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Recent Progress in Bulk Heterojunction Solar Cells: Emerging Strategies for High Performance

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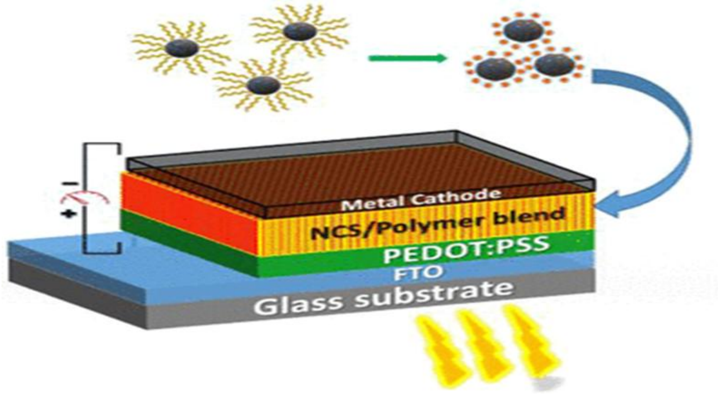
Graphical abstract



Abstract

Bulk Heterojunction (BHJ) solar cells integrate photoactive polymers with quantum dots (QDs) or nanocrystals (NCs) to synergistically combine the advantages of organic and inorganic materials. This hybrid architecture facilitates efficient charge transport and significantly enhances light absorption across the solar spectrum. The tunable optical and electronic properties of NCs allow flexible design strategies to maximize photon capture over a broad wavelength range. In particular, lead chalcogenide-based NCs (PbS, PbSe, PbTe) are notable for their strong near-infrared (NIR) absorption and size-dependent bandgap tunability ranging from 0.3 to 1.5 eV, attributed to their large exciton Bohr radii of approximately 18, 46, and 150 nm, respectively. Despite their

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promising optoelectronic features, the incorporation of lead chalcogenide NCs into polymer-based BHJ architecture remains relatively underexplored. This review highlights recent progress in the integration of these NCs within polymer composites, examines their influence on material properties and device performance, and discusses existing challenges and future research directions for advancing BHJ solar cell technology.

Keywords: BHJ Solar Cells; Quantum Dots; Lead Chalcogenides; Bandgap Tuning; NIR Absorption

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التطورات الحديثة في الخلايا الشمسية ذات الوصلة غير المتجانسة الحجمية: استراتيجيات مبتكرة لتحقيق كفاءة عالية

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ملخص

تدمج الخلايا الشمسية متعددة الوصلات السائبة (BHJ) البوليمرات الضوئية مع النقاط الكمومية (QDs) أو البلورات النانوية (NCs) لتجمع بشكل تآزري مزايا المواد العضوية وغير العضوية .يُسهّل هذا الهيكل الهجين نقل الشحنات بكفاءة، ويُحسّن بشكل كبير امتصاص الضوء عبر الطيف الشمسي .تتيح الخصائص البصرية والإلكترونية القابلة للضبط للبلورات النانوية استراتيجيات تصميم مرنة لتحقيق أقصى استفادة من التقاط الفوتونات عبر نطاق واسع من الأطوال الموجية .على وجه الخصوص، تتميز الخلايا الشمسية متعددة الوصلات السائبة القائمة على كالكوجينيد الرصاص PbS، PbSe ، PbTeبامتصاصها القوي للأشعة تحت الحمراء القريبة (NIR) وقابليتها لضبط فجوة النطاق حسب الحجم، والتي تتراوح بين 0.3 و 1.5 إلكترون فولت، ويعزى ذلك إلى أنصاف أقطار إكسيتون بور الكبيرة التي تبلغ حوالي 18 و46 و150 نانومتر، على التوالي .على الرغم من خصائصها البصرية الإلكترونية الواعدة، إلا أن دمج خلايا الكالكوجينيد الرصاصية النانوية في بنية BHJ القائمة على البوليمر لا يزال غير مستكشف نسبيًا .تُسلّط هذه المراجعة الضوء على التقدم المُحرز مؤخرًا في دمج هذه الخلايا النانوية ضمن مركبات البوليمر، وتدرس تأثيرها على خصائص المواد وأداء الأجهزة، وتناقش التحديات الحالية وتوجهات البحث المستقبلية لتطوير تقنية خلايا BHJالشمسية.

الكلمات المفتاحية: خلايا BHJ الشمسية؛ النقاط الكمومية؛ الكالكوجينيدات الرصاصية؛ ضبط فجوة النطاق؛ امتصاص الأشعة تحت الحمراء القريبة.

1. Introduction and motivation

The increasing global demand for energy, coupled with growing concerns over the depletion of non-renewable fossil fuels, has prompted extensive research into alternative energy sources such as hydropower, wind, geothermal, solar, and hydrogen. Among these, solar energy stands out as the most abundant, cost-effective, and reliable renewable resource. Owing to its vast potential, researchers have developed various methods for harvesting solar energy [1,2]. Photovoltaic (PV) cells have become a leading technology due to their durability, cost efficiency, and wide applicability [1,3–5]. The pursuit of low-cost PV materials and simplified fabrication processes continues to drive innovation in the solar energy sector. Currently, most commercial solar cells are based on silicon (Si), achieving conversion efficiencies of up to 26.1% in monocrystalline devices. However, silicon-based manufacturing remains energy-intensive, costly, and environmentally taxing, motivating researchers to explore alternative, low-cost materials and device architectures [1,2,6].

