

Advanced techniques and methods for organic chemistry applications in nanoenergy materials development

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<https://doi.org/10.46649/ajiea.v2.1.1a.30.6.2026>

Abstract. Recently, interest in nanomaterials has increased, driven by the global trend toward integrating them into modern and advanced industries. This is due to their unique properties, stability, and superior performance, which distinguish them from traditional and classical materials. Among these materials, our research will integrate nanoscale perovskites with nanocomponents to produce a semiconductor nanocomposite with unique chemical and physical properties, particularly when used in catalysis, specifically in photovoltaic systems. This is demonstrated by models and simulation results using MATLAB. Thanks to its ease of fabrication and synthesis, availability, low cost, and the ability to integrate with other components to form a nanocomposite that meets demand, it achieves superior performance and efficiency compared to semiconductors such as silicon and germanium. Furthermore, it is capable of absorbing light and transporting charges, meeting a significant portion of the global energy demand.

Keywords: Photovoltaic systems; Perovskite photovoltaics; nanomaterials; Chemical materials; Nanochemistry.

1. INTRODUCTION

The transition to renewable energy sources is a global challenge that requires innovative solutions. Solar cells are emerging as a leading technology. However, the first and second generations suffer from limitations in efficiency and initial cost [1][2]. Chemical materials have also been utilized in energy storage processes, which has contributed to a new path toward replacing outdated technologies with more advanced ones. Battery chemicals have been introduced as a new challenge, and these technologies have succeeded in changing the course of modern technologies, which in turn will protect the environment and reduce pollutants and gaseous emissions [3] [4].

In contrast, the third generation of solar cells, which relies on Nanochemistry, opens new horizons for the development of materials with unique properties. This research aims to explore the role of chemical engineering in the design and manufacture of advanced nanomaterials and organic materials that form the basis of these cells. The focus will be on interaction mechanisms at the molecular level and how the chemical structures of materials can be manipulated to improve light absorption, charge transport, and stability. The research will also provide a comprehensive comparison between the most prominent materials, proposing a new research approach that combines the strengths of both fields to achieve unprecedented performance.

The discovery and development of perovskites, environmentally friendly and stable materials with a high capacity to absorb solar radiation, has also been noted. They are used in charging and generating energy from solar radiation.

This article, published in 2024, explores the development of perovskites and their organic and inorganic halides to produce materials with desirable properties in this field, particularly for solar panels and chargers. Kumar S, Sharma et al. discussed mitigating the harmful effects and toxicity of lead halides used in the manufacture of solar panels at the end of their lifespan. Researchers in the field of chemical applications in industries and energy production suggest using readily available, environmentally friendly materials without any harmful side effects. Research has been conducted to reduce the toxicity of lead used with perovskites in the manufacture of environmentally friendly solar cells. Work is currently underway to develop solar cells using chemicals that do not leave toxic residues with negative environmental impacts. This includes replacing toxic lead with non-toxic

materials such as silver, copper, germanium, titanium, tin, bismuth, and other chemicals that are less harmful than the toxic effects of hazardous lead.

Researchers in the clean energy cell industry are conducting experiments in collaboration with chemical laboratories to prevent the use of these chemical alternatives, develop efficient alternative methods and materials for energy production, and replace outdated methods for producing photovoltaic cells. Therefore, it is essential to follow safety procedures when using these chemical nanomaterials, which reduces the harmful effects and waste associated with their use and after consumption. These materials produce easy-to-use, low-cost, high-performance, durable, and hazard-free materials[6].

These recent studies and research in 2018, 2023, and 2025 have focused on developing the use of perovskite halides as nanomaterials, given their significant importance as versatile semiconductors in various areas of life[14]. Thanks to their unique chemical and physical properties in the field of electrical power generation, this catalyst is a powerful catalyst in photocatalysis. In this study, these materials were used as active materials in the fabrication of photocatalytic devices, where they were incorporated into ni-p/p-i-n systems, as well as in electrolyte manufacturing processes. Heterogeneous catalyst designs were also investigated to enhance carbon dioxide reduction and hydrogen generation reactions. Photocatalysts have also been used to produce organic compounds and manufacture less harmful or environmentally friendly chemicals. This study proposes an update to halide-perovskite-based photocatalytic systems for solar cell manufacturing. The challenges in photocatalysts based on this material lie in combining suitable active electrode materials and methods. Some advanced studies have been published on the use of halideperovskite, the basic material in photocatalysts. Information on photovoltaic cell encapsulation and packaging has also been published. The use of heterogeneous photocatalysts in hydrogen upgrading and carbon dioxide reduction reactions has also been investigated. The use of photocatalysts has been studied in photocatalysts, as well as in the synthesis of organic chemical compounds and the production of environmentally friendly materials. Their unique properties have been observed, making them one of the most popular and preferred materials for the production of catalytic nanocells. They are also widely used in some organic compound synthesis reactions. Numerous improvements and developments are currently underway to improve the quality and efficiency of nanomaterial production.

Modern centers have moved towards introducing perovskite chemical technology into schools, colleges, and engineering institutes for educational purposes and to educate the next generation about the necessity of using this material. The Indian National Center for Research and Technology has published several books and publications on this material, which will be useful to future generations in the field of electronics and technology.

The available information on this material has shown that it must be approached from multiple perspectives, including structural design, with the goal of future use in energy development. This contributes to the development and diversification of modern energy sources, eliminating pollution and toxicity problems, and making the environment more sustainable.[7].

2. MATERIALS AND METHODS

2.1. MATERIALS

This academic study used a range of advanced materials in solar cells, including:

- Graphene: A nanomaterial with superior electrical and mechanical properties.
- Polymers: Provide flexibility in withstanding mechanical stresses on the processor.
- QD chemicals: Chemicals added to achieve photovoltaic power gains.
- Polymer-perovskite blends: These materials were combined to study the effect of this bonding on performance at temperatures ranging from 25 to 65°C.

