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Design and simulation of perovskite solar cells with ZnO and graphene

Abstract

Today, the need for primary and secondary energies is always increasing to meet the energy needs of mankind. In recent years, solar cells have been used as an alternative to produce renewable, sustainable, and pollution-free energy. Various materials have been used as the transfer layer in cells. TIO2 is one of these materials that has been widely used as the electron transfer layer, but currently, ZnO is another significant material. is more recently used than TIO2. Also, perovskite solar cells are the new generation of solar cells that belong to the nano family. Currently, perovskite solar cells (PSC) as a promising cell in the electronics industry, due to the high power conversion efficiency, as well as the relatively lower cost of manufacturing a silicon solar cell, and such high flexibility that leads to the use of Perovskite is on different types of substrates. Also, the use of graphene as the most important fundamental photovoltaic material for photovoltaic energy conversion has emerged and been used. Graphene is used as a transparent electrode, as an active layer between layers, as an electron and hole transfer layer, or as an electron and hole separator layer in the construction of solar cells. In this article, the goal is to find the best structure with the highest power conversion efficiency in solar cells, and we will see further that by using perovskite, ZnO, and graphene, we will achieve a power conversion efficiency of 16% with a low manufacturing cost.

Keywords: *solar cell; perovskite; simulation; ZnO graphene;*

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Introduction

Global warming caused by the high emission of carbon dioxide and the effects of greenhouse gases is one of the main concerns of humans today(Wang et al., 2022). Carbon oxide in the atmosphere traps the heat reflected from the earth's surface into the atmosphere as a strong aura and as a result makes the earth warmer. In the past decades, continuous efforts have been made in the field of geology and carbon dioxide capture. However, efforts in this field require spending more energy(Shin et al., 2022; Steele et al., 2022; Tarasova et al., 2022). Through research and reports, it has been determined that by 2050, the global energy demand will double with the rapid growth of population and the industrialization of countries, especially in developing countries. Hence, the development of renewable energies without the use of fossil fuels such as thermal wind solar cells, biomass, and hydro-electricity is widely have been studied at global levels. Solar energy is considered a clean energy source. However, the manufacturing cost, size, stability, reproducibility, and high-power conversion efficiency of solar cells are considered an effective approach to improving solar cells(Yamada & Kanemitsu, 2022). A solar cell or photovoltaic cell is a solid state electronic component. which converts a percentage of sunlight energy directly into electricity by the photovoltaic effect, which is a physical and chemical phenomenon. In the past years, various types of solar cells with different functions and structures have been designed and manufactured. The name perovskite is derived from the mineral structure $CaTiO_3$, which was discovered by a German mineralogist named Gustav Rose in 1839. It was proposed in 1792-1856 and he chose the name perovskite for this material, which was often considered a promising material for future generations of solar cells the first halogen-based perovskite structure in cesium halide ($CsPbX_3$) was observed by Moller in 1958, and the conductivity characteristics were adjusted and changed by changing the halogen components to achieve different spectral responses(Lee et al., 2021; H. Xu et al., 2022). The first appearance of organic cation in halogenated perovskite was proposed and developed for I, CL, and Br by Messrs. Weber and Naturforsch in 1978 Perovskite in photovoltaics began its work in 2001 when Miyasaka and his colleagues used $CH_3NH_3PbBr_3$ as a sensitizer. began to be applied on TiO_2 for dye-sensitized solar cells, which reached a power conversion efficiency of 2.2% In 2011, Mr. Park and his colleagues used perovskite nanostructures on TiO_2 as a sensitizer and achieved a power conversion gain of 1.8% to improve absorption performance on conventional dyes. Also, the use of zinc oxide in solar cells has been the focus of researchers in the last decade. The important advantages of ZnO include very good electrical, optical, and mechanical properties, as well as important chemical properties, including thermal stability, and also due to its high availability in the environment, it is widely used for a wide range of practical applications such as sensors. It is used as gas, catalysts, liquid crystal display panels, electronic photodiodes, solar cells, and also as an electrode(Abadi et al., 2019; S. Liu et al., 2022). It should be noted that the most important advantage of zinc oxide is its very low cost compared to other types of materials. For example, in 2015, a perovskite solar cell was made based on ZnO nanorods. ZnO nanorods were grown through the ZnO seed layer in the solution, and the thickness and length of these nanorods were controlled by changing the concentration of the solution and the growth time(Xie et al., 2009). In this method, with perovskite penetration into ZnO nanotubes, the power conversion efficiency reached 11.13%. In this method, by fully comparing the spectral response of ZnO nanorods with TiO2 nanorods, the importance of using ZnO nanorods instead of TiO2 has been considered due to the much higher current concentration in perovskite solar cells based on ZnO nanorods. Also, the assembly of charges in this structure is much faster and more than in the TiO2 structure(Ehtesham et al., 2016; Tabi et al., 2022; Tritt et al., 2008). Due to their unusual electronic properties, graphene-based nanomaterials have led to much research in the field of photovoltaic energy conversion in the last two decades. Following the first discovery of graphene in 1985 by Buckminsterfullerene, the separation of graphene by exfoliation of graphite in 2004 led to many advances in fundamental and applied physics. Since then, graphene has been widely investigated in a wide variety of applications in electronics, photonics, energy-related devices, and sensors. In Figure 1, you can see the trend of research and articles published in the field of graphene, and as it is clear, the use of graphene in articles is increasing day by day(Qu et al., 2021).