In recent years, organic polymer solar cells have attracted growing attention because they are lightweight, flexible, low-cost, environmentally friendly, and amenable to low-temperature, solution-based fabrication [3,7,8]. These characteristics make large-scale production and deployment of polymer-based solar cells particularly promising [1,3]. Moreover, their fabrication is

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significantly less expensive than that of inorganic counterparts, positioning them as an attractive option for sustainable energy generation. Nevertheless, structural imperfections within organic semiconducting polymers often create trap states that hinder efficient charge-carrier transport. Unlike inorganic nanocrystals, where charge carriers move more freely, carrier transport in organic materials primarily occurs through hopping mechanisms [10,11]. Despite these limitations, advancements in polymer design, device architecture, and interfacial engineering have significantly improved performance. While early polymer solar cells achieved efficiencies of only around 7%, recent innovations have led to power conversion efficiencies up to 32.9% in monolithic two-terminal tandem devices [12,13] and 25.7% in single-junction photovoltaic cells [14,5].

The bulk heterojunction (BHJ) technology idea was developed to boost the efficiency of photovoltaic cells [3,15]. With method, organic and hybrid organic–inorganic semiconductors, along with donor and acceptor materials, are joined into one active layer [16,17]. The components to be donated and accepted are dissolved in a suitable solvent and dried into a thin layer. By using this structureAn increased area where the donor and acceptor contact promotes the dissociation of excitons. and moves charges easily. A layer of BHJ, sized at 100–200 nm for sunlight absorption, is perfectly suitable and, since this is far thinner than 1 µm of the standard inorganic layer, leads to better performance [9,11,18]. BHJ formation gives rise to both improved transport of charge carriers and better resistance to heat and the polymer matrix helps keep the light-harvesting NCs working as they should over time [19-21]. For this reason, these architectures are considered highly promoted for the production of HPV cells that join together p-type polymers and inorganic semiconductors [22]. HPV cells may be arranged as expected from polymers mixed with inorganic nanocrystals (NCs)(Figure1). This approach offers better radiation absorption (10^{-17} m^{-1}), versatile solution processing, lower loss of electrons, properly adjustable pathways for charges and better capture of a broader amount of sunlight [23-25].

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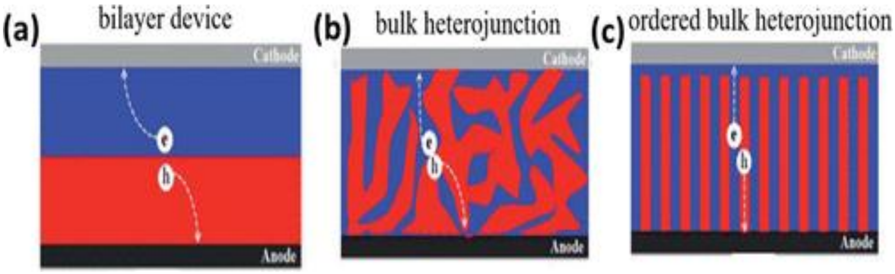

Figure 1. A series of cell layups where the polymer and inorganic NCs provide the donor sites is established with: (a) one device setup, (b) random mixing of the two and (c) orderly mixing of the materials [25].

A p-type conjugated polymer in the hybrid cell gathers light to form holes, which travel to the anode and an n-type inorganic semiconductor deliver electrons to the cathode. At that part of the junction, excitons mix with the free charge carriers. Electricity appears when charged particles head to the electrodes. Mainly, an active layer is built by sandwiching inorganic nanocrystal (NC) layers over the top of the conjugated polymer layer. Certain cells choose to arrange their active elements by layers, while others mix them freely by design. In a number of cases, extra layers, for example, an ETL and HTL, may be put in to raise the performance of the entire device. The main inorganic components used in these cells are nanostructured semiconductors such as metal chalcogenides and metal oxides. Thanks to their exposure over the bulk heterojunction, these substances help faster transmission of electrons into the system. They are also useful because they remain stable under stress from environmental factors, which organic NCs cannot do.

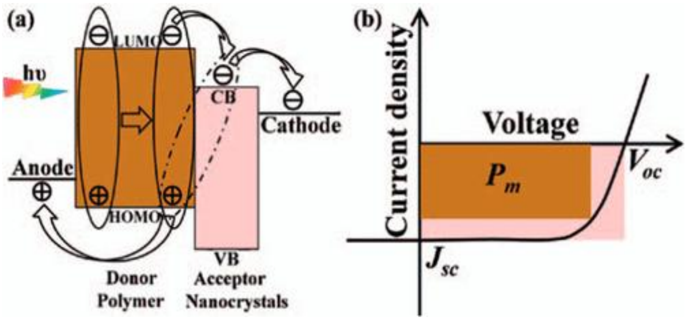

Figure 2. The polymer NSCs energy level diagram, modeled on four main steps for the hybrid solar cell and for a HSC, an example J−V curve is shown after illumination, giving voltage (V), short circuit current density (Jsc) and the point of highest possible power (Pm) [11].