2.2. METHODS

The electronic and optical properties of the studied materials—graphene, polymers, composites, and polymer-perovskite blends—were modeled in MATLAB 2024b using appropriate mathematical formulas derived from academic literature. The research methodology relied on MATLAB 2024b as the primary tool for conducting analyses and simulations, based on the physicochemical parameters of each material's properties. The steps included the following:

- Mathematical Modeling: The properties of the materials (graphene, polymer, multimaterials, and polymer-perovskite) were modeled in MATLAB using codes...

- Thermal Variables: Temperature values from 25°C to 65°C were used as key variables to study the effect of temperature on performance, efficiency, and stability. This was used to evaluate the response of individual and composite materials to temperature changes.
- Performance Analysis: Key Performance Indicators (KPIs) were calculated.
- Validation and Comparison: The results were compared with data published in previous academic studies to ensure the reliability of the models and the validity of the conclusions.

2.2.1 PROPERTIES:

According to the American Chemical Society, perovskite is also known as calcium titanium oxide, and its chemical symbol is CaTiO_3 , named after the Russian nobleman L. Perovski. This compound occurs in the form of colorless, shaped crystals that change color depending on the presence of impurities, such as copper, iron, and other elements.[8] Chemically, this material consists of a cationic part (symbol β), an anionic part, and a halogen. Therefore, its general formula is ABX_3 [5].

It is found in Russia, Italy, Switzerland, and other countries. It has been chosen for use in the electrical industry due to its chemical and physical properties, including electrical conductivity, stability, catalytic properties, insulation, conductivity, and ionic properties.[8]

2.2.2 FEATURES AND PROPERTIES:

The advantages of this material are among the factors that have led to its widespread popularity due to its excellent chemical and physical properties. This makes it ideal for use in current popular applications, such as industrial, electrical, and electronic applications, LED design, sensor manufacturing, as well as magnetic and waveguide electronics. Therefore, it has been chosen for use in the electrical industry due to its chemical and physical properties, as shown in Figure 6, perovskite (CaTiO_3) crystals.

This material has chemical and physical properties that improve efficiency, performance, and stability. These properties include [5] [8]:

- High energy absorption.

- Electrical conductivity
- Stability
- Catalytic properties
- Conductivity and ionic properties
- Ability to transfer dipole charges
- Flexibility in charge transfer
- Insulation: High dielectric constant
- Ability to add elements when needed for improvement
- Ability to adjust and control energy gaps
- Non-hazardous
- Insoluble
- Resistant to thermal effects, with a melting point of 1975°C.
- making it suitable for solar energy applications.
- Pressure resistance
- Photocatalytic and magnetic properties.
- Resistance to magnetic and thermal effects.
- Low oxidation susceptibility.
- Resistance to oxidation under atmospheric conditions.
- Low-cost manufacturing capability.
- Flexible chemical modification.
- Simple synthesis.
- Hybridizability.
- Available in a variety of colors, such as black, orange, and yellow, due to its ability to chemically bond with other materials.

2.2.3 MODERN GLOBAL TRENDS:

According to the National Renewable Energy Laboratory (NREL) team responsible for the modifications and updates to the chart in Figure 5, we note that emerging photovoltaic solar cells made of organic perovskite materials, outlined in red and yellow, have been widely used since 2013 and are expected to reach efficiencies of 27 to 30.1 per cent by 2025. This has made tandem and hybrid photovoltaic cells (perovskite/silicon and perovskite/CIGS) capable of performing two separate absorption processes that capture more solar radiation (perovskite/silicon and perovskite/CIGS)[9].

According to the Financial Times, a leading international newspaper, solar farms in China rely on components between organic perovskites and silicon to manufacture photovoltaic panels coated with a glass layer to absorb the maximum amount of light. These cells, called glass perovskite cells, are developing rapidly.

Japan has turned to multilayer chemical solar cells made from perovskites, which are extremely thin films no more than one millimetre thick and have a high capacity to absorb and utilize large amounts of light [10].

The report, published on the LiveScience news website, presented a discovery by scientists that eliminates the need for batteries when operating devices with dim lights and room lights. This is achieved by using a perovskite cell, which absorbs the most energy and operates with high efficiency, regardless of its small size. It can capture light from indoor lights, alarms, and any other light source by sensing it[12].

2.2.4 RELIABILITY – STABILITY: CHALLENGES AND SOLUTIONS:

- Rapid reaction with some chemicals. Therefore, the behavior of each material must be studied to optimize crystallinity.
- Reducing recombination: This is achieved by manufacturing stable facade coatings, combining them with polymeric materials.
- Reducing material leakage: Double glass barriers are used to trap some leaky materials.
- Preventing oxidation: This is achieved by eliminating or reducing the use of lead.
- Preserving the environment: This is achieved through proper recycling and recovering materials for further use under the supervision of specialists [11].

2.2.5 MAIN ISSUES:

We are seeing significant progress in photovoltaic cells, especially those made from materials (graphene, polymers, quantum dots, and others), which are widely available on the market.

However, there are major obstacles, including:

- ☐ Poor stability
- ☐ Low efficiency
- ☐ Short lifetime of quantum dot cells
- ☐ Low light absorption in graphene cells is limited.

Therefore, scientists have turned to perovskite, which has been found to have an efficiency above 25%.

Despite its good efficiency, the degradation of the individual material due to humidity is the main obstacle to its widespread use.

Therefore, efforts must be made to improve the stability of perovskite cells in conjunction with their high efficiency, so that they can become a leading and reliable alternative to polymer, graphene, and quantum dot technologies. As shown in Figures 4(a), (b), (c), and (d), the efficiencies for polymeric materials, graphene, quantum dots, and perovskite.

