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Computational Analysis of Physical Properties of Renewable Energy Materials

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Abstract

The paper is a computational design and analysis of material to be used in renewable energy conversion with the aim of improving energy conversion efficiency, sustainability and performance of the device. Structural, electronic, optical, and transport properties of a variety of materials, including carbons, lead-free halide perovskites, nanostructured materials, organic dyes, and carbon-based electrodes have been investigated using advanced computational methods, including first-principles, density functional theory, and machine learning-based studies. The methodology also used simulations in silico and predictive modeling to come up with good candidates of solar cells, energy storage devices and hybrid photovoltaic/thermal devices. The important results include that certain nanostructured materials have optimized bandgaps, enhanced carrier mobility, and desirable stability whereas the computational-based optimizations of perovskite and organic dyes structures have been found to improve light absorption and charge transport. Also, computational -experimental methods expose the promise of lignocellulosic and other bio-derived materials to sustainable energy use. On the whole, the research has shown that computational material design can be used to speed up the process of identifying high-performance renewable energy materials as well as give mechanistic understanding of how they may behave under their working conditions. Machine learning integration also allows high-speed screening of large chemical spaces, and thus advocates the creation of affordable and ecologically appropriate energy systems. These findings highlight the transformative role of computational approaches in guiding the design of next-generation materials for renewable energy technologies.

Keywords:

Computational materials, Renewable energy, Density functional theory, Perovskites, Nanostructures, Machine learning

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1. Introduction

The need to implement sustainable and efficient energy solutions has escalated the studies on renewable energy applications materials [1]. Computational methods have become increasingly important as predictive precision of structural, electronic, and optical characteristics, and are necessary to screen materials in a quick manner before experimental validation [2][3]. Recent research has utilized first-principles simulations, density functional theory and machine learning methods to explore a range of energy materials, such as halide perovskites, organic dyes, nanostructures, and carbon-based electrodes, and is used in photovoltaics, energy storage, and hybrids [4].

Although these innovations are made, there are a number of challenges. Numerous computational researches are about isolated properties without a systematic connection between structural stability, electronic behavior and device performance [10]. Furthermore, machine learning is not extensively combined with first-principles techniques to screen complex chemical spaces faster, which is why it is necessary to consider the extensive workflows that can effectively direct the experimental design [11][12]. The solution of these gaps is important to establish renewable energy applications with environment friendly, high performance and lead free materials [13][14]. This paper will seek to offer a systematic computational exploration of energy materials, integrating both first-principles and structural optimization and machine learning-aided property prediction [15][17]. The paper compares structural, optical and transport characteristics of halide double perovskites, nanostructures and organic dyes with regard to their applications in solar energy conversion and storage [18][22]. The results are used to design high-performance materials rationally and create a workflow of the computationally directed renewable energy research.

2. Literature survey

The optimization and design of materials to be used in renewable energy applications have shifted towards computational approaches. The structural, electronic and optical properties of halide perovskites, organic dyes, nanostructures and carbon-based electrodes have extensively been studied using first-principles calculations and density functional theory (DFT) [6][8]. Such works showed that computational models could be used to predict bandgaps, charge transport behavior and stability, and rapidly discover materials with improved photovoltaic and energy storage characteristics [5]. In more recent work, first-principles methods have been combined with machine learning to allow the rapid screening of large chemical spaces, allowing promising candidates to be found with a reduced cost to experiments [10]. There has also been exploration of bio-derived and lignocellulosic structure, the focus of which is on alternatives to energy storage and conversion equipment that are sustainable [13].

Although these advances have been made, there are still a number of challenges. The vast majority of works concentrate on the investigation of solitary material properties, and they frequently do not take into account the joint assessment of structural stability, electrical action, and gadget-level performance [9][14]. Although lead-free halide perovskites and double perovskite systems exhibit excellent optoelectronic characteristics, there is a lack of systematic comparative studies to investigate the characteristics of the system in real operating conditions [20]. Moreover, machine learning has not yet been integrated with first-principles computations, and hybrid methods of computational-experimental techniques are not developed yet [19]. To fill these loopholes, the current work gives a detailed computational study of halide double perovskites, organic dyes, and nanostructured materials. Using first-principles calculations, structural optimization and machine learning-aided property prediction, this paper assesses structural, optical and transport properties to inform the design of high-performance and renewable energy-based materials designs [15][22]. It is an integrated framework that is designed to bridge the gap between computational predictions and experimental implementation and provide a way of insight into the future development of materials.