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From Figure 2 it can be seen that, in a hybrid solar cell, four parts are essential such as capturing light, supported by exciton movements, separating the newly generated electrons, and collecting the resulting charges [11]. Receiving photons by the polymer triggers the creation of excitons. There is no need for a built-in electrical field to make excitons move in devices. The fast movement of excitons in diffusion is required to prevent large amounts of recombination. BHJ structures function through diffusion at the contacts between the materials which occurs by random jumps called hops. Structuring polymers to interact with nanocrystals is necessary to separate the short-diffusion excitons quickly and reduce recombination losses. Energy considerations suggest that dissociating excitons into free charge carriers by transferring the charges is usually most feasible. The NC conduction band and the polymer LUMO need to be separated by at least 0.3 eV for good partition. During splitting apart at the photointiator, the electron and holes travel through the polymer matrix to their assigned electrodes. This type of movement is due to internal electric fields and effective transport of charge [20,33].

Many researchers are interested in making lead chalcogenide nanocrystals because the exciton Bohr radius is broad in both PbS (20 nm) and PbSe (46 nm). which result in large carrier mobility. Since these NCs have strong quantum confinement effects, obtaining NIR luminescence and low-energy photon absorption is straightforward. It has also been noted that such exciton-multipliers may use newly developed methods to extract complex hot charge carriers. Due to these excellent features, using chalcogenide materials in bulk heterojunction hybrid solar cells (HSCs) is recognized as a smart approach to boost benefits. and affordability in solar technology. Yet, using materials with lead poses some environmental issues. However, some of these concerns may be avoided if the lead in NCs is decreased, proper device encasement is used, and safe NC recycling methods are put in place.

Given the rising importance of solar energy as a leading renewable resource, polymer-based solar cells have attracted extensive attention due to their low cost, simple fabrication, and environmental compatibility. The integration of organic polymers with inorganic nanocrystals (NCs) in hybrid photovoltaic (HPV) architectures has emerged as a promising approach to enhance device efficiency through improved exciton dissociation and efficient charge transport within the bulk heterojunction (BHJ) layer. Among the various nanocrystals explored, lead chalcogenide NCs (PbS, PbSe) stand out for their tunable bandgaps, high carrier mobility, and potential to surpass traditional efficiency limits. However, the inherent toxicity of lead-based materials necessitates the development of responsible synthesis, handling, and recycling strategies to ensure environmental safety. This review aims to provide a comprehensive overview of lead chalcogenide-based hybrid polymer solar cells, focusing on their fabrication methods, structural integration, and underlying working mechanisms. Additionally, it highlights the current challenges, environmental considerations, and future research directions essential for advancing this class of next-generation photovoltaic technologies.

2. Chalcogenide nanocrystals

Frequently, various low-bandgap semiconductor QDs made from metal chalcogenide NCs are mixed in bulk heterojunction (BHJ) solar cells with organic semiconductors [37]. These colloidal NCs have gained interest for solar technology because they (i) change their properties with size, (ii) are simple to make, and (iii) are suitable for making solar cells in solution. Because of these qualities, they can be used to build optoelectronic devices that use little energy and are cost-effective. NCs of lead chalcogenides (like PbS, PbSe, and PbTe) attract much interest because They react easily to NIR light and their band gaps can be adjusted to lie between 0.3 and 1.5 eV. The exciton Bohr radius in PbS is 18 nm, PbSe 46 nm and PbTe 150 nm. which let free warm electrons to transfer and carry energy more easily. Research done by Socol et al [40] and others [36,38,39) revealed PbS and PbSe NCs in solar cell active layers boosted both efficiency and device stability over cells that did not contain inorganic NCs [40]. Researchers previously [41,42] mainly worked on solar cells that took advantage of PbS NCs and conjugated polymers to enhance performance. Including inorganic NCs in these layouts has been demonstrated to increase optoelectronic performance by enhancing the ability of charge carriers to travel through a material and boosting the stability of the device. In addition, attaching amines, carboxylic acids, and thiols to NCs improves their solubility in organic solvents and encourages compatibility with polymers in blends. MoreoverExperts found that the character of the NCs plays a role in the customs of light and charge motion within the hybrid setup [43].

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2.1 Researchers have also made hybrid solar cells using lead sulfide nanocrystals as one of the elements.

A major hurdle in using lead sulfide (PbS) semiconductor nanocrystals (NCs) is lowering the number of defects by improving their surface chemistry. To address this problem, we can passivate the electronic traps both inside and along the edges of the material. To learn more about the issue, the team synthesized PbS NCs and observed the changes to their solar cell efficiency from adding 1,2-ethanedithiol (EDT), 3-mercaptopropionic acid (MPA), malonic acid (MA) and tetrabutylammonium iodide (TBAI). According to the findings, the absorption edge of the PbS NCs was 900 nm (Figure 3a), yet the exciton peaked at a shorter wavelength in the PTB1/PbS mix, indicating role by the polymer in addition to the nanocrystals. Changes made to the ligands after the deposition did not alter the properties of the polymer coating. For the most part, investigations from the past would often use short-chain amines or pyridines as substitutes for surface ligands., but these were ineffective at replacing all the original surface ligands or covering surface trap sites, causing PCEs below 4%. Only the treatment with MPA in Colbert's report achieved the greatest PCE, at 2.49%, while all other tests had scores under 2% (Figure 3b).