2.2.6 MATHEMATICAL MODEL FOR CALCULATING:-

- Current-voltage (I-V) characteristics
- Calculating the efficiency (PCE)
- Evaluating the effect of polymers on performance.

Improved performance and efficiency.

Mathematical Model

1. Basic Current - Voltage (I - V) Equation

$$J(V) = J_{sc} - J_0 (e^{\frac{qV}{kT}} - 1) - \frac{V}{R_{sh}} - J_{series}$$

- J_{sc} : Short-circuit current
- J_0 : Reverse saturation current
- R_{sh} , R_s : Shunt and series resistances

2. Power Conversion Efficiency (PCE)

$$\eta = \frac{P_{max}}{P_{in}}$$

- V_{oc} : Open-circuit voltage
- FF : Fill factor
- P_{in} : Incident optical power

3. Chemical Integration Equation (Property Enhancement)

$$V_{oc,new} = V_{oc,ref} (1 + \alpha_{V_{oc}} f_{polymer})$$

$$J_{sc,new} = J_{sc,ref} (1 + \alpha_{J_{sc}} f_{polymer})$$

- $f_{polymer}$: Polymer incorporation fraction
- α : Enhancement coefficients

4. Fill Factor (FF) Equation

$$[FF =]$$

- V_{mp} , J_{mp} : Voltage and current at maximum power point

3. RESULTS AND DISCUSSION

3.1. RESULTS

This research paves the way for direct application in electronics and industry. MATLAB simulations, mathematical modelling, and fundamental analysis of perovskite components used in solar cells were studied and analyzed. Incorporating them with polymers can enhance flexibility and stability, increasing efficiency to 30% or slightly more. This was achieved by directly manipulating the interface gap, as shown below.

- ☐ Stability: According to the simulation results, photovoltaic cells integrated with nanolayers exhibited better stability in the event of thermal degradation compared to conventional cells.
- ☐ Efficiency: It was clearly observed that the efficiency of photovoltaic cells integrated with nanolayers increased when compared to cells made from other materials, exceeding 28-30%, which is higher than other materials. Furthermore, the efficiency increased in the summer due to the abundance of solar radiation, and the cells integrated with nanomaterials performed well, achieving high building efficiency.
- ☐ Reliability: Reliability has always been related to performance, stability, and efficiency, which is evidence that the implemented design is more reliable.
- ☐ Performance: The performance of our design was clearly evident, outperforming conventional cells.
- ☐ Lifespan: The nano-coating cells demonstrated excellent protection against high temperatures, the effects of incident light, and high humidity, resulting in a longer lifespan. Thus, the nano-coating ensures stable performance despite seasonal and long-term fluctuations.

3.2. DISCUSSION

- **Impact of Integration:** Simulation and analysis results demonstrate the clear impact of integrating perovskite with polymer nanomaterials on the performance and efficiency of solar cells. The nanopolymer incorporation contributed to enhanced efficiency, stability, and operational lifespan, overcoming many of the limitations of conventional cells.
- **Efficiency:** The cells also demonstrated high power conversion efficiencies, reaching approximately 28–30%, which is higher than those of graphene, polymers, and quantum dots under the same conditions. Due to the integration of perovskite and polymer layers, it reduces recombination losses, facilitates charge movement, and is effective against environmental factors.

It also enhances light absorption, charge transport, and overall performance.

- **Stability and Reliability:** The study showed that the integrated cells maintain stability under various conditions, including temperature, humidity, light, and chemical degradation. This layer acts as a protective barrier, preventing degradation and prolonging the lifespan of the active perovskite layer. Compared to conventional designs, the results demonstrate higher reliability for long-term operation.
- **Comparison with Previous Studies:** The results are consistent with recent studies confirming the advantages of perovskite-polymer composites in solar cell applications. Unlike conventional silicon or quantum dot technologies, these nanomaterials combine high efficiency with environmental safety, allowing the replacement of toxic materials such as lead with safer alternatives. The results also confirm the potential of halide perovskites in photocatalysis and power generation, highlighting their versatility in energy conversion and catalytic applications.
- **Challenges and Future Prospects:** Despite significant performance improvements, challenges remain regarding very long-term stability in harsher environmental conditions. Therefore, further research is recommended to develop advanced encapsulation strategies, use non-toxic materials, and improve polymer-perovskite interfaces. Alternative nanomaterials, or other types of nanochemicals, should be tested to demonstrate their ability to improve performance, efficiency, reliability, and stability. Modern technologies, such as artificial intelligence, can also be incorporated to achieve a paradigm shift in improving and developing these materials to achieve acceptable results.