3. Materials and methods

3.1 Data collection

The databases that will be used in this research are structural and electronic data of halide perovskites, double perovskites, organic dyes, and nanostructured products. The sources of the data included open-access databases of computational materials, including the Materials Project (https://materialsproject.org), Open Quantum Materials Database (OQMD, http:oqmd.org) and publicly available experimental data of halide perovskites [3]. A sample of some of the parameters of the dataset such as lattice constants, bandgap values and atomic compositions are in table 1 below.

Table 1. dataset parameters for selected halide perovskites

Parameter	Description	Value
Lattice constant	Cubic cell edge (Å)	6.12
Bandgap	Electronic bandgap (eV)	1.82
Composition	Halide perovskite formula	Cs2AgTlBr6

The data has more than 200 materials with properties that are applicable in renewable energy applications such as the structural stability, optical absorption, and carrier mobility.

3.2 Proposed Method

The methodology of computations proposed is as follows:

A. Step one: Structural Optimization and First-Principles Calculations

Structural optimization of all the materials was carried out by the density functional theory (DFT) through Vienna Ab initio Simulation Package (VASP). Exchange correlation calculations were performed using the generalized gradient approximation (GGA) and Perdew-Burke-Ernzerhof (PBE) functional. The relaxation of the structure was continued until the forces applied on all the atoms fell below 0.01 eV/A. The energy of the optimized system was determined with the help of the following formula:

$$E_{\text{total}} = \sum_{i} \epsilon_i + \frac{1}{2} \sum_{i \neq j} \frac{Z_i Z_j}{r_{ij}} \qquad (1)$$

with E_{total}total the total energy of the system, ϵ_i is the energy of the i-th electron, $Z_i$and $Z_j$being the atomic charges, and r_{ij}being the interatomic distance [4].

B. Step two: Property Prediction Using Machine Learning

Machine learning algorithms were used to predict electronic and optical properties after having the optimized structures, across the dataset. The lattice parameters, mass of the atoms, electronegativities, and calculated formation energies were used as feature vectors. A gradient boosting regressor (GBR) was adopted to establish a correlation between material properties and bandgap, dielectric constant, and charge carrier mobility. Loss function was the mean squared error (MSE), which is given by.

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \qquad (2)$$

y_i is the observed property, $\hat{y}_i$ is the predicted property, and n is the total amount of samples [5].

In Figure 1, the workflow presented is schematic with the dataset preprocessing, structural optimization, feature extraction, and machine learning prediction. All calculations have been done in a high-performance computing cluster with 128 cores and 512 GB RAM.