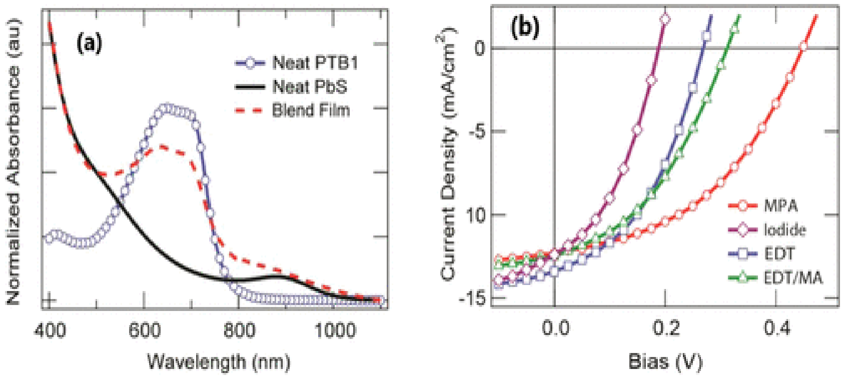

Figure 3. The absorption spectra of PbS NCs, the PTB1 blend and the pure materials (a) before exchange and (b) after exchange [44].

PIA spectroscopy studies proved that in the presence of MPA and TBAI, polaron formation was longer-lasting for the analyzed systems. Where MPA was used, the results were: results show a carrier lifetime of τ ≈ 10 ms, while for those treated with TBAI, the lifetime is about τ ≈ 3 ms. The findings showed that MPA-treated blends have better charge generation and recombination lifetimes compared to untreated blends. Because of this, devices that used

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these MPA-treated PbS nanocrystals performed better, showing better voltage and fill factor and higher overall conversion of power to electricity [44].

Denba-Lu et al. [46] examined how PbS nanocrystals with iodide straps behave in BHJ solar cells. A rapid synthesis technique was used involving replacing the initial ligands with lead iodide (PbI_2) and ammonium iodide (NH_4I). When iodide-based ligands were introduced, the nanocrystals spread better in the solvent and matched better with the polymer base. Exchanging iodide in PbS NCs increased their stability and improved the photovoltaic activity. Unexpectedly, each material had its own pattern of absorption, with the oleate-capped NCs showing a slight drop in energy (lower wavelength) of 37 meV when compared to NCs coated with oleic acid (OA). Only the BHJ cell using PbI_2-passivated PbS nanocrystals in AM 1.5G illumination could reach a PCE of 4.8% among all devices, this being due to their broad NIR response. The analysis of PL lifetime found that photoluminescence from PbI_2-passivated films decayed faster providing a better route for charge movement to reach the external circuit, resulting in improved Jsc for the device.

Piliego and his team [47] built hybrid solar cells using nanocrystalline PbS and the conjugated polymer PDPPTPT. Since they are highly soluble in toluene, a first excitonic absorption peak for the PbS NCs was visible near a wavelength of 1100 nm. When using the PDPPTPT: PbS process, a fleet of electrodes are coated with PbS particles, both PbS particle's and the polymer's absorption were seen. The polymer had features between 600 and 800 nm, but PbS showed a broadened and redshifted peak, both caused by the polymer's cross-linking and the introduction of defects. To increase the electronic connection between NCs, oleate chains were exchanged for benzenedithiol ligands. A weight ratio of 10:90 of PDPPTPT: PbS was shown on ITO, and processes were carried out after deposition. Based on the PCE, Jsc, Voc, and FF measurements, the resulting device achieved 2.9% efficiency, For Jsc, the module gives 12.5 mA/cm^2; Voc measures at 0.47 V and the fill factor is 49%. Both PDPPTPT and PbS contributed significantly to the photocurrent in the measurements (see Figure 4).

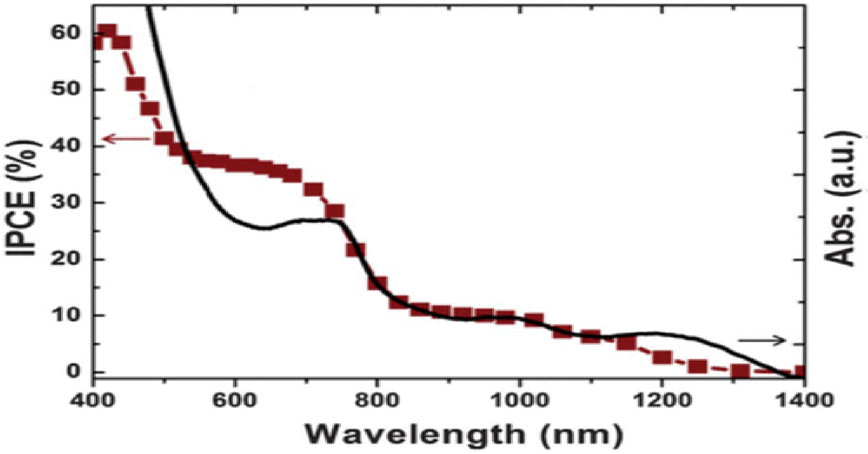

Figure 4. The blend film and its matching solar cell (47)

Research led by Jianyu Yuan and colleagues [48] brought together four DTP-based polymers, PDBF, PDTD, PDFT, and PDTT, and NCs of PbS to create new type II heterojunctions for better open-circuit voltage. Earlier studies showed that the HOMO energy level (5–5.2 eV) of PbS NCs was a barrier to transferring charge to polymers. The researchers fixed this by making the polymers' HOMO energy level −5.0 ± 0.2 eV.

