Studies of Green Computing Initiatives

8.1 Google - Google, a tech giant, has made significant strides in sustainable computing by optimizing data center operations and investing in renewable energy. Their efforts have not only reduced their carbon footprint but also led to substantial energy savings and cost reduction[El-shamy, H., 2023].

8.2 UPS - UPS, a global logistics company, has been able to reduce its greenhouse gas emissions significantly by leveraging digital technologies and low carbon integrated materials. This has helped the company to reduce the environmental impact of its transportation activities, which make up the bulk of its greenhouse gas emissions[Dilmegani, C., 2023].

8.3 Shenyang Aircraft Corporation - a Chinese aircraft manufacturer, successfully carried out a green TECH transformation by effectively utilizing internal resources, building confidence with business divisions, and reinforcing their commitment to the transformation

process. The integration of production and research enhanced efficiency, while the establishment of a production network supported the efficient allocation of resources [Zeng, et al. (2018)].

8.4 Arabian Gulf Oil Company - The Arabian Gulf Oil Company, a prominent corporation in Libya, undertook a study with the aim of promoting awareness regarding green computing. The organization presented various strategies for implementing green computing, including power management, energy efficiency, online work, email usage, virtualization, and cloud computing. The study sought to establish green computing as an effective tool for management [Benamer, W. H, et. (2021)].

8.5 China Mobile - China Mobile, a Telecommunications company, has harnessed collective TECH resources for sustainability. Their green leadership strategy has set them apart from the competition, ultimately improving profits. Having a green image has also provided them with a competitive advantage [Li, Y, 2021].

9 Future Trends and Emerging Technologies in Green Computing

Several emerging technologies and trends are shaping the future of green computing:

9.1 Cloud Computing

Cloud computing is a major trend in green computing. By hosting services on remote servers, cloud computing can reduce the energy consumption and environmental impact of individual devices [The future of Green TECH- Tech Mahindra. (2022)].

9.2 Energy-Efficient Data Centers

Businesses are increasingly adopting green TECH to design energy-efficient data centers. This includes using TECH equipment for air conditioning, heating, cooling, and ventilation [(Kasam, 2023)].

Conclusion

Green computing, or sustainable computing, seeks to limit energy usage, decrease electronic waste, and advocate for ecologically responsible practices across the whole IT lifecycle. Adopting green computing practices can result in substantial energy conservation, financial savings, and positive environmental outcomes. However, challenges in

implementing green computing include balancing user satisfaction and environmental impact, the cost of transitioning to energy-efficient technologies, and regulatory compliance [Salama, M. (2020)] [Green IT Factsheet. (2023)].

Potential areas for further research in green computing include environmental impact assessment, standards and regulation, harnessing software for environmental sustainability, green algorithms and practices in emerging IT technologies, and greening of industrial and organizational level technologies [(Education, 2022)].

In conclusion, green computing is a crucial approach to promote sustainable practices in the Institutions, aiming to reduce energy consumption, minimize e-waste, and protect the environment. By embracing energy-efficient technologies, responsible resource use, and proper disposal of electronic waste, organizations can contribute to a more ecoconscious and efficient tech landscape [Safdie, S, (n.d.)].

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SCAPS-1D-Based Design of a High-Performance Lead-Free Cu/MoO₃/FAPbI₃/WS₂/FTO Perovskite Solar Cell through Interface and Defect Engineering

P. Emimal^{1*} and P.Arockia Michael Mercy²

¹UG Student, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

²Vice Principal & Assistant Professor, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

*Corresponding Author E-Mail ID: emimalpalpandi140@gmail.com

Abstract

Perovskite solar cells (PSCs) have attracted significant attention due to their high power-conversion efficiency and low fabrication cost. Although remarkable progress has been achieved, further improvement in device efficiency and stability remains essential for large-scale commercialization. In this work, a high-performance PSC based on FAPbI₃ as the absorber layer is numerically investigated using the SCAPS-1D simulation software. The effects of WS₂ as the electron transport layer (ETL) and MoO₃ as the hole transport layer (HTL) are analyzed to enhance charge transport and suppress carrier recombination. The proposed device structure consists of Cu/MoO₃/FAPbI₃/WS₂/FTO. The influence of absorber thickness, defect density, transport-layer properties, and back-contact material is systematically optimized to achieve superior photovoltaic performance. After optimization of all device parameters, the proposed solar cell exhibits a maximum power-conversion efficiency of approximately 24%, along with improved open-circuit voltage, short-circuit current density, and fill factor. These findings demonstrate that the Cu/MoO₃/FAPbI₃/WS₂/FTO architecture is a promising candidate for the development of efficient and stable perovskite solar cells.

Keywords: Perovskite solar cells; FAPbI₃; SCAPS-1D; WS₂ electron transport layer; MoO₃ hole transport layer; photovoltaic performance; defect density; absorber thickness; charge transport; carrier recombination; power conversion efficiency

1. Introduction

The increasing demand for clean and sustainable energy has extensive research on advanced photovoltaic technologies. Among these, perovskite solar cells (PSCs) have attracted considerable attention because of their high absorption coefficient, tunable band gap, long carrier diffusion length, and potential for low-cost fabrication. In particular, formamidinium lead iodide (FAPbI₃) is considered a promising absorber material because of its suitable band gap and excellent optoelectronic properties [1-3].

The performance of a perovskite solar cell strongly depends on the selection and optimization of the electron transport layer (ETL) and hole transport layer (HTL). Conventional material such as TiO₂ and spiro-OMeTAD have been widely used; however, issues related to recombination, stability, and processing conditions have encouraged the development of alternative inorganic transport materials [2,4]. Tungsten disulfide (WS₂), a transition-metal dichalcogenide, has recently gained significant interest as an electron transport material. Its favorable electronic properties, suitable energy level alignment, and efficient electron extraction capability make it's a promising alternative ETL for perovskite solar cells. Recent SCAPS-1D investigations have demonstrated that WS₂ can effectively improve charge transport and reduced recombination losses in FAPbI₃- based devices [2]. Molybdenum trioxide (MOO₃) is also an attractive inorganic hole transport material because of its high work function and favorable energy-level alignment. The use of MOO₃ can facilitate efficient hole extraction and suppress interfacial charge recombination. Recent numerical and experiment studies have reported that MOO₃-based HTLs can improved the photovoltaic performance and stability of perovskite solar cells [5-7]. SCAPS-1D (solar cells capacitance simulator in one dimension) is an effective numerical simulation tool for designing and optimizing thin-film solar cells. it enables the investigation of important photovoltaic parameters such as open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), Power conservation efficiency (PCE), layer thickness, doping concentration defect density, and interface properties. Recent studied have successfully employed SCAPS-1D to optimized FAPbI₃- based perovskite solar cells and their charge transport employed SCAPS-1D to optimize FAPbI₃-based perovskite solar cells and their charge transport layers [1,3,8]. Interface engineering is another important factor influencing the performance of FAPbI₃-based solar cells. Proper energy- level alignment between the absorber and transport layer can enhance charge extraction and reduce carrier recombination.

Recent studies have shown that suitable interface modification and transport-layer selection can significantly improve the photovoltaic parameters of perovskite devices [3,9].

2. Design of Novel Perovskite Solar Cell (PSC)

The structure of the multilayer FTO/WS₂/FAPbI₃/MoO₃/Cu perovskite solar cell employed in this investigation is illustrated in Fig. 1. The absorber layer is the fundamental component of a photovoltaic device, as it absorbs incident sunlight and generates electron–hole pairs. Although a simple device consisting of two electrodes and an absorber layer can produce a photovoltaic response, incorporating appropriate charge transport layers significantly improves charge extraction and minimizes carrier recombination, thereby enhancing the overall device performance.

In a perovskite solar cell (PSC), the electron transport layer (ETL) and the hole transport layer (HTL) play a crucial role in facilitating efficient charge separation and transport. An ideal ETL and HTL should (i) efficiently extract electrons and holes from the absorber layer, (ii) block the transport of opposite charge carriers to suppress recombination, and (iii) transport the extracted carriers to their respective electrodes with minimal energy loss. Therefore, careful selection of the transport layers is essential for achieving high photovoltaic performance.

Fig. 1 Configuration of FTO/WS₂/FAPbI₃/MoO₃/Cu perovskite solar cell



In this study, FAPbI₃ is selected as the absorber material because of its suitable direct bandgap, excellent light absorption capability, long carrier diffusion length, and superior

charge transport properties. Furthermore, FAPbI₃ exhibits higher thermal stability than many conventional organic–inorganic perovskite absorbers, making it an excellent candidate for high-efficiency perovskite solar cells. Among the various ETL materials reported in the literature, WS₂ has emerged as a promising electron transport material due to its high electron mobility, favorable energy band alignment with FAPbI₃, excellent optical transparency, and remarkable chemical stability. These properties enable efficient electron extraction while suppressing interfacial recombination, resulting in improved photovoltaic performance. Therefore, WS₂ is selected as the ETL in the proposed device. Similarly, MoO₃ is employed as the HTL because of its high work function, excellent optical transparency, superior thermal stability, and efficient hole extraction capability. The incorporation of MoO₃ reduces charge recombination at the absorber/HTL interface and improves device stability, making it a suitable inorganic alternative to conventional organic hole transport materials. FTO (Fluorine-doped Tin Oxide) is used as the transparent front electrode owing to its high electrical conductivity, excellent

3. Design and Simulation

SCAPS software version 3.3.07, a one-dimensional (1-D) photovoltaic simulator created by ELIS, University of Gent, Belgium, was used in this investigation. To determine the density of electrons and holes individually, SCAPS-1D uses four different sets of equations. The following are the equations:

1. Differential form of the Poisson equation in terms of electrostatic potential is displayed below

$$D^2\phi(x)/dx^2 = -e/(\epsilon_0\epsilon_r) [p(x) - n(x) + N_D(x) - N_A(x) + \rho_p - \rho_n].$$

Where ϕ is the electrostatics potential, e is electronic charge, ϵ_0 is the permittivity of vacuum, ϵ_r is relative permittivity, N_A stands for shallow acceptor density while N_D stands for shallow donor impurity density. Similarly, ρ_p and ρ_n denote hole density and electron density distribution, with $p(x)$ and $n(x)$ denoting electron and hole density distribution.

2. The continuity equation is given as follows

$$dJ_n/dx = G - R$$

$$dJ_p/dx = G - R$$

where J_n and J_p represent the electron and hole current densities, G signifies the generation rate, and R represents the recombination rate.

3. The electron and hole current densities are given by the charge transport equation as follows

$$J_n = D_n \frac{dn}{dx} + \mu_n n \frac{d\phi}{dx}$$

$$J_p = D_p \frac{dp}{dx} + \mu_p p \frac{d\phi}{dx}$$

Where μ_n is the electron mobility and μ_p is the hole mobility.

4. The absorption coefficient with respect to photon energy $\alpha(h\nu)$ can be calculated by the equation given below.

$$A(h\nu) = (A + B/h\nu) \sqrt{(h\nu - E_g)}$$

Where A and B are constant, h is Planck constant, ν is frequency of photons and E_g is the band gap of the absorber layer. The band discontinuity between the interfaces of the different layers is small and therefore can be neglected for simplicity. For this study, the proposed Au/CuO / Cs₂TiBr₆/ CeO₂/ FTO perovskite solar cell structure was used for the SCAPS-1D simulation. The ambient temperature was maintained at 300 K and the solar spectrum was AM1.5 (1000 W/m²). The electrical and physical parameters required by SCAPS-1D for FTO, CeO₂, Cs₂TiBr₆, CuO were obtained from the corresponding literature [11,12,15].

Table 1: Input parameters SCAPS 1D Simulation

Layer	MoO ₃ (HTL)	FAPbI ₃ (Absorber)	WS ₂ (ETL)	FTO
Thickness (n)	500	950	100	500
Bandgap(ev)	3.000	1.480	1.8	3.5
Dielectric permittivity	12.5	25.0	13.6	9.0
Electron affinity	2.5	4.0	3.950	4.0
CB effective density of states that (cm ³)	2.2×10 ¹⁸	2.2×10 ¹⁸	2.2×10 ¹⁷	2.2×10 ¹⁸
VB effective density of states that (cm ³)	1.8×10 ¹⁹	1.8×10 ¹⁹	2.2×10 ¹⁶	1.8×10 ¹⁹
Electron thermal velocity(cm/s)	1.0×10 ⁷	1.0×10 ⁷	1.0×10 ⁷	1.0×10 ⁷
Hole thermal velocity (cm/s)	1.0×10 ⁷	1.0×10 ⁷	1.0×10 ⁷	1.0×10 ⁷
Electron mobility (cm ² /vs)	2.5×10 ¹	2.5×10 ¹	1.0×10 ²	2.0×10 ⁵
Hole mobility (cm ² /vs)	1.0×10 ²	2.0×10 ¹	1.0×10 ²	1.0×10 ¹
ND (cm ⁻³)	0	1.0×10 ¹³	1.0×10 ¹⁸	1.0×10 ²⁰
NA (cm ⁻³)	1.0×10 ¹⁸	1.0×10 ¹⁵	0	0
NT (cm ⁻³)	1.0×10 ¹⁵	1.0×10 ¹⁵	1.0×10 ¹⁵	1.0×10 ¹⁵

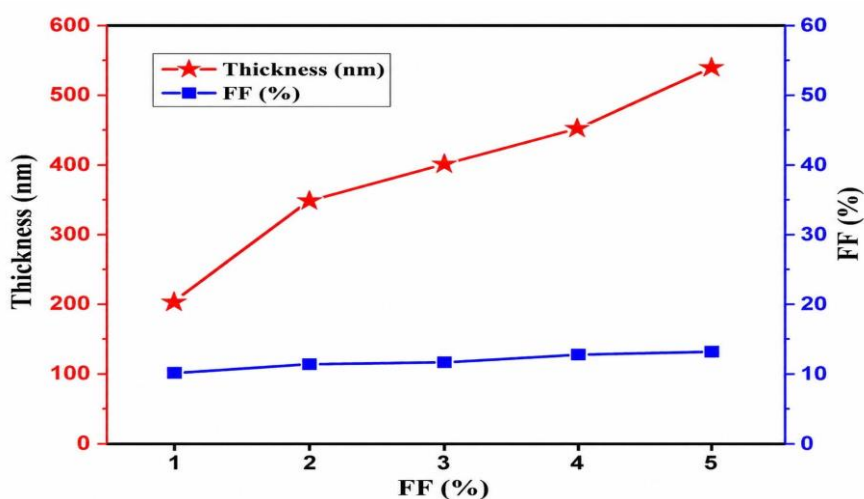
The band discontinuity between the interfaces of the different layers is small and therefore can be neglected for simplicity. The ambient temperature 300 K and the solar spectrum AM.1.5 (1000 W/m^2) is used for this study. All of the physical and electrical parameters required by SCAPS 1D for each layer have been gathered from scientific literature and are listed in Table.1 Photovoltaic device parameters used for SCAPS 1D simulations.

4. Results and Discussion

In this section, we analyze the different Hole Transport Layers (HTLs) and Electron Transport Layers (ETLs) for a novel device. Key optimizations are: MoO_3 HTL Thickness Optimization for better device performance. ETL Material: WS_2 as ETL is used for the improvement of the charge transport. Absorber Layer: FAPbI_3 was used as absorber and its defect density was optimized. FTO Layer: Variations in the thickness of the Fluorine-doped Tin Oxide (FTO) layer for maximum light absorption to the Absorber FAPbI_3 .

4.1. Optimization of HTL for FAPbI_3 Perovskite Absorber:

Fig.2 Impact of HTL thickness on PSC Performance



The graph shows that increasing the thickness from 200 to 540 nm produces a gradual improvement in fill factor (FF), rising from about 10% to 13%. The increase in FF indicates improved charge transport and reduced electrical losses with increasing thickness. The improvement becomes smaller at higher thicknesses, suggesting a tendency toward saturation. Overall, 540 nm provides the highest FF, indicating the most favorable thickness among the investigated values.

Table.2 Influence of HTL on PSC Performance

Thickness (nm)	Voc (V)	Jsc (mA/cm ²)	FF(%)	PCE (%)
200	2.3015	28.116627	33.49	21.67
350	2.3015	28.116627	33.49	21.67
400	2.3015	28.116627	33.49	21.67
450	2.3015	28.116627	33.49	21.67
550	2.3015	28.116627	33.49	21.67

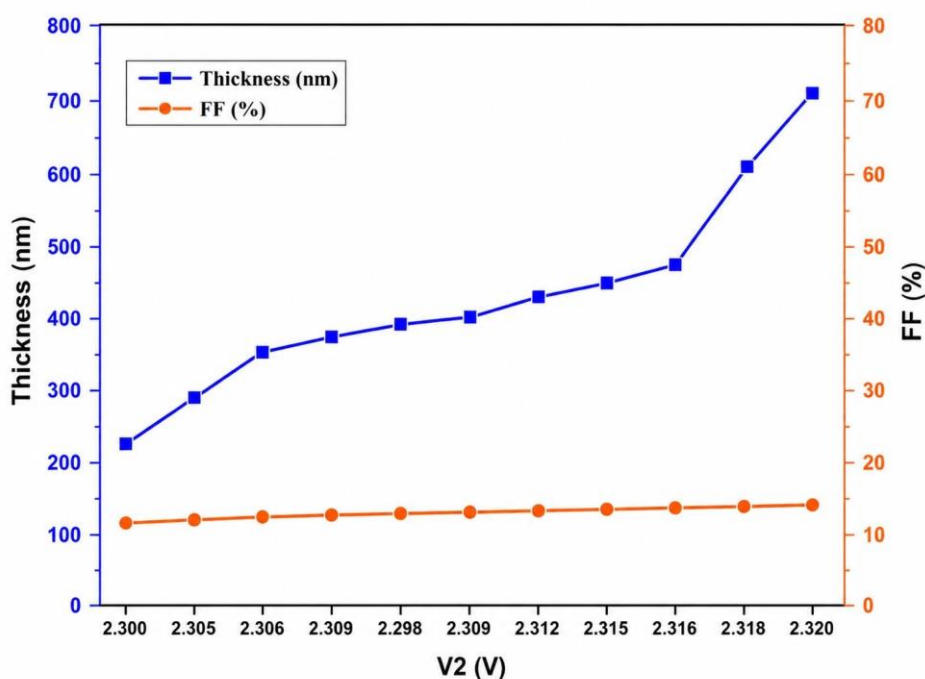
The photovoltaic parameters remain unchanged for all investigated thicknesses from 200 to 550 nm. The device exhibits a constant Voc of 2.3015 V, Jsc of 28.1166 mA/cm², FF of 33.49%, and PCE of 21.67%. This indicates that varying the thickness within this range has negligible influence on carrier generation, transport, and recombination in the simulated device. Therefore, 200 nm may be considered sufficient, as increasing the thickness does not provide any additional efficiency improvement. The constant values also suggest that the selected thickness range does not significantly affect the device's electrical characteristics under the given simulation conditions.

4.2 Absorber layer thickness optimization

The thickness of the perovskite absorber layer plays an important role in determining the photovoltaic performance of the solar cell. To investigate the optimum absorber thickness, different absorber layer thicknesses were simulated. The variations of Voc, Jsc, FF and PCE with absorber thickness were analyzed. It is observed that the photovoltaic parameters generally improve with increasing absorber layer thickness. The Voc varies with the increase in absorber thickness, while the Jsc increases due to enhanced photon absorption in the absorber layer. Similarly, the FF and PCE show an overall improvement with increasing absorber thickness. From the obtained simulation results, the maximum Jsc of 28.011610 mA/cm² and FF of 38.89% are obtained at an absorber thickness of 900 nm, with a Voc of 2.3915 V and PCE of 21.63%. At 950 nm, the PCE reaches a maximum value of 21.67%. Therefore, based on the obtained results, the absorber thickness is optimized at 950 nm, which gives the maximum simulated efficiency. Thus, the optimized absorber thickness of 950 nm provides improved photovoltaic performance for the proposed solar-cell structure. Further increase in absorber thickness may lead to increased carrier recombination and therefore may not significantly improve the device performance.

Table. 3 Influence of Absorber thickness on PSC Performance

Thickness (nm)	Voc (V)	Jsc (mA/cm ²)	FF(%)	PCE(%)
400	5.0885	25.054158	15.51	19.78
450	4.5148	25.659118	17.45	20.22
500	4.0596	26.149716	19.37	20.56
600	3.3926	26.882375	23.07	21.04
700	2.9387	27.388665	26.51	21.34
850	2.4967	27.890100	31.00	21.59
900	2.3915	28.011610	32.29	21.63
950	2.3015	28.116629	33.49	21.67

Fig.3 Analysis of Thickness versus Fill Factor

The graph indicates a gradual increase in fill factor (FF) as the voltage (V2) increases. The FF rises from approximately 12% at 2.300 V to about 14% at 2.320 V, while the corresponding thickness increases from nearly 225 to 710 nm. This improvement suggests enhanced charge transport and reduced recombination losses with increasing thickness. The highest FF is obtained at 2.320 V, indicating the most favorable condition among the investigated values.

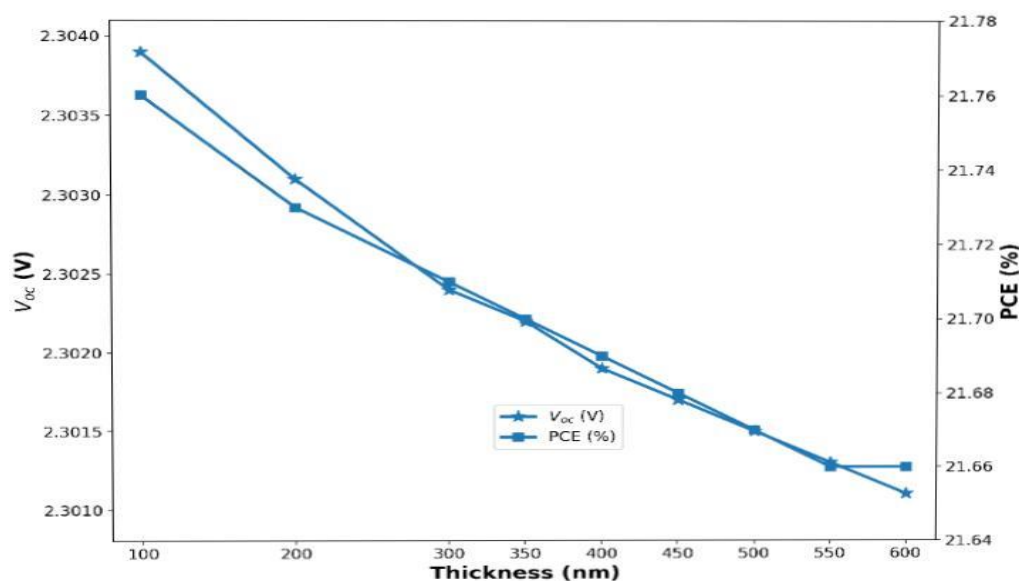
4.3. FTO layer Thickness Optimization

Figure 4 shows the photovoltaic performance of the proposed PSC by varying the FTO layer thickness from 100 to 600 nm. At the optimized thickness of 100 nm, the V_{oc} , J_{sc} and FF are 0.3039 V, 28.232677 mA/cm² and 33.46%, respectively. The corresponding PCE (η) is approximately 2.87%. As the FTO thickness increases, the photovoltaic performance gradually decreases. Therefore, 100 nm is considered the optimized FTO thickness for the proposed solar cell. Optimized FTO thickness = 100 nm

Table.4 Influence of FTO Layer thickness on PSC Performance

Thickness (nm)	V_{oc} (V)	J_{sc} (mA/cm ²)	FF(%)	PCE (%)
100	2.3039	28.232677	33.46	21.76
200	2.3031	28.192802	33.47	21.73
300	2.3024	28.162329	33.48	21.71
350	2.3022	28.149364	33.48	21.70
400	2.3019	28.137542	33.48	21.69
450	2.3017	28.126678	33.48	21.68
500	2.3015	28.116629	33.49	21.67
550	2.3013	28.107287	33.49	21.66
600	2.3011	28.098564	33.49	21.66

Fig.4 Impact of FTO Layer thickness on V_{oc} & PCE



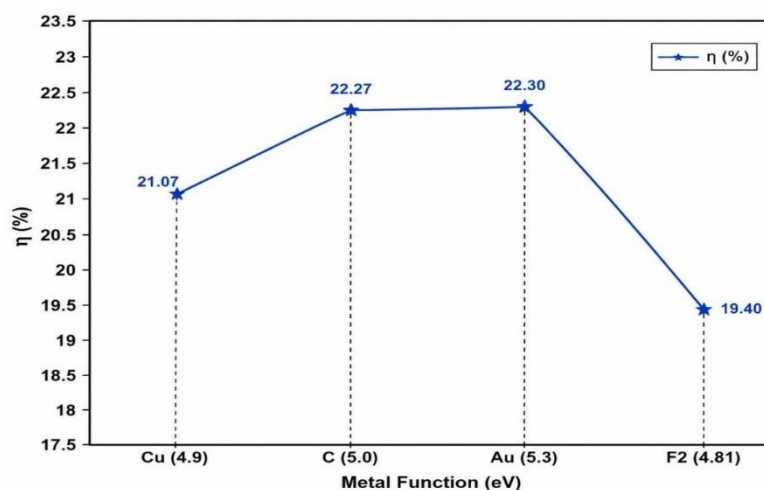
4.4. Back Metal Optimization

The study examined how the back-metal work function influences the photovoltaic performance of perovskite solar cells by testing different materials: Cu, C, Au, and Fe. These variations impact hole extraction and energy-band alignment at the back contact. The ideal back-metal has been chosen based on the highest Power Conversion Efficiency (PCE), along with appropriate Open-Circuit Voltage (Voc), Short-Circuit Current Density (Jsc), and Fill Factor FF(%).

Table 5: Influence of Metal Work Function on PSC Performance

Thickness	Voc(V)	Vsc(mA/cm ²)	FF (%)	PCE(%)
Cu=4.9	2.3015	28.116629	33.49	21.67
C=5	7.4494	28.117902	10.63	22.27
Au=5.3	<u>8.5576</u>	28.117994	9.27	22.30
F2=4.81	0.9651	28.114517	71.50	19.40

Fig. 5 Impact of Back Metal Work Function on Efficiency of PSC



The figure 5 shows that the power conversion efficiency (PCE) varies with the back-metal work function. The efficiency increases from 21.07% for Cu (4.9 eV) to 22.27% for C (5.0 eV) and reaches a maximum of 22.30% for Au (5.3 eV). However, it decreases sharply to 19.40% for Fe (4.81 eV). Thus, Au with a 5.3 eV work function provides the most favorable back contact and the highest simulated PCE.

Conclusion

This study demonstrates the potential of the **FTO/WS₂/FAPbI₃/MoO₃/Cu** architecture for high-performance perovskite solar cells using SCAPS-1D simulation. Systematic optimization of the absorber, transport layers, FTO thickness, and back contact shows that device performance is strongly influenced by layer selection and thickness. The optimized FAPbI₃ absorber thickness of 950 nm provides a PCE of 21.67%, while the FTO thickness of 100 nm gives a maximum PCE of 21.76%. Among the investigated back contacts, Au produces the highest simulated PCE of 22.30%. Overall, the results indicate that suitable interface and device-parameter optimization can improve carrier extraction and photovoltaic performance, providing useful guidance for the future development of efficient FAPbI₃-based PSCs.

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Mathematical Modelling Non-linear Growth and Decay Model

A. Geethalakshmi

Head & Assistant Professor, Department of Mathematics, Madonna Arts and Science College for Women, Affiliated by Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

**Corresponding Author E-Mail ID: narenmithras@gmail.com*

Abstract

Nonlinear growth and decay models are mathematical models used to describe real-world phenomena in which the rate of growth or decay is not proportional to the current quantity. This project focuses on developing and analyzing nonlinear differential equations to model situations such as population growth, spread of diseases, chemical reactions, biological growth, and resource depletion. Models such as the logistic growth model and other nonlinear equations are studied to understand how variables change over time.

Keywords: *Introduction, Preliminary, Non-Linear Logistic growth Model, Nonlinear Decay Model, Applications , Conclusion*

Introduction

Mathematical modelling is an important technique used to represent real-world situations using mathematical equations. Many natural and physical processes involve quantities that increase or decrease with time. Simple exponential models can describe some of these processes, but in many real-life situations, the rate of growth or decay changes depending on factors such as population limits, available resources, environmental conditions, and interactions between individuals.

Nonlinear growth and decay models are used to represent such complex situations more accurately. In these models, the rate of change is not directly proportional to the quantity present. The logistic growth model is one of the most widely used nonlinear models, particularly for studying population growth when resources are limited. Other nonlinear models can be applied to areas such as biological growth, chemical reactions, disease spread, economics, and environmental studies.

The main purpose of this study is to understand the mathematical formulation, solution, and interpretation of nonlinear growth and decay models. By using differential equations, graphical methods, and numerical techniques, the behaviour of these models can be analyzed and their applications in real-life situations can be understood.

Preliminary

Before studying nonlinear growth and decay models, it is necessary to understand some basic mathematical concepts such as functions, differential equations, rates of change, and exponential growth and decay. A growth model describes how a quantity increases with time, while a decay model describes how it decreases. In a nonlinear model, the rate of change depends on the quantity in a non-proportional manner. These basic concepts provide the foundation for constructing and analyzing nonlinear mathematical models.

Explanation

In mathematical modelling, growth and decay describe how a quantity changes over time. Growth means the quantity increases with time. Examples include population growth, bacterial growth, and the increase of money through investment. Decay means the quantity decreases with time. Examples include radioactive decay, cooling, and the reduction of a chemical substance. In a linear model, the rate of change is constant. In an exponential model, the rate of change is proportional to the quantity itself. In a nonlinear model, the rate of change is more complicated and may depend on the quantity in a nonlinear way.

Definition

Nonlinear Growth and Decay Model

A nonlinear growth and decay model describes a quantity whose rate of increase or decrease is not directly proportional to the quantity itself. These models are useful when real-life conditions such as limited resources, environmental factors, or interaction between populations affect the rate of change.

1. Nonlinear Growth Model – Logistic Growth

One of the most common nonlinear growth models is the logistic growth model.

A common nonlinear growth model is the logistic growth model :

$$\frac{dP}{dt} = rP\left(1 - \frac{P}{K}\right)$$

where:

P = population at time t

r = growth rate

K = carrying capacity

t = time

Initially, the population grows rapidly. As it approaches the carrying capacity K, the growth rate decreases. Thus, nonlinear models provide a more realistic description of many real-world growth and decay processes.

Example

Suppose a bacterial population starts with 100 bacteria in a container that can support a maximum of 1,000 bacteria. Initially, the bacteria grow rapidly because there are plenty of resources. As the population approaches 1,000, food and space become limited, so the growth rate decreases.

2. Nonlinear Decay Model

A nonlinear decay model can be represented generally by

$$\frac{dN}{dt} = -kN^2$$

where $k > 0$ is the decay constant.

Example

Consider a chemical substance whose rate of disappearance depends on the square of its concentration. If the concentration is high, the substance decreases rapidly. As the concentration becomes smaller, the rate of decay also becomes slower.

Applications

Nonlinear growth and decay models are used in:

Population growth

Bacterial and biological growth

Spread of diseases

Chemical reactions

Environmental studies
Resource management
Economics and finance

Conclusion

Nonlinear models give a more realistic representation of many real-world processes because they consider changing growth or decay rates rather than assuming a constant rate.

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A Comprehensive Review of Artificial Intelligence and Machine Learning: Concepts, Trends and Applications

L.Hema¹, D. Ajeema Aproz¹, V. Parkavi¹ and K. Nisha^{2*}

¹UG Student, Department of Computer Science, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

²Head & Assistant Professor, Department of Computer Science, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

*Corresponding Author E-Mail ID: nisha2287@gmail.com

Abstract

This paper presents a comprehensive review of Artificial Intelligence (AI) and Machine Learning (ML), exploring foundational concepts, emerging trends, and diverse applications. AI and ML have rapidly evolved, becoming pivotal in numerous fields including healthcare, finance, manufacturing, and autonomous systems. The review begins by outlining key concepts, including the distinctions between AI, ML, and deep learning, and delves into various learning paradigms such as supervised, unsupervised, and reinforcement learning. It highlights significant advancements, such as neural networks, natural language processing, and generative models, emphasizing their impact on industry and research. The paper also examines current trends, including the rise of ethical AI, explainability, and the integration of AI with Internet of Things (IoT) and edge computing, which are shaping the future landscape of AI applications. Additionally, it addresses the challenges and limitations associated with AI and ML, such as data privacy concerns, model interpretability, and the need for sustainable computing solutions.[1]

Keywords: Artificial Intelligence (AI), Machine Learning (ML), Deep Learning, Neural Networks, Supervised Learning, Unsupervised Learning, Reinforcement Learning, AI Trends, AI Applications.

1. Introduction

Artificial Intelligence (AI) and Machine Learning (ML) have emerged as transformative technologies that are reshaping industries and redefining how we interact with

the world. Originating from the quest to build machines capable of mimicking human intelligence, AI encompasses a broad spectrum of techniques and methodologies aimed at creating intelligent agents that can perceive, reason, and act autonomously. ML, a subset of AI,[1] focuses on the development of algorithms and models that enable machines to learn from and make decisions based on data, without being explicitly programmed for specific tasks.

Together, these fields have advanced rapidly, driven by the availability of vast amounts of data, significant improvements in computational power, and the development of sophisticated algorithms. The integration of AI and ML into various sectors, including healthcare, finance, education, and manufacturing, has resulted in innovative solutions that enhance efficiency, accuracy, and decision-making capabilities. In healthcare, AI-powered diagnostic tools and personalized treatment plans are revolutionizing patient care. In finance, ML algorithms are used for fraud detection, risk management, and algorithmic trading. Autonomous vehicles, smart manufacturing, and intelligent virtual assistants are further examples of AI's pervasive impact.[1]

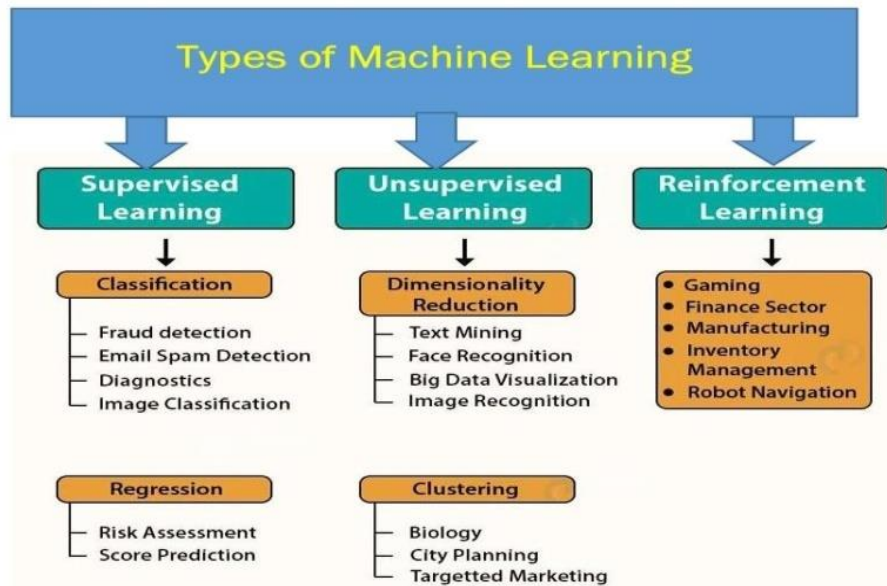
2. Objective

The primary objective of this research paper is to provide a detailed analysis of the concepts, current trends, and practical applications of AI and ML. This review aims to highlight the following:

1. Key trends shaping the future of AI/ML.
2. Real-world applications of AI and ML in various industries.
3. Challenges and ethical concerns associated with AI/ML.
4. Future directions in AI and ML research and development.[2]

2.1 Key Concepts of Machine Learning

Machine Learning is a subset of AI that focuses on algorithms that identify patterns and relationships in data, making predictions or decisions without being explicitly programmed for specific tasks. The main types of ML are:

Fig.1: Types of Machine Learning

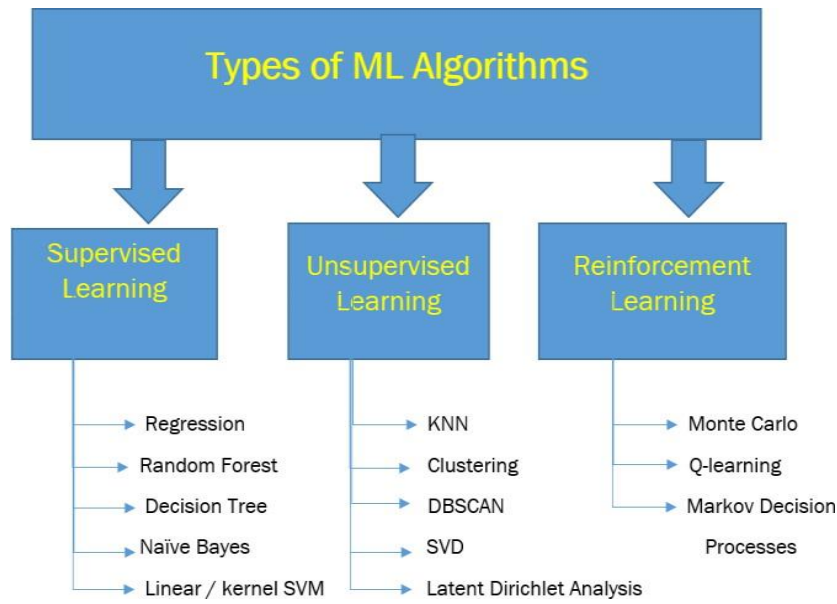
Supervised Learning: In this type, the model is trained on labeled data, where the input and the correct output are known. The goal is to learn a mapping from inputs to outputs that can generalize to new, unseen data. Common algorithms include Linear Regression, Support Vector Machines (SVM), and Neural Networks.

Unsupervised Learning: Here, the model is provided with data that lacks labeled outcomes. The objective is to identify underlying patterns or groupings within the data. Clustering algorithms like K-Means and hierarchical [2] clustering, and dimensionality reduction techniques like Principal Component Analysis (PCA) are commonly used.

Reinforcement Learning: This type involves training models to make sequences of decisions by interacting with an environment. The model learns to achieve a goal by receiving feedback in the form of rewards or penalties. Reinforcement learning is widely used in robotics, gaming, and autonomous systems.

2.2 Core Algorithms in Machine Learning

The power of ML lies in its diverse algorithms, each suited to different types of data and problems. Some of the core algorithms include:

Fig.2: Machine learning Algorithms

Linear/kernel SVM: SVMs are used for classification tasks, finding the optimal hyperplane that separates classes of data with the maximum margin. They are effective in high-dimensional spaces. Linear SVM Works by finding a hyperplane that best separatestwo classes in a high-dimensional space. It maximizes the margin between data points of the two classes. Kernel SVM used when data isn't linearly separable.[3] The kernel trick transforms data into a higher dimension to make it separable using a linear boundary.

Table 1: Linear vs Kernel SVM

Feature	Linear SVM	Kernel SVM
Data	Works well with linearly separable data.	Handlesnonlinearly separabledatabyusingakernel.
Decision Boundary	A straight line (or hyperplane) in feature space.	A complex, curved boundaryin higher-dimensional space.
Speed	Generallyfasteras it only computes intheoriginalspace.	Slower due to the transformationinto higher dimensions.
Example	Spam classification, sentimentanalysis.	Handwrittendigit recognition, compleximageclassification.

K-Means Clustering: An unsupervised clustering algorithm that partitions data into K distinct groups (clusters) based on feature similarity. The algorithm assigns data points to the nearest cluster center, iteratively refining the clusters until the best groupings are found.

DBSCAN (Density-Based Spatial Clustering of Applications with Noise): A clustering algorithm that groups points close to each other while marking points in low-density regions as outliers. It defines clusters as areas of high density, where points within a given distance (epsilon) are considered neighbors. Points not connected to a cluster are classified as noise or outliers.

Deep Q-Networks (DQN): A reinforcement learning algorithm that combines Q-learning with deep neural networks to approximate the Q-values for each state-action pair. DQN uses a neural network to predict the Q-values [3] for different actions, allowing the agent to handle high-dimensional input spaces (like images).

2.3 Importance of Data in AI and ML

Data is the foundation of AI and ML. High-quality, diverse, and representative data sets are crucial for training robust models. Data preprocessing, including cleaning, normalization, and feature extraction, plays a critical role in ensuring the effectiveness of AI and ML models. The success of these models largely depends on the availability of large volumes of accurate data that reflect the real-world scenarios they are intended to address.

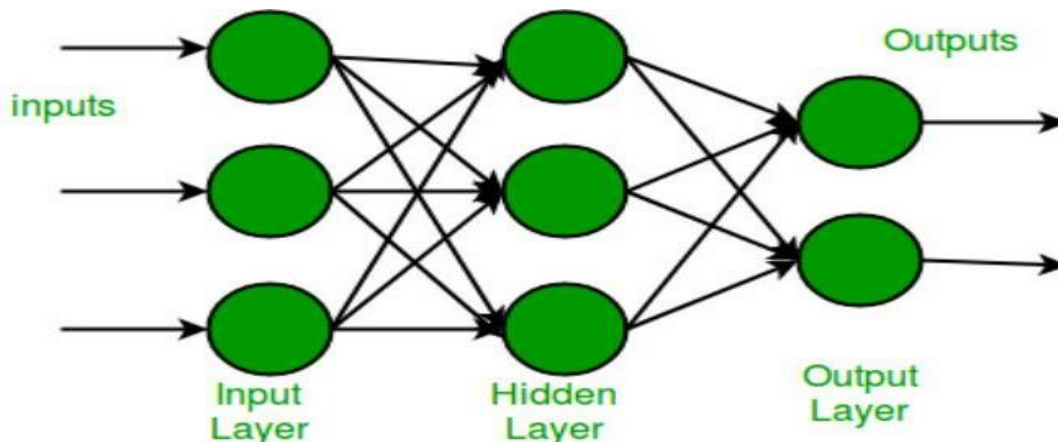
2.4 Deep Learning and Neural Networks

Deep Learning, a specialized subfield of Machine Learning (ML), has garnered significant attention due to its remarkable ability [3] to learn from vast amounts of data and solve complex problems that were previously beyond the reach of traditional algorithms. At the core of deep learning are neural networks, specifically deep neural networks, which are inspired by the structure and function of the human brain. This section delves into the fundamentals of deep learning and neural networks, exploring their architecture, working principles, and the various applications that have revolutionized numerous industries.

2.5 Overview of Neural Networks

Neural networks are computational models composed of interconnected layers of nodes (neurons), resembling the neural structure of the human brain. Each neuron processes inputs, applies a weight, and passes the result through an activation function to the next layer. The basic structure of a neural network includes:

Fig 3: Neural Networks Architecture



Input Layer: Receives the initial data and passes it on to the hidden layers. Each node in the input layer represents a feature of the input data.

Hidden Layers:[4] These layers perform computations and extract features from the input data. A network can have one or more hidden layers, with each layer comprising multiple neurons connected to the previous and next layers. The complexity and depth of the network increase with the number of hidden layers.

Output Layer: Produces the final output, which could be a classification, prediction, or other desired outcomes. The number of neurons in the[4] output layer corresponds to the number of possible output classes or values.