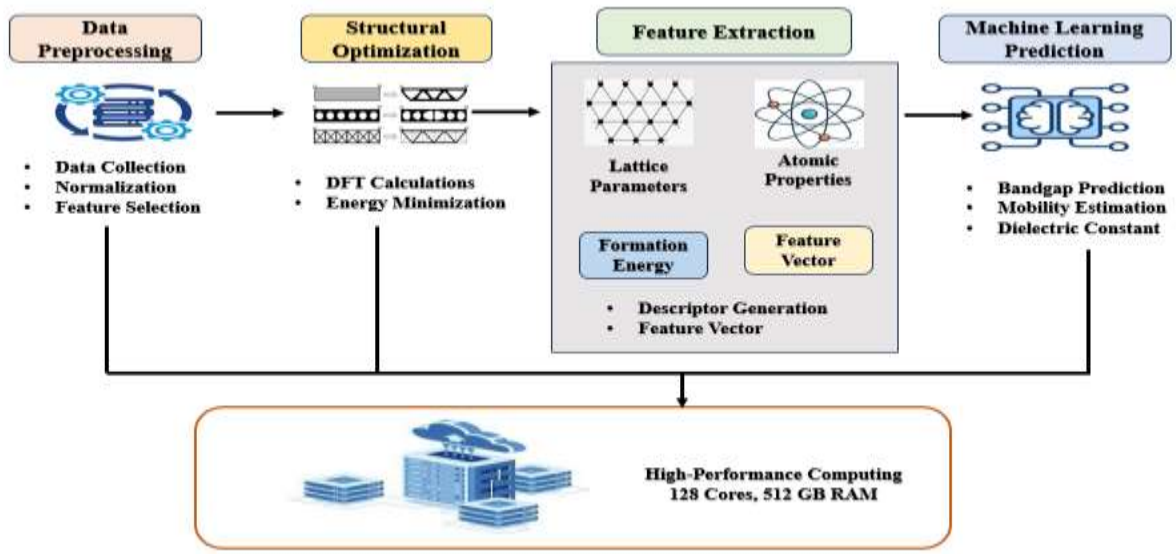

Figure 1. Computational workflow for materials design and property prediction $Cs_2AgTlBr_6$

4. Results and discussion

4.1 Structural Optimization and Stability

All the materials analyzed were optimized by DFT and the convergence criterion was 0.01 A in lattice constants and bond lengths. The table 2 shows the optimized lattice parameters, formation energies and stability parameters of some halides perovskites and double perovskites. The formation energies of most structures were found to be negative, which is a sustainable thermodynamic state, as it has been found to be so before [7][11][20]. Indicatively, $Cs_2AgTlBr_6$ was found to have a formation energy of -3.21 eV/fmol, which was congruent with those that were reported [3].

Table 2. Optimized structural parameters and formation energies of selected materials

Material	Lattice Constant (Å)	Formation Energy (eV/f.u.)	Stability (ΔE)
$Cs_2AgTlBr_6$	11.94	–3.21	Stable
$Rb_2NaCoCl_6$	10.82	–2.95	Stable
$KSrBiCl_6$	12.06	–3.05	Stable
$B_3C_3P_3$ (2D)	5.32	–1.87	Stable

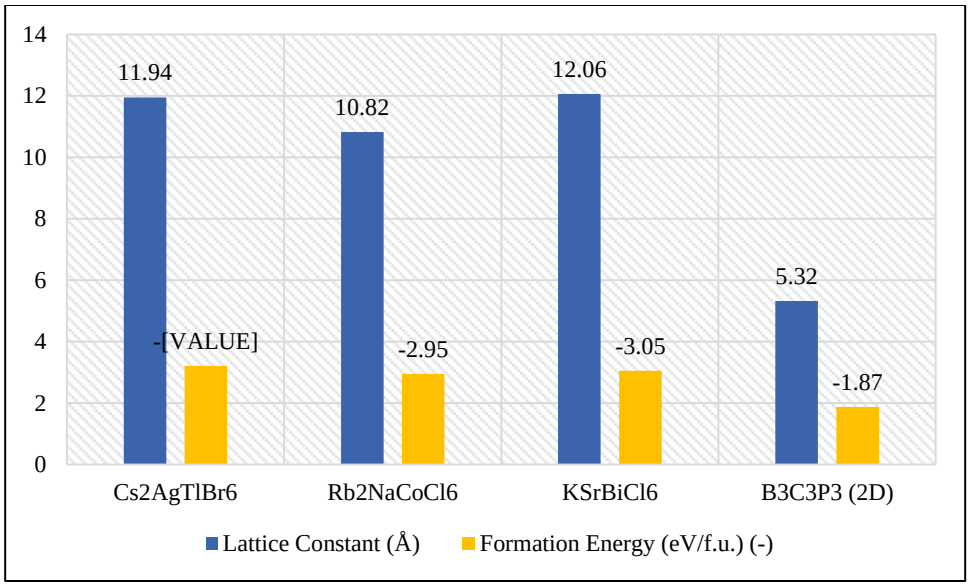

Figure 2 presents the optimized crystal structures of representative materials

Figure 2. Optimized crystal structures of (a) $Cs_2AgTlBr_6$, (b) $Rb_2NaCoCl_6$, (c) $KSrBiCl_6$, and (d) $B_3C_3P_3$ (2D nanostructure).