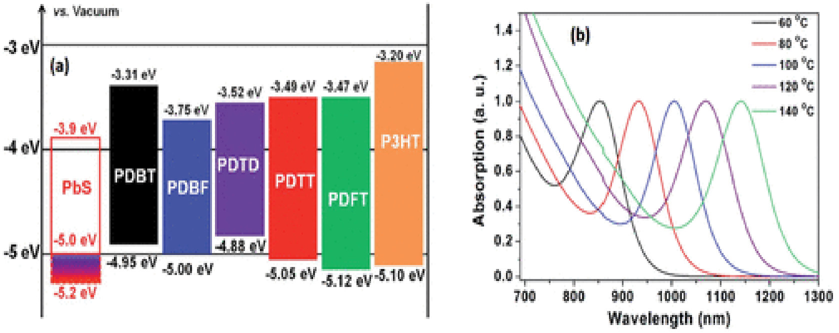

Figure 5. (a) Energy levels within different polymers and PbS nanocrystals and (b) the UV−Vis spectra for QDs produced through the method, at several temperature points [48]

To modify the bandgap of the PbS nanocrystals, the researchers changed the processing temperature from 60 to 140 °C. This also caused changes in the absorption spectra of the NCs, as is shown in Figure 5. Putting PbS NCs in the gaps enhanced the performance of the hybrid film in devices made via the ITO/PEDOT-PSS/polymer-PbS/PbS/LiF/Al structure. Since the layer blocked cracking, it also made electrons move better, so charge recombination rarely

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happened. The hybrid film consisted of 19 times more quantum dots than polymer. For the device formed using the PDBT-PbS blend, the PCE was 4.23%, giving a Voc of 0.55 V, a Jsc of 13.29 mA/cm² and an FF of 56%. The films' top layers did not give much data, a consistent smoothness in those layers supported the desired behavior of the devices. (Figur.6) The film made from PDBT-PbS NCs showed higher uniformity when compared to the other hybrid films. For the other films, polymer aggregations, cracks and phases separated vertically were detected (Figure 6) and since this leads to areas where no contact exists between the NCs and polymer, fewer charge carriers can move and overall device efficiency Suffers.

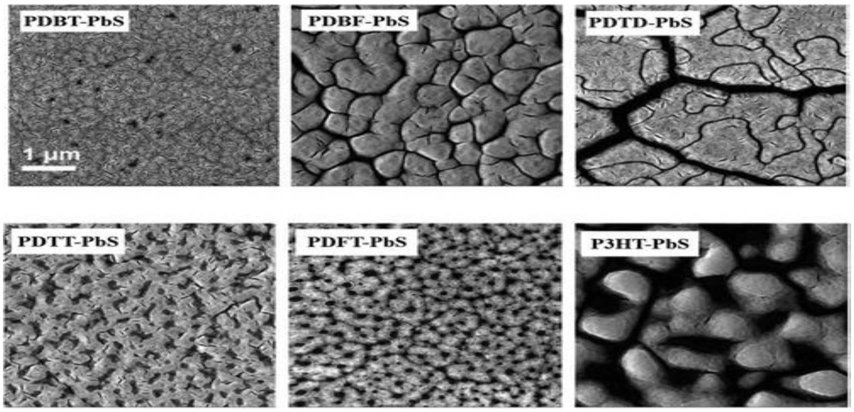

Figure 6. The films composed from merging polymers and PbS NCs at a ratio of 1:19 [48]

To promote mixing in the polymer-nanocrystal system, Dang-Trung Nguyen and fellow scientists made a block copolymer known as P3HT-b-PS [49]. The broader distribution of OA-capped PbS NCs with a 3.09 nm diameter (detected in Figure 7a) in the blend was likely due to the interaction of two networks and it helped promote charge transport during energy conversion in the cell. By employing the 1:20 P3HT-b-PS:PbS ratio, the efficacy of our nanoclicks improved from 3.66% to 4.18%, meaning a 13% increase compared to the P3HT-PbS mixture (Figure 7b). Once P3HT was included at a 0.7:0.3 ratio with P3HT-b-PS, the PCE climbed to 4.91% as a result. The good results were possible thanks to the increased amount of P3HT..

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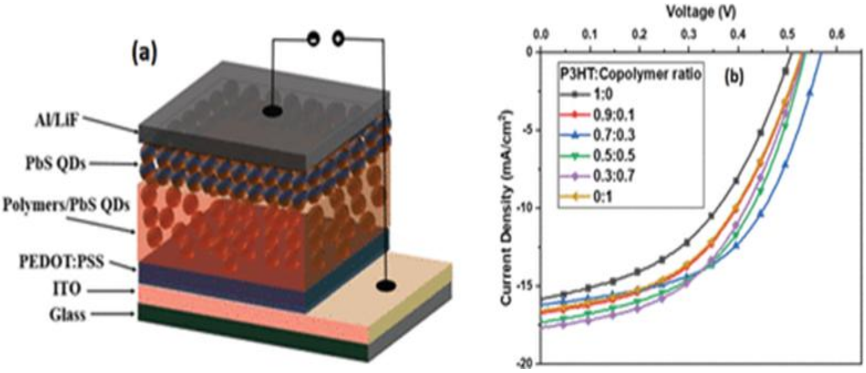

Figure 7. (a) A picture of the BHJ cell is given and (b) the weight percentages of BDT-PbS in the active layers using a current-voltage diagram [49]

Yoshida *et al.* [50] newly used the polymer PNDI-SH and changed from the usual method that involves oleic acid coating of the PbS nanocrystals (NCs). The UV-visible spectra for PNDIBr: PbS-QD (70:30 w/w) were very similar both before and after they were blended. A shift to a lighter band was visible at the wavelength in the NIR region, with λmax moving from 982 nm to 1054 nm. It was considered that replacing a smaller oleic acid with PNDI-SH in liquids allowed the shift. Redshift occurred for both the PbS QDs and the mixed PNDI-SH: PbS-QD, seen when the absorption peak in the mixed film was located at 1195 nm versus 1058 nm for the PNDIBr: PbS-QD sample. Microscopic studies indicate that the clusters formed in the PNDI-SH: PbS-QD blend are larger, averaging a wider diameter, than the clusters found in the PNDI-Br: PbS-QD film. The QDs were secure in PNDI-SH and were still Dispersive after experiencing both air and organic solvents. However, the resulting solar cell outperformed the solar cell just with the polymer which demonstrates the role of compensation. The way the PbS QDs self-assembled caused a delay in current transport and reduced how excitons separated which probably caused poorer photovoltaic performance.