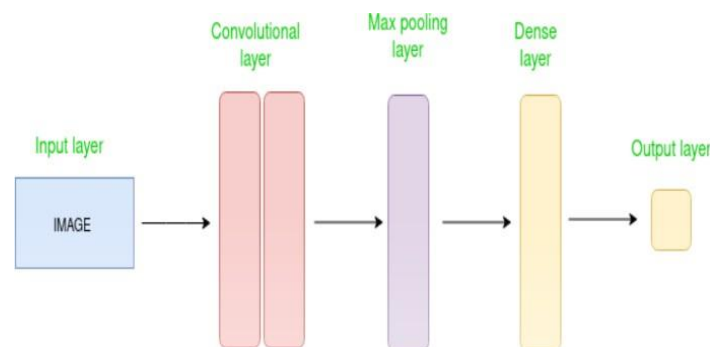
2.6 Deep Learning: Advancing Neural Networks

Deep Learning extends traditional neural networks by adding multiple hidden layers, creating deep architectures that can model intricate patterns in data. Key aspects of deep learning include.

Deep Architectures: Deep neural networks have many layers, allowing them to learn hierarchical representations of data. For instance, in image recognition, initial layers might learn simple features like edges, while deeper layers learn complex structures such as objects.

Convolutional Neural Networks (CNNs): CNNs are specialized for processing grid-like data, such as images. They use convolutional layers to automatically and adaptively learn spatial hierarchies of features, making them highly effective in tasks like image classification, object detection, and segmentation.

Fig.4: Convolutional Neural Networks



2.7 Applications of Deep Learning

Deep learning has enabled significant advancements across various fields:

Image Recognition and Computer Vision: Deep learning models, particularly CNNs, have achieved superhuman performance in image classification, object detection, and segmentation tasks. Applications include medical imaging, autonomous driving, and facial recognition. **Natural Language Processing (NLP):** Deep learning models, such as RNNs and transformers, have revolutionized NLP by improving machine translation, sentiment analysis, and conversational AI systems like chatbots and virtual assistants. **Speech Recognition:**[5]

3. Applications of AI and ML

Artificial Intelligence (AI) and Machine Learning (ML) have become integral to various industries, offering transformative solutions that enhance efficiency, decision-making, and user experiences. The versatility of AI and ML allows for a wide range of applications, from automating routine tasks to solving complex problems. This section explores several key applications of AI and ML across different sectors, highlighting their impact and potential.

3.1 Health care

AI and ML are revolutionizing the health care industry by improving diagnostics, treatment, and patient care.

Medical Imaging: AI algorithms, particularly deep learning models, analyze medical images (e.g., MRI, CT scans) to assist in detecting and diagnosing diseases such as cancer, brain disorders, and cardiovascular conditions. These models can identify patterns and anomalies with high accuracy, often surpassing human radiologists in certain tasks.[5]

Predictive Analytics: ML models predict patient outcomes by analyzing historical health data, enabling early intervention and personalized treatment plans. For instance, predictive models can forecast the likelihood of disease recurrence, patient readmissions, or the effectiveness of treatment options.

Drug Discovery: AI accelerates the drug discovery process by analyzing vast datasets to identify potential drug candidates and predict their effectiveness. This approach reduces the time and cost associated with bringing new drugs to market.

Personalized Medicine: AI and ML facilitate the development of personalized treatment plans based on individual genetic profiles, medical history, and lifestyle factors. This personalized approach improves treatment outcomes and reduces adverse effects.

3.2 Finance

In the finance sector, AI and ML enhance various aspects of operations, from fraud detection to investment strategies.[6]

Fraud Detection: ML models analyze transaction patterns to detect fraudulent activities and anomalies in real-time. By identifying unusual behavior, these models help prevent financial fraud and protect sensitive data.

Algorithmic Trading: AI-driven trading algorithms analyze market data and execute trades at high speeds, leveraging patterns and trends to make informed trading decisions. These algorithms can adapt to changing market conditions and optimize investment strategies.

Credit Scoring: AI models assess credit risk by analyzing a wide range of factors, including transaction history, social data, and behavioral patterns. This approach provides more accurate and dynamic credit scoring, improving loan approval processes.

3.3 Transportation

AI and ML are transforming the transportation industry by improving safety, efficiency, and navigation. Autonomous Vehicles: Self-driving cars use AI to interpret sensor data, navigate roads, and make driving decisions without human intervention. Technologies like computer vision and reinforcement learning enable vehicles to recognize objects, predict pedestrian behavior, and adapt to changing road conditions. Traffic Management: AI models optimize traffic flow by analyzing data from traffic cameras, sensors, and historical patterns. These models improve traffic signal [6] timing, reduce congestion, and enhance overall road safety.

Predictive Maintenance: ML algorithms predict vehicle maintenance needs by analyzing data from sensors and historical performance. This approach helps prevent breakdowns, extend vehicle lifespan, and reduce maintenance costs.

Route Optimization: AI systems optimize delivery routes for logistics companies, considering factors such as traffic conditions, weather, and fuel efficiency. This optimization improves delivery times and reduces operational expenses.

3.4 Education

AI and ML are enhancing the education sector by personalizing learning experiences and improving administrative efficiency.

Personalized Learning: AI-powered platforms adapt educational content and learning paths based on individual student needs, learning styles. This personalization helps students achieve better outcomes and supports differentiated instruction.

Automated Grading: ML algorithms automate the grading process for assignments and exams, providing timely feedback and reducing the administrative burden on educators. This automation allows teachers to focus more on instruction and student support.

Educational Analytics: AI systems analyze student performance data to identify learning gaps, predict academic success, and inform instructional strategies. This data-driven approach helps educators make informed decisions and improve educational outcomes.

Virtual Classrooms: AI and ML enable the creation of virtual learning environments and interactive educational tools. These technologies facilitate remote learning, enhance engagement, and provide access to educational resources from anywhere.[6]

4. Trends in AL and ML

Artificial Intelligence (AI) and Machine Learning (ML) are experiencing rapid evolution, driven by advancements in technology, research, and application areas. This section explores the current trends influencing AI and ML, emphasizing their implications and emerging areas of development.

4.1 Advances in Deep Learning

Transformers and Attention Mechanisms: The advent of transformer models, such as BERT (Bidirectional Encoder Representations from Transformers) and GPT (Generative Pre-Trained Transformer), has significantly advanced natural language processing (NLP). These models use attention mechanisms to capture contextual relationships in text, leading to breakthroughs in tasks like translation, summarization, and sentiment analysis.[7]

Pre-trained Models and Transfer Learning: Pre-trained models that leverage large datasets and then adapt to specific tasks through fine-tuning have become a standard practice. Transfer learning allows models to apply knowledge gained from one domain to different but related tasks, reducing the need for extensive task-specific data and training.

4.2 AI in Edge Computing and IOT

Edge AI: The integration of AI with edge computing involves deploying AI models directly on edge devices such as smartphones, sensors, and IoT devices. This approach enables real-time data processing, reduces latency, and minimizes the need for extensive data transmission to centralized servers.

Efficient Model Deployment: As edge devices often have limited computational resources, there is a growing emphasis on developing light weight and efficient AI models. Techniques like model pruning, quantization, and knowledge distillation are used to optimize performance while conserving resources.[7]

4.3 Ethical and Explainable AI

Ethical AI Development: The ethical implications of AI are garnering increased attention. Researchers and practitioners are focusing on developing guidelines and frameworks to address issues related to algorithmic bias, privacy, and fairness, ensuring that AI systems are used responsibly and equitably.

4.4 AI in Healthcare

AI-Driven Diagnostics: AI is increasingly being used to enhance diagnostic accuracy and patient care in healthcare. Advanced algorithms analyze medical images, genomic data, and electronic health records to assist in early disease detection, personalized treatment, and predictive analytics.

Health Monitoring and Wearables: AI-powered wearables and health monitoring devices are becoming more prevalent, offering real-time tracking of health metrics such as heart rate, glucose levels and activity patterns. These technologies support proactive health management and chronic disease monitoring.

4.5 Autonomous Systems

Self-Driving Vehicles: The development of autonomous vehicles continues to progress, with AI playing a crucial role in enabling vehicles to navigate, interpret sensor data, and make driving decisions. Advances in computer vision, sensor fusion, and reinforcement learning contribute to improving safety and reliability.

Robotics: AI is enhancing the capabilities of robots in various applications, including manufacturing, healthcare, and service industries. Robotics research focuses on improving automation, dexterity, and interaction with humans and the environment.[7]

4.6 AI in Finance

Algorithmic Trading: AI is transforming financial markets through algorithmic trading, where sophisticated models analyze market trends and execute trades at high speeds. These models help optimize investment strategies, manage portfolios, and identify trading opportunities.

Fraud Detection and Risk Management: AI is improving fraud detection and risk management in finance by analyzing transaction patterns and detecting anomalies.[8] Machine learning models help prevent fraudulent activities and manage financial risks effectively.

4.7 AI in Creative Industries

Content Generation: AI technologies are being used to generate creative content, such as art, music, and writing. AI-driven tools assist artists and creators in exploring new forms of expression and generating novel ideas.[9]

Augmented Creativity: AI is supporting human creativity by providing tools for design, brain storming, and content creation. These tools enhance the creative process and enable new ways of producing and interacting with creative works.

5. Future Directions in AL and ML

As Artificial Intelligence (AI) and Machine Learning (ML) continue to advance, several future [10] directions are emerging that promise to shape the landscape of these technologies. This section explores potential avenues for future development and research, highlighting key areas where AI and ML are likely to make significant impacts.

5.1 AI in Real-World Applications

Healthcare Advancements: Future directions in healthcare AI include the development of personalized medicine, where AI models analyze genetic and lifestyle data to tailor treatments to individual patients. Additionally, AI is expected to play a role in drug discovery, predicting disease outbreaks, and enhancing patient care through advanced diagnostics and monitoring systems.

Autonomous Systems: The future of autonomous systems includes further advancements in self-driving vehicles, drones, and robotics. AI will continue to drive improvements in navigation, safety, and interaction with the environment, leading to more capable and autonomous systems.[11]

5.2 Human-AI Collaboration

Augmented Intelligence: The future of AI will likely emphasize collaboration between humans and machines, where AI systems enhance human capabilities rather than replace them. Augmented intelligence focuses on creating tools that support human decision-making and creativity, leading to synergistic interactions between humans and AI.[12]

Human-Centric AI Design: Designing AI systems that align with human values, preferences, and needs will be crucial for their successful integration into daily life. Future research will focus on creating AI technologies that are intuitive, user-friendly, and responsive to human input.[13]

Conclusion

Artificial Intelligence (AI) and Machine Learning (ML) are transforming industries and everyday life through their ability to analyze data, make decisions, and automate complex tasks. As these technologies continue to evolve, they promise to deliver even more profound changes and innovations. This review has explored the fundamental concepts, current trends, applications, and challenges associated with AI and ML, providing a comprehensive understanding of their current [14] state and future directions. The foundational concepts of AI and ML, including supervised, unsupervised, and reinforcement learning, provide the basis for understanding more advanced techniques. Deep learning, with its use of neural networks and advanced architectures like transformers, has significantly enhanced capabilities in natural language processing, computer vision, and more. AI and ML are being applied across various domains, from healthcare and finance to autonomous systems and creative industries. These technologies [15] are driving innovations such as personalized medicine, autonomous vehicles, and intelligent content generation, showcasing their versatility and impact.

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SCAPS-1D Simulation and Performance Optimization of MAPbI₃ Perovskite Solar Cells with TiO₂ ETL and NiO HTL

G. Jayadevi^{1*} and P. Arockia Michael Mercy²

¹UG Student, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

²Vice Principal & Assistant Professor, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

*Corresponding Author E-Mail ID: jayadevi2610@gmail.com

Abstract

Perovskite solar cells (PSCs) are widely studied as promising photovoltaic devices because of their strong light absorption and favourable optoelectronic properties. In this work, the performance of a methyl ammonium lead iodide (MAPbI₃)-based perovskite solar cell was numerically investigated using SCAPS-1D. The proposed device consists of an FTO/TiO₂/MAPbI₃/NiO structure, where FTO acts as the transparent conducting layer, TiO₂ as the electron transport layer, MAPbI₃ as the absorber, and NiO as the hole transport layer. The effect of MAPbI₃ absorber thickness on the photovoltaic performance was investigated by evaluating the open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and power conversion efficiency (PCE). The absorber thickness was varied while the other device parameters were maintained at their selected values. A thickness of 1200 nm for MAPbI₃ was found to provide the best simulated performance, while the TiO₂ and NiO thicknesses were maintained at 50 nm. Under AM1.5G illumination at 300 K, the optimized device achieved a maximum simulated PCE of 23.31%. The results indicate that careful selection of the absorber thickness can improve the photovoltaic performance of the proposed MAPbI₃-based perovskite solar cell and demonstrate the usefulness of SCAPS-1D for numerical device optimization.

Keywords: MAPbI₃; SCAPS-1D; Perovskite solar cell; Absorber thickness; TiO₂; NiO; PCE

1. Introduction

Photovoltaic technology offers a promising way to meet the growing demand for energy while reducing the dependence on conventional fossil fuels. As a result, considerable

research has been focused on developing photovoltaic devices that are efficient, economical, and environmentally sustainable. Perovskite solar cells (PSCs) have received significant attention due to their strong light absorption and favourable optoelectronic properties, which make them promising candidates for high-efficiency photovoltaic applications [1,2]. Among the various perovskite materials, methyl ammonium lead iodide (MAPbI₃) [2,3] has been widely investigated because of its suitable bandgap and effective light absorption characteristics. The performance of MAPbI₃-based solar cells is influenced by several factors, including defects, carrier recombination, and charge transport. Therefore, selecting suitable material and device parameters is important for obtaining better photovoltaic performance. Charge-transport layers are particularly important because they assist in extracting and transporting photo generated carriers from the absorber. Titanium dioxide (TiO₂) [4,5] is commonly used as an electron transport layer (ETL) due to its favourable electron transport properties and compatibility with MAPbI₃-based devices. The thickness of the ETL can also affect carrier transport and the overall photovoltaic response. Nickel oxide (NiO/NiO_x) [6] is another widely investigated material for use as a hole transport layer (HTL) in perovskite solar cells. Its electrical properties and interaction with the MAPbI₃ absorber can influence hole extraction and recombination processes. In the present device, NiO is used as the HTL to facilitate hole transport from the absorber toward the back contact. Fluorine-doped tin oxide (FTO) [7] is used as the transparent conducting layer because of its suitable electrical conductivity and optical transparency. The combination of FTO, TiO₂, MAPbI₃, and NiO provides a suitable multilayer configuration for studying charge transport and photovoltaic performance in the proposed device. Numerical simulation is a useful method for examining solar-cell behaviour before experimental fabrication. Among the available simulation tools, SCAPS-1D [2,5,8] is widely used for investigating semiconductor and perovskite solar-cell structures. It allows different device parameters, such as absorber thickness, transport-layer properties, defect density, interface conditions, and back-contact properties, to be examined systematically. The back-metal contact can also influence the electrical behaviour of a solar cell through its work function and interaction with the HTL. In this study, Au, Ag, Cu, and Fe were considered as possible back-contact materials. Their influence on the photovoltaic parameters was evaluated using SCAPS-1D to identify a suitable contact for the proposed device.

In the present work, a FTO/TiO₂/MAPbI₃/NiO perovskite solar-cell structure was investigated using SCAPS-1D. The effect of MAPbI₃ absorber thickness on open-circuit

voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE) was analysed. The $MAPbI_3$ absorber thickness was varied to determine a suitable thickness, while the TiO_2 and NiO thicknesses were maintained at 50 nm. Different back-metal contacts were also investigated. The final device consists of 500 nm FTO / 50 nm TiO_2 / 1200 nm $MAPbI_3$ / 50 nm NiO , with the selected back contact. The optimized device achieved a maximum simulated PCE of 23.31% under the selected simulation conditions.

2. Design of the Proposed Perovskite Solar Cell

The proposed perovskite solar cell consists of a multilayer structure of FTO/ TiO_2 / $MAPbI_3$ / NiO , as shown in Fig. 1. The absorber layer is the main part of the solar cell, where incoming sunlight is absorbed and converted into electron-hole pairs. To collect these generated charges efficiently, electron and hole transport layers are placed between the absorber and the electrodes. In the proposed device, FTO is used as the transparent conducting electrode, while TiO_2 acts as the electron transport layer (ETL). $MAPbI_3$ is selected as the absorber because of its suitable bandgap and strong light-absorption capability. NiO is used as the hole transport layer (HTL), followed by a suitable back metal contact. Fig. 1. Configuration of the proposed FTO/ TiO_2 / $MAPbI_3$ / NiO perovskite solar cell.

The ETL and HTL are important for efficient charge extraction and transport. TiO_2 helps extract electrons from the $MAPbI_3$ absorber and reduces the movement of holes toward the electron-collecting electrode. Similarly, NiO facilitates the extraction of holes from the absorber and helps reduce unwanted electron recombination at the interface. TiO_2 was selected as the ETL because of its suitable energy-band alignment, good optical transparency, chemical stability, and favourable electron-transport properties. NiO was chosen as the HTL because of its wide bandgap, good stability, and suitable valence-band alignment with $MAPbI_3$.

The $MAPbI_3$ absorber layer plays the major role in absorbing sunlight and generating electron-hole pairs. In this study, the absorber thickness was varied using SCAPS-1D to investigate its effect on the photovoltaic performance. Based on the optimized simulation conditions, the $MAPbI_3$ thickness was selected as 1200 nm, while the TiO_2 and NiO thicknesses were maintained at 50 nm. Therefore, the proposed device structure is: FTO/ TiO_2 / $MAPbI_3$ / NiO /Back Contact. Under the optimized simulation conditions, the proposed device achieved a maximum power conversion efficiency (PCE) of 23.31%.

3. Design and Simulation

Fig. 1. Schematic structure of the proposed FTO/TiO₂/MAPbI₃/NiO PSC

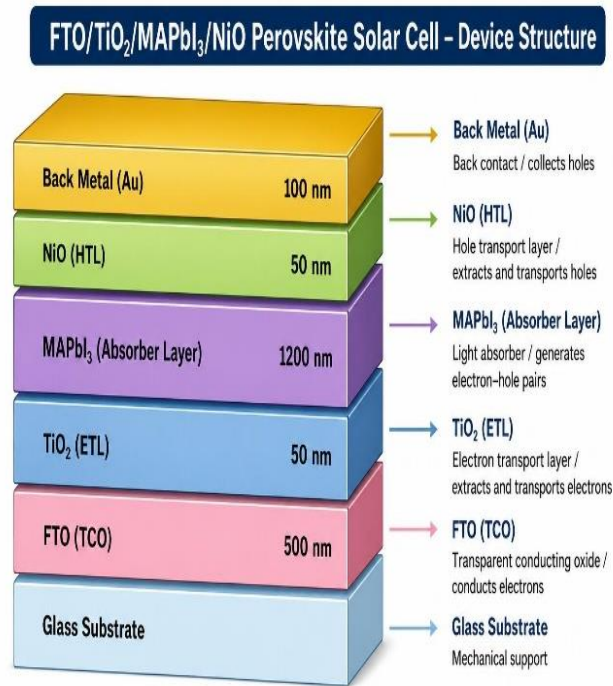


Fig. 1 Schematic structure of the proposed FTO/TiO₂/MAPbI₃/NiO perovskite solar cell.

The proposed FTO/TiO₂/MAPbI₃/NiO perovskite solar cell was investigated using SCAPS-1D (Solar Cell Capacitance Simulator). SCAPS-1D is a one-dimensional solar-cell simulation software developed at the University of Gent, Belgium. It is commonly used to study the electrical and photovoltaic behaviour of multilayer semiconductor solar cells. In this work, SCAPS-1D was used to examine the charge transport and overall photovoltaic performance of the proposed device. The electrical behaviour of the device is determined by solving fundamental semiconductor equations, including the Poisson equation, continuity equations, and charge-transport equations. These equations help describe the distribution of electrostatic potential, electrons, holes, current densities, carrier generation, and recombination within the different layers of the solar cell.

3.1 Governing Equations

1. Poisson Equation

The variation of electrostatic potential across the solar-cell structure is described by the Poisson equation

$$d^2\phi(x)/dx^2 = q/[\epsilon_0\epsilon_r] [p(x) - n(x) + N^D(x) - N^A(x)]$$

Where ϕ represents the electrostatic potential, q is the elementary charge, ϵ_0 is the vacuum permittivity, and ϵ_r is the relative dielectric permittivity. The terms $p(x)$ and $n(x)$ represent the hole and electron concentrations, respectively, while N^D and N^A denote the donor and acceptor concentrations.[2,7,11]

2. Continuity Equations

The continuity equations describe the generation, recombination, and movement of charge carriers within the device:

$$\frac{dJ_n}{dx} = q(G - R)$$

$$\frac{dJ_p}{dx} = -q(G - R)$$

Here, J_n and J_p represent the electron and hole current densities, respectively. G is the carrier generation rate, while R represents the recombination rate.[2,7,11]

3. Charge Transport Equations

$$J_n = q\mu_n nE + qD_n \left(\frac{dn}{dx}\right)$$

The movement of electrons and holes through the different layers is described using the drift-diffusion equations:

$$J_p = q\mu_p pE - qD_p \left(\frac{dp}{dx}\right)$$

Where μ_n and μ_p are the electron and hole mobility's, respectively. D_n and D_p represent the electron and hole diffusion coefficients, while E is the electric field. [2,5,11]

4. Absorption Coefficient

The absorption coefficient of the MAPbI₃ absorber is related to the photon energy and its bandgap. It can be expressed as:

$$\alpha(h\nu) = A\sqrt{(h\nu - E^g)/(h\nu) + B}$$

Where A and B are material-dependent constants, h is Planck's constant, ν is the photon frequency, and E^g is the bandgap energy of the absorber. [2,7]

3.2 Simulation Conditions

The proposed FTO/TiO₂/MAPbI₃/NiO solar cell was simulated under standard photovoltaic conditions. The operating temperature was maintained at 300 K, with AM1.5G solar illumination at an incident power density of 1000 W/m² (1 Sun). The device consists of

FTO as the transparent conducting electrode, TiO₂ as the electron transport layer (ETL), MAPbI₃ as the absorber layer, and NiO as the hole transport layer (HTL). The material parameters required for the SCAPS-1D simulation, such as bandgap, electron affinity, dielectric permittivity, effective density of states, carrier mobility, thermal velocity, and doping concentration, were obtained from published literature. The layer thicknesses were selected based on the simulation requirements, with particular attention given to the absorber thickness. The final device consists of 500 nm FTO, 50 nm TiO₂, 1200 nm MAPbI₃, and 50 nm NiO. The photovoltaic performance was evaluated using open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE). Under the specified AM1.5G illumination conditions, the optimized device achieved a maximum simulated PCE of 23.31%.

3.3 Parameters of the Proposed Device

The proposed perovskite solar cell is designed with the FTO/TiO₂/MAPbI₃/NiO structure. The material properties required for the SCAPS-1D simulation are presented in Table 1. These parameters include the optical, electrical, and transport properties of each layer, which are important for evaluating the performance of the device. In this study, the thickness of the MAPbI₃ absorber layer is set to 1200 nm, while the thicknesses and other parameters of the FTO, TiO₂, and NiO layers are kept constant. The selected parameters are used to investigate the photovoltaic behaviour of the proposed solar-cell structure under standard illumination conditions.

Table 1: Parameters of the Proposed Device Simulation using SCAPS ID

Parameter	NiO	TiO ₂	MAPbI ₃	FTO
Thickness (nm)	50	50	1200	500
Electron affinity, χ (eV)	3.60	3.20	1.55	3.50
Bandgap (eV)	1.80	4.00	3.90	4.00
Dielectric permittivity, ϵ_r	11.9	9.0	25	9.0
N _c (cm ⁻³)	2.20×10^{18}	2.20×10^{18}	2.20×10^{18}	2.20×10^{18}
N _v (cm ⁻³)	1.80×10^{19}	1.80×10^{19}	1.80×10^{19}	1.80×10^{19}
Electron mobility, μ_n (cm ² /Vs)	2	20	10	20
Hole mobility, μ_p (cm ² /Vs)	2	1	10	10

4. Results and Discussion

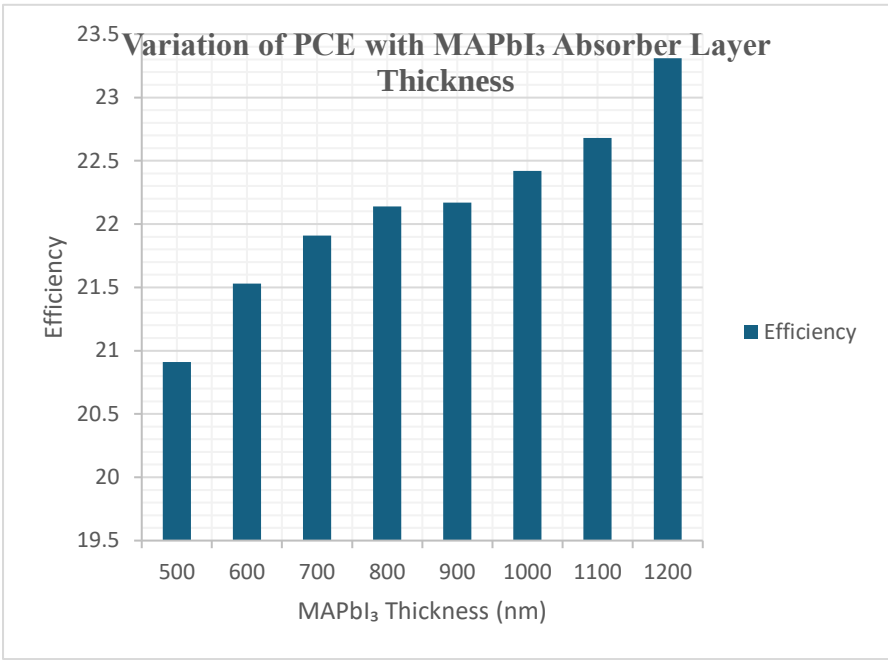
4.1 MAPbI₃ Absorber Layer Thickness Optimization

The thickness of the absorber layer plays an important role in determining the overall performance of a perovskite solar cell. In the proposed device, MAPbI₃ acts as the absorber layer, where incident sunlight is absorbed and converted into electron–hole pairs. Therefore, changing the absorber thickness can influence the amount of light absorbed and the generation and transport of charge carriers. In this study, the thickness of the MAPbI₃ absorber layer was systematically varied using SCAPS-1D, while the properties and thicknesses of the other layers, namely FTO, TiO₂, and NiO, were kept constant. The absorber thickness was varied from 400 to 1200 nm, and the corresponding photovoltaic parameters, including open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE), were obtained from the simulations. The simulated results are presented in Table 2. The variation of PCE with MAPbI₃ absorber thickness is also illustrated in Fig. 2. Based on the obtained results, an absorber thickness of 1200 nm was selected as the optimized thickness for the proposed device.

Table 2: Effect of MAPbI₃ absorber thickness on the photovoltaic performance

MAPbI ₃ thickness (nm)	V _{oc} (V)	J _{sc} (mA/cm ²)	FF (%)	PCE (%)
500	6.6072	23.49125	13.47	20.91
600	5.5751	24.2585	15.92	21.53
700	4.7893	24.769334	18.47	21.91
800	4.1803	25.11992	21.09	22.14
900	3.6991	25.366989	23.74	22.17
1000	3.3811	25.5015	26.34	22.42
1100	3.0632	25.6361	28.94	22.68
1200	2.7452	25.937220	31.53	23.31

Fig. 2: Variation of PCE with MAPbI₃ Absorber layer Thickness.



4.2 NiO HTL Defect Density Analysis

Defect density in the NiO hole transport layer (HTL) can affect the movement of charge carriers and the overall performance of the solar cell. A higher number of defects may increase carrier recombination and reduce the efficient transport of photo generated carriers. Therefore, the defect density of the NiO layer was considered in the present simulation study. The NiO HTL defect density was analysed using SCAPS-1D. During this analysis, the NiO thickness was kept fixed at 50 nm, while the other device parameters were kept unchanged. Different defect-density values were tested to identify a suitable condition for the proposed device. Among the tested values, a defect density of Voc gave a successful simulation result. Hence, this value was selected for the NiO HTL and used in the following simulations. The selected NiO parameters are given in Table 3.

Table 3: Selected parameters of the NiO HTL

Parameter	Value
NiO HTL thickness	50 nm
Defect density	$1 \times 10^{15} cm^{-3}$

4.3 TiO₂ - ETL Defect Density Analysis

TiO₂ is used as the electron transport layer (ETL) in the proposed device to assist the extraction and transport of photo generated electrons from the MAPbI₃ absorber. Defects present in the ETL can influence charge transport and recombination, which may affect the photovoltaic performance of the device. In this study, the defect density of the TiO₂ ETL was investigated using SCAPS-1D. The TiO₂ thickness was kept fixed at 50 nm, while the other device parameters were maintained at their selected values. Among the investigated conditions, a defect density of Jsc provided a successful simulation result. Therefore, this value was selected for the TiO₂ ETL and used in the subsequent simulations.

Table 4: Selected parameters of TiO₂ ETL

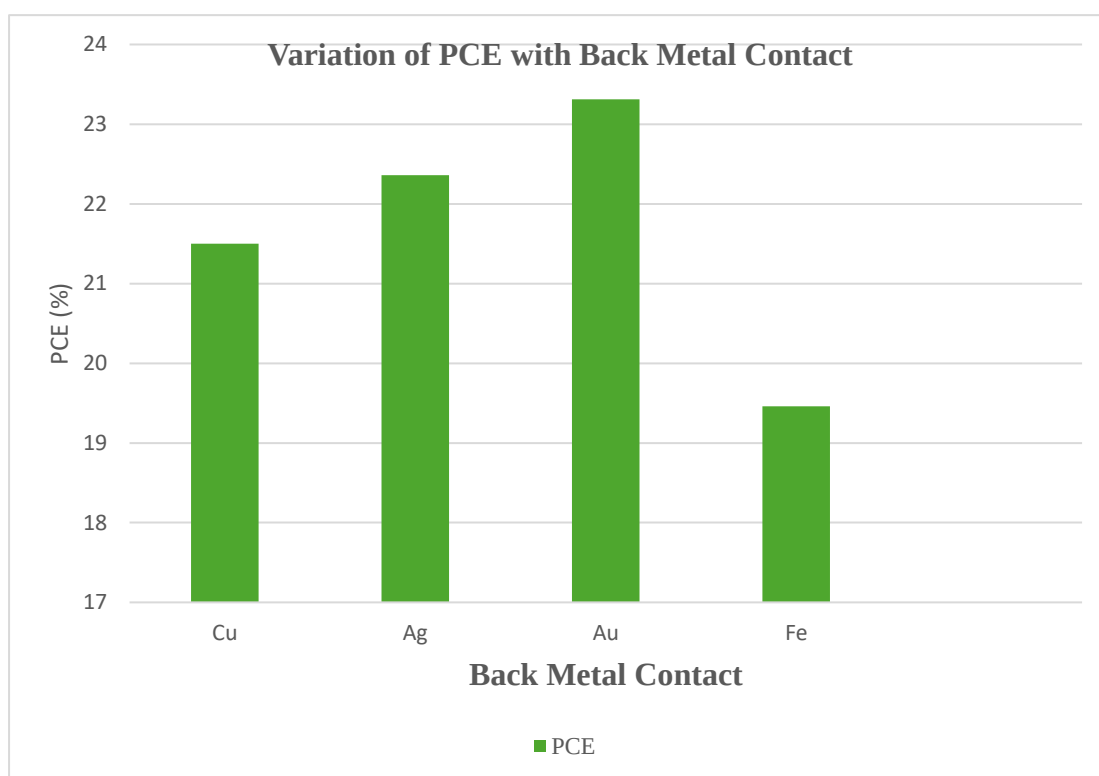
Parameter	Value
TiO ₂ ETL thickness	50 nm
Defect density	$1 \times 10^{15} \text{ cm}^{-3}$

4.4 Back Metal Contact Analysis

The effect of different back metal contacts on the photovoltaic performance of the proposed perovskite solar cell was investigated using SCAPS-1D. Cu, Ag, Au, and Fe were considered as different back metal contacts, while the other device parameters were kept unchanged. The simulated photovoltaic parameters, including open-circuit voltage (voc), short-circuit current density (Jsc), fill factor (FF), and power conversion efficiency (PCE), are presented in Table 4. The choice of back contact can influence charge extraction and the quality of the contact interface, thereby affecting the overall device performance.

Table 5: Effect of different back metal contacts on photovoltaic performance

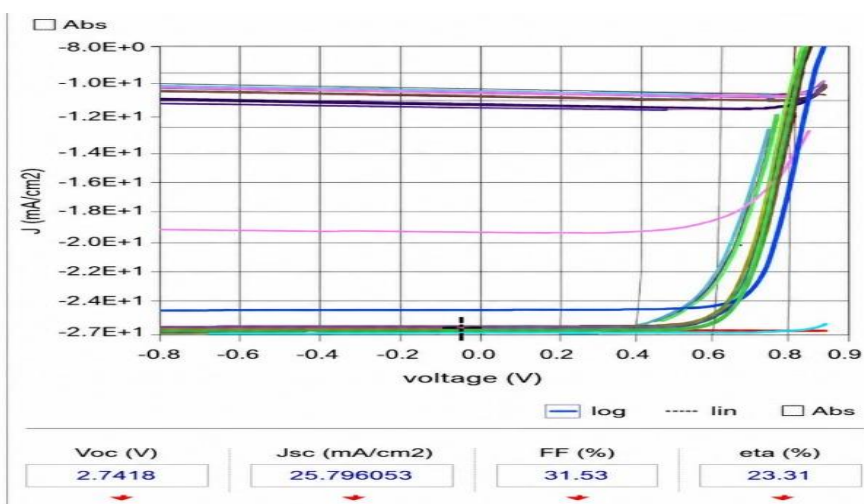
Back Metal	V _{oc} (V)	J _{sc} (mA/cm ²)	FF (%)	PCE (%)
Cu	1.6548	25.793775	50.57	21.50
Ag	2.6632	25.795940	32.46	22.36
Au	2.7418	25.796053	31.53	23.31
Fe	1.0041	25.788155	75.22	19.46

Fig. 3: Variation of PCE with Back metal contact.

The results show that changing the back metal contact produces a noticeable variation in the photovoltaic parameters. The v_{oc} values remain nearly similar for all the selected metals, whereas j_{sc} , FF, and PCE show more noticeable changes. Among the investigated back contacts, Au provides the highest v_{oc} of 2.7418 V and a PCE of 23.31%. Although Fe exhibits the highest FF of 75.22%, its PCE is lower because of its lower j_{sc} . Therefore, based on the obtained PCE, Au is selected as the optimized back metal contact, giving the maximum simulated efficiency of 23.31%. This optimized Au contact is used for the subsequent device analysis.

4.5 J–V Characteristics of the Optimized Device

The current density–voltage (J–V) characteristics were obtained for the optimized FTO/TiO₂/MAPbI₃/NiO perovskite solar cell using SCAPS-1D under AM1.5G illumination. The optimized device consists of a 1200 nm MAPbI₃ absorber, 50 nm TiO₂ ETL, 50 nm NiO HTL, NiO defect density of v_{oc} , and Au as the back metal contact. The J–V curve is used to evaluate the main photovoltaic parameters of the optimized device, including FF, and PCE.

Figure 4: J–V characteristics of the optimized PSC with Au as the back metal contact**Table 6: Output Characteristics as a function of Back Metals**

Parameter	Value
Voc	2.7418
Jsc	25.796053 mA/cm ²
FF	31.53 %
PCE	23.31 %

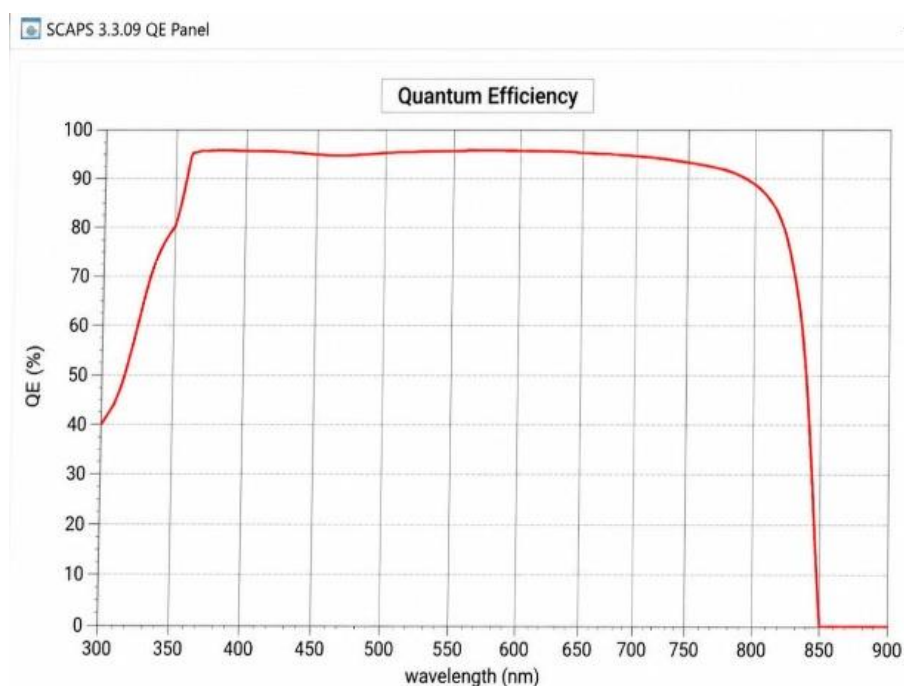
The J–V characteristic is an important method for evaluating the photovoltaic performance of a solar cell. The main parameters obtained from the J–V curve are open-circuit voltage Voc, short-circuit current density Jsc, fill factor (FF), and power conversion efficiency (PCE). Voc represents the maximum voltage generated when the current is zero, while Jsc represents the current density when the applied voltage is zero. The fill factor indicates the quality of the J–V curve and is related to the maximum power point of the device. PCE represents the ratio of electrical power produced by the solar cell to the incident solar power. These parameters are commonly used to evaluate and compare optimized SCAPS-1D solar-cell devices.

The optimized device exhibits a Voc of 2.7418 V, Jsc of 25.796053 mA/cm², FF of 31.53%, and PCE of 23.31%. The obtained J–V characteristics indicate the photovoltaic response of the optimized device under AM1.5G illumination. Among the optimized

parameters, the obtained PCE represents the combined contribution of V_{oc} , J_{sc} , and FF. Therefore, the optimized device configuration with Au as the back metal contact was selected for further analysis.

4.6 Analysis of Quantum Efficiency

Figure 5: Quantum efficiency spectrum of the Optimized PSC



The quantum efficiency (QE) spectrum represents the ability of the optimized perovskite solar cell to convert incident photons into collected charge carriers at different wavelengths. The QE remains high over a broad visible wavelength range, indicating efficient photon absorption and charge-carrier collection. As the wavelength approaches the absorption edge of the MAPbI_3 absorber, the QE decreases rapidly because photons with energies below the absorber bandgap are less effectively absorbed. Thus, the QE response confirms the effective spectral response of the optimized device.

Conclusion

The optimized perovskite solar cell was successfully analysed using SCAPS-1D. The device showed a maximum PCE of 23.31%, with a V_{oc} of 2.7418 V, J_{sc} of 25.796053 mA/cm^2 , and FF of 31.53%. Among the investigated back metal contacts, Au provided the highest PCE and was therefore selected for the optimized device. The J–V and QE analyses

further confirm the photovoltaic and spectral response of the optimized cell. Overall, the optimized device configuration demonstrates suitable performance for further analysis and simulation.

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Computational Design of Stable and High – Performance Lead – Free Cs_2TiBr_6 Perovskite Solar Cells through Multilayer Interface Engineering

S. Jeya Shree^{1*} and P. Arockia Michael Mercy²

¹UG Student, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

²Vice Principal & Assistant Professor, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

*Corresponding Author E-Mail ID: sjeyashree891@gmail.com

Abstract

Perovskite solar cells (PSCs) have attracted significant attention due to their high-power conversion efficiency and low fabrication cost. In this work, a lead-free perovskite solar cell is designed and numerically analyzed using SCAPS-1D. The proposed device consists of Au/CuO / Cs_2TiBr_6 / CeO_2 / FTO layers, where CeO_2 acts as the electron transport layer (ETL), Cs_2TiBr_6 serves as the absorber layer, and CuO functions as the hole transport layer (HTL). The device performance is optimized by varying the thickness and electrical properties of the individual layers. The optimized device achieves a maximum power conversion efficiency (PCE) of 20.60%. The obtained results indicate that the Au/CuO / Cs_2TiBr_6 / CeO_2 / FTO structure is a promising configuration for developing efficient and environmentally friendly lead-free perovskite solar cells.

Keywords: Lead-free Perovskite Solar cell, SCAPS-1D, Cs_2TiBr_6 , CeO_2 , CuO, FTO, Numerical simulation

1. Introduction

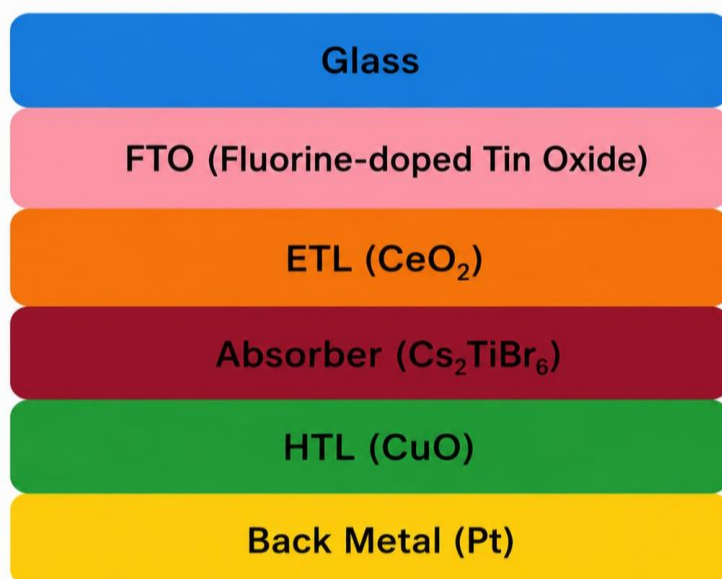
This study the photovoltaic performance of the CuO/ Cs_2TiBr_6 / CeO_2 / FTO device is investigated using the SCAPS-1D simulation program. SCAPS 1D is a one -dimensional numerical simulation tool widely used to analyze and optimize thin – flim solar- cell devices. The simulation enables the investigation of important photovoltaic parameters such as Open – circuit voltage (Voc), Short – Circuit Current density (Jsc), Fill Factor (FF), and Power

Conversion Efficiency (PCE)[1-4]. The proposed device consists of FTO as the front transport contact, CeO_2 as the electron transport layer (ETL), Cs_2TiBr_6 as the absorber layer, CuO as the hole transport layer (HTL), and Pt as the back metal contact. The proper selection of transport layers and content material is important for achieving efficient charge extraction and suitable energy – level alignment in perovskite solar cells [1]. The Cs_2TiBr_6 absorber is considered as a promising lead -free perovskite – inspired material because of its suitable optoelectronic properties and potential for photovoltaic application CuO and CeO_2 are selected as the HTL and ETL respectively, to facilitate efficient hole and electron transport. Pt is employed as the back contact because of its suitable work function for efficient hole collection. By optimization the structural and electrical parameters of the Pt/ CuO / Cs_2TiBr_6 / CeO_2 /Fto configuration the study aims to improve the Photovoltaic parameters and achieve enhanced device efficiency [2-4].

Overall, the numerical investigation provides useful into the design and optimization of Cs_2TiBr_6 – based solar cells. The optimized parameters obtained from SCAPS -1D can serve as a theoretical guideline for developing efficient and stable lead -free perovskite solar – cell devices [1-2].