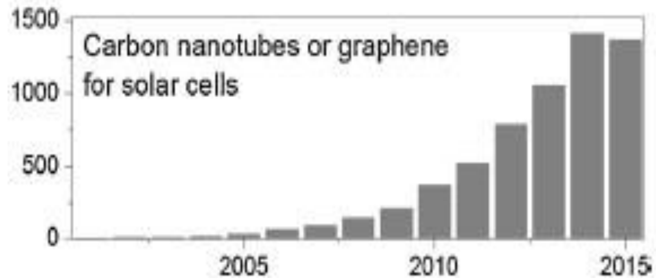

Figure 1. Number of articles published in the field of graphene

Research Methods:

The solar cell structure is designed as shown in Figure 2 and as you can see, a thin layer of glass is placed at the beginning to maximize light absorption. This structure has been created and analyzed using the finite difference time domain (FDTD) simulation method(Agresti et al., 2016; Gharibzadeh et al., 2019). In this method, the simulated part is first gridded and Maxwell's equations are solved in the space of these grids and the electric field (E) and magnetic field (H) are obtained. By obtaining the above values, the value of the Poynting vector in the whole area is obtained by equation (1).

1. $\vec{S} = \vec{E} \times \vec{H}$
2. $A = -\frac{1}{2}(\vec{\nabla}.\vec{S})$

Also, the amount of absorption in the active area of the cell per volume unit (A) is obtained from equation (2).

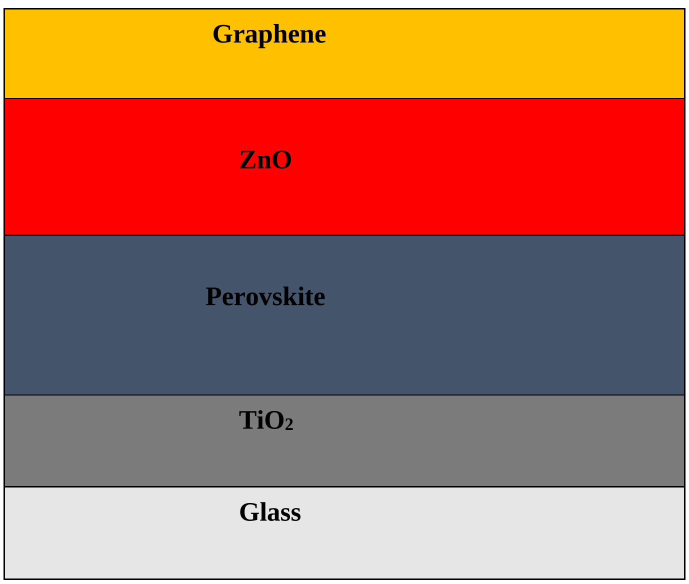

figure 2

Equation (3) has been used to obtain the electron-hole production rate.