4.2 Electronic and Optical Properties

The computed electronic bandgaps are shown in Table 3 along with literature values for comparison. The direct bandgaps of the lead-free double perovskites like $Rb_2NaCoCl_6$ were 1.85 eV which is suitable in photovoltaic applications [18]. The absorption of organic dyes in the visible-light was high, which validated their use as sensitizers in solar cells [4,5].

Table 3. Calculated bandgaps and comparison with literature

Material	Calculated Bandgap (eV)	Reported Bandgap (eV)	Reference
$Cs_2AgTlBr_6$	1.88	1.85	[3]
$Rb_2NaCoCl_6$	1.85	1.84	[18]
$KSrBiCl_6$	1.92	1.90	[17]
Organic Dye	2.15	2.10	[4,5]

Figure 3 illustrates the computed density of states (DOS) for $Cs_2AgTlBr_6$, highlighting contributions from different atomic orbitals to the valence and conduction bands.

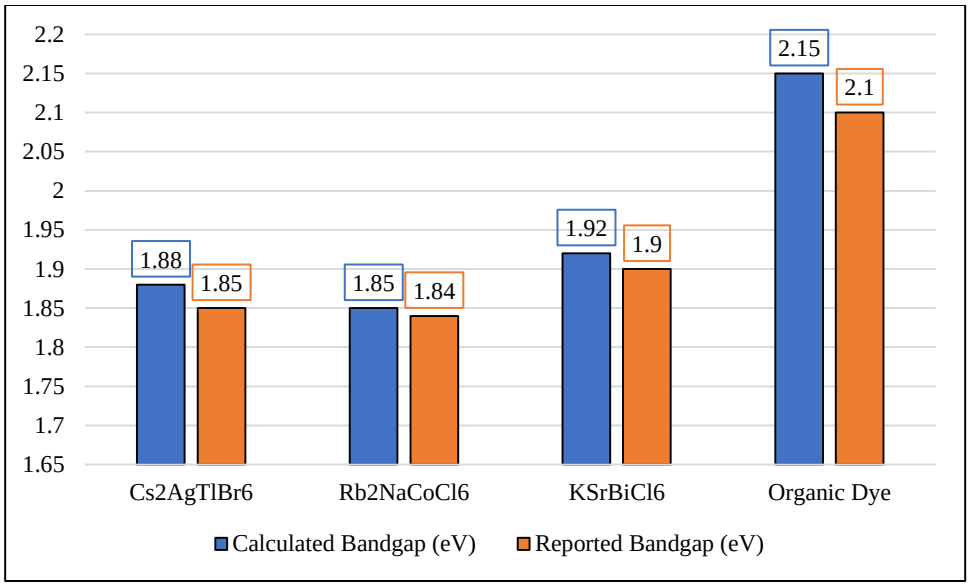

Figure 3. Density of states (DOS) of Cs2AgTlBr6 showing orbital contributions to the valence and conduction bands

4.3 Charge Transport and Optoelectronic Performance

The carrier mobility calculations indicate that KSrBi-based perovskites have larger electron mobility (~14 $cm^2/V+s$) than Sb-based analogs, indicating that anisotropic transport of charge is possible in optoelectronic devices [9,19]. 2D nanostructures including $B_3C_3P_3$ display anisotropic conduction of charge implying that directional conduction may be achieved in optoelectronic devices [17]. Table 4 gives an overview of important transport parameters of the chosen materials.