Engaging low bandgap nonfullerene small molecules with quantum dots at the interface improved the response to visible radiation, increased the separation of charge carriers and improved the way they move through the device. These devices made from QD/SM bridges showed a photovoltaic conversion efficiency of 13.1% and an EQE over 80% in visible light and 60% in NIR wavelengths. The Voc was improved from 0.60 V in QD/polymer-only devices to 0.66 V with the addition of the polymer layer, most likely because it

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encouraged better charge splittings and drove holes out, reducing the chances of recombination. Additional improvement was achieved when PD2FCT-29DPP, a polymer based on diketopyrrolopyrrole (DPP), was applied. This improved how the device extracts and transfers charges. When the hole transport layer (HTL) was PD2FCT-29DPP, PbS-based devices achieved outstanding PCEs of 14%, Along with having a high FF of 70%. Fluorinated benzothiadiazole was introduced to raise the HOMO level of PD2FCT-29DPP, letting the Voc rise and reducing the bimolecular recombination percentage.

2.2 Type of hybrid solar cells made with lead selenide nanocrystals

The high Bohr radius of PbSe at 46 nm is responsible for its carrier mobility of up to 7 cm–2V–1s–1. Just as in PbS, by changing the band gap of PbSe to the NIR, quantum confinement effects help it absorb photons with low energy levels[53-54]. Li et al [55] increased the synthesis time from 3 to 5 minutes in their experiments [55]. While all NCs had strong absorption signals, those that reacted longer showed up as a lighter blue and became larger. When a ligand exchange ($CdCl_2$·TDPA·OLA) occurred, the absorption bands of the passivated NCs were shifted from 1468 to 1475 nm. A bulk heterojunction film was produced by mixing P3HT, PCBM and PbSe in 1,2-dichlorobenzene and letting them react for 10 hours. PCE achieved in devices made from halide-passivated NCs was 3.31% which is 14.5% greater than the PCE of cells built using normal PbSe NCs. Mehta and his colleagues created PbSe nanocrystals covered in oleic acid and oleylamine and the band gaps were found to be 1.15 and 1.05 eV**.** The presence of oleylamine was found to guide the formation and growth of PbSe quantum dots, leading to better consistency in size distribution. Using P3HT: PbSe polymer matrix films provided improved charge transport and higher current compared to studies with different solvents. Enhanced performance by oleylamine-capped PbSe QDs is due to more nucleation occurring, the better protection they offer, and easier removal of their molecules during postsynthesis. An improved current and voltage response is seen in the ({ITO}/PEDOT: PSS/P3HT: PbSe (OA/OLA) QDs) type solar cells. Due to a better particle size and improved charge transport enabled by easier removal of ligands, this process improved contact between the QD layers and the composite layer. More tests on

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composite layer thickness and NC concentration could improve our knowledge of how the device functions.

Different work by Sun et al demonstrates that PbSe NCs can be placed on nine particular semiconducting polymers (PDTPBT, PDTD, PDBF, PDTT, P3HT, PDFT, PBDT-T-FDP, PBDT-TPD and PBDT-T8-TPD) using a technique known as spin-coating. The graph in figure 8a represents each device’s current-voltage curve; the PDTPBT model had the highest PCE at 5.31%. Less energy was lost to recombination and the electric field was stronger in the organic solar cells, leading to a bigger open-circuit voltage than was possible in PbSe Schottky junction solar cells. The quenching process in photoluminescence (PL) experiments was used to observe how the charges moved through the NCs and the polymer (Figure 8b). When polymers were included, PbSe PL was quenched, showing that excitons in PbSe NCs were dissociated and the holes moved to the polymers. By quenching the device, the hole transfer improved, making the device work better.

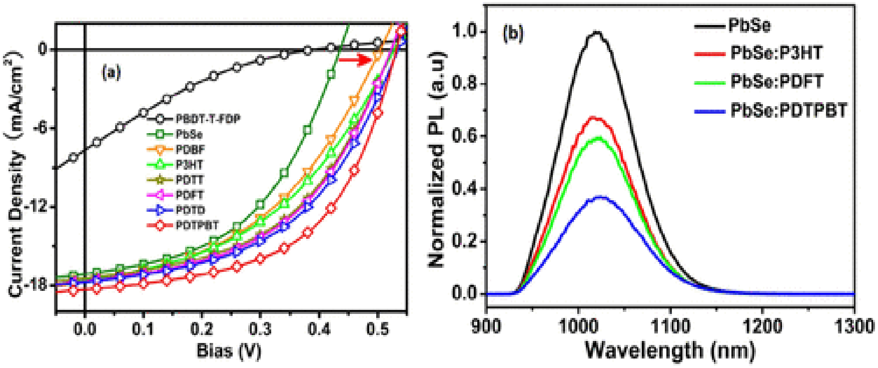

Figure 8. (a) Current–voltage data and (b) the photoluminescence data, normalized for comparison, for PbSe only and the two PbSe−polymer samples [57]