$$GR = \int \left(\frac{\varepsilon'' \left|\vec{E}(\omega)\right|^2}{2\hbar} \right) d\omega \quad 3)$$

Research and findings:

Now, in this part, using table (1), we will show that the use of the three structures of perovskite(Afify et al., 2022; Jia et al., 2022; Nazerian et al., 2017; Tan et al., 2013), ZnO, and graphene in this structure improves the basic parameters of the cell and finally the power conversion efficiency of the solar cell is improved(Chen et al., 2015; F. Xu et al., 2022). In Table 6, each of the three materials perovskites, graphene, and ZnO have been used alone in a solar cell sample and we have shown its basic and important parameters(Cheng et al., 2022; Fakharuddin et al., 2022; P. Liu et al., 2021). As you can see, the amount of current concentration, FF, and power conversion gain is low in them. Now, by comparing these values with the values of this article, you will realize that the above values have been improved by using all the above three materials in the structure of the solar cell presented in this article(Liang & Wang, 2020).

ή (%)	**FF**	**V_{OC} (V)**	**J_{sc} (mA/cm^2)**	Type of solar cell
8.8	83.3	0.1	68.2	Graphene-based
0.82	08	0.7	68.0	**Based on ZnO**
66.68	72	0.2	67.280	**Based on perovskite**
61.28	38.2	0.1118	61.8818	**this article**