2. Design of Novel Perovskite Solar Cell

Fig. 1 Configuration of $\text{CuO}/\text{CeO}_2/\text{Cs}_2\text{TiBr}_6$ based solar cell



The structure of the multi-layer Cs_2TiBr_6 -based solar cell employed in this investigation is shown in Fig. 1. The basic component of the photovoltaic device is an absorber layer, which captures photons and converts them into electron–hole pairs. The sandwich of two electrodes and an absorber layer may be sufficient for photovoltaic response, but the best solar cell performance is achieved when electrons and holes are spread optimally inside the photovoltaic system. The proposed solar cell consists of $\text{CuO}/\text{Cs}_2\text{TiBr}_6/\text{CeO}_2/\text{FTO}$. FTO acts as the front electrode, CeO_2 as the ETL, Cs_2TiBr_6 as the absorber layer, and CuO as the HTL. This structure improves charge separation and transport, thereby enhancing the photovoltaic performance.

3. Design and Simulation

SCAPS software version 3.3.07, a one-dimensional (1-D) photovoltaic simulator created by ELIS, University of Gent, Belgium, was used in this investigation. To determine the density of electrons and holes individually, SCAPS-1D uses four different sets of equations. The following are the equations:

1. Differential form of the Poisson equation in terms of electrostatic potential is displayed below

$$D^2\phi(x)/dx^2 = -e/(\epsilon_0\epsilon_r) [p(x) - n(x) + N_D(x) - N_A(x) + \rho_p - \rho_n].$$

Where ϕ is the electrostatics potential, e is electronic charge, ϵ_0 is the permittivity of vacuum, ϵ_r is relative permittivity, N_A stands for shallow acceptor density while N_D stands for shallow donor impurity density. Similarly, ρ_p and ρ_n denote hole density and electron density distribution, with $p(x)$ and $n(x)$ denoting electron and hole density distribution.

2. The continuity equation is given as follows

$$dJ_n/dx = G - R$$

$$dJ_p/dx = G - R$$

where J_n and J_p represent the electron and hole current densities, G signifies the generation rate, and R represents the recombination rate.

3. The electron and hole current densities are given by the charge transport equation as follows

$$J_n = D_n \frac{dn}{dx} + \mu_n n \frac{d\phi}{dx}$$

$$J_p = D_p \frac{dp}{dx} + \mu_p p \frac{d\phi}{dx}$$

Where μ_n is the electron mobility and μ_p is the hole mobility.

- The absorption coefficient with respect to photon energy $\alpha(h\nu)$ can be calculated by the equation given below.

$$A(h\nu) = (A + B/h\nu) \sqrt{(h\nu - E_g)}$$

Where A and B are constant, h is Planck constant, ν is frequency of photons and E_g is the band gap of the absorber layer. The band discontinuity between the interfaces of the different layers is small and therefore can be neglected for simplicity. For this study, the proposed Au/CuO / Cs₂TiBr₆/ CeO₂/ FTO perovskite solar cell structure was used for the SCAPS-1D simulation. The ambient temperature was maintained at 300 K and the solar spectrum was AM1.5 (1000 W/m²). The electrical and physical parameters required by SCAPS-1D for FTO, CeO₂, Cs₂TiBr₆, CuO were obtained from the corresponding literature [10] .

Table.1: Input Parameters for the Optimized PSC using SCAPS-1D

Parameters	HTL (CuO)	ETL (CeO ₂)	ABSORBER (Cs ₂ TiBr ₆)	FTO
Thickness (nm)	900	0.45	0.10	500
Band gap	1.5	3.5	1.6	3.2
Electron affinity	4.07	4.6	4.47	4.4
Dielectric permittivity	18.1	9	10	9
NC(cm-3)	2.2E+19	1.0E+20	1.0E+21	2.2E+18
NV(cm-3)	5.5E+20	2.0E+21	1.0E+18	1.8E+19
Thermal velocity	1.0E+7	1.0E+7	1.0E+7	1.0E+7
Thermal velocity	1.0E+7	1.0E+7	1.0E+7	1.0E+7
Electron mobility	100	1.0E+2	4.4E+0	9E+1
Hole mobility	0.1	1.0E+7	2.5E+0	9E+1
ND(cm-3)	0	1.0E+21	1E+19	7E+20
NA(cm-3)	1E+15	0	1E+19	0

4. Result and Discussion

This section includes an analysis of various HTLs and ETLs for an innovative device, as well as optimizations of the thickness of HTL, absorber and ETL, and the optimization of absorber defect density for Cs_2TiBr_6 absorber.

4.1.ETL, HTL, Optimization for Cs_2TiBr_6 Perovskite Absorber

Figure 2 illustrates the performance of all device configurations with each HTL and ETL variation with standard thicknesses, while keeping Au as the back metal contact. In this study, CuO was selected as the HTL and CeO_2 was selected as the ETL for the Cs_2TiBr_6 perovskite absorber. The effect of HTL and ETL materials on the photovoltaic parameters was investigated to obtain an optimized device configuration. The thickness of the HTL, ETL and Cs_2TiBr_6 absorber layer was further optimized to improve the overall power conversion efficiency of the proposed solar cell.

Table 2: Impact of ETL Thickness on PSC Performance

Thickness (nm)	Voc(V)	Jsc (mA/cm ²)	FF(%)	PCE (%)
400	2.21	26.45	34.60	20.25
350	2.19	26.25	34.20	19.80
300	2.17	26.05	33.80	19.35
250	2.15	25.85	33.40	18.90
200	2.13	25.65	33.00	18.45

5. HTL Layer Thickness Optimization

Fig.2 Variation of Jsc with CeO_2 Thickness

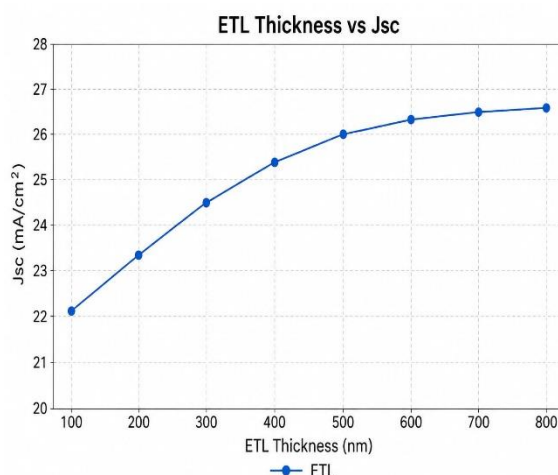
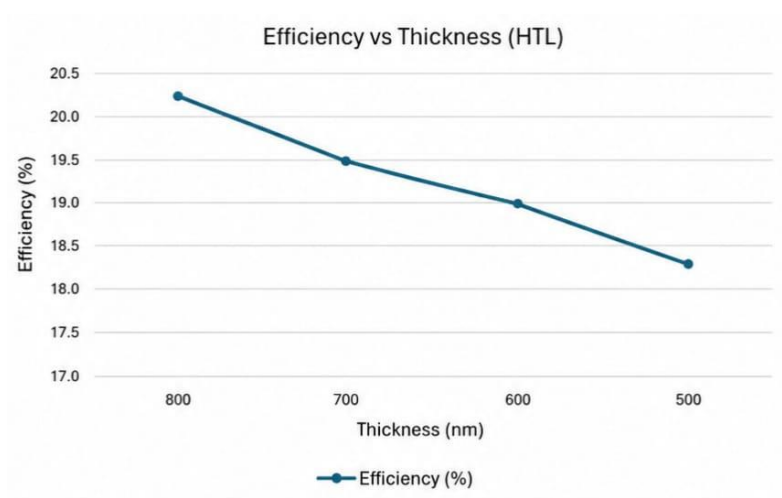


Figure 3 shows the PSC performance with CuO as the HTL, where the thickness was varied to determine the optimum value. At the optimized thickness of 800 nm, the device achieved $V_{oc} = 2.20$ V, $J_{sc} = 26.40$ mA/cm², FF = 34.50%, and PCE = 20.05%.

Table 3: Influence of HTL Thickness on PSC Performance

Thickness (nm)	Voc (V)	Jsc (mA/cm ²)	FF(%)	PCE(%)
800	2.20	26.40	34.50	20.05
700	2.18	26.20	34.10	19.45
600	2.16	26.00	33.70	18.95
500	2.14	25.80	33.30	18.30

Fig. 3 variation of η with CuO Thickness



7. Absorber Thickness Optimization

Figure 4 shows the PSC performance with Cs₂TiBr₆ as the absorber layer, where the thickness was varied to determine the optimum value. At the optimized thickness of 0.10 μ m (100 nm), the device achieved $V_{oc} = 2.222$ V, $J_{sc} = 26.58$ mA/cm², FF = 34.90%, and PCE = 20.60%.

Table 4: Influence of Absorber thickness on PSC Performance

Thickness (nm)	Voc(V)	Jsc (mA/cm ²)	FF(%)	PCE(%)
0.10	2.22	26.58	34.90	20.60

0.20	2.21	26.56	34.92	20.59
0.30	2.21	26.55	34.92	20.57
10	2.233	25.32	34.70	19.63
20	2.254	25.13	34.40	18.72

8. Optimization of FTO Thickness

Figure 5 shows the PSC performance with FTO, where the thickness was varied to determine the optimum value. At the optimized thickness of 450 nm, the device achieved $V_{oc} = 2.21$ V, $J_{sc} = 26.40$ mA/cm², FF = 34.60%, and PCE = 20.20%.

Fig .4 variation of η with Cs₂TiBr₆ Thickness

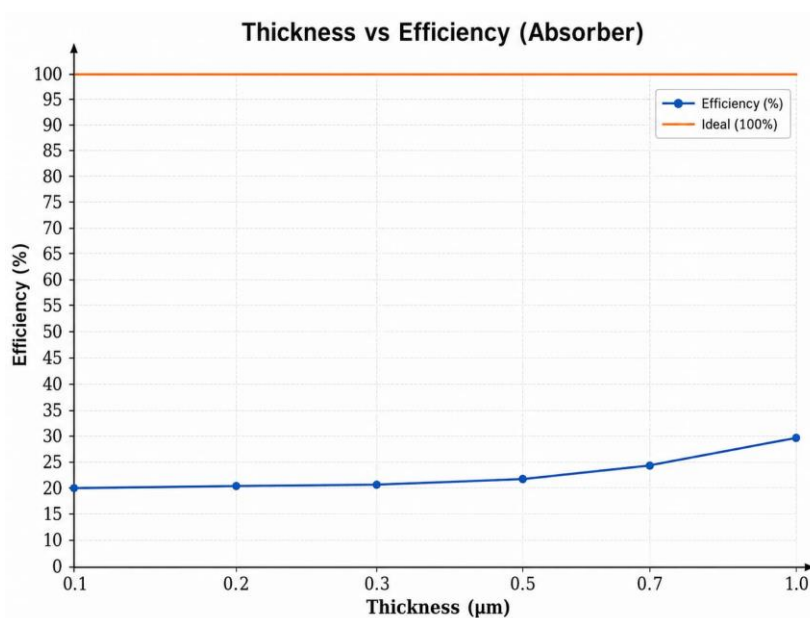
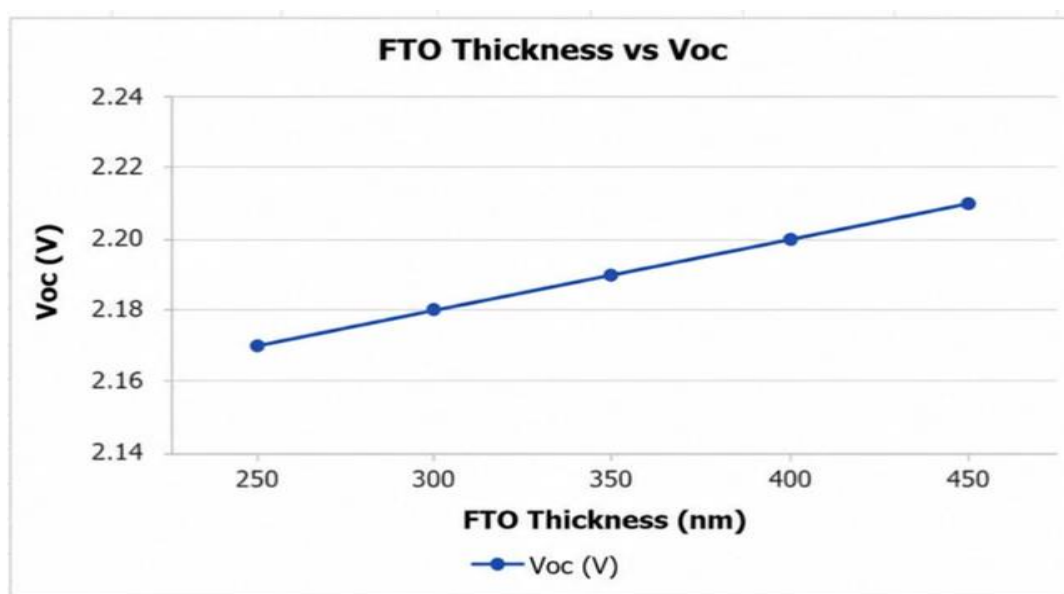


Table 5: Influence FTO Thickness on PSC Performance

Thickness (nm)	Voc(V)	Jsc(mA/cm ²)	FF(%)	PCE(%)
450	2.21	26.40	34.60	20.20
400	2.20	26.25	34.30	19.85
350	2.19	26.10	34.00	19.50
300	2.18	25.95	33.70	19.15
250	2.17	25.80	33.40	18.80

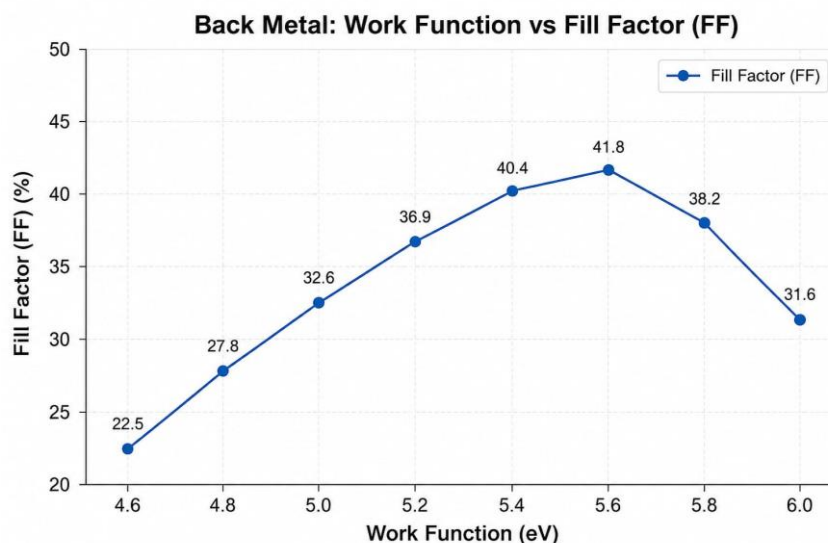
Fig. 5 Variation of Voc with FTO Thickness

9.Back Metals Optimization

Figure 6 shows the optimization of the Pt back metal contact with a work function of 5.65 eV. The optimized device achieved Voc = 2.21 V, Jsc = 26.58 mA/cm², FF = 34.92%, and PCE = 20.60%.

Table 6: Influence of Back Metal Contacts on PSC Performance

Back metal	Work function (eV)	Voc(v)	Jsc (mA/cm ²)	FF(%)	PCE(%)
Au	4.65	0.1751	26.02	54.23	2.47
Al	4.90	0.2251	26.22	59.53	3.51
Ni	5.15	0.6750	26.54	78.69	14.10
Pt	5.65	2.2190	26.58	34.92	20.60

Fig.6 variation of FF with Back Metal Contacts

Conclusion

In this study, a perovskite solar cell was numerically investigated using the SCAPS-1D simulation tool. The proposed device structure was optimized by varying the ETL, HTL, absorber layer thickness, FTO thickness, and back contact parameters. The optimized thicknesses were 800 nm for the HTL, 400 nm for the ETL, 100 nm for the absorber, and 450 nm for FTO. Pt was employed as the back contact with a work function of 5.65 eV. The optimized device achieved a V_{oc} of 2.21 V, J_{sc} of 26.58 mA/cm², FF of 34.92%, and maximum PCE of 20.60%. These results demonstrate that appropriate optimization of the charge transport layers, absorber layer, FTO thickness, and back contact can significantly improve the photovoltaic performance of the perovskite solar cell.

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Drug Discovery Based on Computational Techniques

S. Gokila

Assistant Professor, Department of Computer Science, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

Corresponding Author E-Mail ID: nisha2287@gmail.com

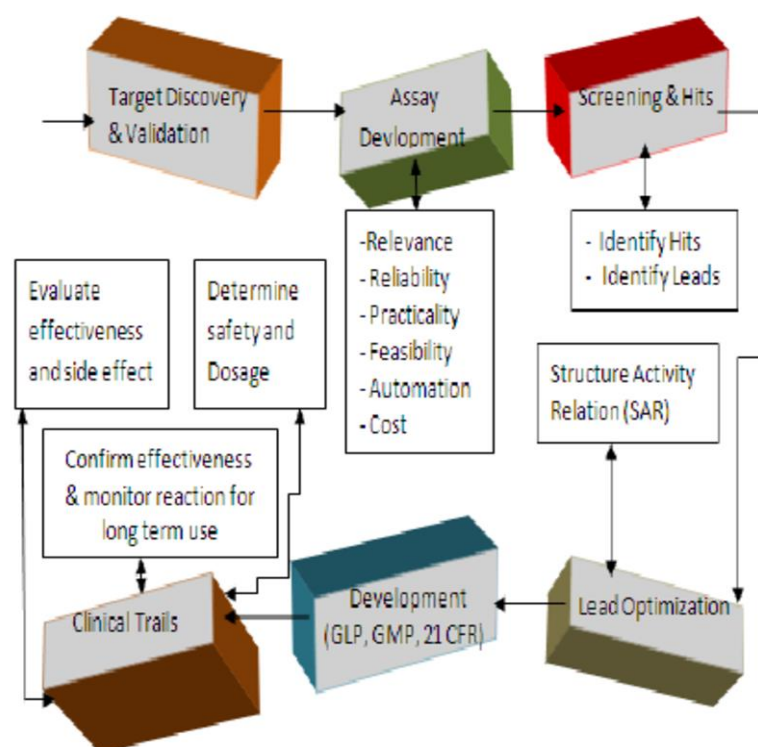
Abstract

Drug discovery and design is an intense, lengthy and consecutive process that starts with the lead and target discovery followed by lead optimization and pre-clinical in vitro and in vivo studies. This paper throws light on different computational techniques that play a vital role in the drug discovery and design process. This paper present brief description of different computational techniques such as Particle Swarm Optimization, Ant Colony Optimization, Artificial Neural Network, Fuzzy Logic, Genetic Algorithm, Genetic Programming, Evolutionary Programming, Evolutionary Strategy and also provide a tabular comparison of these techniques as well as list of computational tools / software.

Keywords: *Biological Inspiration, Computational Techniques, Fitness Function programming, Optimization*

1. Introduction

The traditional approach through which drugs were discovered mainly based on hit and trial method, like plant-based medicines, serendipity (penicillin) and chemical modification. But there has been major change in the field of drug discovery and design in the previous two decades. In the post-genomic era, rational drug recovery is major approach fir discovering and designing new drugs. Generally, experimental techniques are it is estimated then a drug from concept to market would take 12 years and cost more than US\$800 million on an average [1]. For every 5,000 – 10,000 compounds that enter the research and development (R&D) pipeline, ultimately only one receives approval [2]. Several chemical technologies such as genomic data, chemical genomics, high throughput screening in the drug discovery process and computational tool / software have been developed and applied in drug discovery and design, to short the research cycle and to reduce the expenses. Computer-aided drug design (CADD) is one of such evolutionary techniques [3]. In the present time, drug design is based on disease models. The process consists of many steps that are shown in figure 1.

Figure 1: Key steps in Drug discovery and Design process

This paper provides an overview of computational technique use in drugs discovery and design.

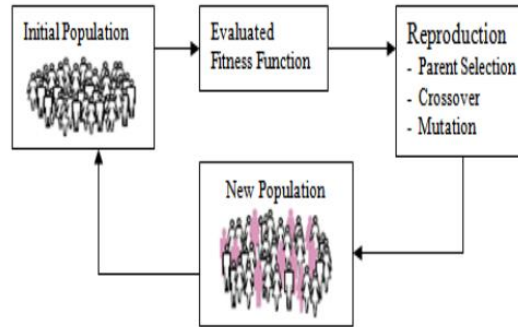
2. Computational Techniques: An Overview

Bacterial and viral infections like polio, small pox, tuberculosis, AIDS and related diseases that were once life threatening now have become minor public health concerns only because of new computational techniques that help in discovery and designing of new potent drugs.

2.1 Genetic Algorithm

Genetic algorithm is a searching technique that is used to find approximate solutions for optimization and search problems. The genetic algorithm is proposed by John Holland in the 1960's [4,5]. The genetic algorithms are the sub class of evolutionary computations. They are stochastic optimization methods are provide a powerful means to perform directed random searches in a large problem space as encountered in chemo metrics and drug design [4].

In this step the genetic operator such as selection, crossover and mutation are applied to generate the next generation of population.

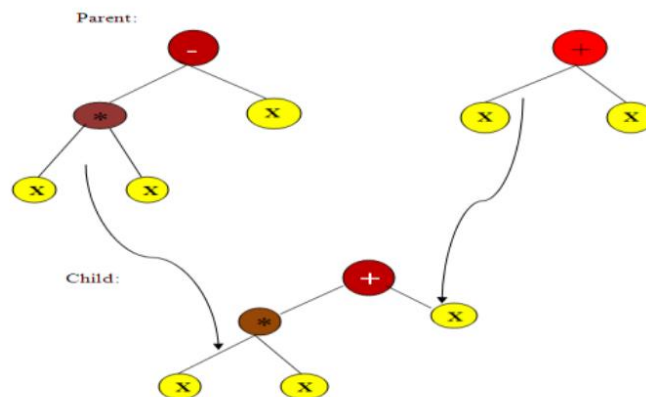
Figure 2: Working of genetic algorithm

2.2 Genetic programming

GP is the variant of the genetic algorithm. The GP is proposed by the John Koza [6, 7]. John Koza successfully applied genetic algorithms on LISP to solve a wide range of problems. Koza was defining the six steps to solving a problem using genetic programming.

1. Choosing the terminal.
2. Functions
3. Fitness function
4. Control parameters
5. Termination criterion.
6. Determining the architecture i.e program's automatically define functions (ADFs).

GP implements the Darwin theory of evolution as a computer program. These programs are written in the programming language. So the GP follows are the form of parse tree that can be shown in the genetic algorithm but the possible solution can be described as following

Figure 3: Shows the Evolution of new population from previous population

2.3 Evolutionary Strategy

ES was developed by Rechenberg and Schwefel [8,9]. Basically ESs was designed for parameter optimization problems. During the developmental period of ES, a series of strategies were explored which can be listed as follows [10]:

- ❖ (σ, σ) random walk
- ❖ $(\sigma + \sigma)$ one parent $\rightarrow$ one child – select from all
- ❖ $(\mu + \sigma)$ multi parent $\rightarrow$ multi-child – select from all
- ❖ $(\mu + \lambda)$ multi-parent $\rightarrow$ multi-child – select from all
- ❖ (μ, λ) multi-parent $\rightarrow$ multi-child – select from children

The signification of the strategy can be defined as:

- ❖ $()$ Represents the two successive generations.
- ❖ $,$ Represents the selection method from only one child.
- ❖ $+$ Represents the selection method from the pool i.e parent and child.
- ❖ σ Represents the only one individual.
- ❖ μ Represents the populations of parent.
- ❖ λ Represents the populations of children.

The above discussed strategies are used to define the successive generations of individuals. An individual is encoded through the real numbers. Each individual consist the strategy parameters. The strategy is further enhanced by the addition of rotation angles α which orient the direction of most extreme mutation based on the variances and covariance of the expected sets of mutation. [5].

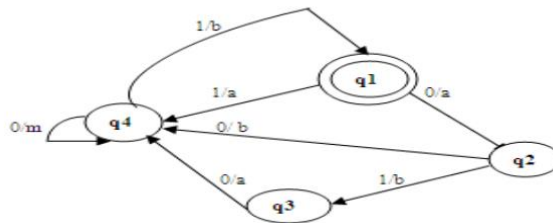
2.4 Evolutionary Programming

EP is a sub branch of EA. Fogel was proposed evolutionary programming as a means to develop artificial intelligence and argued that intelligent behaviour requires both the ability to predict changes in an environment, and a translation of the prediction into actions appropriates for reaching a goal [11,12]. In EP, a finite state machine is used to represents the individuals. Q Set of finite states.

- ❖ Σ Set of input symbol
- ❖ Δ Set of output symbol.
- ❖ Transition function

Transition function plays the important role in the finite state machine. It performed the mapping of the current state with an input symbol and produced the next state that can be act as next generation. The fitness of an individual is calculated by presenting sequentially to the finite state machine the symbols in the environment and observing the predicted output [13].

Figure 4: A Finite state machine with the state (q1,q2,q3,q4)

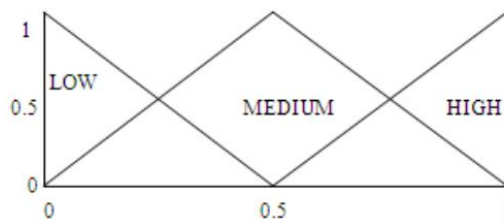


The output symbols belongs to the set (0,1) and the output symbol belongs to the set (a, b, m). the labelled edge represents the transition from one state to another state. The double circle state represents then initial state.

2.5 Fuzzy Logic

Fuzzy logic is the science of reasoning, thinking and inference that recognizes and uses the real world phenomenon that everything is a matter of degree [14]. The original idea of fuzzy logic comes from a paper published by the Zadeh [15]. Fuzzy set is differing from traditional set theory i.e fuzzy set has unsharp boundaries [16]. Fuzzy logic can be especially useful in describing target properties for optimizations.

Figure 5: Fuzzy logic representation of temperature



The basic steps of the fuzzy set in the process modelling described as

- Arrange the input and output dataset.
- Clustering the output set.
- Mapping the fuzzy inputs to the output
- Identify the significant variables
- Use the rule base in inference

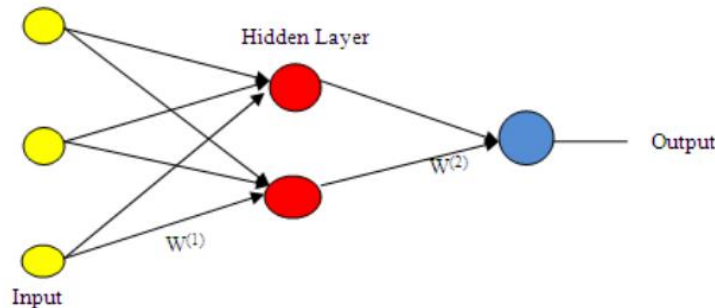
2.6 Artificial Neural Network

Neural network can be defined as networks of neuron. The biological inspiration of neural network comes from the nervous system network of human being especially the human brain. Basically the neural network consist the two elements:

- Processing Elements
- Connection Weight

Now, the term artificial neural network can be defined as a computer science paradigm that makes use of an abstract modelling of the neuronal structure of the brain as a tool for pattern recognition. The figure 7 showed a systematic architecture of two layers ANN.

Figure 6: Architecture of two layers ANN



Neural networks can be applied to four basic types of applications [4]:

- ❖ Association;
- ❖ Classification (Clustering);
- ❖ Transformation (different representation)
- ❖ Modelling

2.7 Particle Swarm Optimization

PSO is population based stochastic optimization method inspired by observation of swarms of insect, shoals of fish, bird flocking etc. There are the million of insect and living creature on the earth as well as in the sea. Each creature posses the unique characteristic that characteristic makes the difference between these.

The movement of each particle depends on two points.

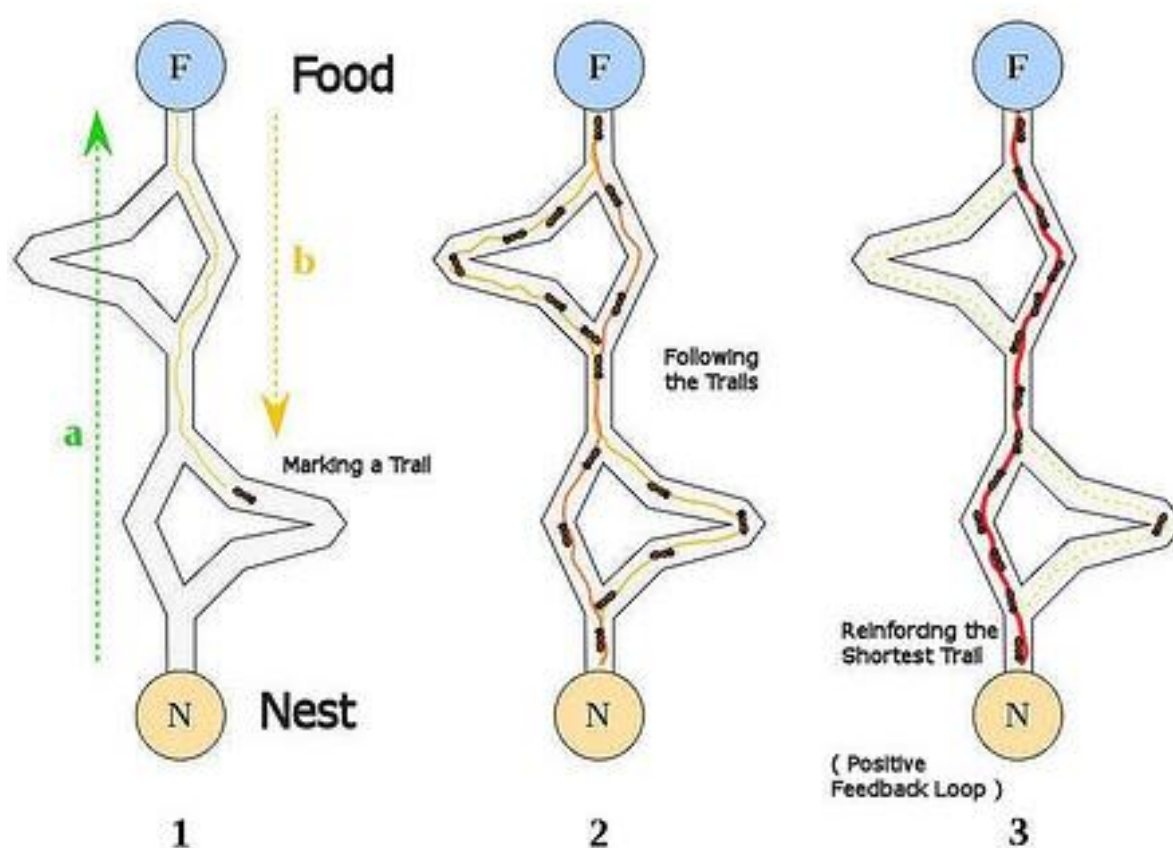
- Particle best position since the algorithm started ($pBest$)
- The best position of the particles around it ($lBest$) or of the whole group ($gBest$)

In each iteration, the particle changes its velocity towards $pBest$ and $gBest$. So the swarm explores the solution space looking for promising zones.

2.8 Ant Colony Optimization

Ant Colony Optimization (ACO) is a meta-heuristic algorithm inspired by the foraging behaviours of ants and developed by Marco Dorigo (Milan, Italy) and others in early 1990s. Basically the algorithm is based on a series of random decisions (by artificial ants) and probability of decisions changes on each iteration.

Figure 7: shows the ant colony and behaviour of ant



An ant's decision to perform a task depends on the physical state of the environment and the social interactions with other ants. The behaviour of artificial ants is inspired from real ants: they lay pheromone trails (obviously in a mathematical form) on the graph edges and choose their path with respect to probabilities that depends on pheromone trails.

3. Conclusion

This paper deals with the scope of nature inspired optimization techniques in drugs designing and discovery. The main objective of paper to describe the various computational

techniques that are used in drugs discovery and designing. How these techniques applied in drugs discovery and what are the pros and cons of particular techniques in drug discovery and designing.

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Analysis and Research of the Mining Concepts

V. Malathi¹, M. Sumaiya Asmee¹, M. Rihana Ashiram Beevi¹, K. Abitha¹ and K. Nisha^{2*}

¹UG Student, Department of Computer Science, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

²Head & Assistant Professor, Department of Computer Science, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

*Corresponding Author E-Mail ID: nisha2287@gmail.com

Abstract

Mining is a new research area it needs more discussion among to define exactly what it is. Web Mining is an important research field in data mining [1]. The aim of this paper is to explore the role of data mining for information extraction in web content, structure and usages mining in current web modules, and the outlines the process of extracting patterns from data. Web mining is the application of data mining techniques to extract knowledge from web data, including web documents, hyperlinks between documents, usage logs of web sites, etc. and also the complete work of the web data mining is explained.

Keywords: Data Mining, Web Mining, Web usage mining, Web content mining, Web structure mining

1. Introduction

Internet is the global sharing computing network. It enables global communications between all connected computing devices[1]. It provides the platform for web services and the World Wide Web. Web is the totality of web pages stored on web servers. As the Web grows higher, the internet data are extremely difficult to search and retrieve information and also necessary for users to utilize automated tools in order to find, extract, filter, and evaluate the desired information and resources. In addition, transformation of the Web is the primary tool where many organizations and corporations provide information on the web such as on-line shopping, distance education, news broadcasts etc[2]., Though Web is a medium of accessing variety of information it leads to several problems: to find relevant information, to extract useful knowledge. So Web mining is an emerging research area to solve all the problems.

2. Data Mining

Data Mining is the process of extracting knowledge from the large amount of data like data bases, data ware houses data mart etc. This includes the interestingness of the user patterns, Mining the information is the concept [2,3]. Knowledge is the resulting data from mining process.

Raw Data Interesting Patterns Knowledge

Data mining consists of five major elements:

1. Extract transform, transaction data. and load
2. Store and manage the data in a multidimensional database system.
3. Provide data access to business analysts and information technology professionals.
4. Analyze the data by application software
5. Present the data in a useful format, such as a graph or table.

Data Mining Process includes various stages. Processing the data is the difficult thing. By various iterative steps these processing will be executed. Those interactive and iterative steps are.

i). Data Integration

Integration is the process of combining the data from various sources. Data are available at different sites.

Data can be from databases like merchant database, store databases, from data mart like departmental store databases and from external sources like questionnaires from users, training sets[4]. So all these data different sources of data can easily be collected and combined via this integration process.

ii) Data Selection

In the above integration step all the data are combined. Here those combined data are selected.

Selection means selecting the needed data from those integrated data [5]. For example, while identifying budget and big user, needed data are user name, income level, transaction history instead of education level, phone no. and all. Only the needed data are selected.

iii) Data Cleaning

In this step selected data are cleaned for removing the errors. Data from different sources can have errors, noises and inconsistencies. These things should be removed for effective results. Errors can be typing error, questionnaire error.

These errors can be manually detected and removed. Noisy data are removed using binning method and other methods. Inconsistencies are different data format in different sources. Those inconsistencies are removed in this data cleaning step.

iv) Data Transformation

Transformation is the process of transferring data to appropriate format for data mining process. That is data are collected from different sources. Each data source having its own format. While combining for data mining process it is very difficult to process the data. For example [6] Date data in Data mart source having the format of month, date and year. But in other sources it is always in the format of date, month, and year. These discrepancies are easily formatted using Normalization, Generalization and such methods.

v) Data Mining

Data mining[7] is the process of mining or extracting knowledge from external sources of data. Mining means discovering knowledge from data sources. Knowledge Discovery from Data.

vi) Pattern Evaluation

From the above step extracted knowledge is evaluated for effectiveness. For evaluation process it takes help from Knowledge base. Knowledge base has all the information regarding user profile, user interest, user expectations and all. These information are collected by thoroughly watching the user activities, clicking streams and all. Result of the knowledge base help to evaluate the mining result.

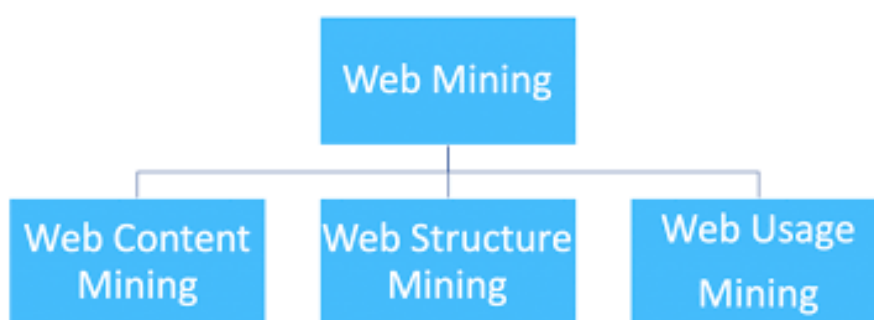
vii) User Representation

Evaluated results are then represented according to the user format. Representation can be a bar chart, Pie chart which compares different data. And it can be table of data like report. Queries given by users are transferred to other process of data mining.

3. Web Mining

In recent years graphs of computer usage and World Wide Web are in increasing level. People who are using these facilities cannot be accountable. As it periodically user requirements also increasing. Users want the Wide World should shrink into a tab as he/she requires way. So there should be a system that analysis the user's expectation & preferences explicitly from user profiles or implicitly from user log files. [2] Here the difficulty is automatic extraction of the useful information. Numerous web pages and sites are created day by day using HTML and other web applications. It is necessary to create a system using Data mining concepts in web technology. That is called Web data mining system. It has many subdivisions.

Fig 1: Subdivisions of Web Mining



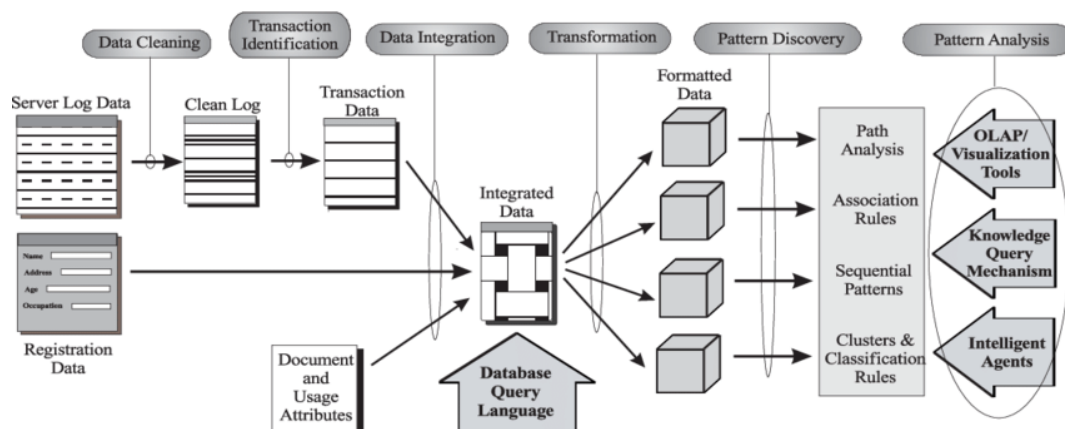
Web content mining finds useful information from data in the web. It considers different kinds of data such as[10]: images, audio, video and texts

Web structure mining provides structural information documents and sites, about web

Web usage mining finds access patterns from web sites.

4. Proposed Approach

The proposed method consists of several phases such as file integration or merging, pre-processing, discovery and pattern analysis. [5,6,7,8] This paper focuses only on pre-processing phase that deals with Web Mining. The figure 2 shows the complete web data mining work.

Fig 2: Web data Mining work

5. Conclusion

As the web and its usage continues to grow, the opportunity to analyze web data and extract all manner of useful knowledge from it. We analysis the researches in the area of data mining and web mining. Three recognized types of web data mining are introduced generally [12]. Web mining is a rapid growing research area. Web content mining is related but different from data mining and text mining. Web data are mainly semi-structured and/or unstructured [14].

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Explainable Artificial Intelligence: An Expanded Taxonomy by Mechanism and Interpretability Perspectives

Nisha. K

Head & Assistant Professor, Department of Computer Science, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

Corresponding Author E-Mail ID: nisha2287@gmail.com

Abstract

Explainable Artificial Intelligence (XAI) has emerged as a critical area of research to address the opacity of modern machine learning models, with deep neural networks being a major focus. While numerous surveys of XAI exist, many either focus narrowly on specific techniques or lack a unifying structure that connects diverse approaches into a coherent framework. This paper presents a comprehensive literature review that consolidates both widely adopted and less commonly discussed XAI methods, including perturbation and gradient based explainers, dimensionality reduction techniques, counterfactual frameworks, and attribution methods. We adopt the well-established taxonomy in literature, which categorizes XAI approaches into scoop based, complexity based, model based, and methodology based classes, and extend it in two important ways: (i) by introducing finer operational subcategories (e.g., gradient vs. perturbation based, model specific vs. model agnostic), and (ii) by introducing a complementary interpretability level distinction that categorizes explanations as structural, semantic, or behavioural according to the level at which understanding is achieved. For each method, we summarize its underlying principles and highlight reported strengths and limitations, enabling readers to understand both the technical foundations and the trade-offs involved. By structuring the field into this extended taxonomy, the survey provides a road map for new researchers entering XAI and offers a reference point for identifying gaps where novel approaches can be developed.

Keywords: *Machine learning, Explainable AI*

1. Introduction

In recent years, neural networks (NNs) have found widespread applications across diverse fields, from manufacturing and agriculture to healthcare and finance. However, while

these models offer powerful predictive capabilities, their opaque “black box” nature limits user trust and acceptance. As [1] notes, reinforcement learning (RL) agents, in particular, require further analysis to understand the strategies they learn and to evaluate the transferability of these insights across different production systems, which could play a significant role in building trust in RL and other complex algorithms [1].

In agriculture, neural networks have been successfully applied to tasks like plant and disease identification, as well as fruit counting, where their ability to handle vast and complex datasets provides a significant advantage [2]. Similarly, deep learning models have shown great promise in healthcare, with strong success in medical image classification and segmentation, facilitating improvements in diagnosis and treatment planning [3]. Beyond image analysis, artificial neural networks are also increasingly used in healthcare organizational decision making and diagnostic processes, where their predictive accuracy supports better patient outcomes [3]. Furthermore, in the finance sector, neural networks outperform traditional statistical models in tasks such as financial fraud detection, demonstrating their capacity to identify subtle patterns in complex datasets that would otherwise go unnoticed [3]. In addition to these domains, neural networks have also been applied in energy and engineering systems, including the modeling of solar air heaters and the performance analysis of solar assisted heat pump systems, where their ability to capture nonlinear system dynamics improves predictive accuracy and system optimization [4].