The composite structure was formed by mixing PbSe nanocrystals with poly[(2-methoxy,5-octoxy)-1,4-phenylenevinylene] at varied ratios. The MOPPV-PbSe composites have a peak UV–vis absorption at 531 nm (as seen in Figure 9). The new band found in this study came from the addition of PbSe to the p-n junction. Purified PbSe NCs added at a level of 50 wt% gave the best outcomes, producing a measuring current density of 3.661 mA/cm3, 0.326 V for the voltage, and a 0.277% photovoltaic conversion efficiency. In a different investigation, Liu et al studied a polymer mixed D–D groups with A-groups to improve the separation and flow of charges. The use of PbS x Se 1−x nanoalloys produced a conversion efficiency of 5.50% and a fill factor of 67%. The development of pure PbS x Se 1−x nanoalloys mostly depended on having sulfur and selenium precursors with the same reactivity. The better performance was due to the addition of a 3D shape, appropriate polymer/NC balance, and vertical alignment of the

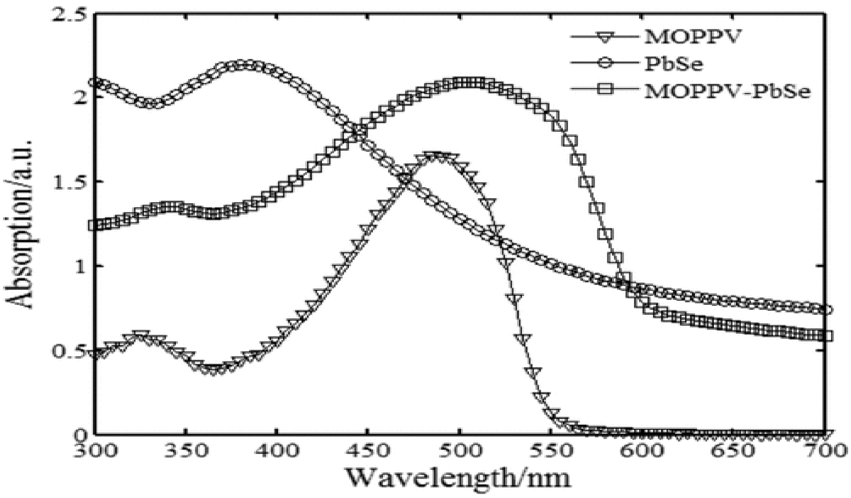

Figure 9. The absorption spectra of the composite PbSe film and each of its components [58]

2.3 The Impact of Ligands

To make nanocrystals (NCs), aliphatic ligands are key because they change solubility, offer access to reactive chemicals, and help NCs keep their stability after being made. Also, they are important in deciding how NCs function. Ligand exchange is regularly applied to adjust the optoelectronic features of NCs. Ligand engineering allows us to control (i) the surface makeup, (ii) the shape of NCs and [71,72] to modify (iii) carrier action, (iv) the point where electrons and holes exist, (v) energy of emission and (vi) better than 2.0 eV changes to the band edge. Table 1 describes some frequently used ligands and the effects they have on the performance of devices. Treating the NCs with MPA led to better performance because the carrier recombination times were increased and the voltage at zero power (VOC) was more positive with TBAI or EDT. Devices treated with TBAI had a VOC of less half that of the devices treated with MPA, with EDT devices lying somewhere in the middle. This change in efficiency might be due to the new arrangement of particles as ligands are exchanged. It should be noted that even though MPA, TBAI and EDT are similar in molecular size and lack mid-gap defects, their structures differ. While considering the two treatments side by side, MPA raised VOC a little but caused a large increase in photocurrent [40]. The vertical optical absorption coefficients are connected to the fact that higher surface dipole moments move both the conduction and valence bands downward. Energy between NCs and polymers is improved by substituting long, insulating oleic acid and trioctylphosphine with smaller and more conductive BDT and EDT during synthesis. Last year, the improvement of efficiency for solar energy conversion led to an average rise of 3% in power conversion rates. In a different work, incorporating CDC_2–CDC_2-tetradecylphosphonic acid (TDPA) significantly raised device efficiency to 14.5%. The better transport of charges from the polymer to NCs was achieved mainly because of improved energy alignment. Using oleic acid and oleylamine to blend PbSe with polymers produced a short-circuit current of 5.6 mA and a VOC of 0.85 V, while just using oleic acid reduced the current to 4.1 mA and the voltage to 0.54 V. Both these outcomes are believed to result from better charge movement and larger numbers of NCs aligning well within the polymer matrix.