3.3. FIGURES AND TABLES:

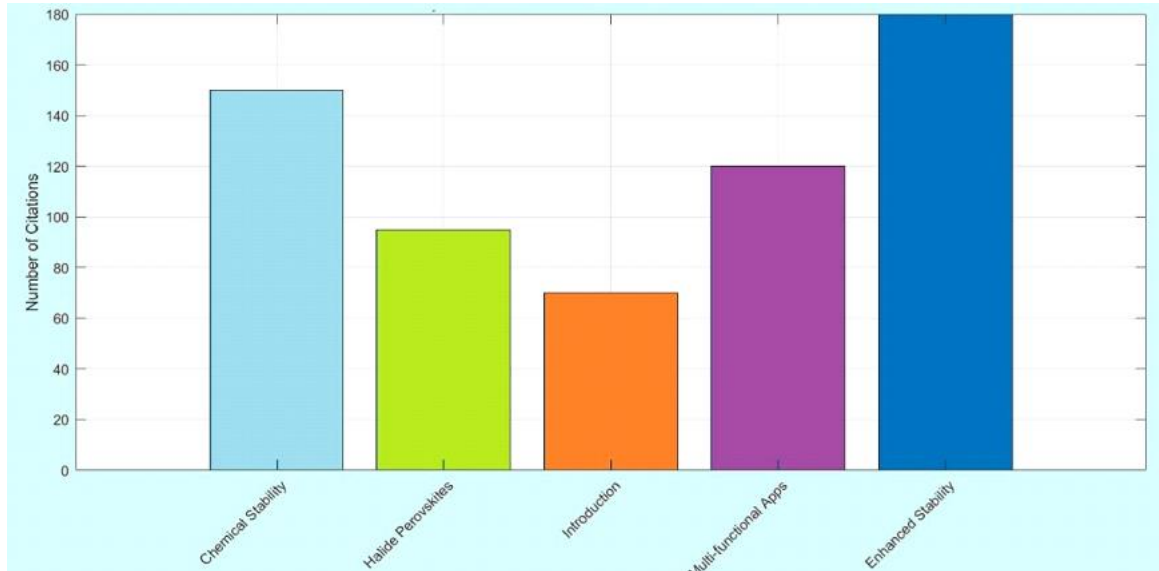


Fig.1. Comparison of the Five Articles Based on Citation Count 2020-2025

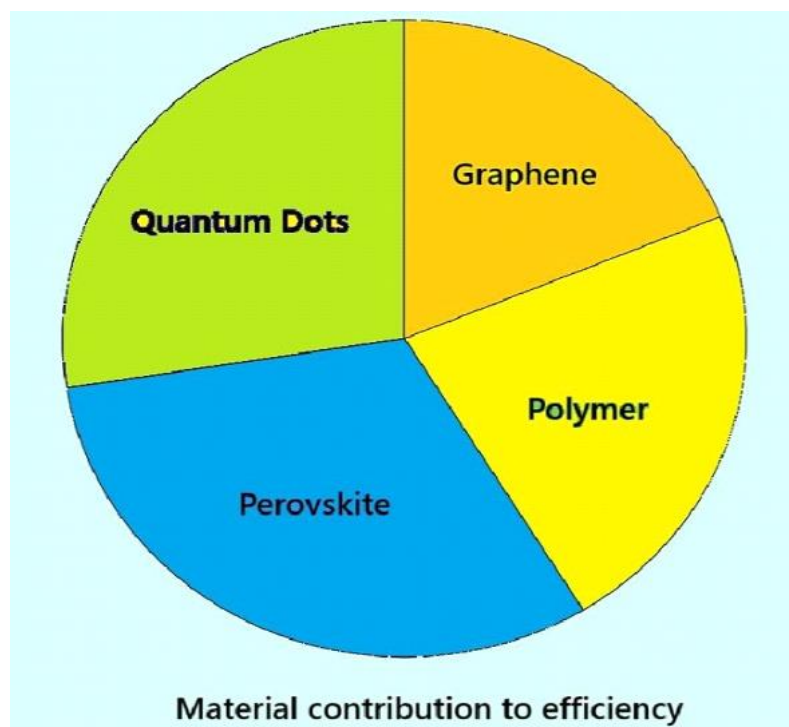


Fig. 2. Contribution of different materials to efficiency.