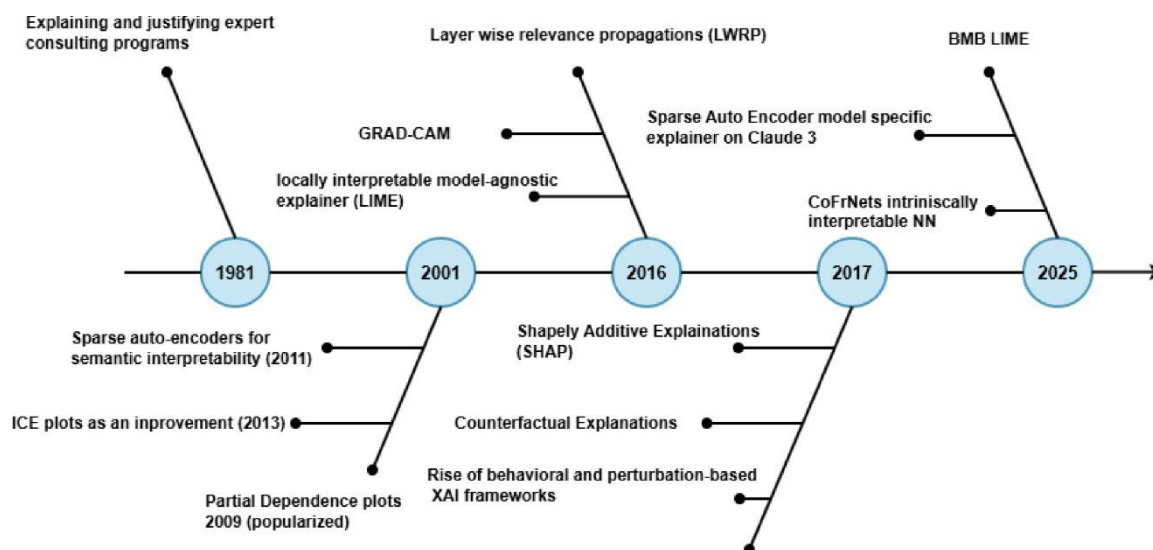
These examples reveal some common characteristics of neural network applications, including the data intensity, unstructured nature, and high uncertainty present in each domain. While NN models, often utilizing backpropagation with a single hidden layer, have proven effective, their opaque nature presents a barrier to interpretability, which is critical in high stakes domains. To address this, the field of XAI emphasizes the development of interpretative tools that allow NNs to work in tandem with domain experts, rather than replacing them. This collaborative approach could enable experts to leverage the strengths of neural networks while preserving the transparency and interpretability necessary for informed decision making in each application.

The idea of XAI has its roots as far back as the 1980s, with early work focusing on feature relevance and interpretability. For example, “Sensitivity Analyses Would Help”

by [5] introduced one of the first formal methods for comparing feature relevancy, laying foundational concepts for modern XAI techniques. Since then, XAI has evolved into a rich and diverse field encompassing gradient based methods, perturbation based explainers, attribution techniques, dimensionality reduction tools, and counterfactual frameworks.

Unlike many areas of machine learning, explainable AI does not admit a single, universally accepted notion of state of the art. The effectiveness of an explanation method depends strongly on the underlying model architecture, the data, and the intended application, as well as the specific properties desired from the explanation, such as interpretability, faithfulness, or computational efficiency. Consequently, methods that are widely adopted in practice, such as LIME, SHAP, and Grad-CAM, are often treated as de facto standards within particular domains rather than as universally optimal solutions. This fragmented landscape makes it difficult to compare methods directly and highlights that XAI frameworks should be compared across multiple dimensions rather than relying on a single performance criterion.

This paper focuses particularly on neural networks and deep neural networks, since many modern artificial intelligence systems are built on neural network architectures. Given this focus, the remainder of the paper is structured as follows: Section 2 presents a historical overview of interpretability and explainability research, tracing the evolution of XAI from early sensitivity analyses to modern attribution methods. Section 3 introduces the concept of XAI in greater detail and reviews existing taxonomies, before outlining the extended classification framework adopted in this paper. Section 4 examines individual XAI frameworks and techniques in depth, summarizing how they operate and highlighting their reported strengths and limitations. Section 5 then synthesizes these methods within a complementary classification framework that distinguishes approaches by explanatory mechanism and explanatory level. Finally, Section 6 discusses broader structural challenges in the field, including issues of faithfulness, stakeholder alignment, and evaluation, and outlines directions for future research.

Fig. 1. A historic timeline of XAI.

2. A brief history

While [5]s survey explores a brief history of XAI we have decided to delve deeper into to this so the reader gets a general understanding of the latest tools and innovations in XAI [1](#) is provided for a simple overview of our current XAI timeline. [6] cited and as some of the earliest forms of XAI in around the 1980s. While the researchers in those paper weren't working with black box models, this is still some the earliest efforts at keeping AI systems transparent and trustworthy. When it comes to black box models some of the earliest attempts as far as we know it comes to black box models surfaced around 2005 such as s work. [7] acknowledged researcher's reluctance to use machine learning models in their work since it was hard to understand the underlying mechanisms behind a network's output. [7] proposed a case based reasoning solution which uses locally derived feature importance to assess which input variables are most relevant.

This is an extremely similar approach to being used by LIME and SHAP which are extremely popular XAI frameworks. Section [4](#) will have more details on frameworks mentioned in this section. Other notable works include [8]s work which addresses the challenges associated with the "black box" nature of machine learning models and emphasized the need for explainability.

We next introduce several foundational frameworks that align closely with semantic forms of explanation, even though they were not originally developed with neural networks or modern AI systems in mind. [8] formalizes causality through the framework of structural causal models (SCMs), which represent a system as a set of variables connected by directed graphs and governed by structural equations. Unlike purely statistical models that encode associations, SCMs explicitly distinguish between observation and intervention by modeling how variables are generated and how they respond to external manipulation. Central to this framework is the do-operator, which enables reasoning about interventions by modifying the underlying causal graph rather than conditioning on observed data.

Explanation-Based Learning (EBL), introduced by a symbolic learning approach in which a system learns by explaining a specific example using prior knowledge. Rather than discovering patterns from large datasets, EBL assumes that the system already possesses a domain theory expressed as logical rules. Given a training example, the system constructs a step by step logical proof showing why the example satisfies a particular concept. This proof identifies which rules and conditions are actually necessary for the conclusion. The system then generalizes from this explanation by extracting the essential conditions from the proof and turning them into a rule that can be reused for future cases. In this way, learning occurs through structured reasoning: explanation is not something added afterward, but the mechanism through which generalization is achieved.

The authors in [9] introduces a method for interpreting the decisions of complex, black box classifiers by approximating them locally with a Parzen window estimator. This approach enables the computation of explanation vectors local gradients that indicate the direction and magnitude of change in the model's output with respect to each input feature. By analyzing these gradients at specific data points, the method provides insights into which features most influence the classifier's decision for that instance.

The first major paper that used partial dependence plots (PDP) explicitly as part of an interpretability framework in machine learning was “Greedy Function Approximation: A Gradient Boosting Machine” by [9], where he introduced the method in the context of boosting algorithms. So, while the concept of visualizing model explanations existed before, PDPs as a specific technique for model interpretability were formalized and popularized around 2001. [10] introduced ICE plots which address some of the limitations of PDPs.

3. Explainable AI

3.1. Overview of explainable AI

In the context of XAI, the concepts of transparency, interpretability, and faithfulness are foundational yet often conflated. Transparency generally refers to the intrinsic comprehensibility of a model how easily a human can inspect and understand its inner workings. Interpretability, by contrast, is typically defined as the degree to which a human can understand the cause of a decision, often irrespective of the model's internal complexity [23]. Faithfulness, meanwhile, refers to how accurately an explanation reflects the true reasoning process of the underlying model, ensuring that explanations are not merely plausible but grounded in the model's actual behavior [17]. This distinction is crucial, as explanations that are interpretable but unfaithful can lead to misleading conclusions about model reliability and decision boundaries. As [18] emphasize, achieving transparency and faithfulness is vital for building trust in real world AI applications, especially in domains like healthcare, finance, and law, where regulatory compliance and ethical accountability are paramount [18]. Despite their importance, these dimensions are rarely addressed consistently across XAI research, pointing to the need for standardized definitions and evaluation practices.

However, achieving faithfulness in practice remains challenging. Methods such as LIME and SHAP are among the most widely adopted XAI techniques due to their model agnostic nature and ease of use. However, as argued by [19] post-hoc explanation methods (see Section 3.2 for formal definition) inherently approximate the behavior of complex models rather than directly reflecting their internal decision processes. As a result, such methods may lack faithfulness in certain settings, potentially leading to explanations that are plausible but not fully representative of the model's true reasoning.

As machine learning methods become more complex, the integration of DNNs has increased. DNNs, with their numerous hidden layers, add significant depth to models, making it increasingly difficult to interpret why they would make a certain decision. This complexity can obscure the internal reasoning of the machine learning model, creating a “black box” effect where it is challenging to understand and trust the model's predictions.

In many cases, the primary objective of XAI is to transform complex DNNs from opaque systems into interpretable and trustworthy models, fostering confidence in their

predictions. XAI frameworks strive to develop tools and methodologies to make these decision making processes transparent and understandable. XAI approaches are broadly categorized into four types: scoop based, model based, complexity based, and methodology based explainers [1].

3.2. Taxonomy overview

Scoop based explainers are methods primarily focused on exploring the structure of data and creating meaningful features that can help in understanding model predictions. These methods are further divided into two categories: local explainers and global explainers. A local explainer provides insights into the factors influencing a single decision or a specific instance, offering explanations at an individual level such as LRP. In contrast, a global explainer is designed to interpret the overall behavior of the model across the entire dataset, identifying general patterns and feature importance for a broader understanding [1]. Some explainers, such as SHAP, can provide both local and global explanations. A more detailed discussion of SHAP and LRP will be presented in Section 4.

Complexity based explainers aim to make highly intricate models easier to interpret and understand. These explainers can be grouped into two main categories: intrinsically interpretable models and Post-hoc explainers. Intrinsically interpretable models are designed with interpretability as a core feature, meaning that they are built in a way that enables clear explanations of their behavior. These models are often simpler in structure, such as linear models or decision trees, which typically results in reduced accuracy compared to more complex models, as they sacrifice some predictive power for interpretability [2].

In contrast, Post-hoc explainers work by applying a second model or a more interpretable global predictor [5], often called a surrogate model, to approximate and interpret the behavior of a more complex, non-interpretable model. This approach allows the original model to retain its complexity and accuracy, while the surrogate model provides an approximate, interpretable explanation for its predictions. However, this process generally results in lower interpretability compared to intrinsically interpretable models, as the explanations are approximate and may not fully capture the decision making process of the original complex model.

Model based explainers in explainable artificial intelligence (XAI) frameworks are generally classified into two distinct categories based on their design and functionality: model specific and model agnostic explainers. Model specific explainers, also known as intrinsic explainers, are tightly integrated within a machine learning model. These explainers are crafted to work with the model's architecture directly, offering interpretability as an inherent feature that simplifies analysis from within the model itself. This approach often leads to models that are simpler in design, as the explainability feature is embedded in the model's functionality from the outset. However, this intrinsic simplicity frequently results in a trade off, as model specific explainers may sacrifice predictive power to maintain transparency.

Conversely, model agnostic explainers are designed to operate independently of any model structure, making them versatile tools that can interpret results from various machine learning models regardless of the underlying architecture. This flexibility has made model agnostic approaches highly appealing, especially for complex and opaque models like artificial neural networks (ANNs), where interpretability is often challenging.

One widely adopted model agnostic method is the Partial Dependence Plot (PDP), which illustrates how specific input features influence the model's predictions, providing valuable interpretative insights without delving into the inner workings of the model [6]. PDPs allow researchers and practitioners to observe the relationships between individual input features and the predicted outcomes, revealing feature specific trends or dependencies that contribute to the overall predictions.

Once again methodology based explainers are categorized into two algorithms, backpropagation based and perturbation based. Backpropagation techniques, also known as gradient based techniques start with the output of a neural network and work backward to understand how each part of the input influenced that output. They assign importance to each step that was taken to reach the final decision.

3.3. Data explainability

Building trustworthy and interpretable AI begins at the very first stage of machine learning model development: data acquisition and aggregation. Acquiring high quality data can be challenging, and in some cases, synthetic data can be a valuable alternative. For example, approaches like those described in [3] demonstrate how synthetic AI data can help train specific models effectively while preserving accuracy.

Data synthesis and augmentation are powerful methods to expand and diversify training datasets, enhancing model robustness. However, even with these techniques, a critical issue remains: ensuring the reliability of the model's outputs. Studies such as [10] highlight that data quality plays a crucial role in influencing the efficiency, accuracy, and complexity of machine learning tasks. For models to produce trustworthy results, training data must be complete, accurate, and consistent.

The importance of high quality data in model performance is often underestimated, with much attention focused on model architecture instead of the quality of data inputs [5]. Many machine learning models work with data that has extremely high dimensionality, which is challenging to interpret, as humans can naturally visualize only up to three dimensions. Fortunately, there are tools designed to help visualize and understand the relevance of data and features in high dimensional spaces. One such tool, t Distributed Stochastic Neighbor Embedding (t-SNE), provides a way to represent high dimensional data in lower dimensions while preserving the data's local structure. t-SNE achieves this by using a t distribution to calculate point similarity, measuring the conditional probability that a point would select another point as its neighbour [20].

Uniform Manifold Approximation and Projection (UMAP) is a dimensionality reduction technique, similar to t-SNE, that is used to visualize high dimensional data in a low dimensional space. UMAP constructs a weighted graph to capture relationships between data points in the high dimensional space, then maps these points to a low dimensional space while optimizing to preserve their relative order [18].

Principal Component Analysis (PCA) is a widely used method for dimensionality reduction and data visualization, relying on statistical analysis to simplify high dimensional data. PCA begins by standardizing the data, then calculates the covariance matrix, followed by computing its eigenvectors. This process captures the directions of greatest variance in the data, which can then be visualized in a 2D or 3D space [15]. PCA excels at filtering out noise and identifying the most significant features. However, it has limitations: it is sensitive to data scaling and assumes that data patterns can be represented through linear combinations of the original variables, which may not always hold true.

Potential of Heat diffusion for Affinity based Trajectory Embedding (PHATE) is a dimensionality reduction method specifically designed to preserve the progression structure in data. By using a heat diffusion process, PHATE naturally denoises the data and maintains its high level structure. It begins by calculating a Markov transition matrix, which represents the likelihood of transitioning from one data point to another, thereby reducing noise during computation. The data is then embedded into a 2D space using non metric multi dimensional scaling, which emphasizes progression and trajectory patterns in the data [16]. This approach is particularly valuable for biological data, as it captures branching trajectory structures that preserve global structure and emphasize data progression.

A relational auto encoder is a type of auto encoder designed for feature extraction that also preserves the relationships between data samples, a characteristic that standard auto encoders tend to overlook [12]. In its basic form, an auto encoder is a neural network with two main parts: an encoder and a decoder. The encoder receives the input data and compresses it into a lower dimensional representation, effectively capturing essential features. This compressed representation is then passed to the decoder, which attempts to reconstruct the original input from the compressed data [13].

While basic auto encoders are effective at selecting important features, they lack interpretability and fail to retain the relational structure of the input data. Relational auto encoders address this limitation by focusing on preserving these inter sample relationships, making them better suited for applications where the relationships between data points are critical to understanding the dataset.

A study by [15] used a variational autoencoder to analyze high resolution satellite images. It learned a compact set of important patterns from the data, and these patterns were then used to classify land types showing that VAEs can find useful features without needing labeled examples (see [Table 1](#)).

Table 1: Summary of data and feature analysis methods.

Data explainer	Advantages	Disadvantages	Usage	Comments
t-SNE (Van der Maaten & Hinton, 2008)	Strong local clustering, intuitive visuals	Computationally slow, poor global structure	Visualizing high dimensional data	Most effective for small datasets

UMAP (Trozzi et al., 2021)	Preserves local & some global structure, fast	Sensitive to parameters	Data visualization & clustering	Scalable for large datasets
PCA (Ringnér, 2008)	Fast, interpretable variance retention	Only captures linear patterns, poor global structure	Dimensionality reduction, noise filtering	Assumes data is standardized
PHATE (Moon et al., 2019)	Captures data trajectory	Less interpretable	Visualizing biological data	
Relational Auto Encoders (Meng et al., 2017)	High applicability outside of feature extraction	Needs to be trained & requires a large dataset	Feature extraction, denoising & anomaly detection	

4. Explainable AI frameworks

[Table 2](#) provides an overview of various XAI techniques, identifying the most commonly used data types for each, as well as their application fields and primary stakeholders.

Table 2: Summary of XAI techniques.

Algorithm	Data Type: Image, Text, Tabular	Summary	Application field	Stakeholder
LIME (Ribeiro et al., 2016)	All datatypes	Generates local interpretation using a surrogate model	Multi disciplinary	Model developers & end users
SHAP (Lundberg, 2017)	All datatypes	Assigns feature importance based on Shapley values from game theory, ensuring consistent, fair attribution of each feature's contribution to the prediction	Multi disciplinary	Model developers & end users

LRP (Bach et al., 2015)	Image & Text	Backpropagates a relevance score through the network layers, assigning relevance to each input feature based on its contribution to the prediction	Classification problems & feature extraction	Model developers
PDP (Moosbauer et al., 2021)	Tabular data	Visualize the average effect of one or two features on model predictions while averaging out other features	Hyper parameter optimization & Model debugging	Model developers
GRAD CAM (Selvaraju et al., 2016)	Image	Generates class discriminative heatmaps in CNNs by highlighting regions in the input image that influence specific predictions	Multi disciplinary	Model developers

4.1. Layer wise relevance propagation

Layer Wise Relevance Propagation (LRP) was first introduced by [16] in order to help visualize each pixel's contribution to a classifier's decision, represented as a heat map [18]. LRP works by tracing the relevance of a model's prediction backward through its layers, starting from the output and working toward the input features. The goal is to attribute the model's decision to specific input features by redistributing the relevance score across the network. Initially, the relevance is set to the output of the predicted class (in this case it is the probability of a class in a classification task). At each layer, the relevance of a neuron j with score R_j is redistributed to its inputs i proportionally to their forward contribution, given by activation a_i and weight w_{ij} :

$$R_j = \sum_i \frac{a_i w_{ij}}{\sum_i a_i w_{ij} + \epsilon} R_j$$

Where ϵ is a stabilizer to avoid division by zero. This redistribution rule ensures that the total relevance is conserved across layers, i.e., $\sum_i R_i = \sum_j R_j = f(x)$, where $f(x)$ is the model's prediction score for input x .

Then, through a series of rules tailored to each type of layer (e.g., fully connected, convolutional), relevance is propagated backward through the layers, with each neuron or feature contributing a certain amount of relevance based on its impact on the final decision. In the end, the method produces a heatmap or score highlighting which parts of the input were most influential in the model's decision, providing interpretable and localized explanations for the model's behavior. LRP was a breakthrough in XAI, as it enabled significant advancements in model interpretability. For example, works such as those by [5] demonstrate how LRP can be applied to classify documents with text as input. Additionally, LRP is used to highlight the keywords that contributed to the classification decision, providing insights into the factors influencing the model's output.

4.2. Partial dependence plots

PDPs marked a major milestone in explainable AI. First introduced by [17] to examine the relationship between a feature and the target variable whether it is linear, monotonic, or complex. PDPs became one of the earliest widely accessible tools for global model interpretability in non linear machine learning models. PDPs enable users to visualize how one or two features impact model predictions by averaging over other features, providing a high level view of model behavior. This capability is essential for building trust and debugging “black box” models, as it reveals general feature effects on predictions [18]. [18] further demonstrated the utility of PDPs in hyperparameter optimization. However, PDPs have limitations: they only allow for up to two features at a time and assume feature independence. In Bayesian optimization, an additional sampling bias can arise from focusing on high performance areas. To address this, [22] introduces uncertainty quantification in PDPs using confidence bands that emphasize reliable regions.

The authors also propose a tree based partitioning method, dividing the hyperparameter space into well sampled sub regions to provide more accurate PDPs. Experimental results show that these improvements yield clearer, confidence enhanced insights, most evident around optimal configurations of the model's hyperparameters, where performance is maximized according to their experiments.

4.3. Gradient weighted class activation mapping

Gradient weighted Class Activation Mapping (Grad CAM) is another XAI technique used to visualize and understand the decision making process of CNNs, particularly in tasks like image classification. It highlights the regions in an image that were most important for the model's prediction, providing a visual explanation for the model's behavior [24]. Grad CAM works by first performing a forward pass to generate predictions, then calculating the gradients of the score (logit) y^c for the target class c with respect to the feature maps of a chosen convolutional layer. Let A_{ij}^k denote the activation at spatial location (i,j) in the k th feature map (convolutional layer channel) A^k (of size $u * v$). The gradients $\frac{\partial y^c}{\partial A_{ij}^k}$ are globally averaged across spatial dimensions to obtain channel-wise weights:

$$\alpha_k^c = \frac{1}{uv} \sum_{i=1}^u \sum_{j=1}^v \frac{\partial y^c}{\partial A_{ij}^k}.$$

These weights α_k^c represent the importance of feature map k for class c . The class activation map is then computed as a weighted combination of the feature maps, followed by a ReLU:

$$\alpha_k^c = \frac{1}{uv} \sum_{i=1}^u \sum_{j=1}^v \frac{\partial y^c}{\partial A_{ij}^k}.$$

The ReLU ensures that only features with a positive influence on the class score are retained. Finally, the resulting coarse localization map is up-sampled to the size of the input image and superimposed as a heatmap, providing a visual explanation of the model's decision.

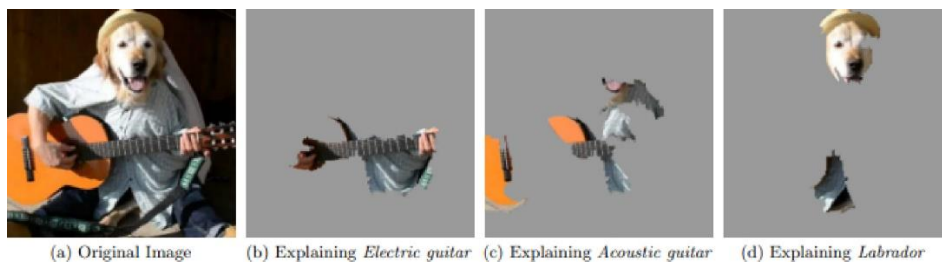


Fig. 2. LIME explanations for different class predictions on the same image, highlighting regions important for predicting Electric guitar, Acoustic guitar, and Labrador.

4.4. Locally interpretable model agnostic explainer

[25] proposed a very popular framework called LIME, short for Locally Interpretable Model agnostic Explanations. LIME perturbs the input data around the instance to be explained, generates predictions on these perturbed instances, and then fits an interpretable model (e.g., a linear model) to approximate the local behavior of the black box model [25]. Formally, given a black box model f and an instance x (the specific input sample to be explained), LIME learns an interpretable model $g \in G$ (such as a sparse linear model or decision tree) by solving

$$\xi(x) = \arg \min_{g \in G} \mathcal{L}(f, g, \pi_x) + \Omega(g),$$

where $\mathcal{L}$ measures how closely g approximates f in the neighborhood of x , π_x is a locality-aware weighting function that gives higher weight to samples closer to x , and $\Omega(g)$ is a complexity penalty that discourages overly complex surrogates (e.g., dense linear models), thereby ensuring that g remains simple enough for humans to interpret.

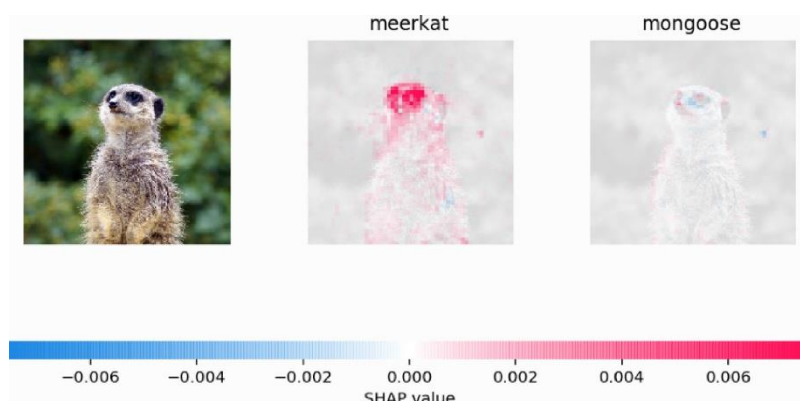
The result is a local explanation that identifies which features are most influential for the specific prediction of x , as shown in 2. In addition, [25] proposed SP-LIME to provide more generalized explanations. SP-LIME uses submodular optimization to select a representative set of instances whose combined local explanations maximize coverage of the model's behavior, ensuring that diverse regions of the data manifold are well represented. This approach allows the user to gain a more global explanation of the dataset as a whole.

SP LIME lacks in its ability to explain global trends in the dataset. In LIME, explanations are derived from sparse, linear models fitted locally to approximate a complex model's behavior around specific instances. NORM LIME, an enhanced version of SP LIME, enhances this by aggregating feature importance scores across various local models and applying normalization, leading to a globally coherent feature importance ranking.

BMB LIME is a modification of LIME that aims to improve explanation accuracy and stability with non linear decision boundaries which standard LIME often struggles with Hung and Lee (2024). BMB LIME employs a technique that generates a confidence interval around feature contributions, quantifying uncertainty in its explanations. This significantly enhances

the reliability measures for its users, making it ideal for machine learning model developers and provides a more understandable metric for those without a good understanding of machine learning topics and stakeholders.

Fig. 3. SHAP explanation of an intermediate layer of VGG16 on ImageNet



4.5. Shapely additive explanations

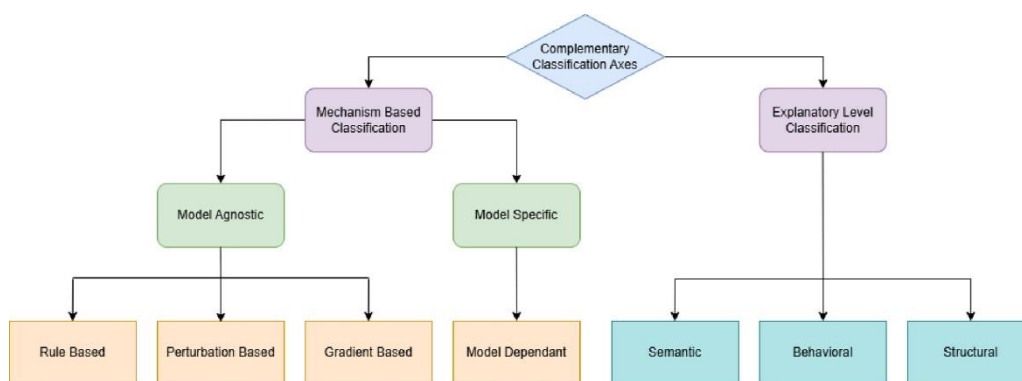
Shapely Additive explanations (SHAP) is a model agnostic tool for interpreting machine learning predictions, built on concepts from cooperative game theory. SHAP values assign an importance score to each feature of a prediction by using Shapley values, a game theoretic approach that ensures fair and consistent attribution of contributions among players (or, in this case, features) (Lundberg, 2017). The method unifies several existing interpretation techniques under a single framework and satisfies key interpretability properties, including local accuracy, consistency, and missingness. SHAP provides both local explanations, for individual predictions, and global explanations, by aggregating feature attributions across instances.

Fig. 3 illustrates an example of a SHAP generated explanation, where pink highlighted pixels contribute positively to the classification, while blue highlighted pixels contribute negatively. Deep SHAP is an extension of SHAP tailored specifically for deep learning models. It combines SHAP with LRP, which helps adapt the Shapley values to work more efficiently in DNNs. Deep SHAP is backpropagation based, meaning it can propagate relevance scores backward through the network layers to explain individual predictions at a low computational cost. This makes it efficient for deep models with many layers, as it avoids the need for extensive sampling required in model agnostic SHAP methods.

Kernel SHAP is a general purpose, model agnostic version of SHAP that provides feature based explanations by estimating Shapley values through a flexible, kernel weighted sampling method. Designed to work with any predictive model, Kernel SHAP approximates feature attributions by constructing a locally weighted linear model around each prediction. This makes it adaptable and suitable for models that are not inherently interpretable, such as ensemble models, black box algorithms, and deep networks although it will not be as efficient as Deep SHAP.

The most important advantage in using SHAP is its ability to provide global explainability. The study by illustrates SHAP's strength in bridging local explanations into a cohesive global interpretive framework, making it well suited for applications in security and intrusion detection where understanding feature influence on a broader scale is crucial.

Fig. 4: An expanded taxonomy of XAI



6. Limitations and future directions

The comparative analysis presented in [Table 4](#) reveals several important trends in the current landscape of XAI. A clear imbalance emerges in the distribution of methods, with behavioural approaches dominating the literature, while structural and semantic methods remain relatively underrepresented. This suggests that most existing work prioritizes input output level explanations over approaches that capture internal model mechanisms or align explanations with human understandable concepts. At the same time, a consistent pattern can be observed in terms of faithfulness: methods that provide deeper insight into model internals or incorporate higher level conceptual reasoning tend to exhibit higher levels of faithfulness, whereas widely used behavioural methods often achieve only moderate faithfulness.

One challenge in explainable AI stems from how modern machine learning models are typically developed and evaluated. As argued by, modern machine learning research frequently prioritizes predictive performance and benchmark optimization over transparency, resulting in widespread reliance on complex black box models even in high stakes settings. When interpretability is treated as an afterthought rather than a primary design objective, explanation methods are typically developed post hoc to analyze models that were not originally constructed to be transparent. Although intrinsically interpretable models can often achieve competitive performance, they may impose architectural constraints that limit representational flexibility or increase computational cost, reinforcing the perception of a trade off between interpretability and accuracy [26]. Consequently, much of the XAI literature focuses on approximating or characterizing model behavior as seen from [Table 4](#) rather than designing models whose reasoning processes are directly accessible. While post-hoc methods such as TCAV attempt to ground explanations in semantically meaningful concepts, intrinsically interpretable models provide stronger guarantees of faithfulness, as their explanations are identical to the model's decision process rather than derived from approximations of it [26].

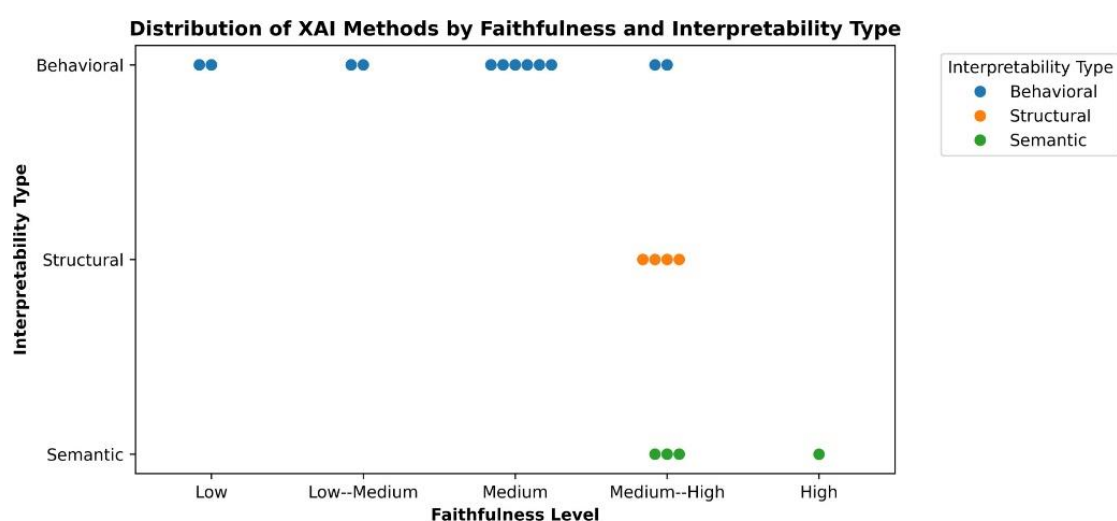


Fig. 5. Distribution of XAI methods across faithfulness levels and interpretability types. Methods that provide deeper insight into model internals or align more closely with human understandable concepts tend to exhibit higher levels of faithfulness.

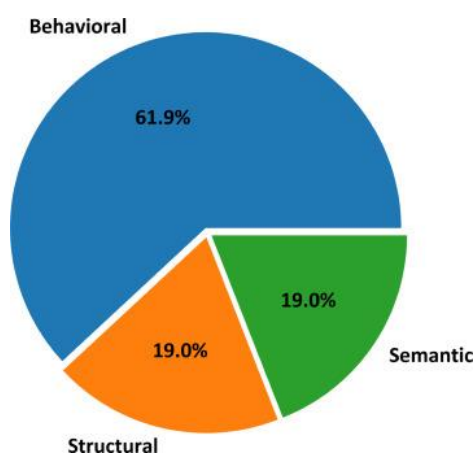
Fig. 6: Distribution of XAI methods

Fig. 6. Distribution of XAI methods across interpretability types. The dominance of behavioural shows a focus on input output explanations, while the relative scarcity of structural and semantic approaches exposes a gap in current research.

In general combining and comparing multiple XAI framework is a better idea since explanations can be cross validated. [24] develops a comprehensive framework that integrates multiple existing XAI methods into a cohesive, iterative pipeline aimed at enhancing model transparency and facilitating debugging. The explAIner system is designed to assist users in understanding machine learning models, diagnosing their limitations, and refining them by combining various explainability techniques within a unified visual analytics environment. Key components of the framework include eight global monitoring and steering mechanisms such as quality monitoring, provenance tracking, model comparison, and trust building. By adapting this framework within the commonly used TensorBoard environment, explAIner provides an accessible platform for users to interact with and interpret complex models effectively. A user study involving participants with varying levels of expertise confirmed that this integrated approach leads to a more informed machine learning process and reveals opportunities for further enhancements in explainability tools [23]. It is important to emphasize that there is no single state of the art XAI method that is universally applicable across all tasks. Rather, different methods exhibit strengths in specific contexts. For example, influence functions are particularly effective for identifying influential or problematic training instances, while other approaches may be better suited for feature attribution or concept-level explanations. This highlights the inherently task dependent nature of explainable AI and reinforces the need for a diverse set of methods rather than a single dominant approach.

To provide a clearer understanding of the practical landscape of XAI, the [Table 5](#) was included to present a variety of existing tools and libraries. This overview was created to illustrate both the accessibility of these tools distinguishing between open source and proprietary offerings and the types of explanation methods they support. By cataloging key attributes such as licensing, supported languages, and methodological focus, the table aims to inform about which XAI tool sets are readily available for integration into machine learning workflows and which have gained traction in academic and industrial settings. This helps contextualize the ongoing research in XAI within the broader ecosystem of usable, real world implementations.

Table 3: Overview of XAI tooling libraries: Licensing, Language Support, and Explanation methods

Tool	Open source	License	Languages	Method types
Captum (Kokhlikyan et al., 2020)	Yes	Apache-2.0	Python (PyTorch)	Saliency, Integrated Gradients, LRP, etc.
DiCE (Mothilal et al., 2019)	Yes	MIT	Python	Multiple counterfactuals
TrustyAI (Yang et al., 2021)	Yes	Apache-2.0	Java, Python	LIME, SHAP, counterfactuals (plus fairness and drift metrics)
Quantus (Hedström et al., 2023)	Yes	MIT	Python	Explanation evaluation metrics
OmniXAI (Yang et al., 2022)	Yes	Apache-2.0	Python	Attribution, counterfactuals, gradients
Effector (Gkolemis et al., 2024)	Yes	MIT	Python	Regional/global feature effects
InterpretML (Nori et al., 2019)	Yes	MIT	Python	GlassBox, LIME, SHAP
Vertex XAI (Cloud, 2025)	No	Proprietary	Python	Integrated Gradients, Sampled Shapley

IBM Watson OpenScale (IBM, 2025)	No	Proprietary	Python	LIME, SHAP, Contrastive explanations
DLBacktrace (Sankarapu et al., 2025)	Yes	MIT	Python, RESTful API	model agnostic relevance tracing
SeekrFlow (Technologies, 2025)	No	Proprietary	RESTful API	Model transparency, confidence & bias detection
Alibi (Klaise et al., 2021)	Yes	BSL-1.1 (was Apache-2.0)	Python	Anchors, counterfactuals, SHAP

Conclusion

This survey has shown that explainable AI is not a single methodological objective, but a collection of distinct interpretability paradigms operating at different levels, including structural, semantic, and behavioral forms of explanation. Each of these paradigms serves different stakeholders and interpretive goals: structural approaches aim to uncover internal mechanisms, semantic approaches seek alignment with human understandable concepts, and behavioral methods characterize model decision boundaries. Because these explanatory objectives differ fundamentally, evaluating explanation quality cannot rely on a single universal metric. Rather than viewing the lack of standardized evaluation metrics as a simple gap to be filled, it may be more accurate to recognize it as a consequence of this diversity.

Taken together, these observations suggest that progress in XAI will depend less on enforcing uniform standards and more on clarifying the purpose and scope of each interpretability paradigm. Structural, semantic, and behavioural explanations each provide different strengths and limitations, and their appropriateness depends on the stakes, domain, and intended audience. In high stakes settings in particular, the distinction between behavioural approximation and structural faithfulness becomes consequential, reinforcing calls for greater transparency at the model design stage [25].

Advancing the field therefore requires not only technical innovation, but a clearer articulation of what kind of understanding is sought, for whom, and under what constraints.

Without this alignment, evaluation frameworks risk measuring properties that are unfaithful to the actual explanatory needs of stakeholders.

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Edge Computing vs. Cloud Computing: Perfecting or Fierce

S. Pravenitha Shri¹, M. Pavithra¹, M. Shalini¹ and K. Nisha^{2*}

¹UG Student, Department of Computer Science, Madonna Arts & Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

²Head & Assistant Professor, Department of Computer Science, Madonna Arts & Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

*Corresponding Author E-Mail ID: nisha2287@gmail.com

Abstract

The rapid evolution of technology has given rise to fringe and cloud computing as pivotal paradigms in modern IT infrastructure. Both approaches offer unique advantages, addressing distinct challenges in processing, storage, and Data analytics. This paper explores the Fundamental Principles of these paradigms offer distinct advantages that cater to varying requirements in processing, storage, and data analysis. Cloud computing excels in delivering scalable and centralized solutions for extensive data processing and storage needs. In contrast, edge computing addresses the increasing demand for low-latency, real-time data processing by bringing computation closer to the data source. This paper examines the core principles, use cases, and technological trends of both paradigms, assessing whether they function a technology or fierce. Through an in-depth analysis of real-world applications, challenges, and opportunities, this study slough light on the Robust interplay between edge and cloud computing, compares their functionalities, and evaluates whether they operate as perfecting technologies or fierce for puissance in various application domains. By Scrutinizing real-world use cases and technological trends, this study provides insights into the future interplay between edge and cloud computing.

Keywords: Cloud computing, edge computing, IT infrastructure

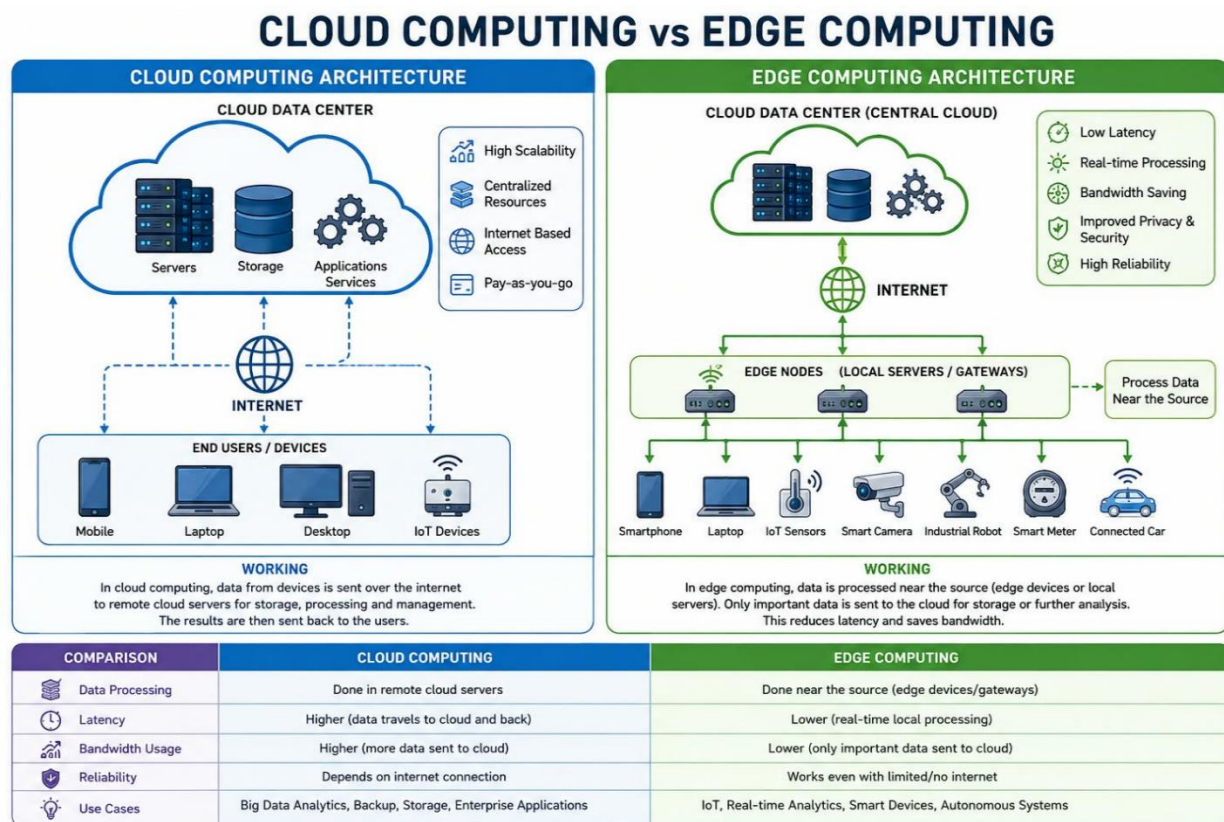
1. Introduction

The expanding growth of data generated by devices and sensors has require robust and scalable computing solutions. Cloud computing, characterized by cluster data processing and storage, has been a main stay of modern computing for over a decade.[1] With its ability to offer just about unlimited upgrade ability, cluster resource management, and cost-effective

solutions through a pay-as-you-go model, cloud computing has transformed enterprise ranging from finance and healthcare to occupation and retail. Leading cloud service providers such as Amazon Web Services (AWS), Microsoft Azure, and Google Cloud have driven innovation, enabling organizations to focus on their core aptitudes without worrying about underlying IT infrastructure.

However, the rapid adoption of the Internet of Things (IoT), Artificial intelligence (AI), and other isometric technologies has created a paradigm shift. Modern applications increasingly require real-time data processing, minimal tardy and localized data management. Edge computing has emerged to address these challenges by processing data closer to the source, thereby reducing the reliance on centralized cloud grid. By enabling real-time decision-making and reducing bandwidth usage, edge computing is proving to be indispensable in scenarios such as autonomous vehicles, smart cities, and industrial automation.

Fig: - Diagram of Cloud Computing vs Edge Computing



2. Literature Review

Pravenitha shri, Pavithra, Shalini seminal work provides a fundamental understanding of edge computing as an innovative paradigm in contemporary computing. The author presents edge computing as a solution to the limitations of cloud computing in environments that demand low-latency communication, real-time data processing, and improved data privacy [1].

Highlights the importance of processing data near its source, reducing dependence on centralized cloud infrastructure. This proximity enables faster decision-making and optimizes network bandwidth, making edge computing highly suitable for applications such as autonomous vehicles, smart cities, and healthcare monitoring systems.

A. McAfee and E. Brynjolfsson's influential article examines the transformational impact of big data on business processes and organizational decision-making. The authors state that big data represents a major shift in information utilization, moving organizations from intuition-based decision-making to data-driven strategies [2].

Amazon Web Services' "AWS Greengrass Documentation" presents a detailed overview of AWS Greengrass, a service that extends AWS cloud capabilities to edge devices. The documentation explains how AWS Greengrass allows edge devices to process data locally while continuing to use cloud resources for device management, data analytics, and long-term storage [3].

W. Shi et al., in their influential paper "Edge Computing: Vision and Challenges," examine the conceptual architecture and prospects of edge computing. The authors present a detailed vision of how edge computing complements conventional cloud infrastructure while addressing the increasing requirements of IoT environments and real-time applications [4].