Table 1.Types of solar cells and checking their parameters

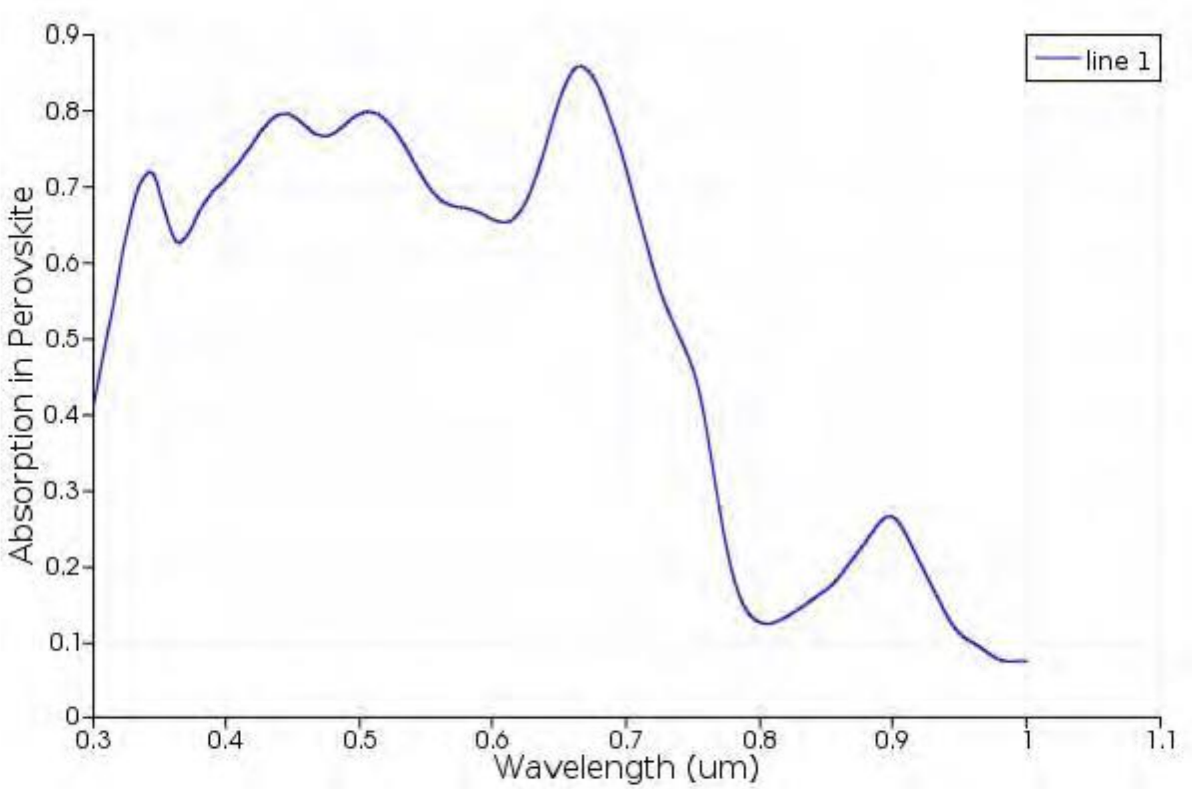

Figure 3. Perovskite solar cell absorption size diagram

Figure 3 shows the absorption coefficient in the spectral range of 0.3 µm to 6 µm for the presented solar cell. As you can see in Figure 3, in the beginning, the absorption at the wavelength of 0.3 micrometers is about 0.4 and the maximum absorption at the wavelength is about 0.7, which is equal to 83%. According to the absorption diagram presented in Figure 3, the amount of absorption decreases with increasing wavelength. Also, as shown in Figure 4, the short circuit current of this structure is about 19,536 mA/cm. As you can see, in this designed solar cell, the amount of current concentration is high and this is due to the use of all three structures of perovskite(Abdollahi Nejand et al., 2022; Vogler-Neuling et al., 2022), ZnO, and graphene, and this is one of the improvement factors in this solar cell compared to other solar cells designed in Articles are passed. As you can see in Figure 5, the value of the solar cell power conversion gain presented in this article is shown. As you can see, the gain in this structure is around 16.25 mW/cm(Dizaj, 2022; Dizaj et al., 2023; Im et al., 2011; Wang et al., 2019).