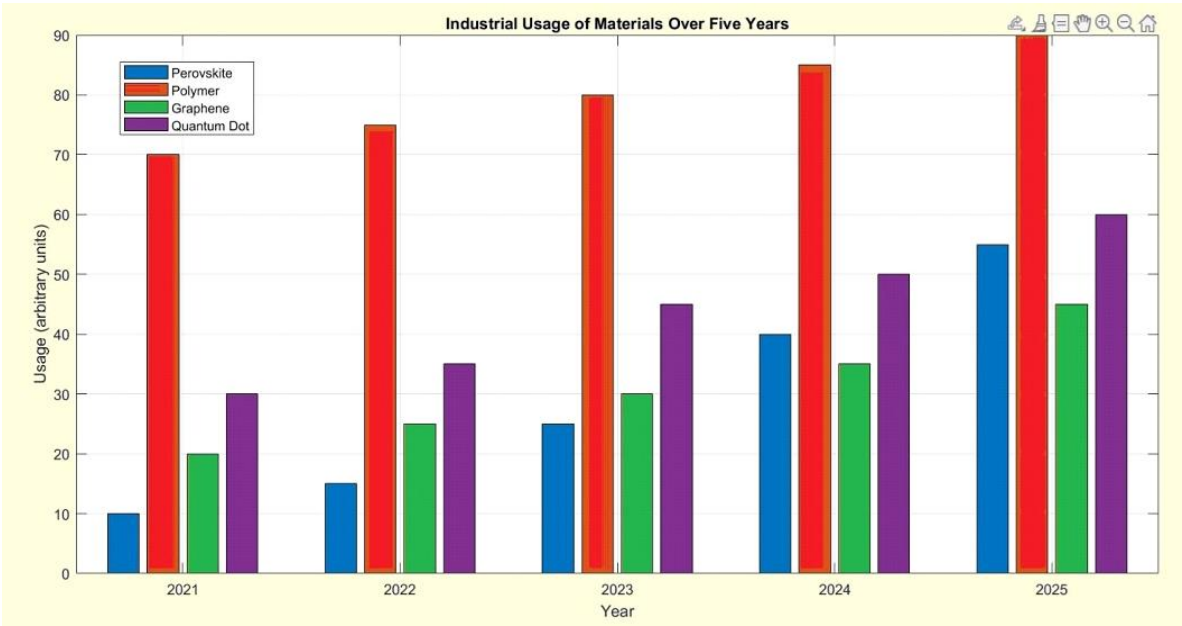


Fig. 3 Use of various materials over the past 5 years

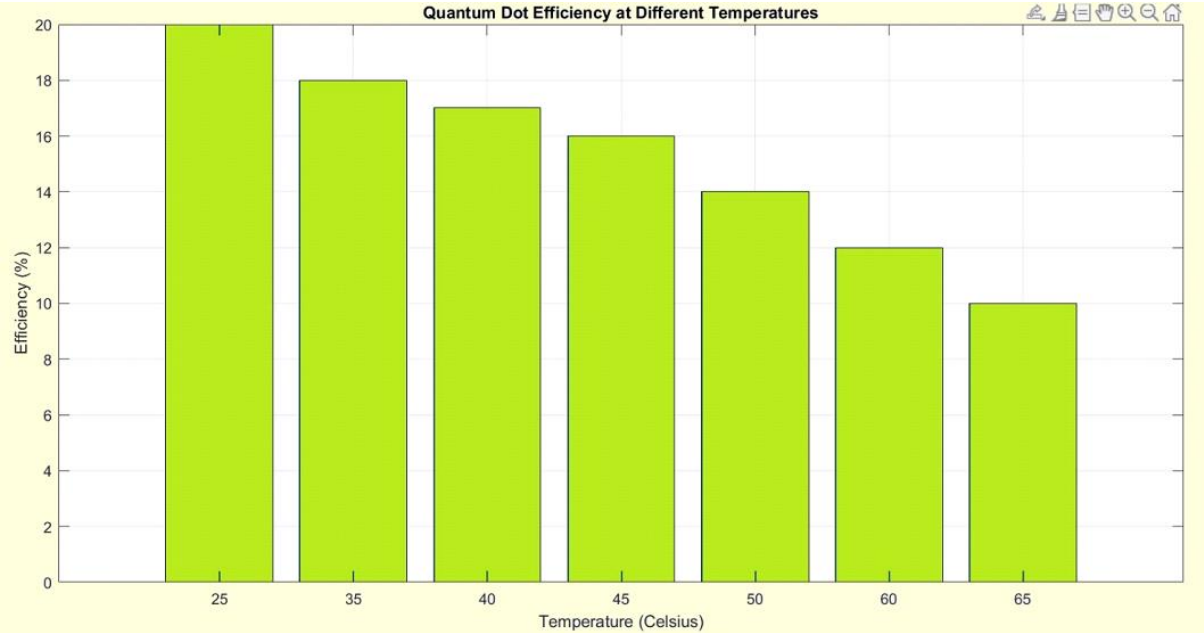


Fig. 4a - The efficiency for QD materials

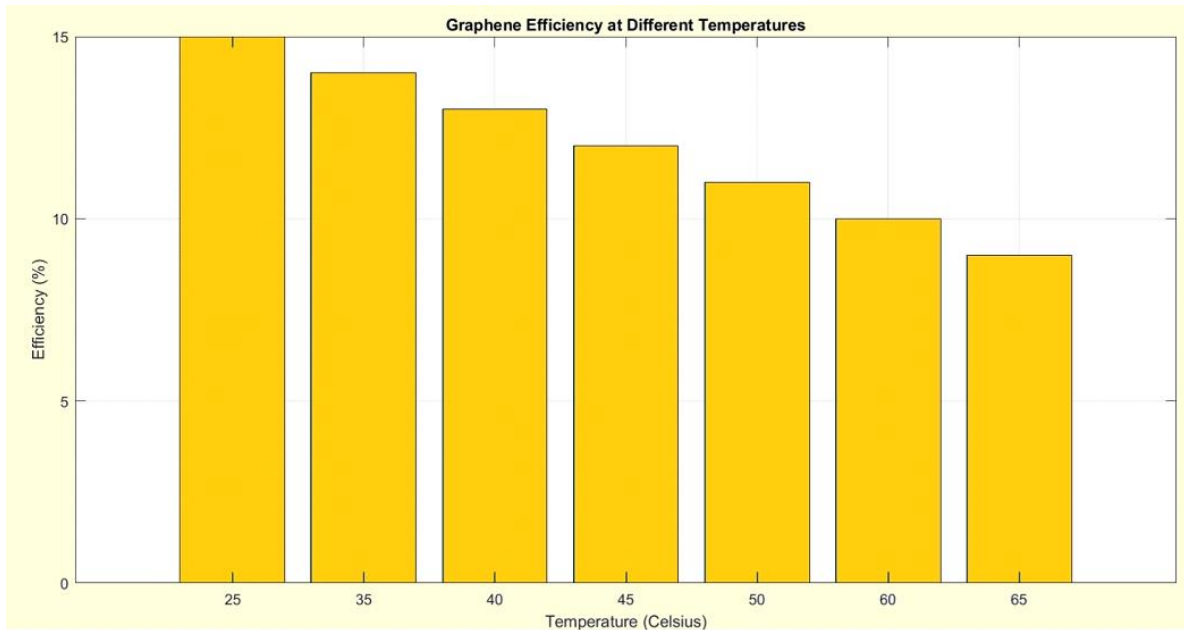