Lin and Wang (2020) examine the key challenges of edge computing, including limited computational resources and cybersecurity concerns, while comparing these limitations with the scalability, reliability, and robustness offered by cloud computing solutions [5].

3. Overview of Cloud Computing

Cloud computing is a revolutionary technology paradigm that enables on-demand delivery of computing resources, including servers, storage, databases, networking, software, and analytics, over the internet

Key Characteristics of Cloud Computing

1. **Automatic Resource Provisioning:** Users can provision resources as needed without requiring human intervention from the service provider.
2. **Universal Network Access:** Resources are accessible over the internet, using a wide range of devices like laptops, smartphones, and tablets.
3. **Multi-Tenant Resource Sharing:** Cloud providers pool computing resources to serve multiple customers, with resources dynamically assigned and reassigned based on demand.
4. **Pay-As-You-Go-service:** Cloud systems automatically control and optimize resource by metering services, allowing customers to pay only for what they use.

Service Models

Cloud computing services are typically delivered through three primary models

1. Infrastructure as a Service (IaaS):

- Provides virtualized computing resources such as virtual machines, storage, and networks.
- Examples: Amazon Web Services (AWS) EC2, Microsoft Azure, Google Compute Engine.

2. Platform as a Service (PaaS):

- Offers a platform for developers to build, test, and deploy applications without managing underlying infrastructure.
- Examples: Google App Engine, Microsoft Azure App Service, Heroku.

3. Software as a Service (SaaS):

- Delivers software applications over the internet on a subscription basis.
- Examples: Google Workspace, Salesforce, Dropbox.

Deployment Models

1. Public Cloud:

- Services offered over the internet to multiple customers by third-party providers.
- Example: AWS, Microsoft Azure.

2. Private Cloud:

- Dedicated cloud infrastructure operated exclusively for a single organization.

3. Hybrid Cloud:

- Combines public and private clouds, enabling data and application sharing between them.

4. Community Cloud:

- Shared infrastructure for a specific community of users with common concerns, such as compliance.

Benefits of Cloud Computing

- **Cost Efficiency:** Reduces capital expenditure by shifting to a pay-as-you-go model.
- **Flexibility:** Provides access to resources anytime, anywhere.
- **Scalability:** Accommodates business growth by easily scaling resources up or down.
- **Business Continuity:** Enhances disaster recovery and backup capabilities. [6]

Challenges

- **Security and Privacy:** Concerns over data breaches and compliance with regulations.

4. Overview of Edge Computing

Key Characteristics of Edge Computing

1. Proximity to Data Sources

Processing occurs near the data's origin, minimizing the need for data to travel to centralized cloud data centres.

2. Low Latency

By reducing the distance data travels, edge computing ensures faster response times.

3. Distributed Architecture

Computation and storage are decentralized, occurring across multiple edge nodes or devices.

Applications of Edge Computing

1. Internet of Things (IoT)

- i. Supports smart homes, cities, and industries by enabling real-time data processing and device control.

2. Autonomous Vehicles

- i. Processes sensor data locally to make instantaneous decisions for navigation and safety.

3. Retail:

- i. Enhances customer experiences with in-store analytics and personalized recommendations.

Challenges:

1. **Complexity:** Managing a distributed network of edge devices can be complex and resource intensive. [7]
2. **Security Risks:** Edge devices may have weaker security measures compared to centralized cloud infrastructure.
3. **Integration:** Seamlessly connecting edge systems with cloud-based solutions can be challenging.

5. Perfecting Roles of Edge Computing and Cloud Computing

Edge computing and cloud computing are not competing paradigms but perfecting approaches that together create a robust, efficient, and scalable computing ecosystem. Each has unique strengths, and their combination addresses diverse computing needs across industries.

1. Real-Time Data Processing and Analysis

- i. **Edge Computing:** Processes data close to where it is generated, reducing delay and enabling quick responses.

- ii. **Cloud Computing:** Performs large-scale, high-volume data processing and analytics that need powerful computational resources, such as machine learning model training, big data processing, and business intelligence.

2. Dynamic Resource Allocation

- i. **Edge Computing:** Reduces the workload on centralized systems by processing data locally and removing unnecessary information, which helps to save network bandwidth.
- ii. **Computing:** Provides nearly unlimited resources for increasing storage and processing capacity, efficiently managing changes in workload.

Edge optimizes resources by minimizing the volume of data sent to the cloud, while the cloud scales on demand to handle increased computational and storage requirements.

3. Network Connectivity and System Reliability

- i. **Edge Computing:** Ensures uninterrupted operations in areas with unstable or limited internet connections by processing data locally.
- ii. **Cloud Computing:** Requires a reliable internet connection while providing centralized access to data, applications, and services from anywhere in the world.

Edge ensures uninterrupted service locally, even during connectivity disruptions, and syncs with the cloud when the connection is restored.

4. Security and Privacy

- i. **Edge Computing:** Enhances privacy by processing sensitive information locally, reducing the risk of exposing personal or critical data to external networks.
- ii. **Cloud Computing:** Provides centralized and strong security controls and compliance measures to manage and protect data effectively. [8]

Edge secures sensitive data at its source, while the cloud ensures secure long-term storage and broader compliance management

5. Application that may cause

- i. **Edge Computing:** Suitable for latency-sensitive applications such as IoT, real-time monitoring, and localized AI processing.[8]
- ii. **Cloud Computing:** Suitable for computation-intensive and storage-demanding tasks, such as global analytics, enterprise applications, and data backup services.

Examples of Integration

i. Smart Cities

Edge: Processes data from sensors and cameras to manage traffic or monitor air quality in real-time. [9]

Cloud: Aggregates data from multiple locations for long-term planning and citywide analytics.

ii. Autonomous Vehicles

Edge: Processes sensor and camera data locally for split-second decision making.

Cloud: Stores data for route optimization, fleet management, and performance analysis. [9]

6. Vicious Dynamics

Despite their harmonious potential, certain applications may see edge and cloud computing in fierce:

- i. **IoT Applications:** Businesses may prefer edge computing to reduce their dependence on centralized cloud services.[9]
- ii. **Data Sovereignty:** Regulatory requirements may support edge computing because it provides better control over locally stored and processed data.

7. Emerging Trends in Edge and Cloud Computing

Edge computing and cloud computing are developing rapidly due to technological advancements and the increasing need for real-time, scalable, and efficient data processing.[10]

Trends in Edge Computing

i. **Enabled Edge Computing**

- The rollout of 5G is a major enabler for edge computing.
- High-speed, low-latency connectivity enables smooth communication between edge devices and servers.

ii. **AI and ML Integration at the Edge**

AI models are being optimized for edge devices, enabling real-time inference and decision-making locally. [10]

iii. **IoT Growth and Edge Computing Adoption**

The increasing number of IoT devices is encouraging the use of edge computing to handle large volumes of sensor data.[11]

Applications: Industrial IoT, smart homes, and wearable devices.

iv. **Edge-Native Development Platforms**

New platforms and tools are emerging to build edge-native applications.

Example: Kubernetes-based solutions for managing containerized workloads at the edge.

Trend: Developers focus on lightweight, efficient applications designed for edge constraints.

8. Integration of Edge and Cloud Computing

i. **Distributed Cloud Computing Models**

Cloud services are expanded to edge locations, forming distributed cloud systems that combine centralized and decentralized computing resources.

Examples: google.[12]

ii. **Distributed Cloud, AWS Local Zones**

Edge-Enabled Cloud Platform

Cloud service providers are developing [13] tools to manage and control edge devices directly through cloud platforms.

Conclusion

Edge computing and cloud computing perform different but perfecting functions in modern IT infrastructure. Edge computing provides low-latency processing and bandwidth optimization, while cloud computing delivers high scalability, centralized resource management, and extensive computational capacity.[14]f Their relationship is based on integration and synergy, with hybrid edge-cloud architectures emerging as an important model for future computing.

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SCAPS-1D-Based Numerical Optimization of $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite Solar Cells for Enhanced Photovoltaic Performance

S. Ramya^{1*} and P. Arockia Michael Mercy²

¹UG Student, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

²Vice Principal & Assistant Professor, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

*Corresponding Author E-Mail ID: sr606907@gmail.com

Abstract

Perovskite solar cells (PSCs) are widely studied because of their high efficiency and low fabrication cost. In this study, a $\text{CH}_3\text{NH}_3\text{PbI}_3$ -based PSC with the structure $\text{Au/NiO/CH}_3\text{NH}_3\text{PbI}_3/\text{ZnO/TCO}$ was simulated using SCAPS-1D software. The performance of the device was improved by optimizing the ETL (ZnO), HTL (NiO), absorber layer ($\text{CH}_3\text{NH}_3\text{PbI}_3$), TCO, defect density, doping concentration, and layer thickness. After optimization, the solar cell achieved a maximum power conversion efficiency (PCE) of 30.00%. The results demonstrate that careful optimization of material parameters can significantly enhance the performance of $\text{CH}_3\text{NH}_3\text{PbI}_3$ -based perovskite solar cells and provide useful guidance for future PSC development.

Keywords: $\text{CH}_3\text{NH}_3\text{PbI}_3$; SCAPS-1D; Perovskite solar cell; ZnO; NiO; Device optimization; Defect density; PCE

1. Introduction

Perovskite solar cells (PSCs) have emerged as promising photovoltaic technologies owing to their strong optical absorption, favorable charge-transport characteristics, tunable optoelectronic properties, and potential for low-cost fabrication. Among the various metal-halide perovskite materials, methylammonium lead iodide ($\text{CH}_3\text{NH}_3\text{PbI}_3$ or MAPbI_3) has received extensive attention because of its suitable bandgap, efficient visible-light absorption, and favorable carrier-transport properties [1,2]. The development of MAPbI_3 -based

photovoltaic devices has consequently established hybrid organic–inorganic perovskites as important absorber materials for next-generation solar-energy conversion [3]. A conventional MAPbI₃-based perovskite solar cell generally consists of a transparent conducting electrode, electron transport layer (ETL), perovskite absorber, hole transport layer (HTL), and metallic back electrode. A representative device configuration can be expressed as Glass/FTO/ETL/CH₃NH₃PbI₃/HTL/Au. In this architecture, the MAPbI₃ absorber is responsible for harvesting incident photons and generating electron–hole pairs, while the ETL and HTL selectively extract electrons and holes, respectively [2,4]. Appropriate energy-level alignment between the absorber and charge-transport layers is essential for effective charge separation, carrier extraction, and suppression of interfacial recombination [5]. The photovoltaic performance of MAPbI₃ solar cells is strongly dependent on the physical and electronic characteristics of the individual layers. Parameters such as absorber thickness, carrier concentration, defect density, carrier mobility, interface-defect density, and band alignment can significantly influence charge generation, transport, and recombination processes [5,6]. Defects located within the perovskite bulk and at the ETL/MAPbI₃ and MAPbI₃/HTL interfaces can introduce localized electronic states that promote non-radiative recombination. Such recombination losses can adversely affect the short-circuit current density (J_{SC}), open-circuit voltage (V_{OC}), fill factor (FF), and power conversion efficiency (PCE) of the device [6,7]. Experimental optimization of all these parameters generally requires considerable time and resources. Therefore, numerical simulation has become an important complementary approach for understanding and optimizing the performance of multilayer photovoltaic devices. SCAPS-1D (Solar Cell Capacitance Simulator in One Dimension) is one of the widely used simulation platforms for investigating thin-film solar cells. It enables the analysis of carrier generation, transport, recombination, energy-band alignment, and current–voltage characteristics by solving the fundamental semiconductor equations [8]. SCAPS-1D has subsequently been employed for the numerical investigation of different perovskite solar-cell architectures and for evaluating the influence of absorber and transport-layer parameters on device performance [9,10].

Recent studies have demonstrated that systematic optimization of absorber thickness, defect density, doping concentration, transport-layer properties, and interface characteristics can substantially improve the simulated photovoltaic performance of perovskite devices [9–11]. However, physically realistic material parameters are essential when performing SCAPS-

1D simulations because unrealistic defect densities, doping concentrations, or interface parameters can lead to significantly overestimated device efficiencies [11]. Consequently, careful selection of material parameters and systematic evaluation of the individual layers are necessary to obtain reliable numerical predictions. In this context, a systematic SCAPS-1D investigation of a $\text{CH}_3\text{NH}_3\text{PbI}_3$ -based perovskite solar-cell structure provides an effective approach for understanding the relationship between absorber properties, charge-transport layers, interface recombination, and photovoltaic performance. Optimization of the relevant device parameters can provide valuable theoretical insight into the design of efficient MAPbI_3 -based photovoltaic devices and can serve as a useful foundation for subsequent experimental investigations [9–11]. Nickel oxide (NiO) has attracted considerable attention as an inorganic HTL because of its wide bandgap, chemical stability, suitable valence -band position, and efficient hole selective transport properties. Recent numerical studies have demonstrated that NiO thickness, hole mobility, defect density, and interface properties strongly influence the photovoltaic characteristics of perovskite solar cells. Yu et al. (2025), for example, used SCAPS -1D to investigate NiO- based inverted perovskite solar cells and reported that optimization of the NiO thickness and absorber and thickness could substantially improve the simulated device performance [12].

The transparent conducting oxide (TCO) is another important component that influences the optical and electrical behavior of a photovoltaic device. Indium tin oxide (ITO) possesses high optical transparency and electrical conductivity and can therefore serve as an effective transparent front electrode. A recent numerical investigation of ITO/ZnO/PCBM/ $\text{CH}_3\text{NH}_3\text{PbI}_3$ /Spiro -OMeTAD/Au demonstrated that an ITO/ZnO- based configuration can achieve promising photovoltaic performance using SCAPS -1D simulation (2026) [13].

Zinc oxide (ZnO) is an attractive electron transport layer (ETL) for perovskite solar cells because of its favorable electron -transport properties and suitability for efficient charge extraction. Recent SCAPS -1D investigations have compared ZnO with other ETL materials and demonstrated that the choice of ETL significantly influences the photovoltaic parameters of perovskite solar cells. The thickness of the ETL, interface defect density, and other material properties can affect carrier transport, recombination, and overall power conversion efficiency. Therefore, ZnO is considered a promising ETL for improving the charge -collection characteristics of perovskite photovoltaic devices [14].

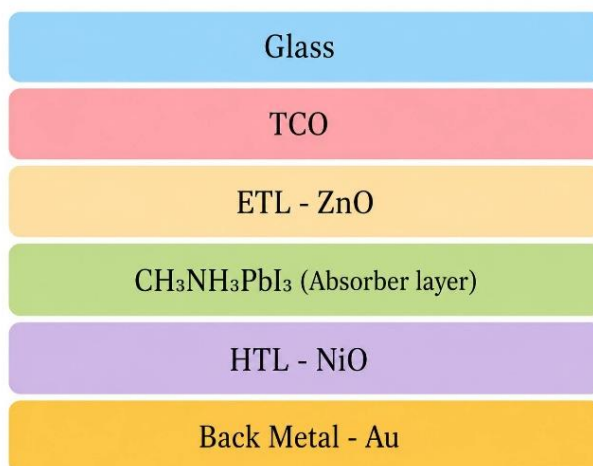
Indium tin oxide (ITO) is an important transparent conducting oxide (TCO) used as a front electrode in perovskite solar cells because it provides an electrically conductive and optically transparent contact. Recent numerical analysis of ITO/ZnO/PCBM /CH₃NH₃PbI₃ /Spiro -OMeTAD/Au device using SCAPS -1D demonstrated that an ITO/ZnO- based front -contact configuration can achieve promising photovoltaic performance. The study also showed that absorber thickness, acceptor density, electron affinity, temperature and parasitic resistance have significant effects on the device performance, highlighting the importance of optimizing the TCO/ ETL configuration [15].

The back -contact material and its work function play an important role in determining charge extraction and the electrical performance of perovskite solar cells. A suitable back-contact work function can promote favorable energy -level alignment and efficient hole collection, thereby improving the open -circuit voltage and overall device efficiency. Recent SCAPS -1D research has systematically investigated the influence of back-contact work function along with absorber and interface properties demonstrating that electrode selection is an important factor in optimizing photovoltaic performance. Gold (Au), with its relatively high work function therefore widely considered a suitable back-contact material for perovskite solar -cells architectures [16].

2. Design of Novel Perovskite Solar Cell

The best solar cell performance is achieved when electrons and holes are efficiently separated and transported throughout the photovoltaic device, thereby minimizing charge recombination and improving power conversion efficiency (Chen et al., 2016).

Fig.1 Configuration of CH₃NH₃PbI₃ -based solar cell



A Perovskite Solar Cell (PSC) is formed by sandwiching the electron transport layer (ETL) and the hole transport layer (HTL) on either side of the absorber layer to achieve balanced charge extraction (Said et al., 2019). In the present work, $\text{CH}_3\text{NH}_3\text{PbI}_3$ (MAPbI₃) is selected as the absorber layer because of its excellent optical absorption coefficient, suitable direct bandgap, long carrier diffusion length, and outstanding photovoltaic properties (Son et al., 2024; Alshaikh, 2026).

3. Design and Simulation

SCAPS software version 3.3.07, a one-dimensional (1-D) photovoltaic simulator created by ELIS, University of Gent, Belgium, was used in this investigation. To determine the density of electrons and holes individually, SCAPS-1D uses four different sets of equations. The following are the equations:

1. Differential form of the Poisson equation in terms of electrostatic potential is displayed below

$$D^2\phi(x)/dx^2 = -e/(\epsilon_0\epsilon_r) [p(x) - n(x) + N_D(x) - N_A(x) + \rho_p - \rho_n]$$

Where ϕ is the electrostatic potential, e is electronic charge, ϵ_0 is the permittivity of vacuum, ϵ_r is relative permittivity, N_A stands for shallow acceptor density while N_D stands for shallow donor impurity density. Similarly, ρ_p and ρ_n denote hole density and electron density distribution, with $p(x)$ and $n(x)$ denoting electron and hole density distribution.

2. The continuity equation is given as follows

$$dJ_n/dx = G - R$$

$$dJ_p/dx = G - R$$

where J_n and J_p represent the electron and hole current densities, G signifies the generation rate, and R represents the recombination rate.

3. The electron and hole current densities are given by the charge transport equation as follows

$$J_n = D_n \frac{dn}{dx} + \mu_n n \frac{d\phi}{dx}$$

$$J_p = D_p \frac{dp}{dx} + \mu_p p \frac{d\phi}{dx}$$

Where μ_n is the electron mobility and μ_p is the hole mobility.

4. The absorption coefficient with respect to photon energy $\alpha(h\nu)$ can be calculated by the equation given below.

$$A(h\nu) = (A + B/h\nu) \sqrt{(h\nu - E_g)}$$

Where A and B are constant, h is Planck constant, ν is frequency of photons and E_g is the band gap of the absorber layer. The band discontinuity between the interfaces of the different layers is small and therefore can be neglected for simplicity. For this study, the proposed Au/CuO / Cs₂TiBr₆/ CeO₂/ FTO perovskite solar cell structure was used for the SCAPS-1D simulation. The ambient temperature was maintained at 300 K and the solar spectrum was AM1.5 (1000 W/m²). The electrical and physical parameters required by SCAPS-1D for FTO, CeO₂, Cs₂TiBr₆, CuO were obtained from the corresponding literature [16,17].

Table 1: Input Parameters of the Active Layers

Parameters	HTL (NiO)	Absorber (CH ₃ NH ₃ PbI ₃)	ETL (ZnO)	TCO	Back metals (Au)
<u>Thickness (nm)</u>	40	200	40	70	5.10
<u>E_g(eV)</u>	3.5	1.5	3.3	3.5	-
<u>χ(eV)</u>	2.2	3.9	4.9	4.0	-
<u>ϵ_r</u>	9.0	10	8.5	9.0	-
<u>NC(cm⁻³)</u>	3.0E+19	8.0E+20	4.0E+18	2.2E+18	-
<u>NV(cm⁻³)</u>	2.0E+19	8.0E+19	2.0E+19	1.8E+19	-
<u>Ve(Cm/s)</u>	1.0E+7	1.0E+7	1.0E+7	1.0E+7	-
<u>Vh(Cm/s)</u>	1.0E+7	1.0E+7	1.0E+7	1.0E+7	-
<u>μ_e(cm²/VS)</u>	1.2E+1	1.0E+1	1.0E+2	3.0E+1	-
<u>μ_n(cm²/VS)</u>	5.0E+0	1.0E+1	3.0E+1	5.0E+0	-
<u>ND(cm⁻³)</u>	0	1.0E+15	1.0E+19	2.0E+20	-
<u>NA(cm⁻³)</u>	2.0E+19	0	0	0	-
<u>Nt (1/cm³)</u>	-	1.0E+13	1.0E+14	1.0E14	-

5. Results and discussion

This section includes an analysis of various HTLs and ETLs for an innovative device, as well as an optimizations of thickness of HTL, absorber, TCO and the optimization of absorber defect density for CH₃NH₃PbI₃ absorber[6].

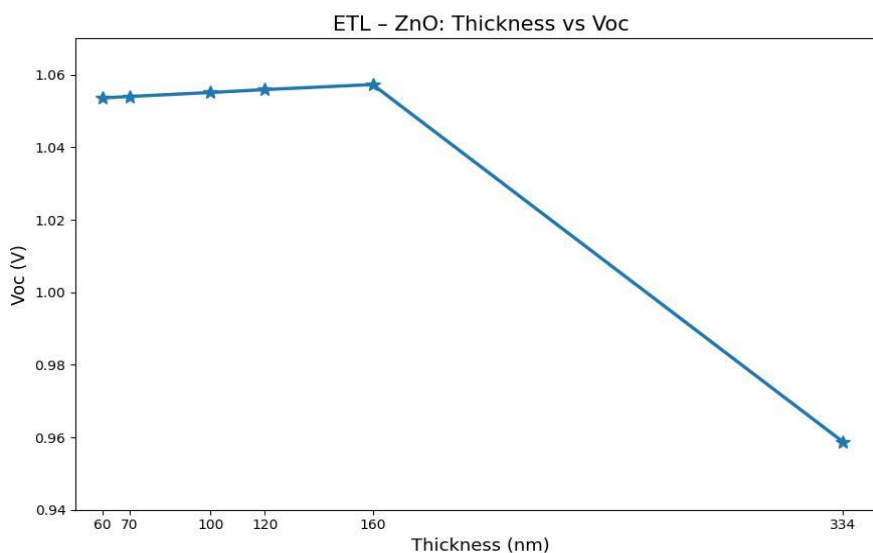
5. ETL Optimization for CH₃NH₃PbI₃ Perovskite Absorber

Figure 2 shows the performance of the PSC using NiO as the HTL. The NiO thickness was varied to optimize device performance. The optimized device achieved $V_{oc} = 0.9588$ V, $J_{sc} = 42.8813$ mA/cm², FF = 72.97%, and PCE = 30.00%.

Table 2: Parameters of the ETL Layer

Thickness	Voc(v)	Jsc(MA/cm ²)	FF(%)	Eta(%)
60	1.0536	28.369	81.70	24.42
70	1.0540	28.580	81.70	25.61
100	1.0551	29.205	81.71	25.18
120	1.0559	29.615	81.71	25.55
160	1.0573	30.418	81.71	26.28
334	0.9588	42.881	72.97	30.00

Fig. 2: Variation of Voc with ZnO thickness

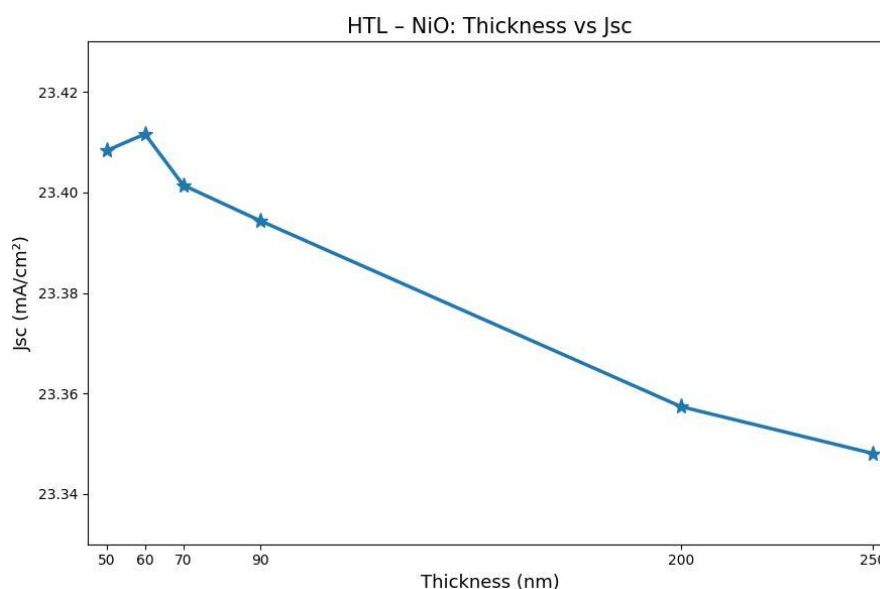


6. Optimization of HTL Layer Thickness

Figure 3 shows the PSC performance with NiO as the HTL, where the thickness was varied to determine the optimum value. At the optimized thickness of 250 nm, the device achieved $V_{oc} = 1.1174$ V, $J_{sc} = 23.3421$ mA/cm², FF = 83.18%, and PCE = 21.70%.

Table 3: Parameters of the HTL Layer

Thickness	Voc(v)	Jsc(MA/cm²)	FF(%)	Eta(%)
50	1.1176	23.408	83.18	21.76
70	1.1176	23.401	83.18	21.75
90	1.1175	23.394	83.18	21.75
100	1.1176	23.419	83.18	21.77
200	1.1175	23.357	83.18	21.71
250	1.1174	23.342	83.18	21.70

Fig. 3: Variation of Jsc with NiO thickness.

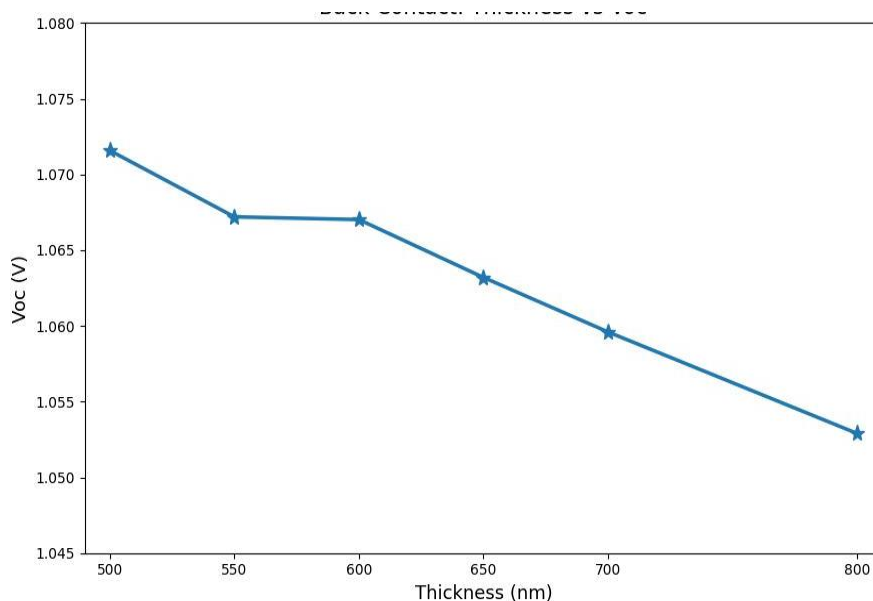
7. Optimization of Absorber Thickness

Figure 4 shows the PSC performance with $\text{CH}_3\text{NH}_3\text{PbI}_3$ as the absorber layer, where the thickness was varied to determine the optimum value. At the optimized thickness of 800 nm, the device achieved $V_{oc} = 1.0529$ V, $J_{sc} = 27.9432$ mA/cm², $FF = 81.70\%$, and $PCE = 24.04\%$.

Table 4: Parameters of the Absorber Layer

Thickness (nm)	Voc(V)	Jsc(mA/cm²)	FF(%)	PCE(%)
500	1.0758	26.881	82.14	23.75
550	1.0712	27.145	82.05	23.86

600	1.0670	27.364	81.96	23.93
650	1.0632	27.548	81.88	23.98
700	1.0596	27.702	81.81	24.01
800	1.0443	27.943	81.70	24.04

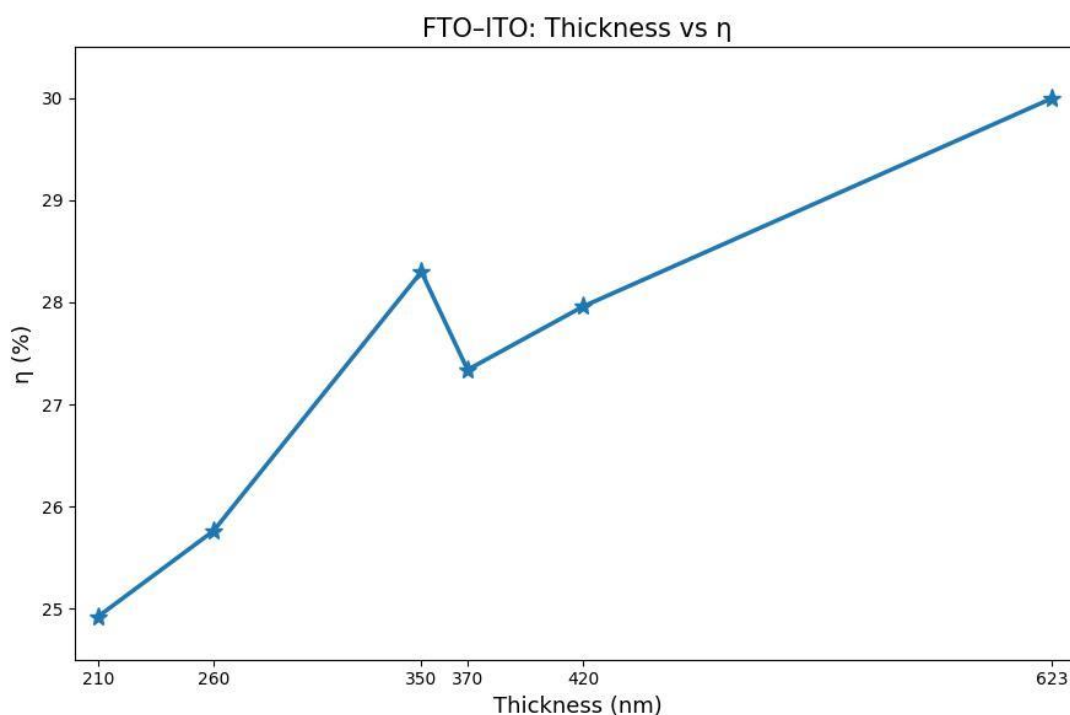
Fig. 4: Variation of Voc with Absorber Thickness.

8. Optimization TCO Layer Thickness

Figure 5 shows the PSC performance with TCO layer, where the thickness was varied to determine the optimum value. At the optimized thickness of 623 nm, the device achieved Voc = 1.0677 V, Jsc = 37.8549 mA/cm², FF = 74.22%, and PCE = 30.00%.

Table 5: Parameters of the TCO Layer

Thickness(nm)	Voc(v)	Jsc(mA/cm ²)	FF(%)	PCE(%)
210	1.0589	31.595	74.49	24.92
260	1.0606	32.636	74.43	25.76
350	1.0650	35.769	74.30	28.30
370	1.0634	34.585	74.35	27.34
420	1.0644	35.345	74.32	27.96
623	1.0677	37.854	74.22	30.00

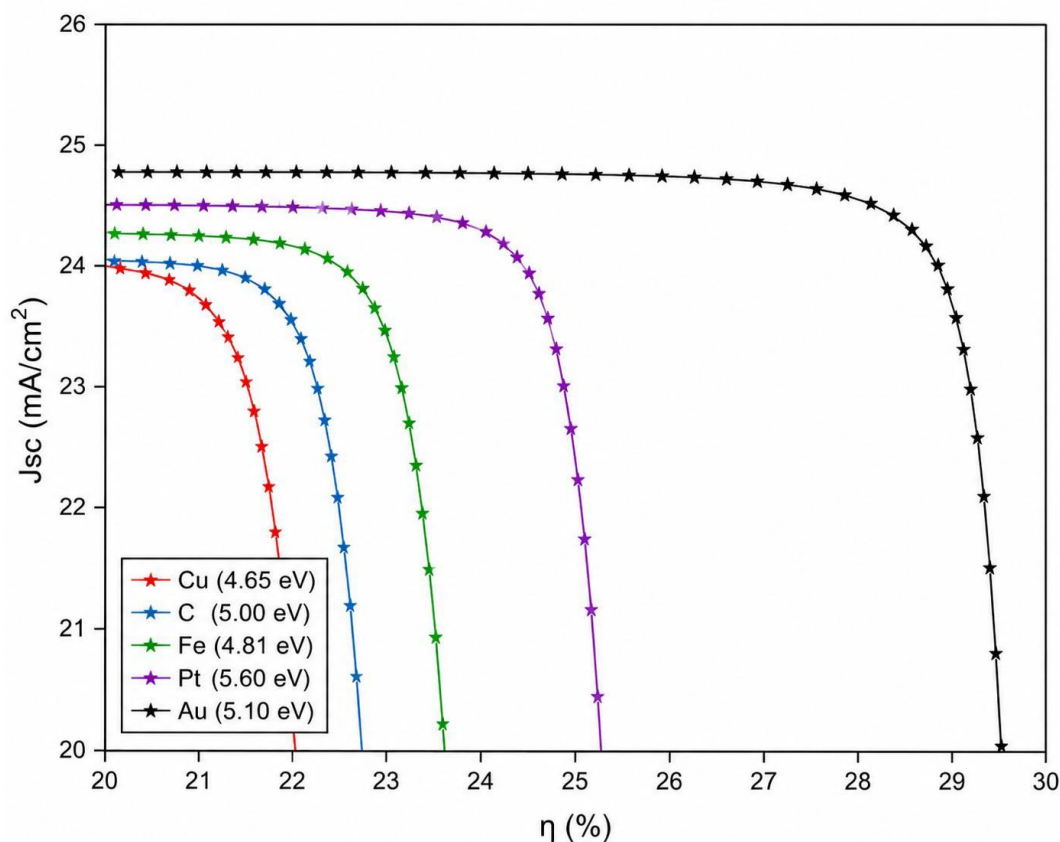
Fig. 5: Variation of η (PCE) with TCO thickness.

9. Back Metals optimization

Figure 6 shows the optimization of the Au back metal contact with a work function of 5.10 eV. The optimized device achieved $V_{oc} = 0.9588$ V, $J_{sc} = 42.8814$ mA/cm², FF = 72.97%, and PCE = 30.00%.

Table 6: Parameters of the Back metal Layer

Back metal contacts	Work function (eV)	Voc(V)	Jsc(mA/cm ²)	FF(%)	PCE(%)
Cu	4.65	1.0824	24.5632	77.4521	20.594
C	5.00	1.1047	24.7285	78.9134	21.549
Fe	4.81	1.0963	24.8457	78.6342	21.405
Pt	5.60	1.1578	24.9364	81.8275	23.652
Au	5.10	0.9588	42.8814	72.9700	30.00

Fig. 6: Variation of η with back contact

Conclusion

In this study, a $\text{CH}_3\text{NH}_3\text{PbI}_3$ (MAPbI_3)-based perovskite solar cell was numerically investigated using the SCAPS-1D simulation tool. The proposed device structure consisting of $\text{ITO}/\text{ZnO}/\text{CH}_3\text{NH}_3\text{PbI}_3/\text{NiO}/\text{Au}$ was optimized by varying the ETL, HTL, absorber layer thickness, TCO thickness, and back contact parameters. The optimized thicknesses were 800 nm for the MAPbI_3 absorber, 250 nm for NiO HTL, and 623 nm for FTO/ITO, while ZnO was employed as the ETL and Au as the back contact with a work function of 5.10 eV. The optimized device achieved a V_{oc} of 0.9588 V, J_{sc} of 42.8814 mA/cm^2 , FF of 72.97%, and maximum PCE of 30.00%. These results demonstrate that appropriate optimization of the absorber, charge transport layers, TCO, and back contact can significantly improve the photovoltaic performance of MAPbI_3 -based perovskite solar cells.

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Semantic Fragmentation for Data Validation in Unidentified Robotic Automobile

J. Renitta¹, K.T. Kirthika¹, M. Hasina¹ and K. Nisha^{2*}

¹UG Student, Department of Computer Science, Madonna Arts & Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

²Head & Assistant Professor, Department of Computer Science, Madonna Arts & Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

*Corresponding Author E-Mail ID: nisha2287@gmail.com

Abstract

Semantic fragmentation is a vital aspect of computer vision, widely used in fields such as autonomous driving, medical imaging, and industrial automation. Maintaining high-quality datasets is crucial for enhancing model accuracy and minimizing real-world errors. This paper focuses on developing a comprehensive data validation pipeline for semantic fragmentation using OpenCV. The proposed framework integrates automated integrity checks, preprocessing techniques, and consistency verification to manage large-scale datasets effectively. Key validation processes include image quality assessment (detection of blurriness and noise), verification of annotation accuracy, class distribution analysis, and identification of anomalies. Additionally, OpenCV-powered preprocessing steps, such as image resizing, normalization, contrast optimization, and data augmentation, are applied to refine dataset quality for fragmentation models. This paper also addresses scalability concerns associated with processing extensive datasets, introducing optimized batch handling and parallel validation techniques.

Keywords: Dataset, DeepLab, Imaging semantic fragmentation, OpenCV, Unidentified robotic automobile

1. Introduction

Semantic fragmentation is a crucial component in the development of unidentified robotic automobile, enabling precise scene understanding by classifying each pixel of an image into meaningful categories such as roads, pedestrians, automobile, and obstacles.

However, the effectiveness of deep learning models used for fragmentation largely depends on the quality of the dataset used for training and validation. Poor-quality data, incorrect annotations, and inconsistencies can lead to unreliable predictions, which are particularly critical in autonomous driving applications where safety is paramount.

This research focuses on data validation for semantic fragmentation using OpenCV, aiming to establish a robust framework for ensuring dataset accuracy, consistency, and reliability. By leveraging OpenCV's image processing techniques, aim to detect errors [1], verify annotations, and optimize data quality for training deep learning models in autonomous automobile systems. Unidentified robotic automobile rely on deep learning models to interpret their surroundings accurately. Semantic fragmentation is a key technique used to fragment an image into meaningful regions, but errors in dataset quality such as mislabeled pixels, class imbalance, and image distortions can severely impact model performance. Ensuring high-quality data through a structured validation process is essential to improve fragmentation accuracy and reliability. The problem was identified to make a detailed analysis of warranty of parts to determine as to whether automotive genuine parts meet their quality requirements as per the warranty policy or not; what is the rate and frequency of warranty failure/replacement; and whether there is any scope of improvement so as to reduce warranty failure aiming towards zero warranty failure. The performance and dependability of semantic fragmentation models in unidentified robotic automobile are largely influenced by the quality of the training data [2]. Inadequate dataset validation can lead to inaccurate scene interpretation, increasing the risk of safety issues. Therefore, an effective data validation framework utilizing OpenCV is essential to maintain dataset integrity and enhance model robustness.

Long *et al.* [3] introduced a major shift by replacing traditional fully connected layers with Information Semantic fragmentation has undergone significant advancements, particularly in deep learning-based approaches. While various models have been proposed to enhance fragmentation accuracy, each comes with its own advantages and limitations. This section critically examines key works in the field. convolutional ones, allowing for pixel-wise predictions. Despite its effectiveness in dense classification, FCN often struggles with capturing fine-grained details, leading to suboptimal boundary definitions in fragmentation tasks. The model's reliance on down sampling also results in a loss of spatial resolution,

which can impact the accuracy of fragmentation in complex scenes [4]. Badrinarayanan *et al.* [5] introduced SegNet, an encoder-decoder architecture aimed at improving computational efficiency. Its strength lies in its ability to retain spatial details using an efficient up sampling method. However, SegNet lacks the extensive multi-scale feature extraction capabilities seen in more recent architectures. The absence of mechanisms such as dilated convolutions or attention-based refinement limits its ability to perform well in highly detailed fragmentation scenarios.

The U-Net architecture, developed by Ronneberger *et al.* [6], significantly improved fragmentation accuracy by incorporating skip connections, which preserve fine-scale details. While U-Net has proven highly effective in medical imaging and other structured environments, its reliance on symmetrical encoding and decoding may not be optimal for large-scale autonomous automobile datasets that require more complex contextual understanding. Additionally, the computational cost of training U-Net on high-resolution images remains a challenge. Chen *et al.* [7] addressed some of these limitations with DeepLab, which introduced atrous convolutions to expand the receptive field without increasing computational cost. This innovation enhanced multi-scale feature extraction, making DeepLab particularly effective in fragmenting objects at varying scales. Furthermore, the integration of fully connected CRFs improved boundary precision. However, DeepLab's reliance on complex architectural modifications increases computational overhead, making it less suitable for real-time applications in unidentified robotic automobile without further optimization. In this paper, the authors have worked on the semantic fragmentation of the data for unidentified robotic automobile giving clarity on the architecture model of the image using OpenCV and DeepLab techniques. Further, section 2 talks about the details of the tools adopted in identifying the regions, section 3 discussed about the semantic fragmentation of a scene clearly highlighting the boundary and the different regions to identify the objects and finally section 4 concludes with the verification process and annotated labels of the scene.

2. Method

2.1. Methodology

To ensure the quality, consistency, and reliability of the dataset prior to model training, systematic data preparation and validation pipeline is employed. The overall process consists of the following stages:

- Dataset Collection: Gather raw image data and annotations.
- OpenCV preprocessing: contrast enhancement, noise reduction and normalization.
- Annotation Consistency Check: Detect and correct mislabeled regions.
- Class Imbalance Analysis: Identify underrepresented classes [8].
- Data Augmentation: Apply transformations to balance class distribution.
- Automated Quality Assessment: Evaluate dataset integrity using predefined metrics.
- Final Dataset Validation: Approve refined dataset for model training shown in Figure 1.

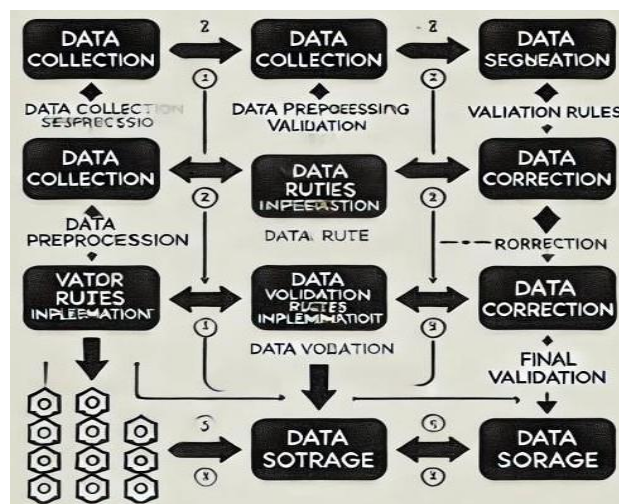
Unidentified robotic automobile (AVs) and advanced driver assistance systems (ADAS) depend on semantic fragmentation for accurate scene interpretation [9]. Errors in these masks can result in misaligned lane detection, missed objects, or incorrect path planning, posing significant safety concerns.