Table1 Both PbSe and PbSe-NCs are made stable by ligands in the PbSe and PbSe-type BHJ solar cells [44-51,55]

Ligand used during synthesis	The first ligand used before film deposition	The second ligand exchanged after film deposition
PbSe/Polymer Solar Cells		
Oleic acid	Butylamine	(I)1,2-ethanedithiol (EDT) (II), 3-mercaptopropionic acid (MPA) (III), malonic acid (MA) (IV), tetrabutylammonium iodide (TBAI)
Oleic acid	(I) leadiodide (II)ammoniumiodide (III)n-butylamine	
Oleic acid, trioctylphosphine (TOP)	BDT (benzothiophene)	EDT
Oleic acid	BDT	BDT
Oleic acid	BDT	

Oleic acid	BDT, oleylamines (OLA)	BDT, MPA, MA
Oleic acid	1-ethyl-3-methylimidazoliumiodide	(I)ammoniumacetate (II)PbX2 (Cl, Br, I)
Oleic acid	PbSe/ Polymer Solar Cells	tetradecylphosphonic acid
Oleic acid	OLA	Trioctylphosphine
Oleic acid	BDT	

Table 2. Data on Cell Parameters of PbSe Nanocrystal-Incorporated BHJ Solar Cells. [46-50]

Cell structure	**Jsc ($mAcm^{-2}$)**	**Voc (V)**	**FF (%)**	**PCE (%)**	**Year**
ITO/PEDOT-PSS/polymer-PbS/PbS/LiF/Al	13.49	0.55	57	4.23	2015
Si-PCPDTBT: PbS-PbI_2	18.2	0.48	55	4.78	2016
PEDOT:PSS :P3HT:P3HT-b-PS (0.7:0.3:20)	16.21	0.57	53.2	4.91	2021
PDPPTPT: PbSe-OA (10:90) wt.%	12.5	0.47	49	2.3	2012
PNDI-SH: PbS-QD (70:30)	7.29	0.83	58.71	3.64	2022

3. What users are worried about and what they expect

The examination finds that lead chalcogenide NCs show high performance in solar cells when paired with other materials. Overcoming big difficulties will be necessary for it to stay on par with popular photovoltaic methods. Tasks include optimizing the way electrons are carried from the polymer to the NCs in the device, improving its shape and performance, achieving uniformity in thin-film coating, modifying the exchange of outer layers on the NCs, and finding new organic molecules suited to optoelectronic purposes. Some of these problems are found in the literature already [3]. Since lead, a dangerous heavy metal, is often found in these solar cells, they still face restrictions in large-scale production. Even so, perovskite solar cells have inspired efforts to design materials similar to PbS, which have equal efficiency and can absorb light from a wider spectrum [2,3]. For hybrid solar cells to succeed, their

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cost must be competitive at the watt-peak (Wp) level. Printing on rolls, spraying material or blade coating at low temperature could efficiently generate many flexible hybrid devices at a low cost. Using these techniques, along with the similar energy payback periods of all three types, makes hybrid solar cells a great advantage. Even so, you can still count on your phone for only about two years which is a major problem. How well batteries hold up under real conditions of heat and light plays a big role in deciding their efficiency and how much they cost to use. The contact they have with other parts of the cell can eventually break down lead chalcogenide NCs. For this reason, researchers should work to improve our knowledge of photovoltaic operations and pin down why devices wear out, so that they can create devices that work more reliably. As shown in Tables 2 and 3, solar cells made with PbS and PbSe nanocrystals in a BHJ show high efficiency and important characteristics. Near-infrared detection is superb for perovskites, but there is limited research on them. Also, the PCEs in these hybrid BHJ solar cells are lower than both pure QD and completely polymer cells [64]. The results from various literature sources reveal that important factors, including ligand exchange, polymer-NC mix, and deposition method, all influence overall function. Even though BHJ solar cells could be both greatly efficient and stable, much work needs to be carried out by scientists. Continually improving the manufacturing process and minimizing errors are necessary to fully utilize what polymer-NC-based BHJ solar technologies can provide.

Table 3. Analysis of Cell Parameters in BHJ Solar Cells That Attach PbSe Nanocrystals. [53-56]

Cell structure	Jsc (mAcm^{-2})	Voc (V)	FF (%)	PCE (%)	Year
ITO/PEDOT: PSS/P3HT: PCBM: PbSe/Al	13.5	0.64	39.2	3.31	2021
ITO/PEDOT: PSS/PDTPBT/PbSe/LiF/Al	16.86	0.58	49.4	4.83	2015
ITO/PEDOT: PSS/MOPPV-PbSe/LiF/Al	3.661	0.23	27.7	0.277	2021
P3HT: PbSe-(OLA)	5.6	0.85	26	1.18	2021

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Conclusion

Lead chalcogenide nanocrystals, owing to their strong infrared response and broadly tunable optical bandgaps, have emerged as highly promising materials for next-generation photovoltaic systems. Their sensitivity to near-infrared light and ability to be integrated with organic polymers make them attractive candidates for hybrid polymer–nanocrystal (BHJ) solar cells. However, despite notable progress in understanding their synthetic chemistry, optical properties, and device performance, the practical implementation of these materials in large-scale solar technologies remains at an early stage. Although lead chalcogenide-based solar cells contain significantly less lead than conventional lead-acid batteries, ensuring safe synthesis, handling, encapsulation, and recycling is essential to minimize environmental risks. Future research should prioritize enhancing device stability and operational lifetime, developing scalable and low-cost fabrication methods, and employing environmentally benign materials without compromising efficiency. Comprehensive studies on charge transport mechanisms, degradation pathways, and interfacial engineering will be key to optimizing performance and ensuring sustainability. With continued innovation in material design and device architecture, polymer–lead chalcogenide hybrid solar cells hold strong potential to contribute meaningfully to the advancement of high-performance, eco-friendly photovoltaic technologies.

Data Availability

No primary research results, software or code have been included and no new data were generated or analysed as part of this review.

Conflicts of interest

There are no conflicts to declare.

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