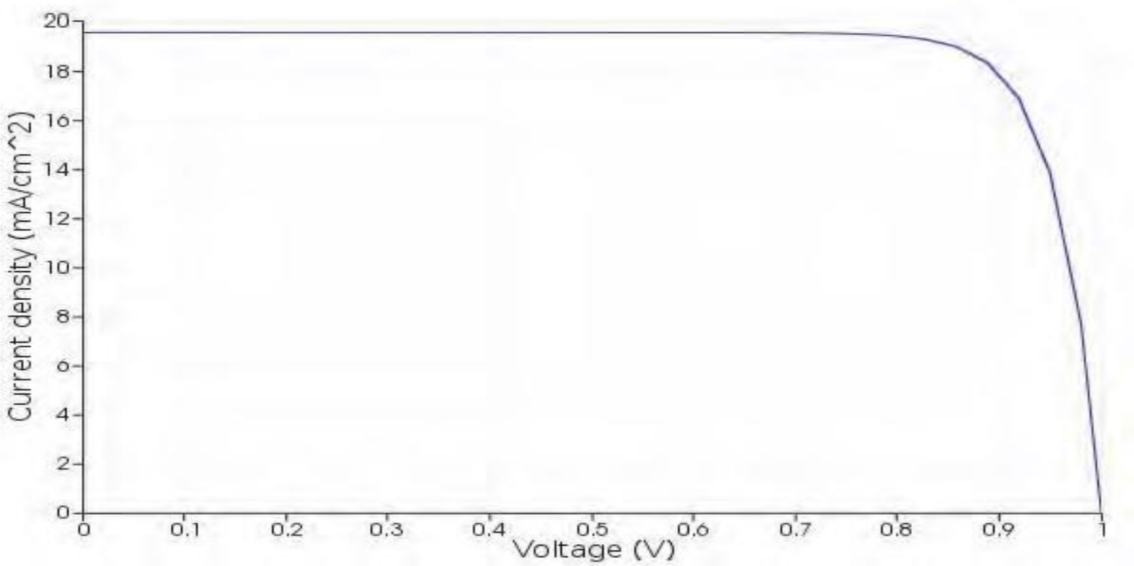

Figure 4. Voltage and current diagram

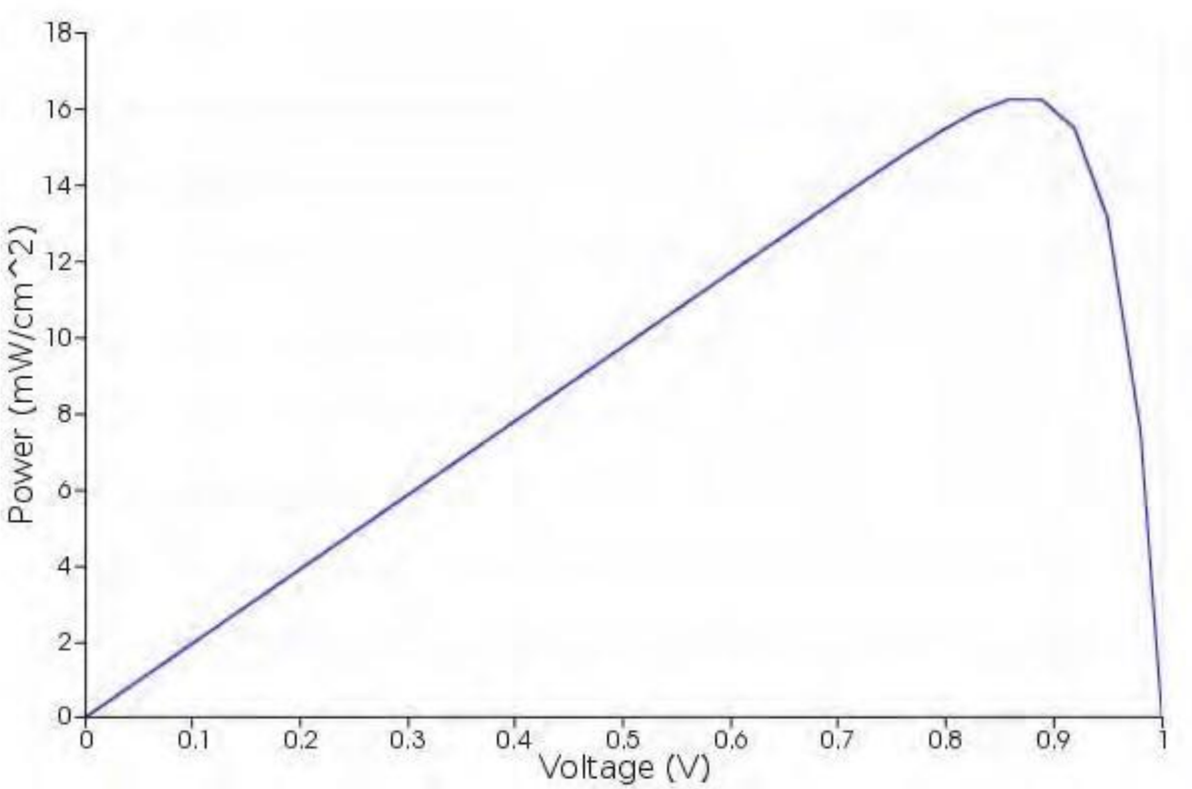

Figure 5.Voltage and power diagram

Conclusion:

In the past years, various solar cells have been presented with various methods, each of which has different structures and as a result, various benefits have been taken. In this article, we presented a solar cell based on perovskite, ZnO, and graphene and showed that this method has not been used in any of the articles. The use of graphene is considered an advantage for this cell due to its abundance in the surrounding environment and its cheapness. Also, the use of graphene, due to its favorable charge transfer capability and its photochemical stability, clearly states the reason for using this material in the structure of this cell. Also, the use of ZnO causes a decrease in the composition of electron-hole pairs and as a result, the current concentration in the cell structure increases, which also improves the performance of the solar cell. It should be noted that the speed of ZnO deposition on FTO is very important. In such a way, the higher the layering speed and its accuracy lead to more uniformity and more regular arrangement of ZnO nanoparticles, and as a result, it leads to an increase in the electron-hole transfer rate. Also, the use of perovskite plays a significant role in the promotion of this cell due to the unique feature of this material in its high absorption power, as well as reducing its losses and its transparency. In this presented structure, we showed that this structure has not been used in any of the articles and we achieved a power conversion gain of 82.61%. Because the use of perovskite structures has been especially noted in solar cells, conducting more research in this field can be very important to increase the power conversion efficiency in solar cells. Also, the use of ZnO is very important because of its anti-reflective properties, and it should be tested on the deposition of ZnO on different types of substrates, and finally, the use of graphene due to the increase in the current concentration of the structures and the increase in this type of currency. It can be further researched as an idea to increase the performance of solar cells.

Result:

In this article, we came to the conclusion that the use of graphene in perovskite solar cells significantly increases the efficiency. Also, the use of Zno reduces the destruction of electron-hole pairs. The use of 2d materials for the layer the 2d method also significantly increases the stability of the solar cell. When we use Zno on the FTO layer, the deposition rate is lower and the uniformity of the Zno nanoparticles is included. In this structure, we have shown that due to the unique feature of Individual graphene plays an excellent role in absorption, as well as the reduction of losses and its transparency. We have been able to create a uniform structure of perovskite solar cells.

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None.

Conflict of interest

None.

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Ethics statement

None

Sources:

Abadi, N. M. S., Banihashemi, M., & Kashaninia, A. (2019). Simulation and Analysis of a Perovskite Solar Cell with (FAPbI 3) 0.85 (MAPbBr 3) 0.15 as Absorber Layer. *2019 27th Iranian Conference on Electrical Engineering (ICEE)*, 173–177.

Abdollahi Nejand, B., Ritzer, D. B., Hu, H., Schackmar, F., Moghadamzadeh, S., Feeney, T., Singh, R., Laufer, F., Schmager, R., & Azmi, R. (2022). Scalable two-terminal all-perovskite tandem solar modules with a 19.1% efficiency. *Nature Energy*, *7*(7), 620–630.

Afify, H. A., Rehm, V., Barabash, A., These, A., Zhang, J., Osvet, A., Schüßlbauer, C., Thiel, D., Ullrich, T., & Dierner, M. (2022). Shape-Controlled Solution-Epitaxial Perovskite Micro-Crystal Lasers Rivaling Vapor Deposited Ones. *Advanced Functional Materials*, *32*(45), 2206790.

Agresti, A., Pescetelli, S., Taheri, B., Del Rio Castillo, A. E., Cinà, L., Bonaccorso, F., & Di Carlo, A. (2016). Graphene–perovskite solar cells exceed 18% efficiency: a stability study. *ChemSusChem*, *9*(18), 2609–2619.

Chen, Q., De Marco, N., Yang, Y. M., Song, T.-B., Chen, C.-C., Zhao, H., Hong, Z., Zhou, H., & Yang, Y. (2015). Under the spotlight: The organic–inorganic hybrid halide perovskite for optoelectronic applications. *Nano Today*, *10*(3), 355–396.

Cheng, S., Sun, Z., Lim, K. H., Gani, T. Z. H., Zhang, T., Wang, Y., Yin, H., Liu, K., Guo, H., & Du, T. (2022). Emerging Strategies for CO2 Photoreduction to CH4: From Experimental to Data-Driven Design. *Advanced Energy Materials*, *12*(20), 2200389.

Dizaj, M. H. (2022). *2D perovskite solar cells and layering with 2D and 3D materials*. https://www.researchgate.net/profile/Mehran-Hosseinzadeh-Dizaj/publication/365322203_2D_perovskite_solar_cells_and_layering_with_2D_and_3D_materials/links/636f3bee431b1f53008fb280/2D-perovskite-solar-cells-and-layering-with-2D-and-3D-materials.pdf

Dizaj, M. H., Shishvan, S. C., & Shahnavaz, F. (2023). *Design and construction of single cation perovskite solar cell and its stability in a solar cell system and their efficiency*.