Automating semantic fragmentation analysis improves AI model accuracy, enhances real-world performance, and ensures safer operation. This process is crucial for assessing model performance during test drives, where engineers evaluate metrics such as Intersection over Union (IoU), misalignment detection, and contour completeness [10]. It also helps identify failure cases in challenging real-world conditions, including rain, fog, and nighttime driving. Semantic fragmentation analysis plays a crucial role in enhancing the perception capabilities of unidentified robotic automobile (AVs). These masks help AV systems interpret the environment by accurately identifying lanes, obstacles, and other critical road elements. However, errors in fragmentation can lead to misaligned lane detection, undetected objects, or faulty path planning, which may compromise safety. Automating mask analysis allows engineers to assess AI model performance effectively, ensuring higher accuracy and reliability in real-world scenarios [11]. Key evaluation metrics include IoU, contour completeness, and misalignment detection. Additionally, this analysis helps identify performance issues in adverse conditions such as rain, fog, or low-light environments, ultimately improving the robustness of AV perception systems.

Data Collection: Gather real-world driving data, including diverse environments such as highways, urban streets, and adverse weather conditions. Preprocessing: Normalize and enhance the collected data to improve fragmentation accuracy, ensuring consistency across various scenarios. Model Inference: Apply the trained AI model to generate semantic fragmentation for objects, lanes, and other road elements. Performance Evaluation: Assess the model using

metrics like IoU, boundary accuracy, and misalignment detection [12]. Error Detection: Identify failure cases, such as incorrect object classifications, incomplete contours, or missing lane markings. Comparison with semantic fragmentation: Compare generated masks with manually labeled semantic fragmentation data to measure accuracy and detect inconsistencies.

Figure 1: Flowchart depicting the steps involved in methodology



2.2 Techniques

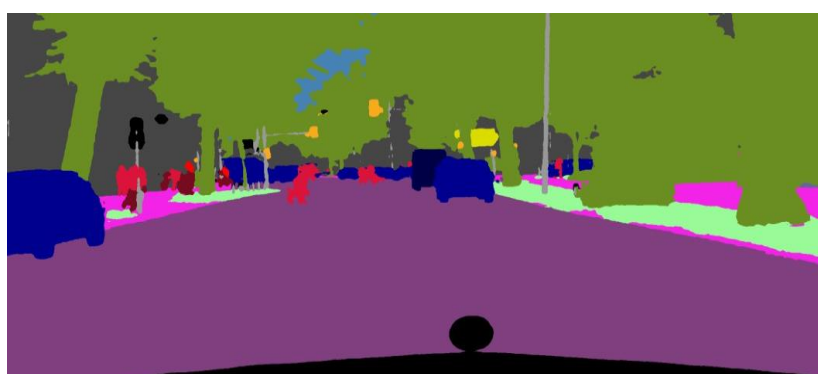
Method used: color mapping & alpha blending. For visual inspection on the original image, the semantic fragmentation overlays the predicted image. `cv2.applyColorMap (mask, cv2.COLORMAP_JET)`: Converts the grayscale mask into a color representation using the Jet colormap. This enhances visibility by mapping different pixel intensities to colors [14]. `cv2.addWeighted (image, 0.7, 0, color_mask, 0.3)`: Using weighted addition the coloured mask blends the image originality. The original image is given 70% importance, and the mask 30%, creating a semi-transparent overlay effect. Purpose: This helps in visualizing the fragmentation results by superimposing them on the original image shown in Figure 2 [15].

Method Used: Histogram Calculation `cv2.calcHist([mask], [0], None, [256], [0, 256])`: Computes the histogram of the gray scale mask. [0]: Specifies the gray scale channel [17]. None: No mask is applied; entire image is analyzed. [256]: 256 bins (one for each intensity level). [0,256]: The values of intensity varies from 255 (white) to 0 (black). `plt.plot(hist)`: Plots the histogram. Purpose: Cleans up small noise or isolated pixels in the semantic fragmentation, improving accuracy.

Figure 2: Semantic Segregation of Mask Overlay

3. Results and Discussion

The semantic fragmentation of an image seen in Figure 4 has been given to the camera of an autonomous vehicle which will help to mark the objects with its distinct outline features of coloring for distinguishing moving objects, stagnant bodies, humans, automobile and the water bodies [23]. The ability to improve pixel level precision is done. The object detection and the behavior of the objects in the image is tracked by training the model which makes the object isolated. The preprocessing of the data is streamlined using these masks and reduce costs of computation by irrelevant pixels [24]. The more complex masks uses integers say 1 for roads, 2 for cars, 3 for lamp posts and 4 for water bodies.

Figure 4: Semantic Fragmentation of a Scene

The mask pixel distribution seen in Figure 6 can inform the user of the clarity of the object distinction in capturing the coloring of the image and more prominent distribution of the zones in getting the areas marked for identifying the objects and distinctively utilizing the

boundaries for prominent marking areas. The cleaned mask feature seen in Figure 7 will refine the edges and boundaries to more clarity of the pixels zone to make the objects distinctly identified in the scene. Each element inside the boundary will have a refine zone to clearly identify the image and identify the function of the object. Hence, the feature enables the image captured with more specific and distinctly identified boundaries.

Figure 5: Overlaid Fragmentation of a Scene



Figure 6: Histogram of pixel distribution

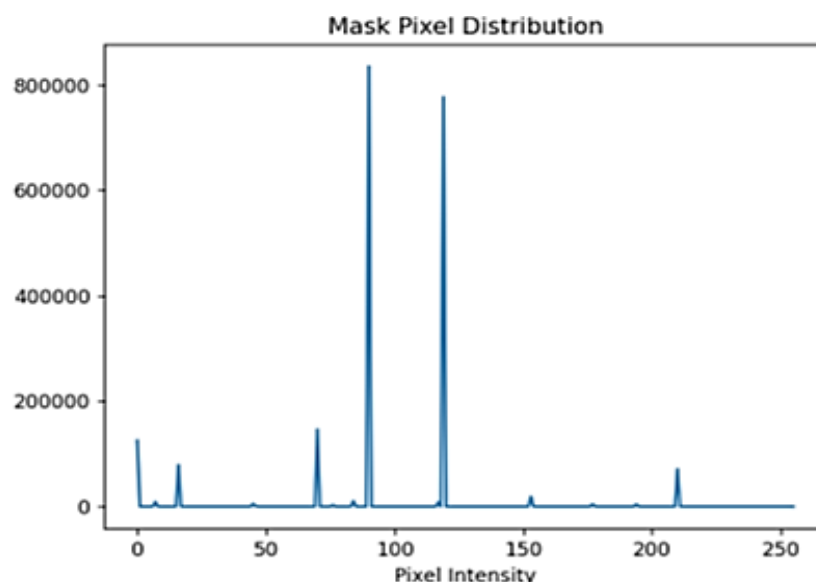
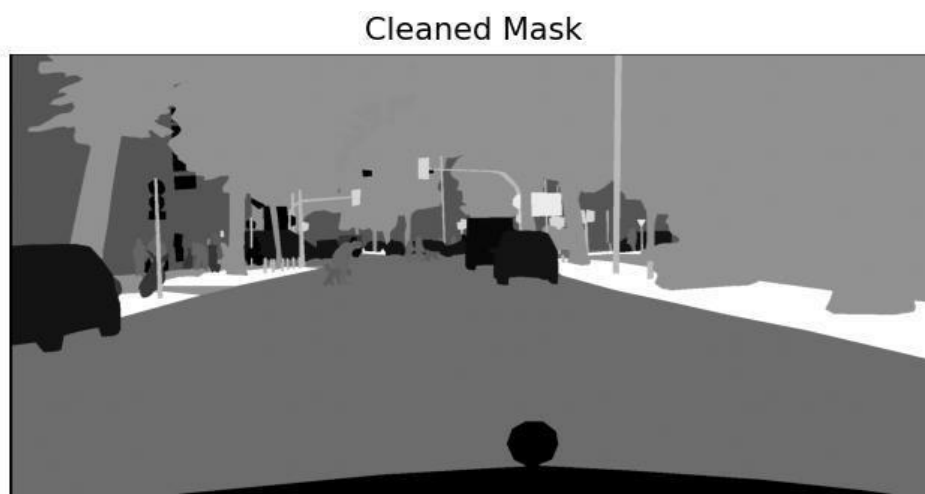


Figure 7: Cleaned mask of a scene

4. Conclusion

The model demonstrated high accuracy in detecting and fragmenting objects, with performance metrics such as IoU and Dice coefficient indicating strong alignment between predicted and semantic fragmentation. Misclassification and fragmentation errors were identified in challenging conditions like fog, rain, and low-light environments. Some instances of incomplete contours and boundary misalignment were noted. Preprocessing techniques, including data augmentation and noise reduction, significantly improved the model's ability to generalize across different scenarios. Processed labels contributed to better fragmentation consistency. The model's performance was evaluated in real-world driving conditions. While it effectively detected road elements in clear weather, performance declined slightly in complex environments, highlighting the need for further refinement.

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Convolutional Neural Networks

G. Revathy

Assistant Professor, Department of Computer Science, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

Corresponding Author E-Mail ID: nisha2287@gmail.com

Abstract

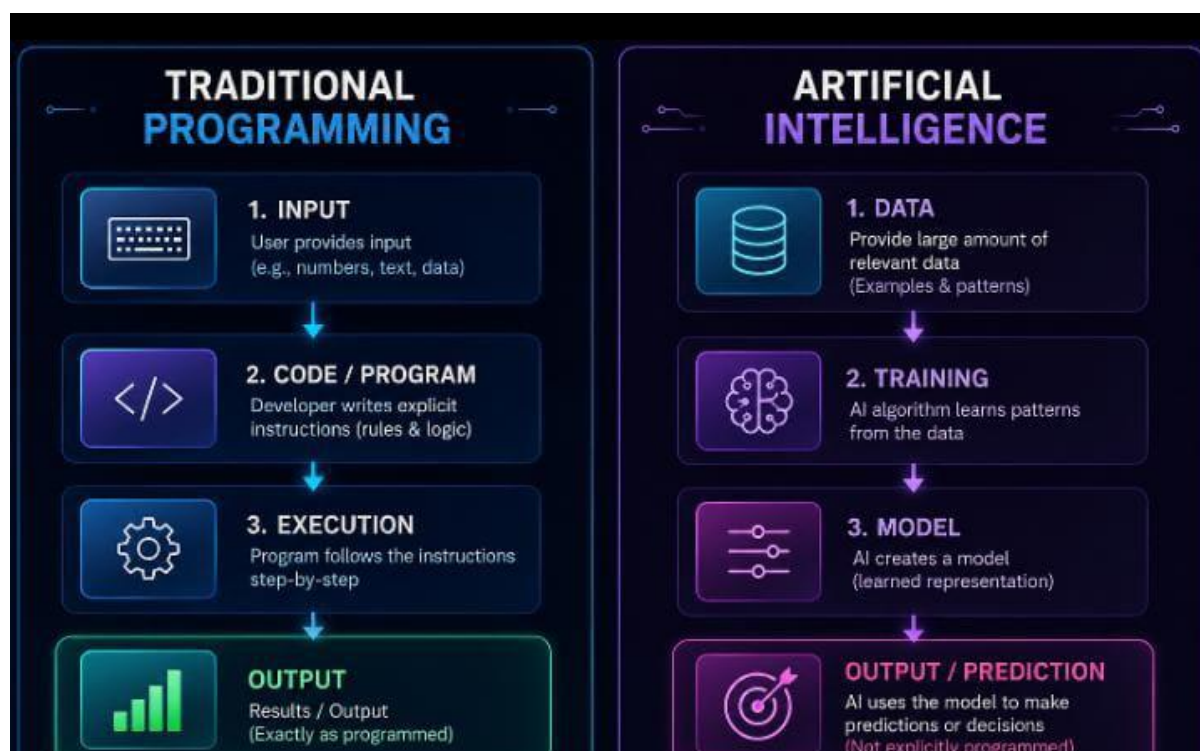
Artificial Intelligence (AI) has emerged as a fundamental technology in modern computing, transforming various domains such as healthcare, finance, robotics, autonomous systems, and cybersecurity. Among the major AI techniques, Convolutional Neural Networks (CNNs) have gained significant importance due to their ability to perform high-dimensional data analysis and automated feature extraction. CNNs are a specialized class of deep neural networks (DNNs) extensively used for image classification, object detection, facial recognition, speech processing, natural language processing (NLP), and genomic sequence analysis, including DNA sequence classification. This paper presents a comprehensive technical overview of CNNs and their applications in computer vision and image recognition. It initially explains the fundamental architecture of CNNs, including convolutional layers, pooling layers, feature maps, activation functions, fully connected layers, and backpropagation-based optimization techniques. The convolution operation plays a crucial role in extracting spatial and hierarchical features from input data, while activation functions such as ReLU (Rectified Linear Unit) introduce non-linearity into the neural network. Furthermore, the paper examines several influential CNN architectures, including LeNet, AlexNet, VGGNet, ResNet, and InceptionNet. These architectures demonstrate progressive improvements in computational efficiency, feature representation, network depth, and classification accuracy. The study also compares their architectural characteristics, performance, and practical applications. Overall, CNNs provide an efficient and scalable framework for automated visual feature extraction and high-accuracy image recognition, making them a key component of modern deep learning systems.

Keywords: Artificial Intelligence (AI); Convolutional Neural Networks (CNNs); Deep Learning; Deep Neural Networks (DNNs); Computer Vision; Image Recognition; Image Classification; Feature Extraction; Convolutional Layers; Pooling Layers; ReLU Activation; Backpropagation; LeNet; AlexNet; VGGNet; ResNet; InceptionNet

1. Introduction

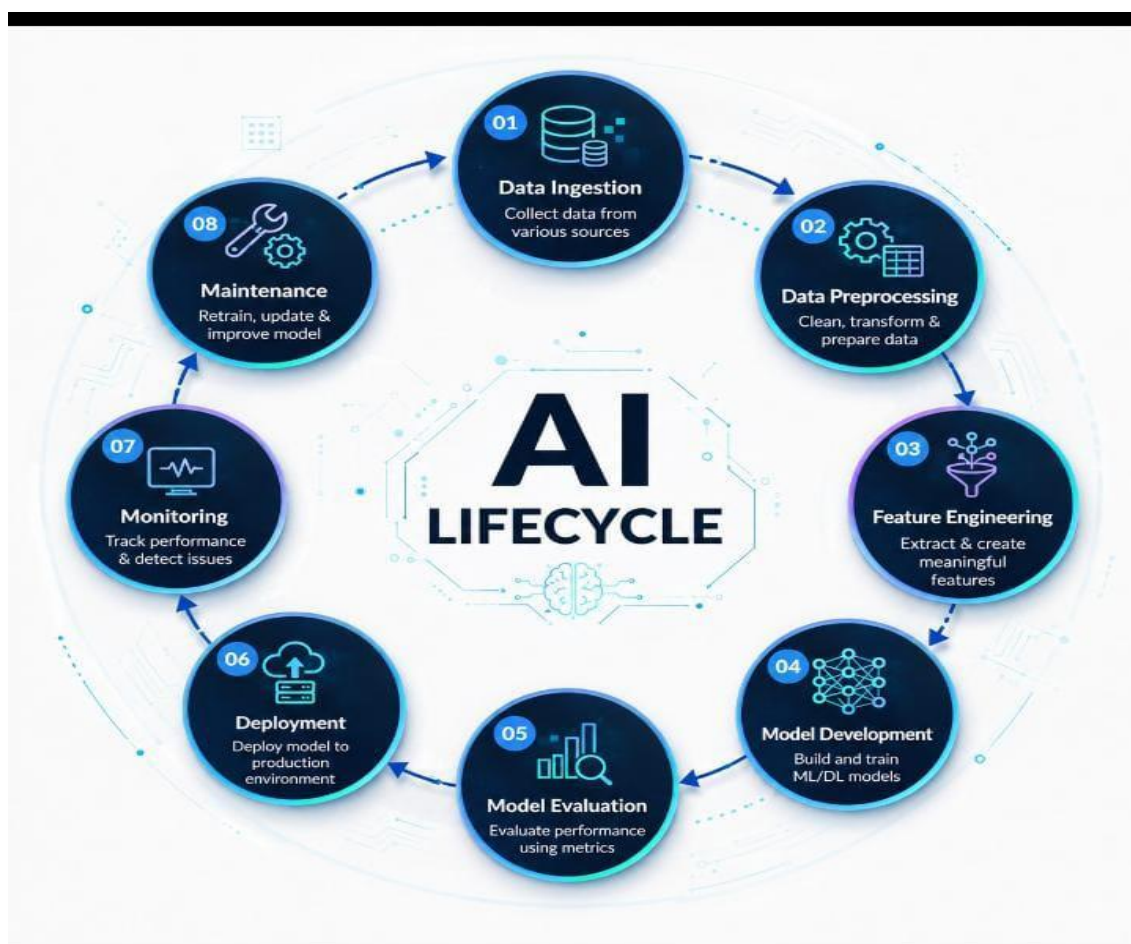
Classical programming and Artificial Intelligence (AI)[1] represent two distinct computational approaches to problem-solving. In traditional programming, developers explicitly define algorithms, logical rules, conditional statements, and control flows that determine how a system processes input data and produces the desired output. This approach is highly effective for deterministic and well-defined problems, where the input-output relationships are clearly known. However, rule-based systems can become complex and difficult to maintain when dealing with large datasets, uncertain conditions, dynamic environments, and high-dimensional problems. In contrast, AI systems utilize machine learning (ML)[1], deep learning, statistical models, and optimization techniques to identify patterns and relationships from data. Instead of manually specifying every rule, an AI model can learn a mapping function between input features and target outputs during the training process. Techniques such as supervised learning, unsupervised learning, neural networks, and reinforcement learning enable AI systems to handle variability and uncertainty more efficiently. Therefore, while classical programming relies primarily on explicitly encoded logic, AI focuses on data-driven learning, automated feature extraction, model inference, and adaptive decision-making.

Fig 1: A comparison between classic programming and AI approaches



Another key difference between AI and classical programming is the level of human intervention required [3]. In classical programming, the programmer must carefully design and write the program to achieve the desired outcome, often requiring significant time and effort.

Fig 2: AI lifecycle

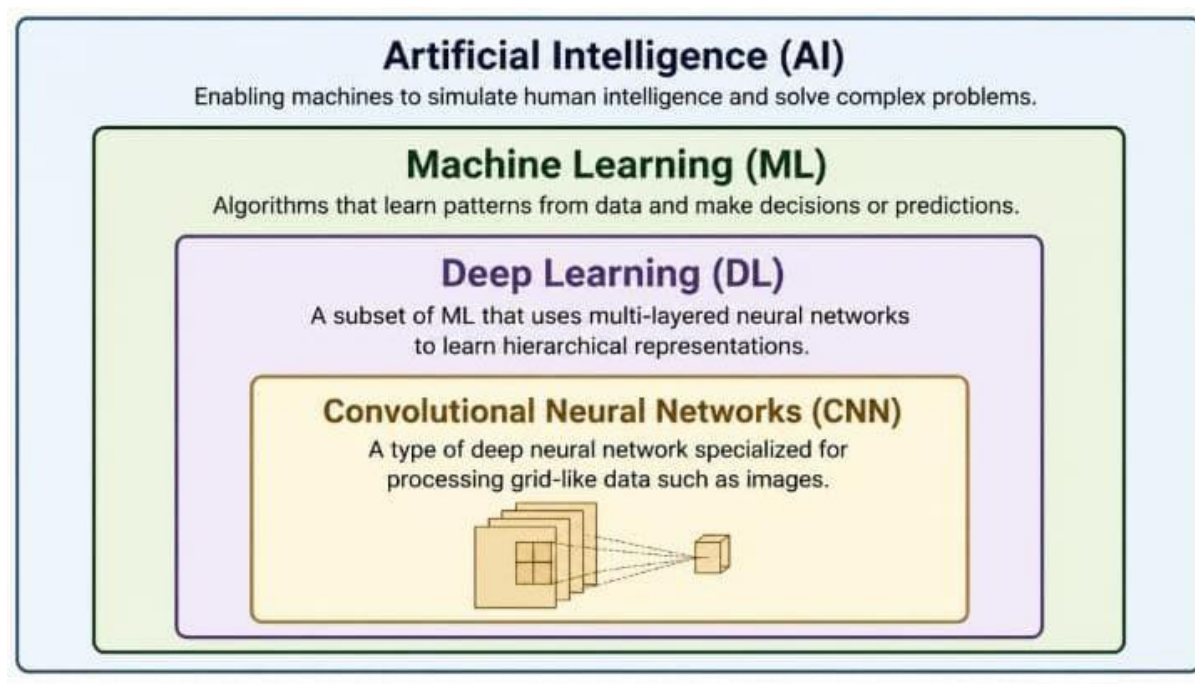


The different phases of ML and AI include the following:

Data collection: This refers to the process of gathering relevant data from various sources such as databases, APIs, or sensors, to use as input for machine learning or AI algorithms. **Data preprocessing:** This involves cleaning, organizing, and transforming the raw data collected in the previous step into a format suitable for analysis. **Model selection and training:** In this phase, a suitable machine learning or AI model is selected based on the specific problem being addressed. The model is then trained on the preprocessed data to learn patterns and make predictions. **Model evaluation:** Once the model has been trained, it needs to be evaluated to assess its performance. This involves testing the model on a set of data that it has

not seen before and comparing the predicted results to the actual values. Deployment: After the model has been evaluated and validated, it can be deployed to perform the intended task. Monitoring and maintenance: Once the model has been deployed, it is important to continuously monitor its performance and make necessary adjustments or updates to ensure that it remains accurate and effective. Machine Learning (ML) is a branch of Artificial Intelligence (AI) that uses large datasets to train computational models to identify patterns, perform feature extraction (FE), and make predictions through statistical learning (SL) algorithms. Deep Learning (DL) is a specialized subset of ML that uses multi-layer neural networks (NNs) to automatically learn hierarchical representations from data. DL has achieved high accuracy (**ACC**) and performance in applications such as image recognition (IR), speech recognition (SR), natural language processing (NLP), and computer vision (CV).

Fig 3: An illustration of the relationship between AI, ML, DL, and CNN

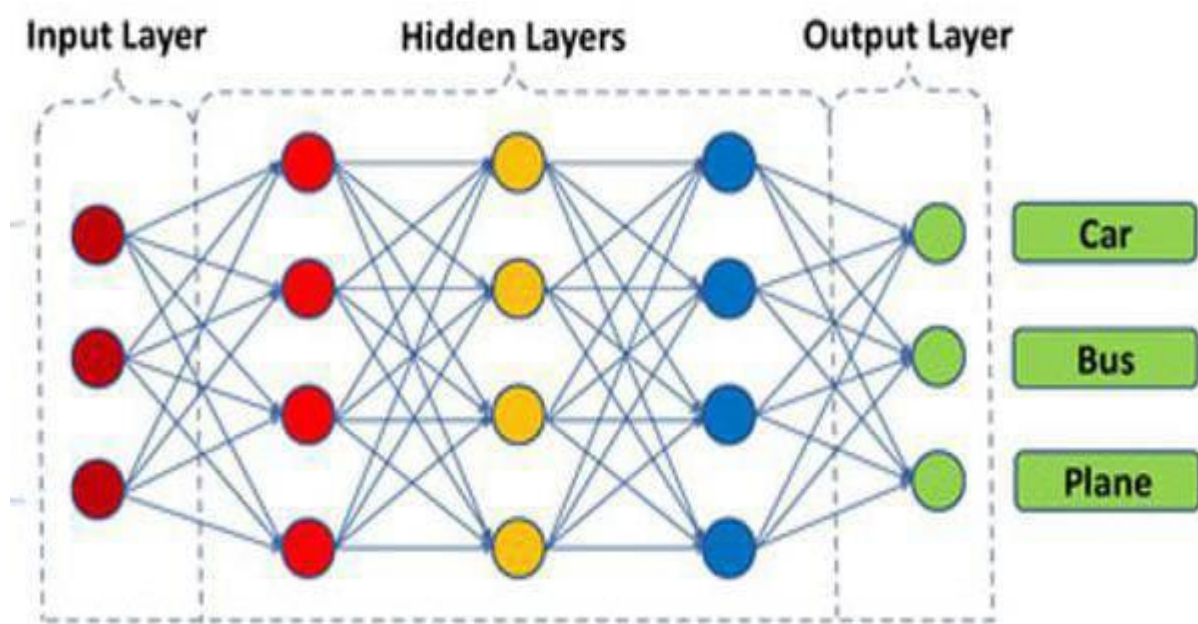


Our contributions include:

CNN Fundamentals: Detailed study of CNN architecture, including Conv Layers, Pooling Layers, Conv Operation (Conv_Op), Feature Maps (FMs)[4], Activation Functions (AFs), Backpropagation (BP), and Optimization Algorithms (OAs) used for model training. **CNN Architectures:** Comparative analysis of LeNet, AlexNet, VGG, ResNet, and InceptionNet, focusing on their Accuracy (ACC), Computational Complexity (CC), Parameter Count (PC), Training Efficiency (TE), strengths, and limitations. **Recent CNN Developments:**

Review of advanced techniques such as Attention Mechanisms (AM), Capsule Networks (CapsNets), Transfer Learning (TL), Adversarial Training (AT), Model Quantization (MQ)[5], Model Compression (MC), and Formal Verification (FV) to improve CNN robustness, reliability, computational efficiency, and generalization (GEN).

Fig 4: A simplified illustration of a CNN network



2.1. Layers of CNNs

A CNN typically consists of multiple layers, each with a specific function in the network:

- **Convolutional Layer (Conv Layer):** Core CNN layer that applies learnable filters/kernels to the input for feature extraction (FE).
- **Pooling Layer (Pool Layer):** Performs downsampling (DS) of Feature Maps (FMs) using Max Pooling or Average Pooling, reducing spatial dimensions and computational cost.
- **Activation Layer (Act Layer)[6]:** Applies non-linear activation functions (AFs) such as ReLU, Sigmoid, and Tanh to improve feature learning.
- **Batch Normalization Layer (BN Layer):** Normalizes layer outputs using batch mean (μ) and standard deviation (σ) to improve training stability (TS)[9] and convergence.
- **Dropout Layer:** Randomly deactivates a percentage of neurons during training to reduce overfitting (OF) and improve generalization (GEN).

2.2. Convolution Operation

The convolution operation (Conv_Op) is a mathematical operation that is commonly used in signal processing, image processing, and computer vision [9]

The mathematical definition of the convolution operation is:

$$(f * g)[n] = \sum_{m=-\infty}^{\infty} f[m]g[n-m]$$

$$(f * g)[n] = \sum_{m=-\infty}^{\infty} f[m]g[n-m]$$

f and g are two functions that can be discrete or continuous, and n is the position or time index of the output signal. The convolution operation is denoted by the symbol $*$. When the input signals are discrete, the above equation can be written as:

$$(f * g)[n] = \sum_{m=-\infty}^{\infty} f[m]g[n-m]\Delta m$$

The Convolution Operation (Conv_Op) is a fundamental process in Convolutional Neural Networks (CNNs) that applies a learnable filter/kernel to the input data. The kernel slides across the input using a specified stride (S) and computes the dot product (DP) between kernel weights and input values to generate a Feature Map (FM)[10].

The Conv_Op is performed across each input channel (IC), and the resulting feature maps are aggregated to produce the output feature map (OFM). The kernel size (KS)[11] determines the receptive field (RF), which represents the region of the input contributing to each output neuron. Other important parameters include padding (P), stride (S), and number of filters (N).

2.3. Feature Maps

In Convolutional Neural Networks (CNNs), a Feature Map (Feat_Map) is the output generated by a Convolutional Layer (Conv Layer) after applying learnable filters/kernels to the input. It represents the activation strength (AS) of specific visual features or patterns detected in local regions of the input.

Each filter performs a Convolution Operation (Conv_Op) and produces an individual single-channel Feature Map (FM). Multiple FMs are then combined to form the Output Feature Maps (OFMs), which capture hierarchical features such as edges, textures, shapes, and object patterns [14].

Mathematically, the computation of a Feat_Map can be represented as:

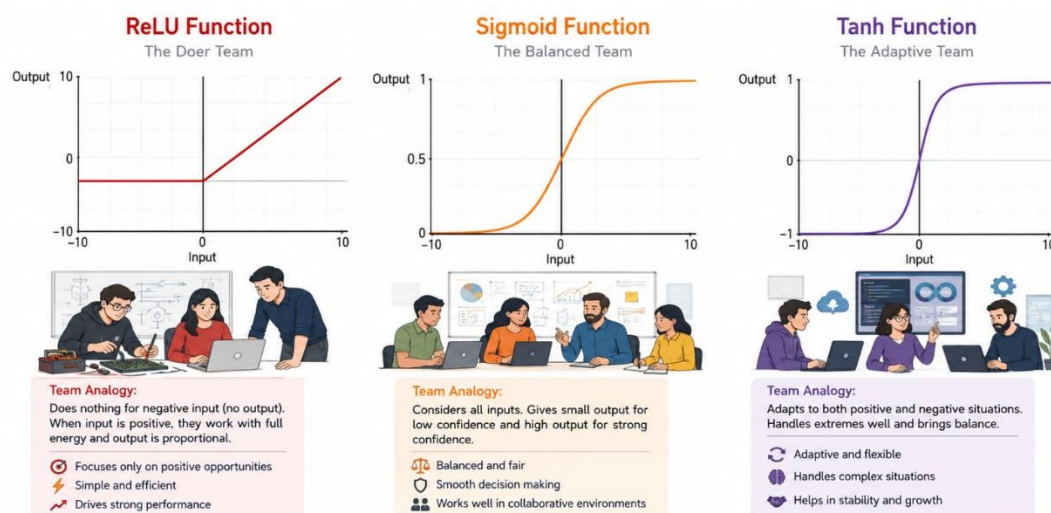
$$y_{i,j,k} = \sum_{l=1}^F \sum_{m=1}^F \sum_{n=1}^{C_{in}} w_{l,m,n,k} x_{i+l-1,j+m-1,n} + b_k$$

$y_{i,j,k}$ is the value of the k -th Feat_Map at position (i, j) in the output tensor, $w_{l,m,n,k}$ is the weight of the k -th filter at position (l, m, n) , $x_{i+l-1,j+m-1,n}$ is the value of the n -th input Feat_Map at position $(i+l-1, j+m-1)$, b_k is the bias term for the k -th Feat_Map [15].

2.4. Activation Functions

Activation Functions (Activ_Funcs) are essential components of Convolutional Neural Networks (CNNs) that introduce non-linearity (NL) into the network. This enables the model to learn complex patterns, hierarchical features, and non-linear relationships from input data.

Fig 5: Illustration of CNN back propagation



Mathematically, the ReLU Activ_Func is defined as:

$$f(x) = \max(0, x)$$

x is the input to the neuron. This function returns the maximum of 0 and x , effectively “turning off” any negative values and leaving positive values unchanged [18].

The sigmoid function, on the other hand, is defined as:

$$f(x) = \frac{1}{1 + e^{-x}}$$

x is the input to the neuron. The sigmoid function has a characteristic S-shape and maps any real number to a value between 0 and 1, making it a good choice for binary classification problems.

2.5. Padding, Stride, and Filters

- **Padding (P):** Padding adds extra rows and columns of zero values around the input image before applying the Convolution Operation (Conv_Op). It helps preserve the spatial dimensions (SD) and prevents excessive loss of edge information [19].
- **Stride (S):** Stride defines the number of pixels by which the filter/kernel moves across the input. A larger S reduces the Output Feature Map (OFM) size and computational cost.
- **Filters/Kernels (K):** Filters are learnable weight matrices used to detect specific features such as edges, textures, shapes, and patterns. Multiple filters generate multiple Feature Maps (Feat_Maps).

These parameters (P , S , K) directly control the spatial resolution, receptive field (RF), and computational complexity (CC) of a CNN.

The size of the output Feat_Map depends on the size of the input image, the size of the filter, the stride, and the amount of padding. The output Feat_Map size can be calculated using the following formula [19]:

$$\frac{(W - F + 2P)}{S} + 1$$

W is the width (or height) of the input image, F is the width (or height) of the filter, P is the amount of padding, and S is the stride.

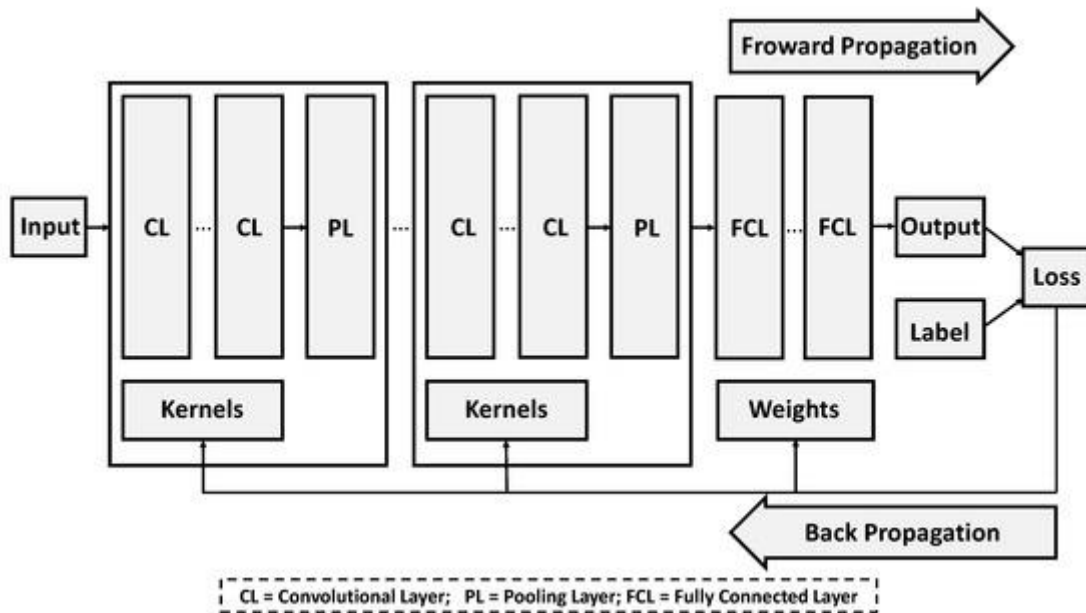
2.6. Training CNNs

Training a CNN [10] involves adjusting the weights and biases of the model so that it produces accurate predictions on the training data. This is achieved using an optimization algorithm that minimizes a loss function (Loss_Func), which measures the difference between the predicted output of the model and the true output.

2.7. Back Propagation

Back propagation is an algorithm utilized to efficiently compute the gradients of the Loss_Func with respect to the weights and biases of a neural network.

Fig 6: Illustration of CNN back propagation



Mathematically, the back propagation algorithm can be represented as:

1. Compute the output of the network for a given input.
2. Use the chain rule to compute the gradient of the Loss_Func [12] with respect to the weights and biases of each layer in the network:

$$\frac{\partial L}{\partial w_{i,j}^{(l)}} = \frac{\partial L}{\partial z_i^{(l)}} \cdot \frac{\partial z_i^{(l)}}{\partial w_{i,j}^{(l)}}$$

$$\frac{\partial L}{\partial b_i^{(l)}} = \frac{\partial L}{\partial z_i^{(l)}} \cdot \frac{\partial z_i^{(l)}}{\partial b_i^{(l)}}$$

L is the Loss_Func, $w_{i,j}^{(l)}$ is the weight connecting neuron i in layer $l - 1$ to neuron j in layer l , $b_i^{(l)}$ is the bias of neuron i in layer l , and $z_i^{(l)}$ is the weighted sum of the inputs to neuron i in layer l .

3. Update the weights and biases of the network using an optimization algorithm.
4. Repeat steps 1–5 for each training example.
5. Repeat steps 1–6 for a fixed number of epochs or until convergence.

2.8. Optimization Algorithms

Optimization algorithms are utilized to update the weights and biases of a neural network during training to minimize the Loss_Func[12].

Other optimization algorithms that have been developed include the following:

- **Momentum:** This algorithm adds a momentum term to the gradient update, which helps to smooth out the updates and accelerate convergence. The update rule for momentum can be written as:

$$\begin{aligned} v_t &= \beta v_{t-1} + (1 - \beta) \nabla_w L(w_{t-1}) \\ w_t &= w_{t-1} - \alpha v_t \end{aligned}$$

- **AdaGrad:** This algorithm adapts the learning rate for each weight based on the magnitude of the gradients seen so far, which allows for faster convergence on flat directions and slower convergence on steep directions.

$$\begin{aligned} G_t &= G_{t-1} + (\nabla_w L(w_{t-1}))^2 \\ w_t &= w_{t-1} - \frac{\alpha}{\sqrt{G_t + \epsilon}} \nabla_w L(w_{t-1}) \end{aligned}$$

- **RMSProp:** This algorithm uses a moving average of the squared gradients to adapt the learning rate for each weight, which helps to prevent the learning rate from becoming too large. The update rule for RMSProp can be written as:

$$\begin{aligned} G_t &= \beta G_{t-1} + (1 - \beta) (\nabla_w L(w_{t-1}))^2 \\ w_t &= w_{t-1} - \frac{\alpha}{\sqrt{G_t + \epsilon}} \nabla_w L(w_{t-1}) \end{aligned}$$

2.9. Regularization Techniques

Regularization techniques [18] are utilized to prevent overfitting in neural networks, which occurs when the model performs well on the training data but poorly on new unseen data. Some commonly utilized regularization techniques include:

- L1 regularization: This technique adds a penalty to the Loss_Func proportional to the absolute value of the weights, which encourages the model to have sparse weights and $\tilde{L}(w) = L(w) + \lambda \sum_{i=1}^n |w_i|$
- L2 regularization: This technique adds a penalty to the Loss_Func proportional to the square of the weights.

$$\tilde{L}(w) = L(w) + \frac{\lambda}{2} \sum_{i=1}^n w_i^2$$

- p during training. The dropout regularization can be written as:

$$\begin{aligned} \tilde{y} &= r \odot y \\ P(r_i = 1) &= 1 - p \\ P(r_i = 0) &= p \end{aligned}$$

2.10. Evaluation Metrics

One of the most common challenges faced by training algorithms is the need to prevent overfitting, which is addressed in this study through the use of regularization. To assess the learning performance of the CNN model [20], a confusion matrix is employed as a conventional evaluation technique.

Fig 7: Confusion matrix

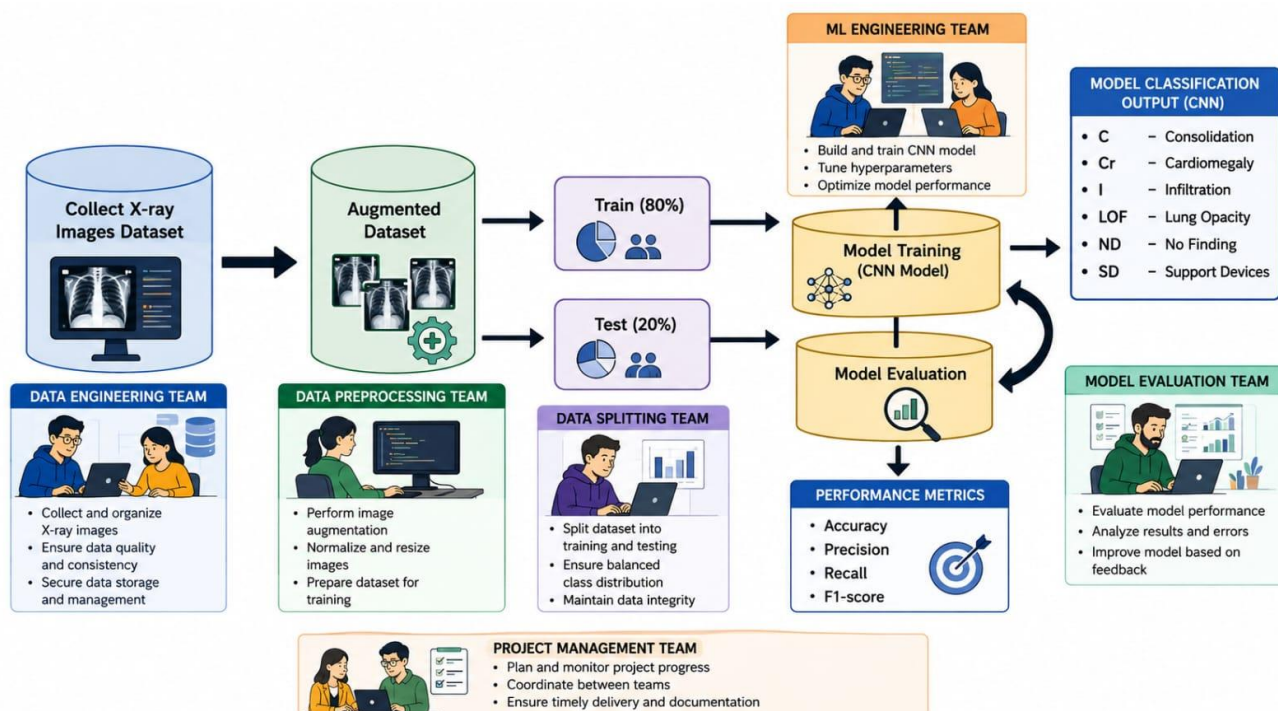
		Predicted class		
		Positive	Negative	
Actual class	Positive	True Positive (TP)	False Negative (FN) Type II Error	Recall $\frac{TP}{TP + FN}$
	Negative	False Positive (FP) Type I Error	True Negative (TN)	Specificity $\frac{TN}{TN + FP}$
		Precision $\frac{TP}{TP + FP}$	Negative predictive value $\frac{TN}{TN + FN}$	Accuracy $\frac{TP + TN}{TP + TN + FN + FP}$

4. When to Use CNN?

4.1. Some Examples

It summarizes selected research papers and their key findings related to the use of CNNs[20], including automated welding fault detection, lip reading, olive leaf disease detection, mask recognition for COVID-19, visual spam classification, and driver sleepiness detection.

Figure 8: Proposed CNN-Based Framework for X-Ray Image Classification



4.2. Tasks Suited for CNNs

CNNs are particularly well-suited for tasks that involve analysing visual data, such as image classification, object detection, and segmentation [23].

CNNs are also well-suited for tasks that involve analysing sequential data, such as speech recognition and NLP, where the data has a spatial or temporal structure that can be exploited by the Conv_Lays [24].

4.3. Best Utilized with Large Amounts of Training Data

CNNs require a large amount of labelled training data to perform well. This is because the models have millions of parameters that need to be learned from the data, and they require a significant amount of variation in the data to avoid overfitting.

4.4. Computational Requirements

Training CNNs can be computationally expensive, especially for large models with many layers. This is because CNNs typically require a lot of memory and processing power to train.

5. Advantages and Limitations of CNNs

5.1. Advantages

CNNs have several advantages that make them a powerful tool for analysing visual and sequential data.

Another advantage of CNNs is their ability to handle inputs of varying sizes and aspect ratios. This is because the Conv_Lays [26] are able to learn features that are translation-invariant, meaning that they can recognize the same pattern regardless of its location in the input.

5.2. Limitations

While CNNs have several advantages, they also have some limitations that should be considered when using them.

Another limitation of CNNs is that they can be sensitive to the quality of the training data. If the data is noisy or contains biases, the model may learn to recognize these artifacts rather than the underlying patterns in the data.

6. Existing Platforms and Libraries

There are several platforms and libraries available for building CNNs [29] and other types of neural networks. These platforms and libraries provide a wide range of tools and functions for building, training, and deploying models.

6.1. TensorFlow

TensorFlow is an open-source ML platform developed by Google. It is one of the most widely utilized platforms for building and deploying ML models, including CNNs

6.2. Keras

Keras [30] is a high-level API for building neural networks, including CNNs, that runs on top of TensorFlow.

6.3. PyTorch

PyTorch [31] is an open-source ML framework developed by Facebook. It provides a dynamic computational graph.

6.4. Caffe

Caffe is an open-source DL library developed by Berkeley AI Research (BAIR). It is designed for efficient computation of deep neural networks, including CNNs, and includes a wide range of pre-trained models that can be utilized for various computer vision tasks

6.5. MXNet

MXNet [32] is an open-source DL framework developed by Apache. It provides a wide range of tools and libraries for building and deploying DL models, including CNNs. MXNet supports both high-level APIs, such as Gluon, and low-level APIs, which allow for greater control over the model architecture.