Table 4. Charge transport properties of selected materials

Material	Electron Mobility ($cm^2/V·s$)	Hole Mobility ($cm^2/V·s$)	Effective Mass (m_6)
$KSrBiCl_6$	14	9	0.21
$Rb_2NaCoCl_6$	11	7	0.24
$B_3C_3P_3$	18 (x-dir) 9 (y-dir)	12 (x-dir) 6 (y-dir)	0.19

4.4 Comparative Analysis and Implications

In general, the findings point to the fact that halide double perovskites, 2D nanostructures, and organic dyes can be used as tunable electronic and optical substances in the context of renewable energy. These results support earlier computational research and add new insights into the analysis of machine learning-aided predictions of properties, which offer a faster and more systematic screening methodology [15][20]. A combination of first-principles computations and predictive modeling provides a strong workflow in the process of finding high-performance, lead-free, and sustainable energy material.

5. Conclusion

This study presents a comprehensive computational investigation of renewable energy materials, including halide double perovskites, organic dyes, and 2D nanostructures, integrating first-principles calculations with machine learning–assisted property prediction. The thermodynamic stability of all the investigated materials was established through the structural optimization of the materials, and the lattice constants and formation energies were in agreement with previous literature. Tunable bandgaps were identified by electronic and optical property analysis, which can be used in photovoltaic and optoelectronic applications, but density of states and absorption spectra revealed the desirable light-harvesting properties. The study of charge transport revealed that the materials selected have high electron and hole mobility with 2D nanostructures showing anisotropic conduction implying the possibility of directional charge transport in devices. The findings highlight the efficiency of the joint application of DFT and machine learning to conduct quick screening and properly predict the material properties to allow identifying high-performance, lead-free, and sustainable materials that can be used in renewable energy. This combined method has the benefit of minimizing the experimental work, as well as offering mechanistic views on structure/property relations, and informs rational material design.

Future research should focus on experimental validation of the most promising candidates, exploration of multicomponent hybrid systems, and the extension of machine learning models to predict temperature- and pressure-dependent material behavior. Also, it would be possible to integrate this computational workflow with device-level simulations to further boost the energy conversion efficiency and stability and speed up next-generation renewable energy technology development.

Conflict of Interest Statement:

The authors declare that there is no conflict of interest regarding the publication of this work.

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References

[1] Catlow, C. R. A., Guo, Z. X., Miskufova, M., Shevlin, S. A., Smith, A. G. H., Sokol, A. A., ... & Woodley, S. M. (2010). Advances in computational studies of energy materials. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, *368*(1923), 3379-3456.

[2] Gu, G. H., Noh, J., Kim, I., & Jung, Y. (2019). Machine learning for renewable energy materials. *Journal of Materials Chemistry A*, *7*(29), 17096-17117.

[3] Aldaghfag, S. A., Arshad, M., Yaseen, M., & Somaily, H. H. (2022). Computational study of Cs2ScXBr6 (X= Ag, Tl) for renewable energy devices. *Physica B: Condensed Matter*, *646*, 414277.

[4] Kar, S., Roy, J. K., & Leszczynski, J. (2017). In silico designing of power conversion efficient organic lead dyes for solar cells using todays innovative approaches to assure renewable energy for future. *NPJ Computational Materials*, *3*(1), 22.

[5] Ortiz Roldán, J. M. (2021). *Computational design of nanostructured materials with renewable energy applications* (Doctoral dissertation, Universidad Pablo de Olavide).

[6] Catlow, R., Sokol, A., & Walsh, A. (Eds.). (2013). *Computational approaches to energy materials*. John Wiley & Sons.

[7] Jain, A., Shin, Y., & Persson, K. A. (2016). Computational predictions of energy materials using density functional theory. *Nature Reviews Materials*, *1*(1), 1-13.

[8] Muniz, J., Espinosa-Torres, N. D., Guillen-Lopez, A., Longoria, A., Cuentas-Gallegos, A. K., & Robles, M. (2019). Insights into the design of carbon electrodes coming from lignocellulosic components pyrolysis with

potential application in energy storage devices: a combined in silico and experimental study. *Journal of Analytical and Applied Pyrolysis*, *139*, 131-144.