Ehtesham, A., Wong, W., Wong, H. Y., & Zaman, M. (2016). Recent Advances in Fabrication Techniques of Perovskite Solar Cells: A Review. *American Journal of Applied Sciences*, *13*(11), 1290–1314.

Fakharuddin, A., Gangishetty, M. K., Abdi-Jalebi, M., Chin, S.-H., bin Mohd Yusoff, A. R., Congreve, D. N., Tress, W., Deschler, F., Vasilopoulou, M., & Bolink, H. J. (2022). Perovskite light-emitting diodes. *Nature Electronics*, *5*(4), 203–216.

Gharibzadeh, S., Abdollahi Nejand, B., Jakoby, M., Abzieher, T., Hauschild, D., Moghadamzadeh, S., Schwenzer, J. A., Brenner, P., Schmager, R., & Haghighirad, A. A. (2019). Perovskite Solar Cells: Record Open-Circuit Voltage Wide-Bandgap Perovskite Solar Cells Utilizing 2D/3D Perovskite Heterostructure (Adv. Energy Mater.

21/2019). *Advanced Energy Materials*, *9*(21), 1970079.

Im, J.-H., Lee, C.-R., Lee, J.-W., Park, S.-W., & Park, N.-G. (2011). 6.5% efficient perovskite quantum-dot-sensitized solar cell. *Nanoscale*, *3*(10), 4088–4093.

Jia, F., Xiao, X., Nashalian, A., Shen, S., Yang, L., Han, Z., Qu, H., Wang, T., Ye, Z., & Zhu, Z. (2022). Advances in graphene oxide membranes for water treatment. *Nano Research*, *15*(7), 6636–6654.

Lee, M., Choi, E., Soufiani, A. M., Lim, J., Kim, M., Chen, D., Green, M. A., Seidel, J., Lim, S., & Kim, J. (2021). Enhanced Hole-Carrier Selectivity in Wide Bandgap Halide Perovskite Photovoltaic Devices for Indoor Internet of Things Applications. *Advanced Functional Materials*, *31*(16), 2008908.

Liang, T., & Wang, B. (2020). Interlayer Covalently Enhanced Graphene Materials: Construction, Properties, and Applications. *Acta Phys. Chim. Sin.*, *38*, 2011059.

Liu, P., Han, N., Wang, W., Ran, R., Zhou, W., & Shao, Z. (2021). High-quality Ruddlesden–Popper perovskite film formation for high-performance perovskite solar cells. *Advanced Materials*, *33*(10), 2002582.

Liu, S., Wang, J., Shao, J., Ouyang, D., Zhang, W., Liu, S., Li, Y., & Zhai, T. (2022). Nanopatterning technologies of 2D materials for integrated electronic and optoelectronic devices. *Advanced Materials*, *34*(52), 2200734.

Nazerian, V., Nasrabadi, A. T., & Dizaj, M. H. (2017). *Picosecond Optical Pulse Narrowing Using Multi Stack Semiconductor Optical Amplifier*. https://www.researchgate.net/profile/Mehran-Hosseinzadeh-Dizaj/publication/348735093_Picosecond_Optical_Pulse_Narrowing_Using_Multi_Stack_Semiconductor_Optical_Amplifier/links/600dd3f492851c13fe355f69/Picosecond-Optical-Pulse-Narrowing-Using-Multi-Stack-S

Qu, X., Ma, J., Jia, S., Wu, Z., Liu, P., Wang, K., & Sun, X.-W. (2021). Improved blue quantum dot light-emitting diodes via chlorine passivated ZnO nanoparticle layer. *Chinese Physics B*, *30*(11), 118503.