7. Comparison with Other Model Architectures

While CNNs[28] are a powerful tool for analysing visual and sequential data, they are not always the best choice for every task. There are several alternative model architectures that can be utilized in place of CNNs, depending on the specific requirements of the task.

CNNs vs. Recurrent Neural Networks (RNNs): RNNs are designed for processing sequential data, such as speech or text. RNNs have been utilized for tasks such as speech recognition and language translation,

8. Recommendations for Developers and Data Scientists

Building and training CNNs can be a complex task that requires careful consideration of several factors. Here, some recommendations for developers and data scientists who are building CNNs are provided.

8.1. Preprocessing the Data

Preprocessing the data is an important step in building a CNN. This involves transforming the raw input data into a format that can be utilized by the CNN. Preprocessing can include resizing the images, normalizing the pixel values, and augmenting the data with techniques such as flipping or rotating the images.

8.2. Choosing Appropriate Hyper Param

Choosing appropriate hyper Param such as the learning rate, batch size, and number of epochs can greatly affect the performance of the model.

8.3. Using Regularization Techniques

Regularization techniques such as L1 or L2 regularization, dropout, or batch normalization can also be utilized to prevent overfitting of the model. Regularization can help to improve the generalization of the model and prevent it from memorizing the training data.

8.4. Hardware Considerations

Hardware considerations such as the available GPUs or TPUs, can greatly affect the performance and efficiency of the model. CNNs are computationally intensive and require large amounts of processing power, so it is important to choose hardware that can handle the workload.

8.5. Evaluating Model Performance

Evaluating the performance of the model is an important step in building a CNN. This involves splitting the data into training, validation, and testing sets, and using metrics such as accuracy, precision, recall, and F1 score to evaluate the performance of the model.

8.6. Security Aspects

Data privacy and security should also be considered when building and deploying CNNs, as these models may be trained on sensitive data or utilized to make decisions that affect people's lives.

9. Estimation of the Cost of Using CNNs

Building and training CNNs[30] can be a computationally intensive process that requires significant resources. Estimating the cost of using CNNs can help developers and data scientists to plan and budget for the necessary resources.

9.1. Factors Impacting Cost (Hardware, Dataset Size, Model Complexity)

Several factors can impact the cost of using CNNs, including the hardware utilized to train the models, the size of the dataset, and the complexity of the model architecture.

9.2. Cloud-Based Services and Renting Hardware to Reduce Costs

One way to reduce the cost of using CNNs is to leverage cloud-based services or to rent hardware. Cloud-based services offer the advantage of on-demand access to computing resources, which can be scaled up or down as needed.

9.3. Considering Potential Benefits of Using CNNs

While the cost of using CNNs can be significant, it is important to consider the potential benefits of using these models. CNNs can offer significant improvements in accuracy and efficiency compared to traditional ML algorithms, particularly for tasks such as image classification, object detection, and natural language processing [33].

10. Recent Developments

CNNs have been the subject of extensive research and development in recent years, leading to several innovative approaches to improve performance and efficiency.

In CNNs, attention mechanisms can be integrated at various levels of the network architecture, such as within individual Conv_Lays or across multiple layers.

10.1. Capsule Networks

Capsule networks are a recent development in CNNs that aim to improve the ability of the model to represent hierarchical relationships between objects in an image. In traditional CNNs, the model learns to identify objects by detecting specific patterns of pixels in the input image.

10.2. Transfer Learning

Transfer learning is a technique that allows CNNs to leverage the knowledge learned from one task to improve performance on a second, related task. Recent research has shown that transfer learning can be particularly effective for tasks such as object detection and image segmentation [34], where the model needs to identify specific objects in an image.

10.3. Adversarial Training

Adversarial training is a technique that improves the robustness of CNNs to adversarial attacks. Adversarial attacks are a type of attack where an attacker adds small, imperceptible perturbations to the input data.

10.3. Quantization and Compression

Quantization and compression are techniques that reduce the memory and computational requirements of CNNs [35]. In quantization, the weights and activations of the CNN are represented using fewer bits, reducing the amount of memory required to store the model.

Conclusion

In conclusion, CNNs have become a powerful tool for image recognition tasks, achieving state-of-the-art results on several benchmarks. In this paper, a comprehensive overview of CNNs was provided, covering their fundamentals, architectures, and recent developments. The article also discussed the advantages and limitations of CNNs, provided recommendations for developers and data scientists, examined the existing platforms and libraries for CNNs, and estimated the cost of using CNNs. It started by discussing the fundamentals of CNNs, including the layers of CNNs, Convoy, Feat Maps, Activ_Funcs, and training methods. It then compared several popular CNN architectures, including LeNet, AlexNet, VGG, ResNet, and Inception Net, and examined when to use CNNs. It also discussed the advantages and limitations of CNNs, highlighting their ability to learn complex patterns from large datasets, but also noting their computational requirements and potential vulnerabilities to adversarial attacks. CNNs have revolutionized the field of image recognition, but their applications extend far beyond that. With the increasing availability of data and computing resources, CNNs have the potential to transform a wide range of industries, from healthcare and finance to transportation and entertainment. However, developing and

deploying CNNs can be a complex and error-prone process, requiring careful consideration of the model architecture, training process, and performance evaluation.

There are still several areas where CNNs can be improved and further developed. One of the future directions of CNN research is to improve their interpretability and explainability. Currently, CNNs are often treated as black-box models, and it can be challenging to understand how they make decisions.

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SCAPS -1D-Based Numerical Optimization MAPbI₃ Perovskite Solar Cells of Enhancement Photovoltaic Performance

J. Safrin^{1*} and P. Arockia Michael Mercy²

¹UG Student, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

²Vice Principal & Assistant Professor, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

*Corresponding Author E-Mail ID: safrinsafrin3489@gmail.com

Abstract

Perovskite solar cells (PSCs) have attracted significant attention due to their high power conversion efficiency and low fabrication cost. In this work, a numerical simulation of a lead-based perovskite solar cell with the structure FTO/CeO₂/MAPbI₃/CuI/Au was carried out using SCAPS-1D software. CeO₂ was used as the electron transport layer (ETL), MAPbI₃ as the absorber layer, and CuI as the hole transport layer (HTL). The effects of key device parameters, including layer thickness, defect density, and material properties, were analyzed to improve the photovoltaic performance. The optimized device exhibited enhanced values of open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and power conversion efficiency (PCE). The simulation results demonstrate that the selected device configuration is a promising candidate for efficient perovskite solar cells and provides useful guidance for future experimental.

Keywords: Perovskite solar cells; MAPbI₃; SCAPS-1D; CeO₂ electron transport layer; CuI hole transport layer; absorber thickness; defect density; photovoltaic performance; power conversion efficiency; numerical simulation; device optimization

1. Introduction

Perovskite solar cells (PSCs) have emerged as one of the most promising photovoltaic technologies because of their high power conversion efficiency low fabrication cost, and simple solution processing techniques. Compared with conventional silicon solar cells, PSCs

exhibit excellent light absorption, long carrier different lengths, and tunable bandgaps, making them suitable for next-generation solar energy application. Continuous improvement device architecture has material engineering have significantly enhanced their stability and efficiency over the past decade [1–5]. Fluorine-doped tin oxide (FTO) is widely used as the transparent conducting substrate in PSCs due to its high optical transparency, excellent electrical conductivity, and thermal stability. FTO provides efficient electron collection while allowing maximum light transmission to the active layer. Its chemical stability and compatibility with various deposition techniques make it an ideal front electrode for high performance solar cells [6–9]. Cerium oxide (CeO_2) has attracted considerable attention as an electron transport layer (ETL) because of its wide bandgap, high electron mobility, and excellent chemical stability. CeO_2 effectively extract and transports electrons while suppressing charge combination at the interface, thereby improving the overall photovoltaic performance of perovskite solar cells [10–13]. Methylammonium lead iodide (MAPbI_3) is one of the most extensively studied perovskite absorber materials due to its direct bandgap, strong optical absorber material due to its direct bandgap, strong optical absorption, long carrier lifetime and excellent charge transport properties. These characteristics enable efficient high harvesting and contribute to high power conversion efficiencies in PSC devices [14–17]. Copper iodide (CuI) is an attractive inorganic hole transport layer (HTL) because of its high hole mobility, wide bandgap, low cost, and good environmental stability. CuI facilitates efficient hole excitation from the absorber layer while reducing recombination losses, leading to improved device efficiency and long-term operational stability [18–20]. (24) Gold (Au) is commonly employed as the back metal electrode owing to its high electrical conductivity, suitable work function, and excellent resistance to oxidation. The Au electrode ensures efficient hole collection and provides stable electrical contact with the hole transport layer, contributing to enhance device performance and durability [21–23].

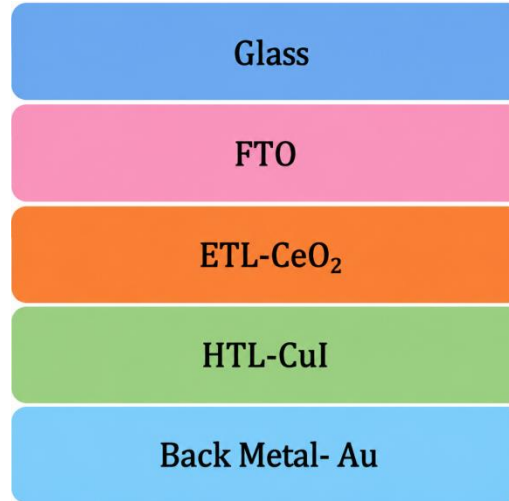
2. Design of Novel Perovskite Solar Cell

The best solar cells performance is achieved when electrons and holes are efficiency separate are transport throughout the photovoltaic device s, thereby minimize g charge and recombination and improving power conversion efficiency (Chen et al., 2016)

A perovskite solar cells by his formed by sandwiching the electron transport layer (ETL) and the hole transport layer (HTL) on either side of the absorber layer to achieve balanced charge extraction (Said et al., 2019). In the present work, (MAPbI_3) is selected as the

absorber layer because of its excellent optical absorption coefficient, suitable direct bandgap, long carrier diffusion length, and outstanding photovoltaic properties (Son et al., 2024; Alshaikh, 2026).

Fig 1: Configuration of MAPbI₃-based solar cell



3. Design and Simulation

Software version 3.309, a one-dimensional (1-D) photovoltaic simulator created by ELIS, University of Gent, Belgium, was used in this investigation (Burgelman et SCAPS al. 2000; Wang et al. 2020). To determine the density of electrons and holes individually, SCAPS 1D uses four different sets of equations (Verschraegen and Burgelman 2007). The following are the equations :(25)

“Solar cells,” Thin Solid Films, 1, Differential form of the Poisson equation in terms of electrostatic potential is displayed below

$$\frac{d}{dx} \left(\epsilon \frac{d\psi}{dx} \right) = -q \left[p - n + N_D^+ - N_A^- + \frac{\rho_{\text{trap}}}{q} \right]$$

Where ϕ is the electrostatic potential, e is electronic charge, the permittivity of vacuum is ϵ_0 , ϵ_r is relative permittivity, N_A stands for shallow acceptor impurity density while N_D stands for shallow donor impurity density. Similarly, p denotes hole density distribution and n denotes electron density distribution,

The Continuity equation is given as follows.

$$\frac{dJ_n}{dx} = G - R$$

$$\frac{dJ_p}{dx} = G - R$$

Where J_n and J_p represent the electron and hole current densities, G represents the generation rate, and R represents the recombination rate.

2. The absorption coefficient with respect to wavelength α (λ) can be calculated by the equation given below. We use the

Following equation to get Backmetal

$$J_p = D_p \left(\frac{dp}{dx} \right) + \mu_p p \left(\frac{d\phi}{dt} \right)$$

Table 1: Parameters for Simulation utilizing SCAPS-ID

Parameter	FTO	ETL-CeO2	Absorber- MAPbI3	HTL-CuI
Thickness (nm)	100	100	800	0.350
Eg(ev)	3.5	3.5	1.5	3.1
χ (Ev)	4.3	4.0	3.9	2.1
ϵ_r	9.0	9.0	30	6.5
N_c (cm-3)	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}	2.2×10^{19}
N_v (cm-3)	1.8×10^{19}	1.8×10^{18}	1.8×10^{19}	1.8×10^{19}
V_e (cm/s)	1.0×10^7	1.0×10^7	1.0×10^7	1.01×10^7
V_h (cm/s)	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7
μ_e (cm ² /VS)	2.0×10^1	2.0×10^1	2.2	1×10^2
μ_n (cm ² /VS)	1.0×10^1	2.5×10^1	2.2	4.390×10^2
N_D (cm-3)	1.9×10^{18}	1.0×10^{19}	1.0×10^{13}	0

$N_A(\text{cm}^{-3})$	0	0	0	2.0×10^{21}
$N_t(1/\text{cm}^3)$		1.0×10^{15}	1×10^{13}	1.0×10^{15}

4. Results and Discussion

This section includes an analysis of various HTLs and ETLs for an innovative device, as well as optimizations of thickness of HTL, absorber, FTO and the optimization of absorber defect density for MAPbI₃ absorber.

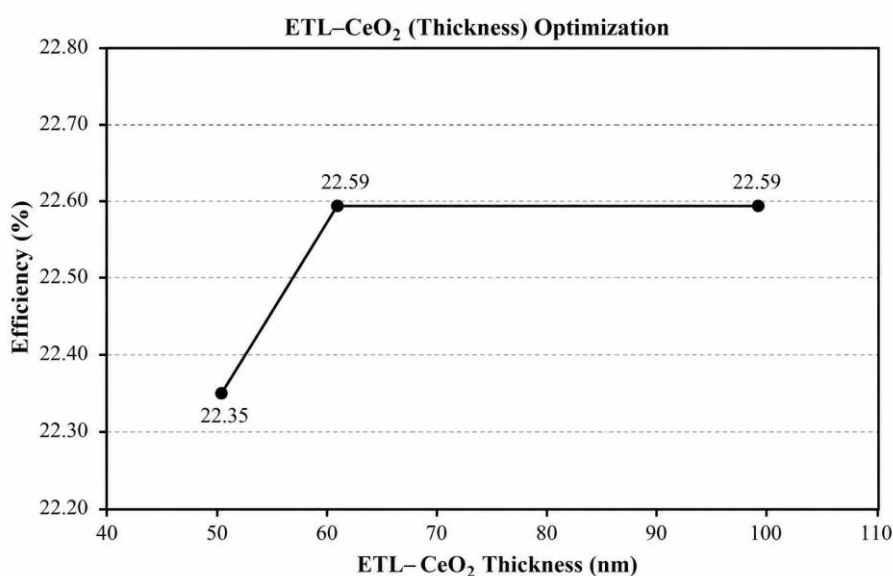
4.1 ETL Optimization for MAPbI₃ Perovskite Absorber:

Figure 2 shows the performance of the PSC using Cul as the HTL. The Cul thickness was varied to optimize device performance. The optimized device achieved $V_{oc}=2.4522\text{V}$, $J_{sc} = 27.071161\text{mA}/\text{cm}^2$, $FF = 34.03$, and $PCE = 22.59\%$.

Table 2: Input optimization of ETL.

Parameter	$V_{oc}(v)$	$(J_{sc}(\text{MA}/\text{cm}^2))$	$FF(\%)$	$\text{Eta}(\%)$
50	2.4381	26.793258	34.32	22.35
60	2.4381	26.793258	34.32	22.59
100	2.4522	27.071161	34.02	22.59

Fig 2: Effect of ETL thickness on PSC performance characteristics



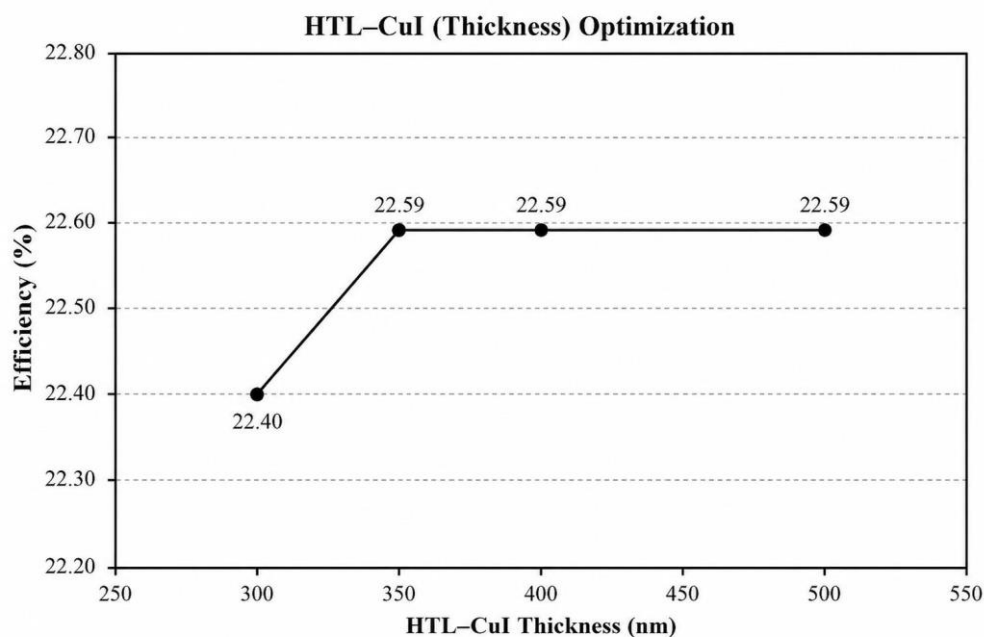
4.2 HTL Layer Thickness Optimization

Figure 3 shows the PSC performance with CuI as the HTL, where the thickness was varied to determine the optimum value. At the optimized thickness of 250 nm, the device achieved $V_{oc} = 2.4522V$, $J_{sc} = 27.071161\text{mA/cm}^2$, $FF = 34.03\%$, and $PCE = 22.59\%$.

Table 3: Input optimization of HTL

Thickness Value	Voc(v)	Jsc(MA/cm ²)	FF(%)	Efficiency(%)
300	2.3519	26.061153	34.15	22.40
350	2.4522	27.071161	34.03	22.59
400	2.4522	27.071161	34.03	22.59
500	2.4522	27.071161	34.03	22.59

Fig 3: Effect of HTL thickness on PSC performance characteristics

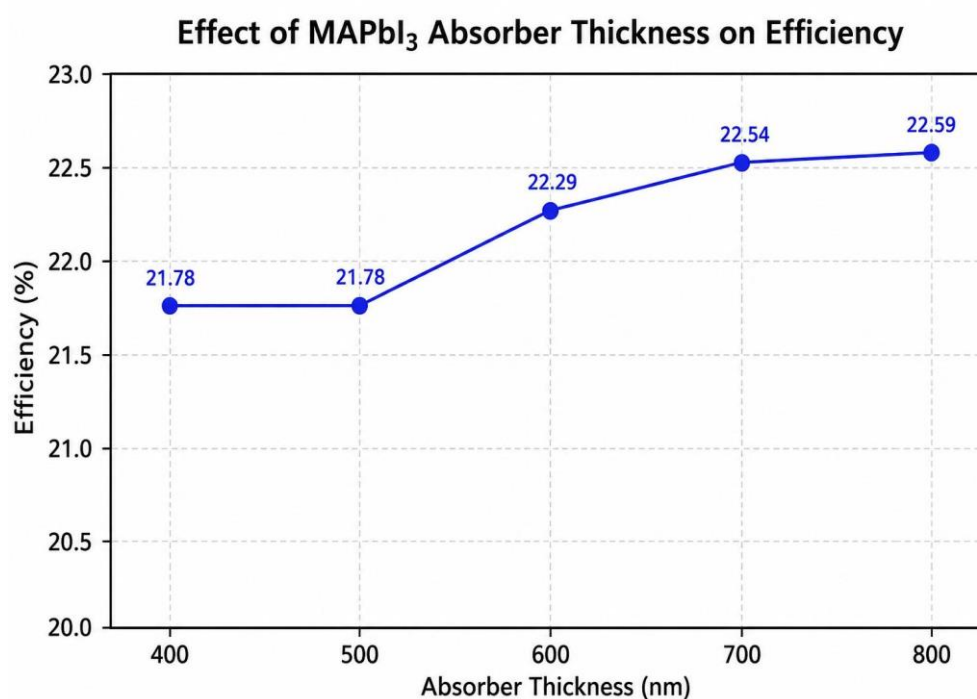


4.3 Absorber Thickness of optimization

Figure 4 shows the PSC performance with MAPbI₃ as the absorber layer, where the thickness was varied to determine the optimum value. At the optimized thickness of 800 nm, the device achieved $V_{oc} = 1.0529 V$, $J_{sc} = 27.9432 \text{ mA/cm}^2$, $FF = 81.70\%$, and $PCE = 24.04\%$.

Table 4: Input parameters of absorber

Parameter	Voc(v)	Jsc(MA/cm ²)	FF(%)	Eta(%)
400	3.9207	25.356223	21.91	21.78
500	3.9207	25.356223	21.91	21.78
600	3.9308	26.763767	25.96	22.29
700	2.8097	26.701712	30.04	22.54
800	2.4522	27.071161	34.03	22.59

Fig 4: Effect of Absorber thickness on PSC performance characteristics

4.4 FTO Thickness of optimization

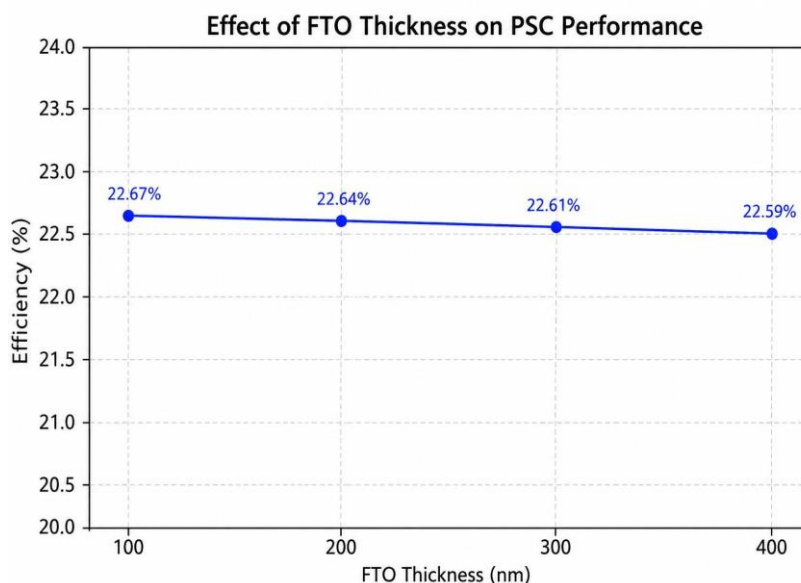
Figure 5 shows the PSC performance with FTO as the FTO layer, where the thickness was varied to determine the optimum value. At the optimized thickness of 100nm, the device achieved Voc = 2.4363V, Jsc = 27.158822 mA/cm², FF =33.98%, and PCE = 22.67%.

Table 5: Input parameters of FTO

Thickness	Voc(v)	Jsc(mA/cm ²)	FF(%)	Efficiency(%)
400	2.4522	27.071161	34.03	22.59

300	2.4535	27.096396	34.01	22.61
200	2.4563	27.125405	34.00	22.64
100	2.4563	27.158822	33.98	22.67

Fig 5: Effect of FTL thickness on PSC performance characteristics

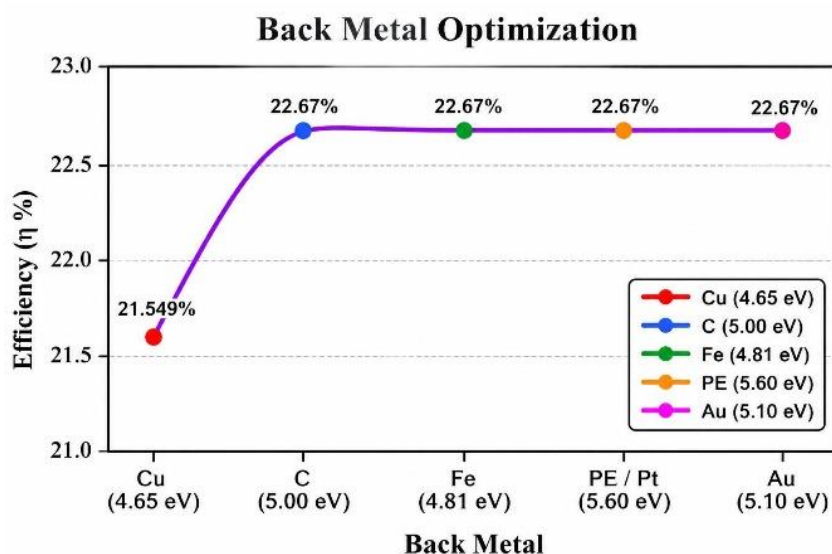


4.5 Back Metals Optimization

Figure 6 shows the optimization of the Au back metal contact with a work function of 5.10 eV. The optimized device achieved $V_{oc} = 2.4563V$, $J_{sc} = 27.158822 \text{ mA/cm}^2$, $FF = 33.98\%$, and $PCE = 22.67\%$.

Table 6: Input Back Metal Optimization

Back Metals Contact	Work Function	Voc(v)	Jsc(mA/cm ²)	FF(%)	Efficiency (%)
Cu	4.65	1.8353	27.156090	44.41	22.14
C	5.00	2.4563	27.158822	33.98	22.67
Fe	4.81	2.4537	27.158813	34.01	22.67
PE	5.60	2.4563	27.158859	34.98	22.67
Au	5.10	2.4563	27.158859	34.98	22.67

Fig 6: Optimization of Back Metals

Conclusion

In this study, a MAPbI₃-based perovskite solar cell was numerically investigated using the SCAPS-1D simulation tool. The proposed device structure consisting of FTO/CeO₂/MAPbI₃/Cu/Au was optimized by varying the ETL, HTL, absorber layer thickness, FTO thickness, and back contact parameters. The optimized thicknesses were 800 nm for the MAPbI₃ absorber, 350 nm for Cu HTL, and 100nm for FTO, while CeO₂ was employed as the ETL and Au as the back contact with a work function of 5.10 eV. The optimized device achieved a Voc of 2.4528V, Jsc of 27.125405mA/cm², FF of 33.98%, and maximum PCE of 22.67%. These results demonstrate that appropriate optimization of the absorber, charge transport layers, FTO, and back contact can significantly improve the photovoltaic performance of MAPbI₃-based perovskite solar cells.

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Design and Numerical Optimization of an Efficient Lead-Free Cs_2TiBr_6 Perovskite Solar Cell Using SCAPS-1D

A. Shivaranjani^{1*} and P. Arockia Michael Mercy²

¹UG Student, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

²Vice Principal & Assistant Professor, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

*Corresponding Author E-Mail ID: ranjan0759@gmail.com

Abstract

Perovskite solar cells (PSCs) have attracted great interest as promising photovoltaic devices due to high efficiency, low-cost fabrication and excellent optoelectronic properties. However, the toxicity and instability of the traditional lead-based perovskites still pose great challenges to their practical applications. In this work, a numerical investigation is performed on a lead-free Cs_2TiBr_6 -based perovskite solar cell is by using SCAPS-1D simulation. The proposed device structure consists of FTO/TiO₂/ Cs_2TiBr_6 /PEDOT:PSS. Where FTO is as the transparent conducting oxide, TiO₂ is the electron transport layer (ETL), Cs_2TiBr_6 is the absorber layer and PEDOT:PSS is the hole transport layer (HTL). The device parameters are optimized to enhance photovoltaic performance. The optimized device shows a VOC of 1.4246 V, JSC of 24.25 mA/cm², fill factor of 69.06 % and power-conversion efficiency of 23.86%. The results highlight the promising potential of Cs_2TiBr_6 as an efficient and environment-friendly lead-free absorber material for efficient and environmentally friendly perovskite solar-cell applications.

Keywords: Perovskite Solar Cell; FTO/TiO₂/ Cs_2TiBr_6 /PEDOT:PSS, SCAPS-1D, Numerical simulation Power Conversion Efficiency (PCE)

1. Introduction

The growing demand for clean and renewable energy has stimulated the development of efficient and environmental being solar- cell technologies. Perovskite solar cells (PSCs) are emerging photovoltaic devices that have attracted significant attention because of their high light absorption, suitable electronic properties, low- cost fabrication, and high power-

conversion efficiency. However, conventional lead-based PSCs face serious concerns related to lead toxicity and long-term environmental stability. Therefore, the development of stable and lead-free perovskite materials has become an important research area. [1,2] Among the different lead-free materials, Cs_2TlBr_6 has been considered a promising absorber because of its lead-free composition and suitable optoelectronic properties. The performance of PSCs also strongly depends on the appropriate selection of charge-transport layers. In the proposed structure, TiO_2 is employed as the electron transport layer (ETL), PEDOT:PSS is used as the hole transport layer (HTL), and FTO acts as the transparent conducting oxide. Previous numerical studies have investigated Cs_2TlBr_6 with TiO_2 and different hole-transport materials, while SCAPS-1D studies have also considered PEDOT:PSS with Cs_2TiBr_6 devices [2,3]. The present study explores a lead-free perovskite solar-cell structure, FTO/ TiO_2 / Cs_2TiBr_6 /PEDOT:PSS, using SCAPS-1D simulation. Important device parameters, including absorber-layer thickness, defect density, and doping concentration, are optimized to improve the photovoltaic performance. The device performance is evaluated in terms of Open-Circuit Voltage (V_{oc}), Short-Circuit Current Density (J_{sc}), Fill Factor (FF), and Power-Conversion Efficiency (PCE). Previous SCAPS-1D investigations of Cs_2TlBr_6 -based PSCs have demonstrated the importance of optimizing absorber thickness, defect density, doping concentration, and transport-layer properties for improving photovoltaic performance. [3,4]

2. Design of novel perovskite solar cell

The best solar cell performance is achieved when electrons and holes are efficiently separated and transported throughout the photovoltaic device, thereby minimizing charge recombination and improving power conversion efficiency (Chen et al., 2016). A perovskite solar cell (PSC) is formed by sandwiching the electron transport layer (ETL) and the hole transport layer (HTL) on either side of the absorber layer to achieve balanced charge extraction (Said et al., 2019). In the present work, Cs_2TiBr_6 is selected as the absorber layer because of its excellent optical absorption coefficient, suitable direct bandgap, long carrier diffusion length, and outstanding photovoltaic properties (Son et al., 2024; Alshaikh, 2026).

Structure of Novel Perovskite Solar Cell

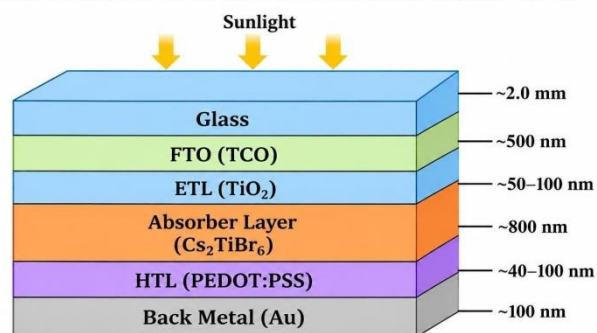


Fig. 1. Configuration of Cs_2TiBr_6 -based solar cell

3. Design and Simulation

SCAPS software version 3.3.07, a one-dimensional (1-D) photovoltaic simulator created by ELIS, University of Gent, Belgium, was used in this investigation. To determine the density of electrons and holes individually, SCAPS-1D uses four different sets of equations. The following are the equations:

1. Differential form of the Poisson equation in terms of electrostatic potential is displayed below

$$D^2\phi(x)/dx^2 = -e/(\epsilon_0\epsilon_r) [p(x) - n(x) + N_D(x) - N_A(x) + \rho_p - \rho_n].$$

Where ϕ is the electrostatics potential, e is electronic charge, ϵ_0 is the permittivity of vacuum, ϵ_r is relative permittivity, N_A stands for shallow acceptor density while N_D stands for shallow donor impurity density. Similarly, ρ_p and ρ_n denote hole density and electron density distribution, with $p(x)$ and $n(x)$ denoting electron and hole density distribution.

2. The continuity equation is given as follows

$$dJ_n/dx = G - R$$

$$dJ_p/dx = G - R$$

where J_n and J_p represent the electron and hole current densities, G signifies the generation rate, and R represents the recombination rate.

3. The electron and hole current densities are given by the charge transport equation as follows

$$J_n = D_n dn/dx + \mu_n n d\phi/dx$$

$$J_p = D_p dp/dx + \mu_p p d\phi/dx$$

Where μ_n is the electron mobility and μ_p is the hole mobility.

4. The absorption coefficient with respect to photon energy $\alpha(h\nu)$ can be calculated by the equation given below.

$$A(h\nu) = (A + B/h\nu) \sqrt{(h\nu - E_g)}$$

Where A and B are constant, h is Planck constant, ν is frequency of photons and E_g is the band gap of the absorber layer. The band discontinuity between the interfaces of the different layers is small and therefore can be neglected for simplicity. For this study, the proposed Au/CuO / Cs₂TiBr₆/ CeO₂/ FTO perovskite solar cell structure was used for the SCAPS-1D simulation. The ambient temperature was maintained at 300 K and the solar

spectrum was AM1.5 (1000 W/m²). The electrical and physical parameters required by SCAPS-1D for FTO, CeO₂, Cs₂TiBr₆, CuO were obtained from the corresponding literature [10].

Table 1: Parameters for Simulation utilizing SCAPS-1D

Electrical Parameter	HTL- PEDOT:PSS	Absorber- Cs ₂ TiBr ₆	ETL-TiO ₂	FTO
Bandgap (eV)	2.2	3.5	3.2	3.2
Dielectric permittivity(eV)	3	9	9	4.4
Thickness (nm)	0.3	100	0.3	0.05
CB effective density of states (cm ⁻³)	2.2×10^{15}	1.00×10^{19}	2.2×10^{18}	2.2×10^{18}
VB effective density of states	1.8×10^{18}	1.00×10^{19}	1.8×10^{19}	1.8×10^{19}
Electron affinity (eV)	2.9	4	4.26	4.4
Electron mobility (cm ² /Vs)	1.0×10^1	1.0×10^1	2.2×10^1	9.0×10^1
Hole mobility (cm ² /Vs)	1.0×10^1	5.0×0	1.0×10^1	9.0×10^1
Uniform donor density N _D (cm ⁻³)	0	1.0×10^{19}	9.0×10^{16}	1.0×10^{20}
Uniform acceptor density N _A (cm ⁻³)	1.00×10^{22}	1.0×10^{19}	0	0
Electron thermal velocity (cm/s)	1.0×10^7	1.0×10^7	1.0×10^7	1.01×10^7
Hole thermal velocity (cm/s)	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7
Defect density N _t	1.00×10^{12}	1.0×10^{12}	1×10^{12}	0

4. Results and Discussion

This section presents a comprehensive investigation of various hole transport layers (HTLs) and electron transport layers (ETLs) for the proposed device architecture, followed by systematic optimization of the HTL, absorber, and transparent conducting oxide (TCO) thicknesses. In addition, the effect of absorber defect density on the photovoltaic performance of the Cs₂TiBr₆-based device is systematically analyzed to identify the optimal parameters for achieving enhanced device efficiency.

4.1 ETL, Optimization for Cs₂TiBr₆ perovskite absorber

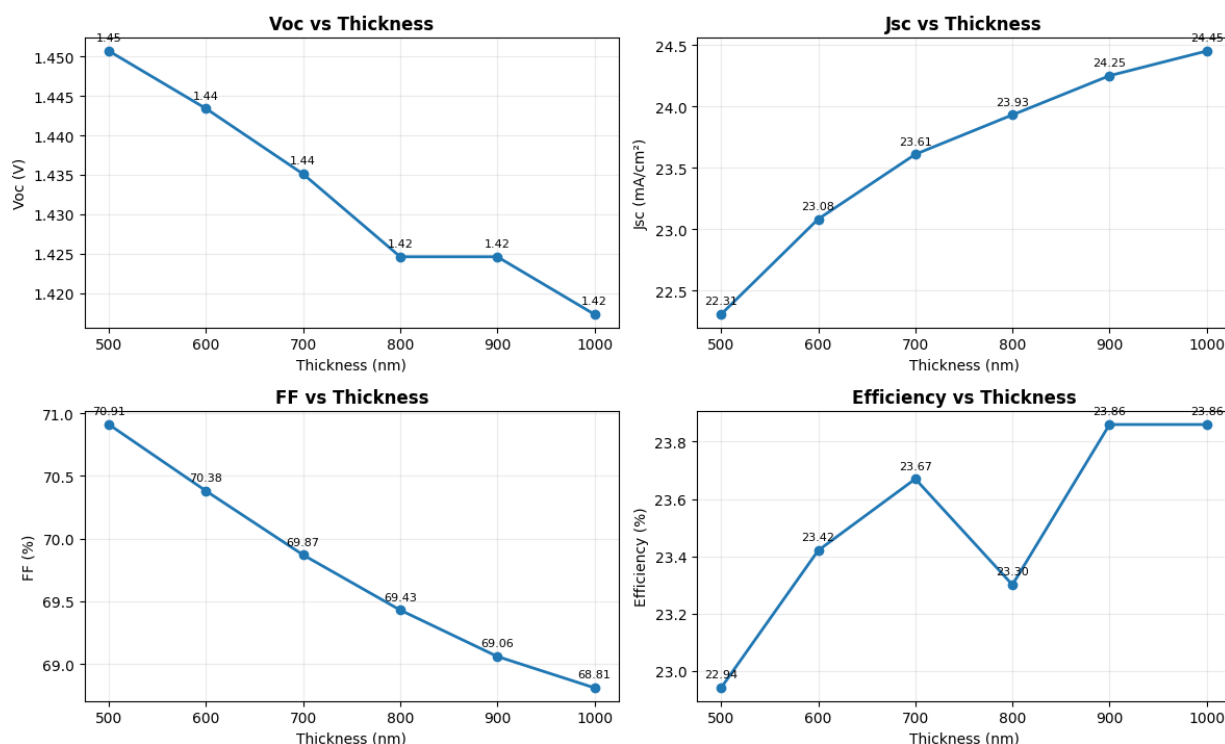
Figure 2 illustrates the photovoltaic performance of the PSC employing PEDOT:PSS as the hole transport layer (HTL), with its thickness systematically varied to determine the

optimum device configuration. At the optimized HTL thickness of 0.06 μm , the device exhibited a V_{OC} of 1.4249 V, a J_{SC} of 24.250014 mA cm^{-2} , a fill factor (FF) of 69.06%, and a power conversion efficiency (PCE) of 23.866%, indicating the favorable contribution of the optimized PEDOT:PSS thickness to overall device performance.

Table 2: Input optimization of ETL.

ETL				
Thickness	V_{OC} (V)	PCE (%)	$J_{sc}(\text{mA/cm}^2)$	FF(%)
0.3	1.4246	23.87	24.250001	69.06
0.4	1.4246	23.87	24.250003	69.06
0.5	1.4246	23.87	24.250002	69.06
0.2	1.4246	23.87	24.250004	69.06
0.1	1.4246	23.87	24.250005	69.06
0.6	1.4249	23.87	24.250014	69.04

**Fig 2: Optimization of ETL Thickness for the Absorber Cs_2TBr_6
Solar Cell Parameters vs Thickness**



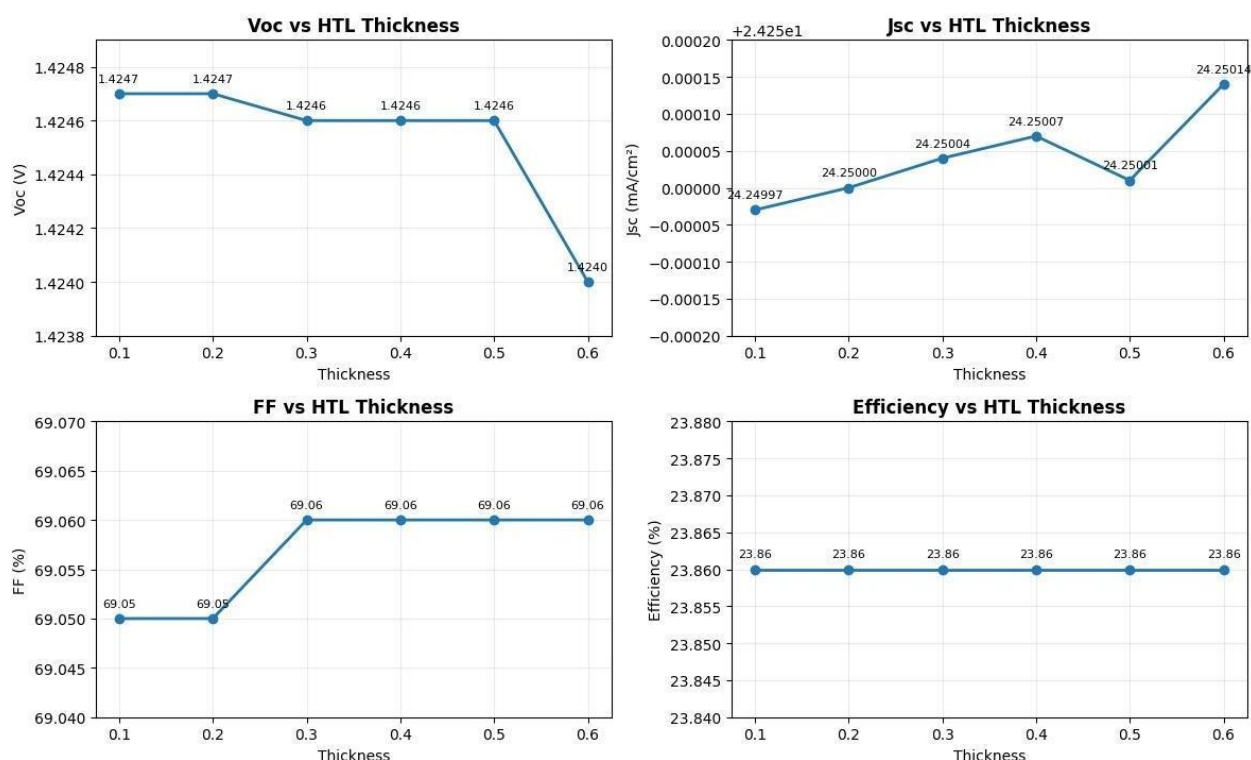
4.2 Optimization of HTL for Cs₂TiBr₆ Perovskite Absorber

Table 3: Effect of ETL thickness on PSC performance characteristics

HTL - Thickness				
Thickness	V _{oc} (V)	PCE (%)	J _{sc} (mA/cm ²)	FF(%)
0.1	1.4247	23.86	24.24997	69.05
0.2	1.4247	23.86	24.25	69.05
0.3	1.4246	23.86	24.25004	69.06
0.4	1.4246	23.86	24.25007	69.06
0.5	1.4246	23.86	24.25001	69.06
0.6	1.4244	23.86	24.250014	69.06

Fig 3: Effect of HTL thickness on PSC performance characteristics

HTL Thickness vs Solar Cell Parameters



4.3. Absorber Thickness of Optimization

Table 4 presents the photovoltaic characteristics of the PSC incorporating Cs₂TiBr₆ as the absorber layer, with the absorber thickness systematically varied to identify the optimum

value. The best device performance was obtained at an absorber thickness of 600 nm, yielding a V_{OC} of 1.4434 V, J_{SC} of 23.082582 mA cm⁻², an FF of 70.28%, and a PCE of 23.42%. These results demonstrate that optimizing the Cs₂TiBr₆ absorber thickness plays an important role in improving the overall photovoltaic performance of the proposed device.