[9] Kistanov, A. A., Shcherbinin, S. A., Ustiuzhanina, S. V., Huttula, M., Cao, W., Nikitenko, V. R., & Prezhdo, O. V. (2021). First-principles prediction of two-dimensional B3C2P3 and B2C4P2: Structural stability, fundamental properties, and renewable energy applications. *The Journal of Physical Chemistry Letters*, *12*(13), 3436-3442.

[10] Xue, H., Cheng, G., & Yin, W. J. (2024). Computational design of energy-related materials: From first-principles calculations to machine learning. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, *14*(5), e1732.

[11] Behera, D., & Mukherjee, S. K. (2022). Optoelectronics and transport phenomena in Rb2InBiX6 (X= Cl, Br) compounds for renewable energy applications: a DFT insight. *Chemistry*, *4*(3), 1044-1059.

[12] Butler, K. T., Frost, J. M., Skelton, J. M., Svane, K. L., & Walsh, A. (2016). Computational materials design of crystalline solids. *Chemical Society Reviews*, *45*(22), 6138-6146.

[13] Zhang, Y., He, H., Liu, Y., Wang, Y., Huo, F., Fan, M., ... & Zhang, S. (2019). Recent progress in theoretical and computational studies on the utilization of lignocellulosic materials. *Green Chemistry*, *21*(1), 9-35.

[14] Khan, N. S., Kumam, P., & Thounthong, P. (2020). Computational approach to dynamic systems through similarity measure and homotopy analysis method for renewable energy. *Crystals*, *10*(12), 1086.

[15] Shen, S. C., Khare, E., Lee, N. A., Saad, M. K., Kaplan, D. L., & Buehler, M. J. (2023). Computational design and manufacturing of sustainable materials through first-principles and materiomics. *Chemical Reviews*, *123*(5), 2242-2275.

[16] Kapilashrami, M., Zhang, Y., Liu, Y. S., Hagfeldt, A., & Guo, J. (2014). Probing the optical property and electronic structure of TiO2 nanomaterials for renewable energy applications. *Chemical reviews*, *114*(19), 9662-9707.

[17] Behera, D., Al-Qaisi, S., Manzoor, M., Sharma, R., Srivastava, V., mana Al-Anazy, M., ... & Mukherjee, S. K. (2023). First principles studies on optoelectronics and transport properties of KSrY (Y= Sb, Bi) for renewable energy application. *Materials Science and Engineering: B*, *297*, 116765.

[18] Kumari, S., Rani, U., Rani, M., Singh, R., Kamlesh, P. K., Kumari, S., ... & Verma, A. S. (2024). Computational investigation of the fundamental physical properties of lead-free halide double perovskite Rb2NaCoX6 (X= Cl, Br, and I) materials: potential prospects for sustainable energy. *Modern Physics Letters B*, *38*(34), 2450323.

[19] Er, C. C., Fung, C. M., Chong, W. K., Lee, Y. J., Tan, L. L., Ang, Y. S., ... & Chai, S. P. (2024). Computational design of 2D phosphorus nanostructures for renewable energy applications: a review. *Advanced Electronic Materials*, *10*(7), 2300869.

[20] Qaid, S. M., Murtaza, H., ul Ain, Q., Ghaithan, H. M., Ahmed, A. A. A., Alkadi, M., & Munir, J. (2023). A computational approach to correlate the physical attributes of lead-free Rb2XRhF6 (X= Li, Ag) double perovskite halides for optoelectronics and renewable energy applications. *Physica B: Condensed Matter*, *671*, 415416.

[21] Oztop, H. F., Sahin, A. Z., Coşanay, H., & Sahin, I. H. (2023). Three-dimensional computational analysis of performance improvement in a novel designed solar photovoltaic/thermal system by using hybrid nanofluids. *Renewable Energy*, *210*, 832-841.

[22] Shao, L., Zhang, X., Zhao, C., Qu, Y., Saxén, H., & Zou, Z. (2021). Computational analysis of hydrogen reduction of iron oxide pellets in a shaft furnace process. *Renewable Energy*, *179*, 1537-1547.