Fig. 4-b- The efficiency for graphene materials

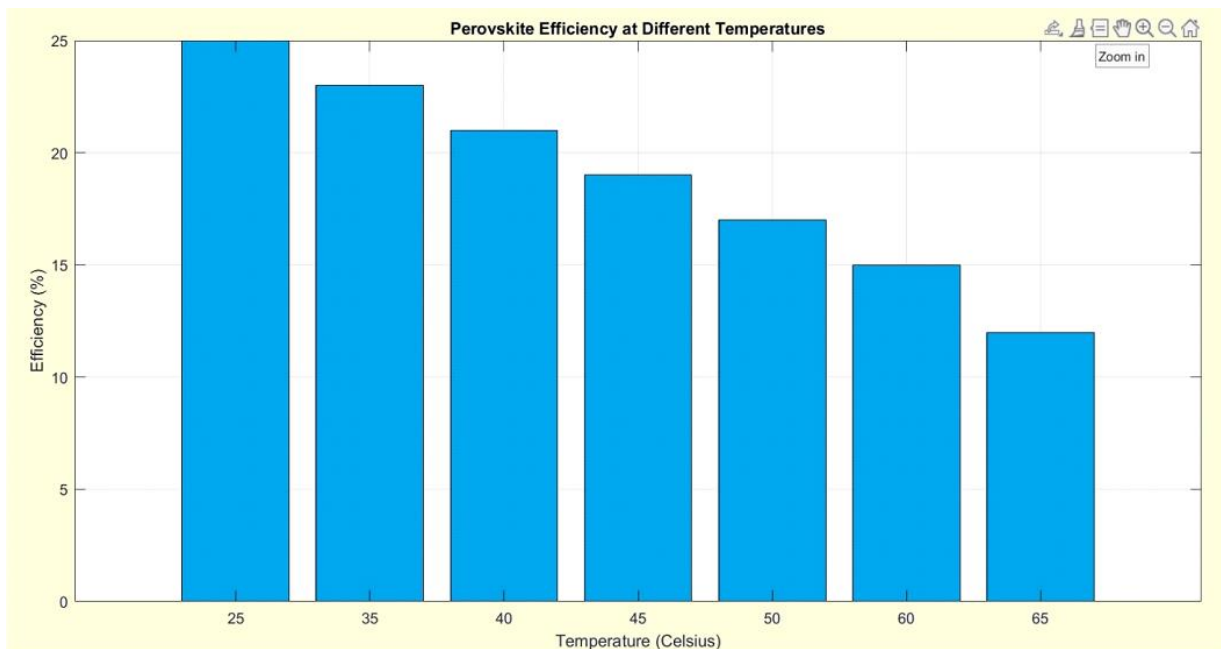


Fig. 4-c- The efficiency for perovskite materials

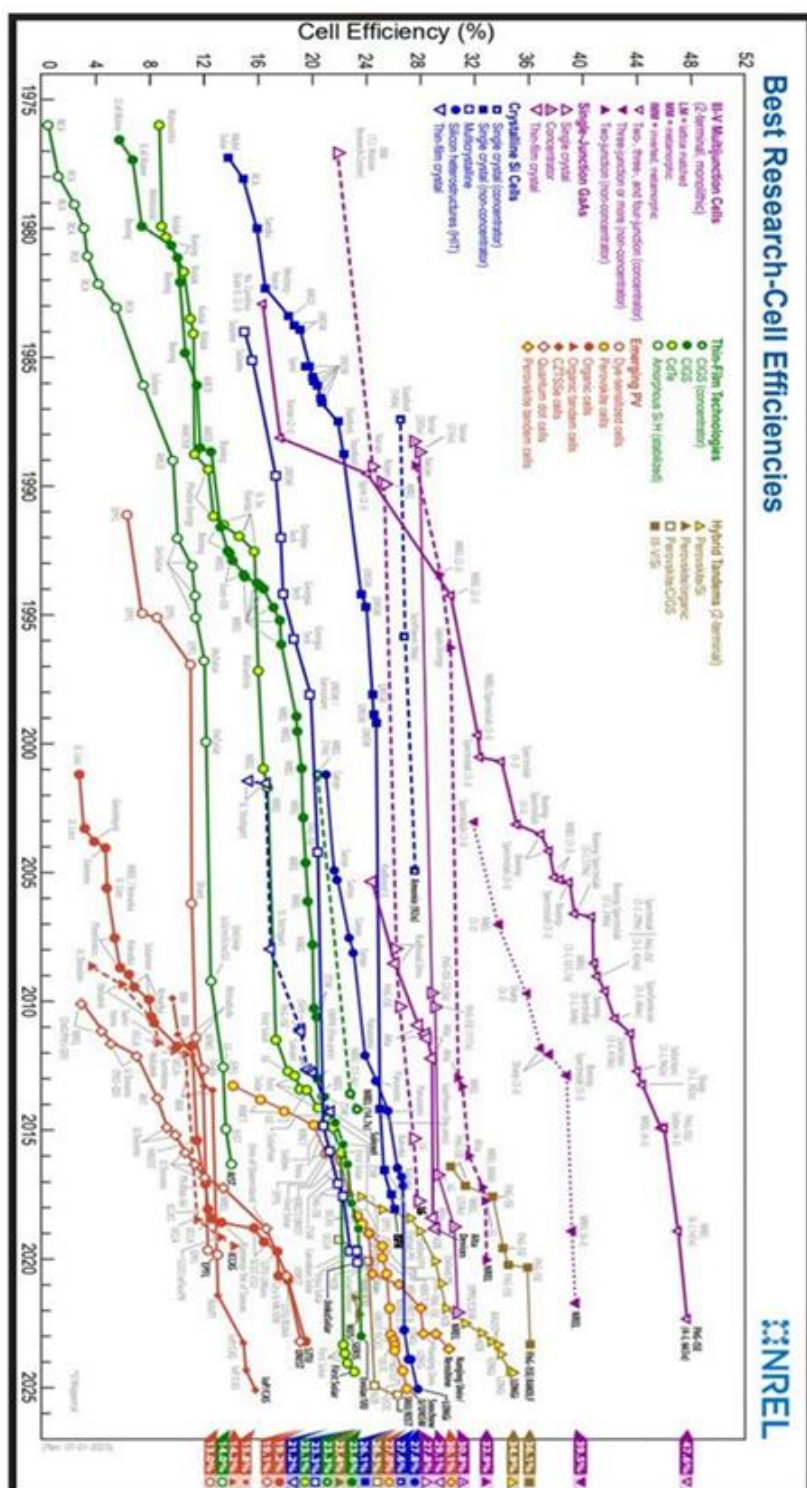


Fig. 5, NREL live diagram