Shin, S. J., Alosaimi, G., Choi, M. J., Ann, M. H., Jeon, G. G., Seidel, J., Kim, J., Yun, J. S., & Kim, J. H. (2022). Strategic Approach for Frustrating Charge Recombination of Perovskite Solar Cells in Low-Intensity Indoor Light: Insertion of Polar Small Molecules at the Interface of the Electron Transport Layer. *ACS Applied Energy Materials*, *5*(11), 13234–13242.

Steele, J. A., Braeckevelt, T., Prakasam, V., Degutis, G., Yuan, H., Jin, H., Solano, E., Puech, P., Basak, S., & Pintor-Monroy, M. I. (2022). An embedded interfacial network stabilizes inorganic CsPbI3 perovskite thin films. *Nature Communications*, *13*(1), 7513.

Tabi, G. D., Pham, H. T., Zhan, H., Walter, D., Mayon, A. O., Peng, J., Duong, T., Shehata, M. M., Shen, H., & Duan, L. (2022). LiI doping of mixed-cation mixed-halide perovskite solar cells: Defect passivation, controlled crystallization and transient ionic response. *Materials Today Physics*, *27*, 100822.

Tan, L.-L., Ong, W.-J., Chai, S.-P., & Mohamed, A. R. (2013). Reduced graphene oxide-TiO2 nanocomposite as a promising visible-light-active photocatalyst for the conversion of carbon dioxide. *Nanoscale Research Letters*, *8*(1), 1–9.

Tarasova, N., Bedarkova, A., Animitsa, I., & Verinkina, E. (2022). Synthesis, Hydration Processes and Ionic Conductivity of Novel Gadolinium-Doped Ceramic Materials Based on Layered Perovskite BaLa2In2O7 for Electrochemical Purposes. *Processes*, *10*(12), 2536.

Tritt, T. M., Böttner, H., & Chen, L. (2008). Thermoelectrics: Direct solar thermal energy conversion. *MRS Bulletin*, *33*(4), 366–368.

Vogler-Neuling, V. V., Karvounis, A., Morandi, A., Weigand, H., Dénervaud, E., & Grange, R. (2022). Photonic Assemblies of Randomly Oriented Nanocrystals for Engineered Nonlinear and Electro-Optic Effects. *ACS Photonics*, *9*(7), 2193–2203.

Wang, L., Chang, B., Li, H., Wu, Y., Liu, Z., Pan, L., & Yin, L. (2022). [PbX 6] 4− modulation and organic spacer construction for stable perovskite solar cells. *Energy & Environmental Science*, *15*(11), 4470–4510.

Wang, L., Zhou, H., Hu, J., Huang, B., Sun, M., Dong, B., Zheng, G., Huang, Y., Chen, Y., & Li, L. (2019). A Eu3+-Eu2+ ion redox shuttle imparts operational durability to Pb-I perovskite solar cells. *Science*, *363*(6424), 265–270.

Xie, W., Tang, X., Yan, Y., Zhang, Q., & Tritt, T. M. (2009). Unique nanostructures and enhanced thermoelectric performance of melt-spun BiSbTe alloys. *Applied Physics Letters*, *94*(10), 102111.

Xu, F., Gong, K., Fan, W., Liu, D., Li, W., Wang, L., & Zhou, X. (2022). J-Aggregated Dyes for Dye-Sensitized Solar Cells: Suppressing Aggregation-Induced Excited-State Quenching by Intramolecular Charge Separation. *ACS Applied Energy Materials*, *5*(11), 13780–13790.

Xu, H., Torres Merino, L., Koc, M., Aydin, E., Zhumagali, S., Haque, M. A., Yazmaciyan, A., Sharma, A., Rosas Villalva, D., & Huerta Hernandez, L. (2022). Metal-Free Interconnecting Layer for Monolithic Perovskite/Organic Tandem Solar Cells with Enhanced Outdoor Stability. *ACS Applied Energy Materials*, *5*(11), 14035–14044.

Yamada, Y., & Kanemitsu, Y. (2022). Electron-phonon interactions in halide perovskites. *NPG Asia Materials*, *14*(1), 48.