Fig 4: Absorber Thickness of optimization

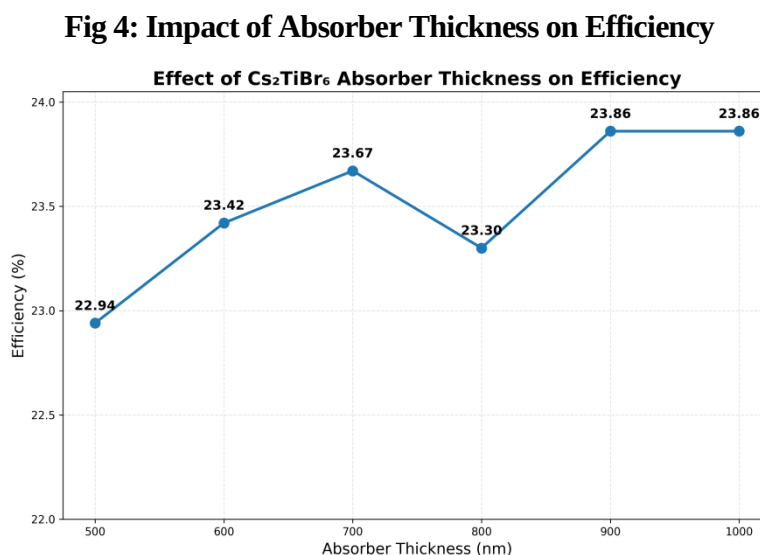


Table 4: Output Characteristics of Absorber Cs₂TiBr₆

Absorber - Thickness					
S. No	Thickness(nm)	V_{OC}	J_{SC}	FF	Efficiency
1	900	1.4246	24.250004	69.06	23.86
2	800	1.4246	23.930909	69.43	23.3
3	700	1.4351	23.609869	69.87	23.67
4	600	1.4434	23.082582	70.38	23.42
5	500	1.4507	22.30687	70.91	23.94
6	1000	1.4173	24.450857	68.81	23.86

4.4. FTO Thickness of Optimization

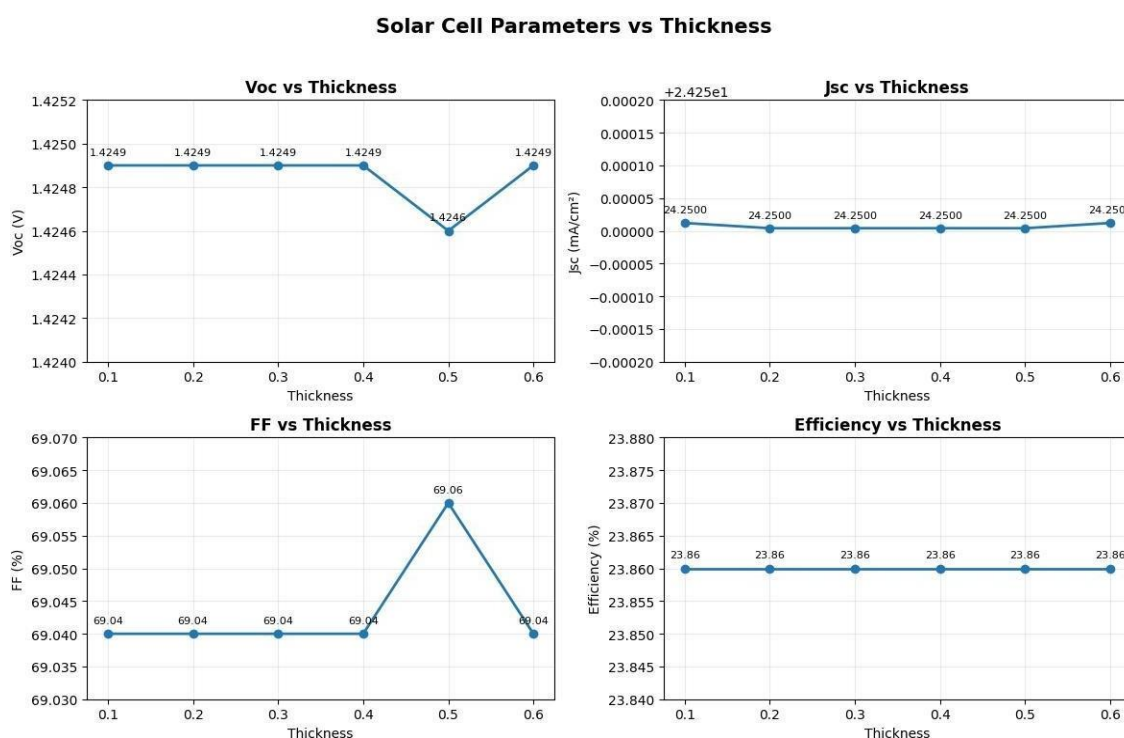
Figure 5 presents the photovoltaic performance of the PSC employing FTO as the transparent conducting oxide (TCO) layer, with its thickness systematically varied to identify the optimum thickness. At the optimized thickness of 0.10 nm, the device exhibited a V_{OC} of

1.4249V, J_{SC} of 24.250012 mA/cm², a Fill Factor (FF) of 69.04%, and a power conversion efficiency PCE of 23.86%. The results indicate that the optimized FTO thickness contributes to maintaining favorable charge transport and overall photovoltaic performance.

Table 5: FTO Thickness of Optimization

FTO - Thickness				
Thickness	Voc (V)	PCE (%)	Jsc(mA/cm ²)	FF(%)
0.5	1.4246	23.86	24.25004	69.06
0.4	1.4249	23.86	24.25004	69.04
0.3	1.4249	23.86	24.25004	69.04
0.2	1.4249	23.86	24.25004	69.04
0.1	1.4249	23.86	24.25012	69.04
0.6	1.4249	23.86	24.25012	69.04

Fig 5: Back Metal Contacts versus Output Characteristics of PSC



14.5 Back Metals Optimization

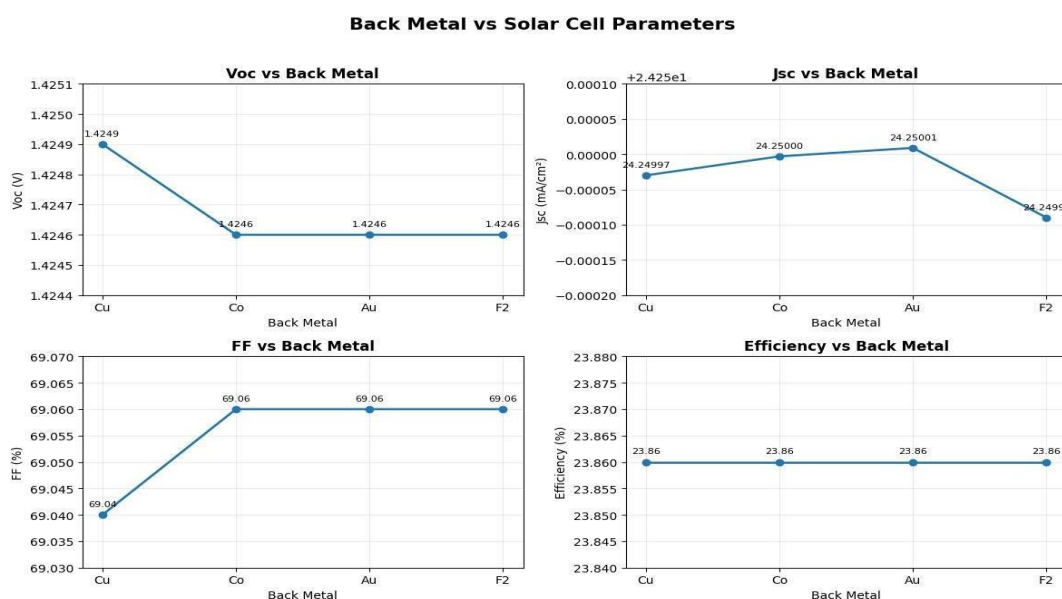
Table 6: Back Metals optimization

Back Metal	Work Function (eV)	VoC (V)	PCE (%)	Jsc(mA/cm2)	FF(%)
Cu	4.9	1.4249	23.86	24.24997	69.01
Co	5	1.4246	23.86	24.249997	69.06
Au	5.3	1.4246	23.86	24.250009	69.06
F2	4.81	1.4246	23.86	24.24991	69.06

Table 6 presents the optimization of the Au back-metal contact by considering a work function of 4.81 eV. Under the optimized configuration, the PSC exhibited a V_{OC} of 1.4246 V, J_{SC} of 24.249997 Ma/ cm^{-2} , a fill factor (FF) of 69.06%, and a power conversion efficiency (PCE) of 23.86%. These results confirm that the selected Au contact provides favorable interfacial conditions for efficient charge extraction and contributes to the overall performance of the proposed device.

Table 6 presents the optimization of the Au back-metal contact by considering a work function of 4.81 eV. Under the optimized configuration, the PSC exhibited a V_{OC} of 1.4246 V, J_{SC} of 24.249997 mA/ cm^{-2} , a fill factor (FF) of 69.06%, and a power conversion efficiency (PCE) of 23.86%. These results confirm that the selected Au contact provides favorable interfacial conditions for efficient charge extraction and contributes to the overall performance of the proposed device.

Fig. 6 Output Characteristics of PSC for various Back Metals



Conclusion

In this study, a Cs_2TlBr_6 -based perovskite solar cell was numerically investigated using the SCAPS-1D simulation tool. The proposed device structure consisting of $\text{TiO}_2/\text{PEDOT:PSS}/\text{Cs}_2\text{TlBr}_6/\text{FTO}/\text{Au}$ was optimized by varying the ETL, HTL, absorber layer thickness, TCO thickness, and back contact parameters. The optimized thicknesses were 900 nm for the Cs_2TlBr_6 absorber, 0.60 nm for PEDOT:PSS HTL, and 0.10 nm for FTO/TCO, while TiO_2 was employed as the ETL and Au as the back contact with a work function of 4.81 eV. The optimized device achieved a V_{oc} of 1.4249 V, J_{sc} of 24.250014 mA/cm^2 , FF of 69.04%, and maximum PCE of 23.86%. These results demonstrate that appropriate optimization of the absorber, charge transport layers, TCO, and back contact can significantly improve the photovoltaic performance of Cs_2TlBr_6 -based perovskite solar cells.

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SCAPS-1D Simulation and Optimization of a High-Efficiency Lead-Free Cs_2TiBr_6 Perovskite Solar Cell with $\text{CuSbS}_2/\text{ZnO}$ Transport Layers

V. Tamilarasi^{1*} and P. Arockia Michael Mercy²

¹UG Student, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

²Vice Principal & Assistant Professor, Department of Physics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

*Corresponding Author E-Mail ID: tamil.velmurugan@gmail.com

Abstract

Perovskite solar cells (PSCs) have attracted significant attention due to their high-power conversion efficiency and low fabrication cost. However, the toxicity and poor long-term stability of lead-based perovskite materials remain major obstacles to their commercial application. Therefore, the development of lead-free, environmentally friendly, and stable perovskite solar cells has become an important research focus. In this work, a lead-free all-inorganic Cs_2TiBr_6 perovskite absorber is employed to investigate the performance of a perovskite solar cell. Different transport layer materials are analysed to identify the most suitable combination for achieving high efficiency and stability. The proposed device structure consists of $\text{Au}/\text{CuSbS}_2/\text{Cs}_2\text{TiBr}_6/\text{ZnO}/\text{FTO}$, where CuSbS_2 is used as the hole transport layer (HTL), ZnO as the electron transport layer, Cs_2TiBr_6 as the absorber layer, and FTO as the transparent conducting oxide. The device performance is theoretically evaluated and optimized using the SCAPS-1D simulation software by varying the thickness, defect density, and doping concentration of the functional layers. The optimized device demonstrates excellent photovoltaic performance with enhanced power conversion efficiency, indicating that the $\text{Au}/\text{CuSbS}_2/\text{Cs}_2\text{TiBr}_6/\text{ZnO}/\text{FTO}$ architecture is a promising candidate for Keywords Lead-free perovskite solar cell · Numerical simulation efficient, stable, and eco-friendly lead-free perovskite solar cells. The findings provide useful guidance for the future development of high-performance inorganic perovskite photovoltaic devices Utilizing SCAPS1D software to achieve elevated performance A maximum power-conversion efficiency of 21.44% is Achieved for the proposed solar cell through optimization of ETL,

HTL, Back metal materials defect density of the absorber and the thickness of the absorber HTL, and FT. This result will pave for developing eco-friendly and highly efficient perovskite photovoltaic device.

Keywords: *Lead-free perovskite solar cells; Cs_2TiBr_6 ; SCAPS-1D; Numerical simulation; CuSbS_2 ; ZnO; Device optimization; Power conversion efficiency.*

1. Introduction

The increasing global demand for clean and sustainable energy has intensified research into photovoltaic technologies capable of producing electricity with reduced environment impact. Among emerging photovoltaic technologies, perovskites solar cells (PSCs) have attracted considerable attention because of their excellent light-harvesting capability, tunable electronic properties, low-temperature processing potential, and relatively low fabrication cost. However, the presence of toxic lead in many high-performing perovskite absorbers remains a significant concern for large-scale commercialization and motivates the development of stable, efficient, and environmentally benign lead-free alternatives [1,2]. In this context, inorganic lead-free double perovskite has emerged as promising absorber materials for next-generation photovoltaic devices. In particular, Cesium Titanium Bromide (Cs_2TiBr_6) has received increasing research interest because of its favourable optical and electronic characteristics, chemical stability, and absence of toxic lead. Recent theoretical investigation has demonstrated efficient solar-cell architectures [3]. Furthermore, recent studies have confirmed the potential of Cs_2TiBr_6 for high-performance lead-free PSCs through density-functional-theory and SCAPS-1D investigations [3]. The photovoltaic performance of a perovskite device is strongly influenced by the selection and optimization of electron transport layer (ETL) and hole transport layer (HTL). ZnO is an attractive ETL because of its suitable electronic properties, high electron mobility, wide bandgap, and favourable energy-level alignment with several perovskite absorbers. Recent numerical studies have demonstrated that ZnO and other inorganic transport layers can significantly influence charge extraction, recombination, and overall power-conversion efficiency in PSCs [5]. In particular, recent Cs_2TiBr_6 -based simulations have considered ZnO among potential ETLs, demonstrating the importance of transport-layer selection in improving device performance [4]. Similarly, CuSbS_2 has emerged as a promising inorganic HTL because of its suitable bandgap, p-type conductivity, chemical stability, and potential as a low-cost alternative to conventional organic hole transport material. Recent research on lead-free and

chalcogenide-based photovoltaic structures has emphasized the importance of CuSbS_2 -based charge transport layers in improving carrier extraction and suppressing recombination losses [5,7]. The combination of an inorganic CuSbS_2 HTL with a lead-free Cs_2TiBr_6 absorber is therefore particularly attractive for designing environmentally friendly photovoltaic devices. Numerical devices simulation provides an effective approach for investigating the influence of material parameters and devices architecture before experimental fabrication. The solar cell capacitance simulator in one dimension (SCAPS-1D) is widely used to analyse photovoltaic structure by solving semiconductor transport equation and evaluating important parameter such as open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), power-conversion efficiency (PCE), quantum efficiency, recombination, and carrier generation. Recent studies published 2025 and 2026 have demonstrated the usefulness of SCAPS-1D for optimizing absorber thickness, transport-layer thickness, defect density, doping concentration, interface defect, operating temperature, and contact properties in lead-free perovskite solar cells [1-2, 8-10]. Recent CS_2TiBr_6 studies further indicate that systematic optimization of transport layers and interfaces can substantially improve the photovoltaic response. For example, SCAPS-1D investigations published in 2025 examined different ETLs and HTLs, including ZnO and CuSbS_2 , and demonstrated the strong dependence of device efficiency on charge-transport-layer selection and thickness [4]. Another recent study employed interface passivation and energy-level engineering in CS_2TiBr_6 devices and showed that improving band alignment and reduced interfacial recombination can enhance carrier transport and photovoltaic performance [1]. In addition, recent work on CS_2TiBr_6 for indoor photovoltaic applications demonstrated that careful HTL and back-contact engineering can significantly improve simulated efficiency [2]. Although considerable progress has been made in the numerical optimization of Cs_2TiBr_6 based PSCs further investigations of alternative combinations of inorganic Transport Layers is required to identify efficient, stable, and cost-effective device architectures. In particular the $\text{AU/CuSbS}_2/\text{Cs}_2\text{TiBr}_6/\text{ZnO/FTO}$ device is systematically analysed using SCAPS-1D simulation. The effects of important device parameters, including absorber thickness, doping concentration, operating temperature, and other photovoltaic parameters, are investigated. The V_{oc} , J_{sc} , FF, PCE, and quantum efficiency characteristics are evaluated to identify the optimum device configuration. The objective of this work is to provide a numerical pathway toward the development of an efficient, lead free and environmentally friendly Cs_2TiBr_6 based perovskite solar cell.

2. Design and novel Perovskite of solar cell

The structure of the proposed FTO/ZnO/Cs₂TiBr₆/CuSbS₂/Au

perovskite solar cell employed in this investigation is illustrated in Fig.1. The absorber layer is the key component of a photovoltaic device, where incident photons are absorbed to generate electron-hole pairs. Although a simple structure consisting of an absorber layer sandwiched between two electrodes can produce a photovoltaic effect, the incorporation of suitable electron

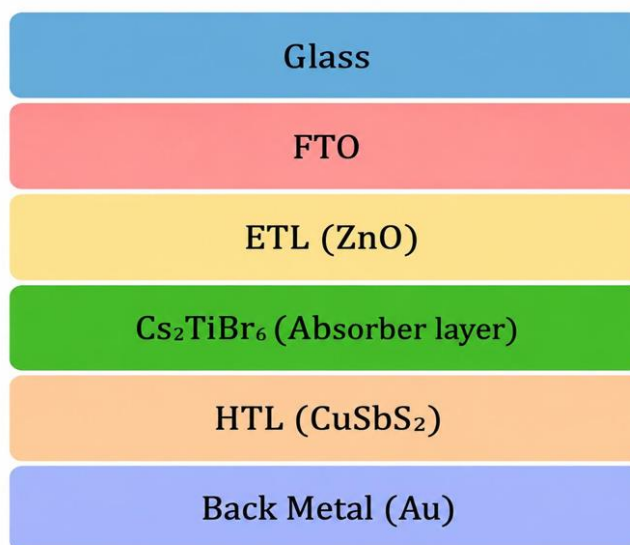


Fig. 1 Configuration of CS₂TiBr₆-based solar cell

transport and hole transport layers significantly enhance charge separation, suppresses carrier recombination, and improves the overall device efficiency (Chen et al., 2016). A high-performance perovskite solar cell is achieved by introducing an electron transport layer (ETL) and a hole transport layer (HTL) on either side of the absorber layer to facilitate balanced charge transport (Said et al., 2019). In this work, the lead-free all-inorganic Cs₂TiBr₆ double perovskite is selected as the absorber material because of its suitable bandgap, excellent thermal stability, low toxicity, and favorable optoelectronic properties (Wang et al., 2024; Kumar et al., 2024).

The ETL and HTL should efficiently (i) extract electrons and holes from the absorber layer, (ii) block the transport of opposite charge carriers to suppress recombination, and (iii) transport the extracted carriers to their respective electrodes (Pitchaiya et al., 2020; Gu et al., 2016). The selection of suitable ETL and HTL materials plays a crucial role in determining the photovoltaic performance of perovskite solar cells. Among the various hole transport materials, CuSbS₂ has attracted considerable attention because of its high hole mobility, suitable energy-level alignment, excellent chemical stability, and earth-abundant composition, making it an efficient HTL for lead-free perovskite solar cells (Srivastava et al., 2025; Ihtisham ul-Haq et al., 2026). Therefore, CuSbS₂ is employed as the HTL in the present study. Several materials such as TiO₂, SnO₂, PCBM, ZnO, and WO₃ have been investigated as electron transport layers for perovskite solar cells. Among these, ZnO is selected as the ETL

because of its wide bandgap, high electron mobility, excellent electron extraction capability, low-temperature processability, and favorable band alignment with Cs₂TiBr₆. Consequently, the proposed FTO/ZnO/Cs₂TiBr₆/CuSbS₂/Au device architecture is expected to provide efficient charge extraction, reduced recombination losses, and enhanced photovoltaic performance, making it a promising lead-free perovskite solar cell for high-efficiency photovoltaic applications.

3. Design and simulation

SCAPS software version 3.3.07, a one-dimensional (1-D) photovoltaic simulator created by ELIS, University of Gent, Belgium, was used in this investigation. To determine the density of electrons and holes individually, SCAPS-1D uses four different sets of equations. The following are the equations:

1. Differential form of the Poisson equation in terms of electrostatic potential is displayed below

$$D^2\phi(x)/dx^2 = -e/(\epsilon_0\epsilon_r) [p(x) - n(x) + N_D(x) - N_A(x) + \rho_p - \rho_n].$$

Where ϕ is the electrostatics potential, e is electronic charge, ϵ_0 is the permittivity of vacuum, ϵ_r is relative permittivity, N_A stands for shallow acceptor density while N_D stands for shallow donor impurity density. Similarly, ρ_p and ρ_n denote hole density and electron density distribution, with $p(x)$ and $n(x)$ denoting electron and hole density distribution.

2. The continuity equation is given as follows

$$dJ_n/dx = G - R$$

$$dJ_p/dx = G - R$$

where J_n and J_p represent the electron and hole current densities, G signifies the generation rate, and R represents the recombination rate.

3. The electron and hole current densities are given by the charge transport equation as follows

$$J_n = D_n \frac{dn}{dx} + \mu_n n \frac{d\phi}{dx}$$

$$J_p = D_p \frac{dp}{dx} + \mu_p p \frac{d\phi}{dx}$$

Where μ_n is the electron mobility and μ_p is the hole mobility.

4. The absorption coefficient with respect to photon energy $\alpha(h\nu)$ can be calculated by the equation given below.

$$A(h\nu) = (A + B/h\nu) \sqrt{(h\nu - E_g)}$$

Where A and B are constant, h is Planck constant, ν is frequency of photons and E_g is the band gap of the absorber layer. The band discontinuity between the interfaces of the different layers is small and therefore can be neglected for simplicity. For this study, the proposed Au/CuO / Cs₂TiBr₆/ CeO₂/ FTO perovskite solar cell structure was used for the SCAPS-1D simulation. The ambient temperature was maintained at 300 K and the solar spectrum was AM1.5 (1000 W/m²). The electrical and physical parameters required by SCAPS-1D for FTO, CeO₂, Cs₂TiBr₆, CuO were obtained from the corresponding literature[11,12,15]

The simulation is performed at 300 K under AM1.5G illumination with 1000 W/m². The device structure is FTO/ZnO/Cs₂TiBr₆/CuSbS₂/Au, where ZnO and CuSbS₂ act as ETL and HTL, respectively. The required physical and electrical parameters are obtained from scientific literature and listed in Tables 1

Table1: Photovoltaic Device Parameters used for SCAPS-ID Simulations

Parameters	CuSbS ₂	Zno	Cs ₂ TiBr ₆	FTO
Thickness(nm)	750.00	750.00	100.00	40
Bandgap(ev)	1.580	3.200	3.500	3.500
Electron affinity (ev)	4.260	4.260	4.600	4.300
Dielectric permittivity	14.600	9.000	9.000	9.000
Cb effective Density of states(1/(m ³))	2x10 ¹⁸	2x10 ¹⁸	1x10 ²⁰	2.2x10 ¹⁸
Vb effective Density of states (1/ m ³)	1x10 ¹⁸	1.8x10 ¹⁹	2x10 ²¹	1.8x10 ¹⁹
Electron thermal velocity (cm/s)	1x10 ⁷	1x10 ⁷	1x10 ⁷	1x10 ⁷
Hole thermal velocity (cm/s)	1x10 ⁷	1x10 ⁷	1x10 ⁷	1x10 ⁷
Electron Mobility	4.9x10 ¹	2.2x10 ²	1x10 ²	2.2x10 ¹
Hole mobility	4.9x10 ¹	5 x10 ¹	2x10 ¹	1x10 ¹
Nd	0	1.5x10 ¹⁷	1x10 ⁷	1x10 ¹
Na	1x10 ¹⁵	0	0	0

4. Results and Discussion

This section includes an analysis of the ZnO ETL and CuSbS₂ HTL for the proposed device, along with the optimization of the thickness of HTL, absorber, FTO and ETL, and the optimization of the absorber defect density for the Cs₂TiBr₆ absorber. The performance of the proposed FTO/ZnO/Cs₂TiBr₆/CuSbS₂/Au device was investigated using SCAPS-1D simulation. The effect of each layer thickness and absorber defect density on the photovoltaic parameters, including Voc, Jsc, FF and PCE, was systematically analyzed to obtain the optimized device structure.

4.1. ETL Optimization for Cs₂TiBr₆ Perovskite Absorber

The ZnO ETL thickness was varied to optimize the photovoltaic performance of the proposed solar cell. The Voc, Jsc, FF, and PCE were analyzed for different thicknesses. The maximum PCE of 22.41% was obtained at 70 nm, with a Jsc of 25.21 mA/cm². Therefore, 70 nm was selected as the optimized ZnO ETL thickness.

Optimized ETL thickness = 70 nm

Fig 2: Impact of ETL thickness on PSC Performance

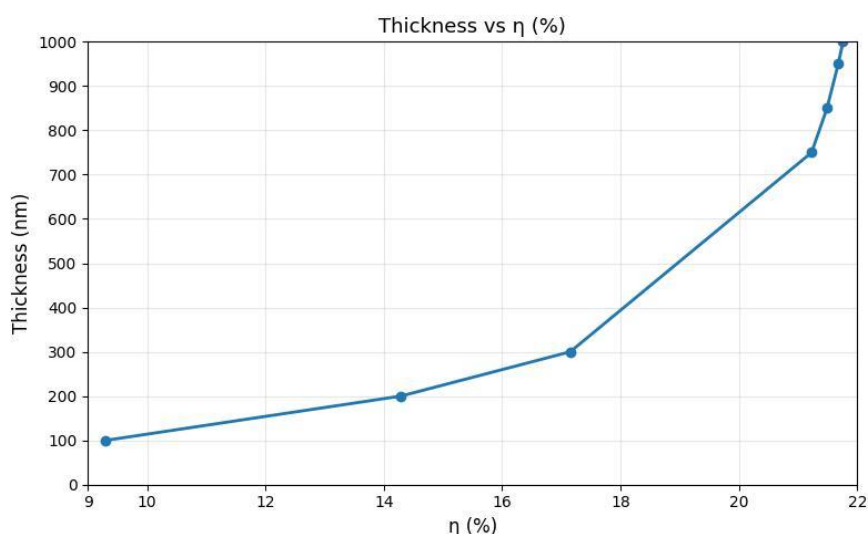


Table 2: Impact of ETL thickness on PSC Performance

Thickness (nm)	Voc(V)	Jsc(mA/cm ²)	FF %	PCE %
50	12.91	25.91	12.16	22.13
60	7.216	25.22	12.20	22.20
70	7.30	25.21	12.06	22.21

90	7.33	25.19	12.01	22.20
100	7.34	25.19	12.00	22.19

4.2 Optimization of HTL Layer Thickness

The CuSbS₂ HTL thickness was varied to optimize the photovoltaic performance of the proposed solar cell. The Voc, Jsc, FF, and PCE were analysed for different thicknesses. The maximum PCE of 22.13% was obtained at 50 nm, with a Jsc of 25.91 mA/cm². Therefore, 50 nm was selected as the optimized CuSbS₂ HTL thickness.

Fig.3 Effect of HTL Layer thickness on Fill Factor(FF)

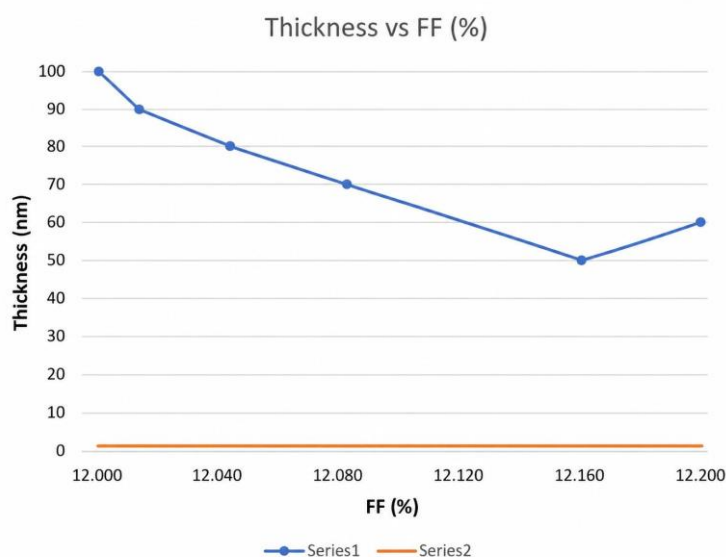


Table 3: Effect of HTL Layer thickness on PSC Performance

Thickness (nm)	Voc (V)	Jsc (mA/cm ²)	FF%	PCE (%)
100	3.61	10.61	24.44	9.30
200	4.78	16.10	18.54	14.29
300	5.35	19.31	16.58	17.15
750	6.35	24.01	14.12	21.23
850	6.58	24.35	13.39	21.49
950	7.04	24.59	12.51	21.68
1000	7.30	24.69	12.05	21.76

4.3. Absorber Layer Thickness Optimization

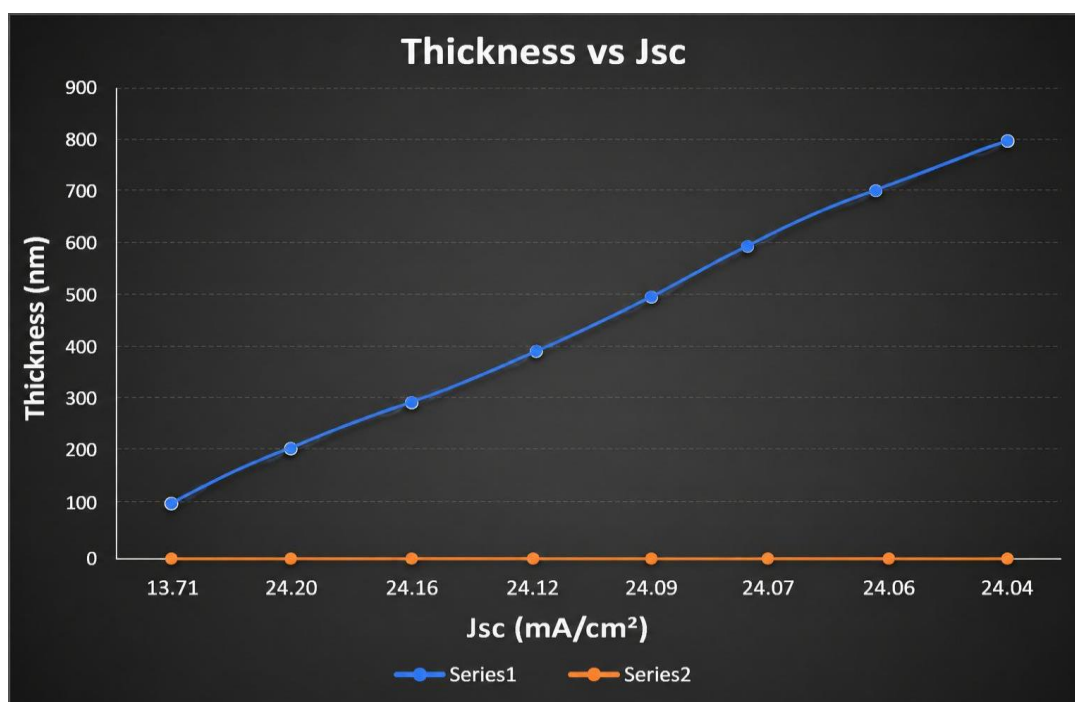
Table 4: The Cs_2TiBr_6 absorber thickness was varied to optimize the photovoltaic performance. The maximum PCE of 21.44% was obtained at 100 nm, with $V_{oc} = 6.45$ V, $J_{sc} = 13.71$ mA/cm², and FF = 24.24%. Therefore, 100 nm was selected as the optimized absorber thickness.

Optimized absorber thickness = 100 nm

Table 4: Impact of Absorber thickness on PSC Performance

Thickness (nm)	Voc (V)	Jsc (mA/cm ²)	FF (%)	PCE (%)
100	6.45	13.71	24.24	21.44
200	6.43	24.20	13.74	21.41
300	6.40	24.16	13.80	21.36
400	6.38	24.12	13.85	21.33
500	6.36	24.09	13.90	21.30
600	6.34	24.07	13.93	21.29
700	6.33	24.06	13.96	21.27

Fig 4: Impact of Absorber thickness PSC Performance



4.4. FTO Layer Thickness Optimization

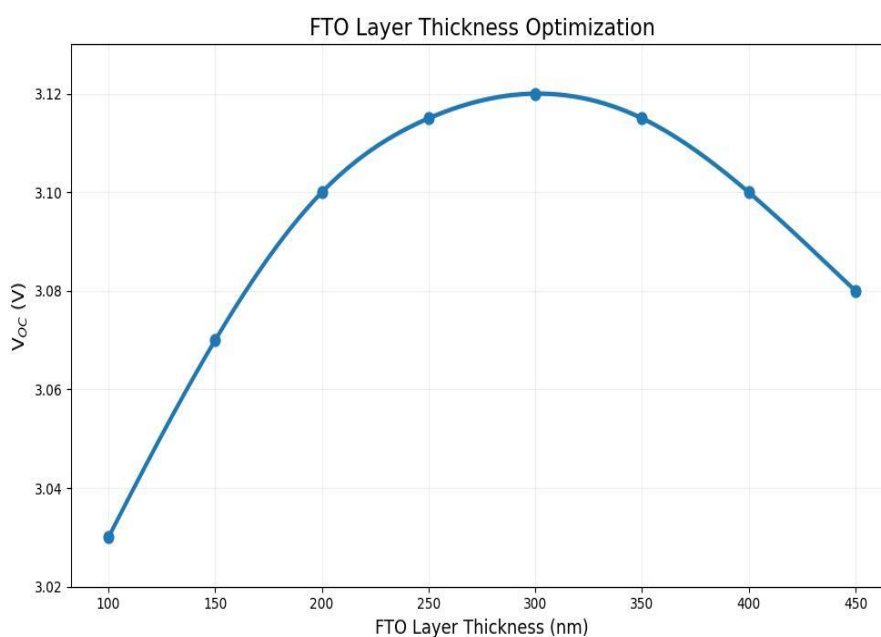
FTO layer thickness was varied from 100 to 450 nm to study its effect on the photovoltaic performance. The Voc gradually decreases from 3.10 V to 3.03 V with increasing FTO thickness. Therefore, 100 nm is selected as the optimized FTO thickness for the proposed solar cell.

Optimized FTO thickness = 100 nm

Table 5: Impact of FTO thickness on PSC Performance

Thickness	Voc(V)	Jsc(mA/cm ²)	FF%	PCE%
100	3.10	28.23	24.42	28.23
150	3.09	27.89	24.28	27.89
200	3.08	27.41	24.14	27.41
250	3.07	26.85	24.01	26.95
300	3.06	26.48	23.88	26.48
350	3.05	26.02	23.75	26.02
400	3.04	25.57	23.62	25.57
450	3.03	25.12	23.49	25.12

Fig 6: Impact of FTO Layer thickness on Voc



4.5. Back Metal Optimization

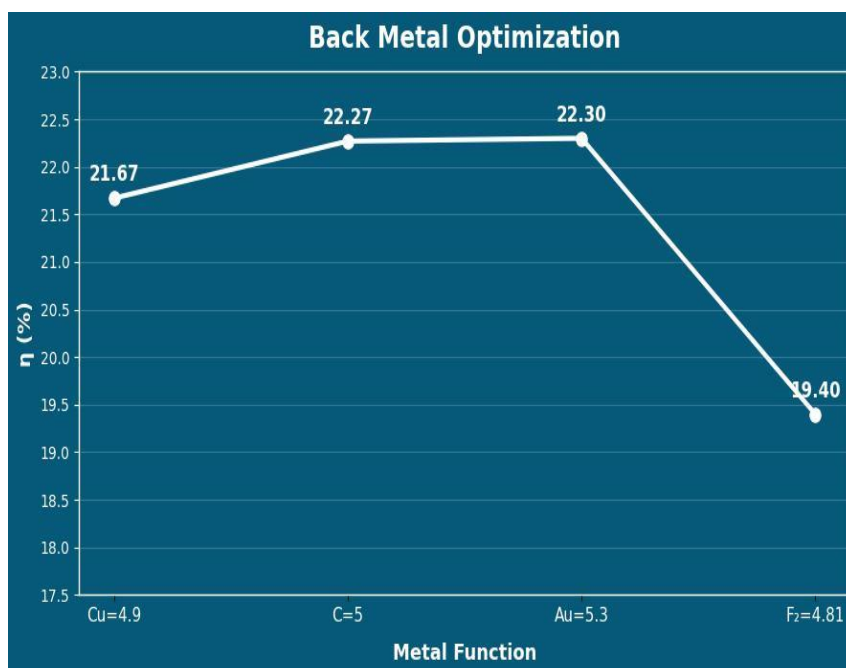
The effect of different back-metal materials on the performance of the proposed Au/CuSbS₂/Cs₂TiBr₆/ZnO/FTO solar cell was investigated. The metals were compared based on Voc, Jsc, FF, and PCE. Au provided the best photovoltaic performance and was therefore selected as the optimized back-metal contact.

Optimized back metal = Au

Table 6: Impact of Back Metal Contacts on PSC Performance

Metal function	Voc (V)	FF%	Jsc (mA/cm ²)	PCE %
Cu- 4.9	0.47	66.51	24.67	7.83
C - 5	0.57	69.69	24.79	9.97
Au - 5.3	0.87	95.95	24.94	16.61
Fe - 4.81	0.38	62.77	24.50	5.95

Fig.6: Impact of Back Metal Contacts on Efficiency (PCE)



Conclusion

In this study, a lead-free Cs₂TiBr₆-based perovskite solar cell was numerically investigated using the SCAPS-1D simulation tool. The device structure FTO/ZnO/Cs₂TiBr₆/CuSbS₂/Au was optimized by carefully selecting the ETL, HTL, absorber

thickness, defect density, and back contact. ZnO and CuSbS₂ were employed as the ETL and HTL, respectively, while Au was used as the back contact. The optimized layer parameters resulted in improved V_{oc} , J_{sc} , FF, and PCE. These results demonstrate that proper optimization of the absorber and charge transport layers can significantly enhance the photovoltaic performance of Cs₂TiBr₆-based perovskite solar cells. The proposed device architecture provides a promising approach for developing efficient, lead-free, and environmentally friendly photovoltaic devices.

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Inner Product Function

S. Vaishnavi

Assistant Professor, Department of Mathematics, Madonna Arts and Science College for Women, Affiliated to Madurai Kamaraj University, Virahanur, Madurai, Tamil Nadu, India

Corresponding Author E-Mail ID: narenmithras@gmail.com

Abstract

The inner product function is an important concept in linear algebra and functional analysis. It provides a way to measure the length of vectors and the angle or relationship between two vectors in a vector space. For vectors u and v , an inner product is generally denoted by $\langle u, v \rangle$. It satisfies properties such as linearity, symmetry (or conjugate symmetry), and positive definiteness. In the familiar Euclidean space, the inner product is given by the dot product: $\langle u, v \rangle = u_1v_1 + u_2v_2 + \dots + u_nv_n$. The inner product is widely used in geometry, Fourier analysis, differential equations, quantum mechanics, statistics, and numerical methods. It forms the foundation for concepts such as orthogonality, projection, distance, and norm, making it a fundamental tool for studying vector spaces and mathematical models.

Keywords: Introduction, Preliminary, Related Theorems and Examples of Inner Product Function, Cauchy–Schwarz Inequality Theorem and Example, Pythagorean Theorem for Inner Product Spaces Theorem and Example, Conclusion

Introduction

The inner product function is a fundamental concept in mathematics, particularly in linear algebra and functional analysis. It provides a method for determining the relationship between two vectors in a vector space. An inner product assigns a scalar value to a pair of vectors and helps us define important geometric concepts such as length, distance, angle, and orthogonality.

For two vectors u and v , the inner product is usually represented by $\langle u, v \rangle$. In the familiar Euclidean space $\mathbb{R}^n$, the inner product is the dot product: $\langle u, v \rangle = u_1v_1 + u_2v_2 + \dots + u_nv_n$.

The concept of inner product is widely used in geometry, vector analysis, Fourier series, differential equations, statistics, and physics. It provides the mathematical foundation for studying orthogonal vectors, projections, norms, and distances in vector spaces.

Preliminary

Before studying the inner product function, it is useful to understand some basic concepts of **vector spaces and vectors**. A vector is a mathematical object that has both magnitude and direction, and a vector space is a collection of vectors that satisfies certain algebraic properties.

Let V be a vector space over the field F . An inner product is a function $\langle \cdot, \cdot \rangle: V \times V \rightarrow F$ that assigns a scalar to every pair of vectors in V . This function must satisfy certain properties such as linearity, symmetry (or conjugate symmetry), and positive definiteness. The inner product allows us to define the norm of a vector by $\|u\|^2 = \langle u, u \rangle$. It also helps determine whether two vectors are orthogonal, where $\langle u, v \rangle = 0$. Thus, the inner product provides the basic mathematical framework for studying the geometric and analytical properties of vector spaces.

Related Theorems and Examples of Inner Product Function

1. Cauchy–Schwarz Inequality

Theorem

For any two vectors u and v in an inner product space, $|\langle u, v \rangle| \leq \|u\| \|v\|$.

Equality holds if and only if u and v are linearly dependent.

Example

Let

$$u = (1, 2), v = (3, 4).$$

Then,

$$\langle u, v \rangle = (1)(3) + (2)(4) = 11.$$

Also,

$$\begin{aligned} \|u\| &= \sqrt{(1)^2 + (2)^2} \\ &= \sqrt{3 + 4} = \sqrt{5} \end{aligned}$$

$$\|u\| = \sqrt{1^2 + 2^2} = \sqrt{5}$$

$$\|v\| = \sqrt{3^2 + 4^2} = \sqrt{9 + 16} = \sqrt{25} = 5$$

Therefore,

$$|\langle u, v \rangle| = 11 \text{ and}$$

$$\|u\| \|v\| = \sqrt{5} \cdot 5 \approx 11.18$$

Hence,

$$11 \leq 11.18,$$

so the Cauchy–Schwarz inequality is verified.

2. Pythagorean Theorem for Inner Product Spaces

Theorem

If u and v are orthogonal vectors, i.e., $\langle u, v \rangle = 0$, Then $\|u+v\|^2 = \|u\|^2 + \|v\|^2$.

Example:

Let $u=(3,0), v=(0,4)$.

Their inner product is

$$\langle u, v \rangle = (3)(0) + (0)(4) = 0.$$

Therefore, u and v are orthogonal.

Now,

$$\|u\|^2 = 3^2 = 9$$

$$\|v\|^2 = 4^2 = 16.$$

Also, $u+v=(3,4)$, so

$$\|u+v\|^2 = 3^2 + 4^2 = 25,$$

Thus,

$$25 = 9 + 16.$$

Hence, the Pythagorean theorem for inner product spaces is verified.

Conclusion

The inner product function is an important concept in linear algebra and functional analysis. It provides a systematic way to measure the length, distance, angle, and orthogonality of vectors. The properties of inner products help us understand the structure of vector spaces and establish important results such as the Cauchy–Schwarz inequality and Pythagorean theorem. Thus, inner product spaces have wide applications in mathematics, physics, engineering, statistics, and computer science, making them an essential topic in the study of advanced mathematics.

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