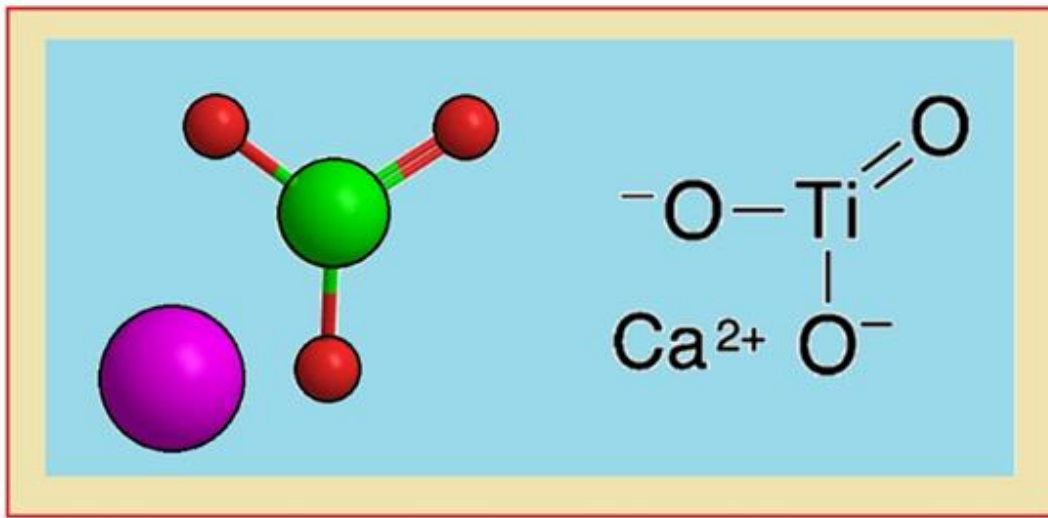


Fig. 6 Perovskite (CaTiO₃) crystals

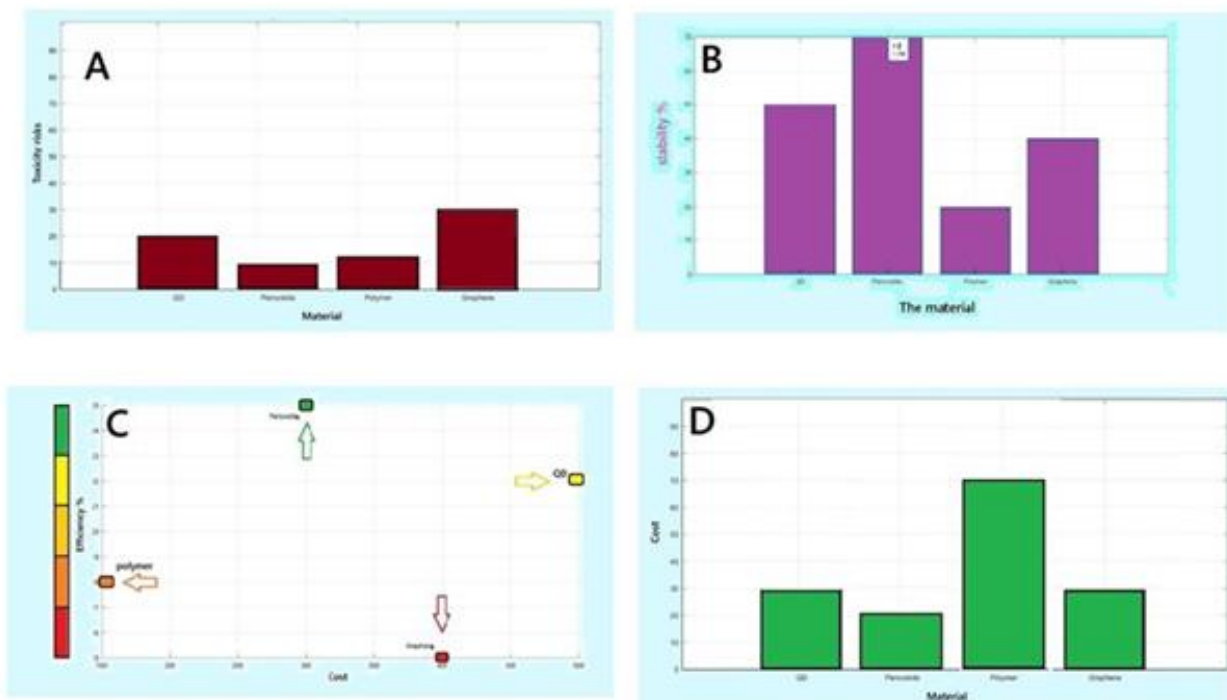


Fig. 7. shows the materials mentioned below: (A- Toxicity and risks, B- Stability, C- Efficiency, D- Cost)

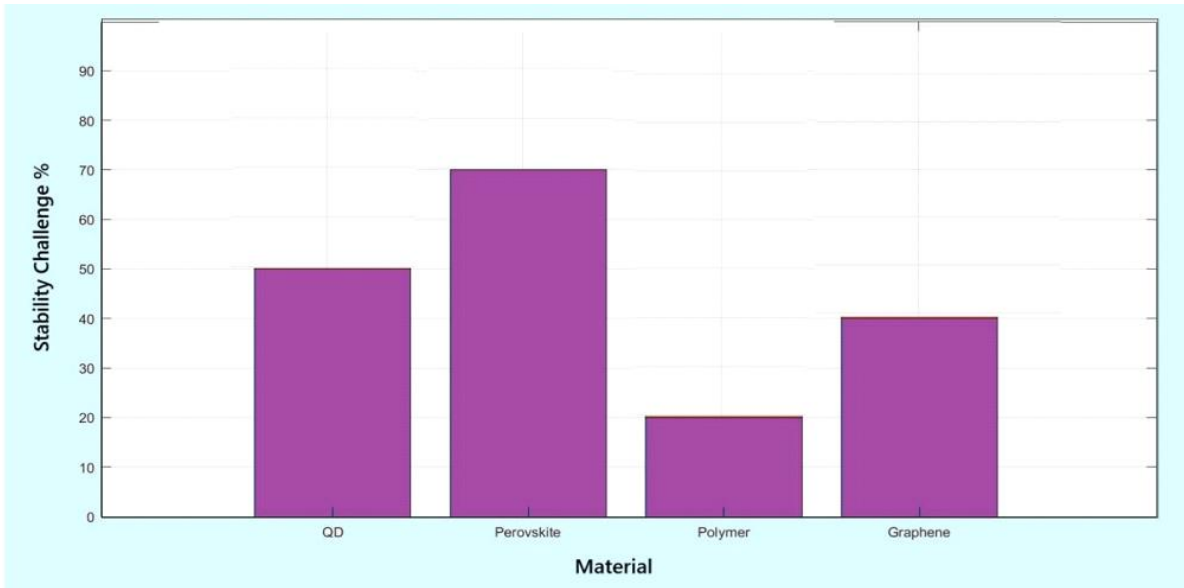


Fig. 8 shows the materials mentioned in CHALLENGER Stability

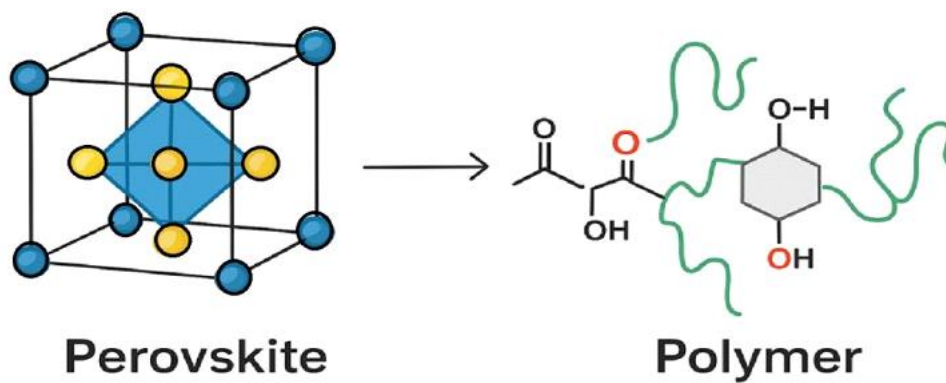


Fig. 9 illustrates the chemical integration of perovskite and polymers

Table 1: Statistical results of solar cell efficiency simulations (perovskite + different materials)

Tempe (°C)	Conventional perovskite ($\eta \pm \sigma$)	Perovskite + polymers ($\eta \pm \sigma$)	Perovskite + graphene ($\eta \pm \sigma$)	Perovskite + QD ($\eta \pm \sigma$)	Perovskite coated with polymers (proposed) ($\eta \pm \sigma$)	%
25	28.5 $\pm$ 0.6	29.1 $\pm$ 0.5	29.3 $\pm$ 0.5	29.0 $\pm$ 0.4	30.2 $\pm$ 0.4	
35	27.9 $\pm$ 0.7	28.6 $\pm$ 0.6	28.8 $\pm$ 0.5	28.5 $\pm$ 0.6	29.8 $\pm$ 0.5	
40	27.4 $\pm$ 0.8	28.2 $\pm$ 0.7	28.4 $\pm$ 0.6	28.1 $\pm$ 0.7	29.5 $\pm$ 0.5	
45	26.8 $\pm$ 0.9	27.7 $\pm$ 0.8	28.0 $\pm$ 0.6	27.6 $\pm$ 0.7	29.1 $\pm$ 0.6	
50	26.1 $\pm$ 0.9	27.1 $\pm$ 0.8	27.5 $\pm$ 0.7	27.0 $\pm$ 0.8	28.7 $\pm$ 0.7	
60	25.3 $\pm$ 1.0	26.3 $\pm$ 0.9	26.8 $\pm$ 0.8	26.2 $\pm$ 0.8	28.1 $\pm$ 0.7	
65	24.8 $\pm$ 1.1	25.9 $\pm$ 1.0	26.3 $\pm$ 0.9	25.7 $\pm$ 0.9	27.7 $\pm$ 0.8	

Note: η represents the average efficiency (%), and σ represents the standard deviation.

Table 2: Performance before and after consolidation at different temperatures (25-65 °C)

PCE (%) before <u>Timp</u>	Perovskite+Polymer	Graphene	Polymer	Multi-materials
25	31.308	26.698	18.525	23.8
35	30.764	26.301	18.245	23.427
40	30.493	26.104	18.105	23.242
45	30.224	25.907	17.966	23.057
50	29.955	25.711	17.828	22.873
60	29.422	25.321	17.552	22.507
65	29.157	25.127	17.416	22.325
PCE after <u>Timp</u>	Perovskite+Polymer	Graphene	Polymer	Multi-materials
25	34.433	26.698	18.525	23.8
35	33.841	26.301	18.245	23.427
40	33.547	26.104	18.105	23.242
45	33.254	25.907	17.966	23.057
50	32.963	25.711	17.828	22.873
60	32.383	25.321	17.552	22.507
65	32.095	25.127	17.416	22.325

4. CONCLUSIONS

To improve the stability, performance, and efficiency of photovoltaic cells, we utilized perovskite, a chemical material distinguished by its unique chemical and physical properties in terms of absorption and charge transfer.

- ☐ The cells were treated by incorporating a Nano polymer and coating the perovskite to extend their lifespan, as the pure perovskite material is sensitive to relative humidity.
- ☐ This combination was proven through real simulations under varying conditions, factors, and climates.
- ☐ This confirms the effectiveness of the proposed integrated layer, which is expected to provide a tangible performance improvement.

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