



# Advances in Theoretical Calculation of Halide Perovskites for Photocatalysis

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Photocatalysis, which includes water splitting for hydrogen fuel generation, degradation of organic pollutants, and CO<sub>2</sub> reduction using renewable solar energy, is one of the most promising solutions for environmental protection and energy conversion. Halide perovskite has recently emerged as a new promising material for photocatalytic applications. The exploration of new efficient halide perovskite-based photocatalysts and understanding of photocatalytic reaction mechanisms can be revealed using theoretical calculations. The progress and applications of first-principles atomistic modeling and simulation of halide perovskite photocatalysts, including metal halide perovskites, halide perovskite heterojunctions, and other promising perovskite derivatives, are presented in this review. Critical insights into the challenges and future research directions of photocatalysis using halide perovskites are also discussed.

**Keywords:** first-principles calculations, photocatalysis, halide perovskites, density functional theory, heterojunctions

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## INTRODUCTION

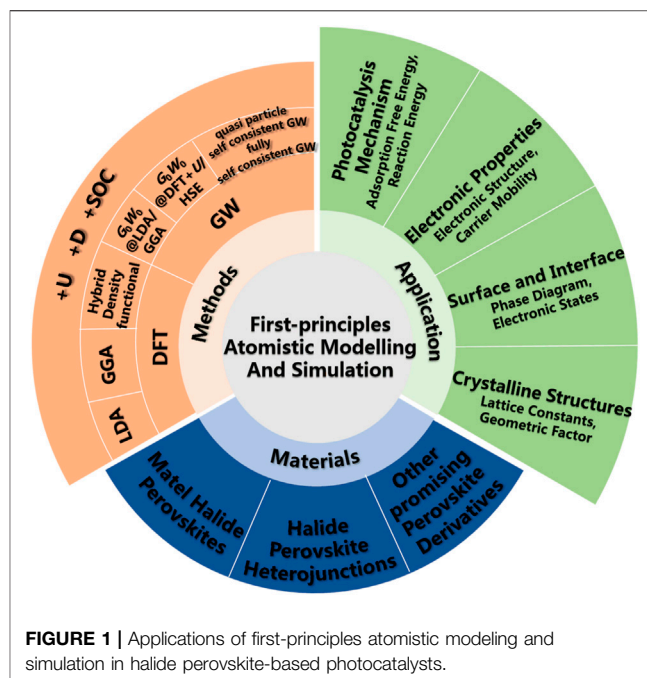
As sustainable, inexhaustible, clean, and renewable energy, solar energy has been considered an attractive alternative for applications of heating systems and electricity production in the past decades. Driven by solar energy, photocatalysis is considered one of the most important routes for using solar energy since the pioneering work on TiO<sub>2</sub> for water splitting in 1972 (Fujishima and Honda, 1972). Photocatalytic processes are applied in four fields: water splitting, CO<sub>2</sub> reduction, degradation of organic compounds, and organic synthesis. Semiconductors have been the most used photocatalysts because of their intrinsic optical and electronic properties, from conventional binary semiconductor photocatalysts (i.e., g-C<sub>3</sub>N<sub>4</sub>, TiO<sub>2</sub>, ZnO, CdS) (Yu et al., 2013; Jin et al., 2015; Ye et al., 2015; Adhikari et al., 2016; Cheng et al., 2018; Jaramillo-Páez et al., 2018; Yu et al., 2018) to ternary photocatalysts (i.e., BiVO<sub>4</sub>, SrTiO<sub>3</sub>, BaTi<sub>4</sub>O<sub>9</sub>) (Inoue et al., 1992; Kato and Kudo, 2002; Zeng et al., 2018; Andrei et al., 2020). However, conventional photocatalysts have drawbacks, such as large bandgap, high carrier recombination rate, and low light-absorption ability. It is critical to develop new photocatalysts with high photo-conversion efficiency.

Metal halide perovskites with a chemical formula of ABX<sub>3</sub> (A = CH<sub>3</sub>NH<sub>3</sub>, CH(NH<sub>2</sub>)<sub>2</sub>, Cs; B = Pb, Sn; X = I, Br, or Cl) have recently attracted extensive research attention because of their extraordinary photophysical properties and performance, such as high visible-light absorption coefficients, long charge carrier diffusion lengths, high photoluminescence quantum yield, tunable bandgap, etc (Park et al., 2016; Zhang et al., 2018a; Shi and Jayatissa, 2018). Furthermore, combined with a diversity of A and B sites and ferroelectric and piezoelectric effects (Frost et al., 2014; Kanhere and Chen, 2014; Sun et al., 2016; Ji et al., 2017; Zhu et al., 2019), ABX<sub>3</sub> halide perovskites are indubitably one of the most promising alternatives in photocatalytic applications (Zhu and Podzorov, 2015; Lee et al., 2018; Hong et al., 2019; Zhu et al., 2019; Chen et al., 2020).

First-principle atomistic modeling and simulation, such as density functional theory (DFT) and Green's function-based many-body perturbation theory (GW), are fundamental means to investigate material properties by inputting the initial lattice structure and known atomic information. The DFT method is a calculation method based on Hohenberg-Kohn theorem and Kohn-Sham equation (Hohenberg and Kohn, 1964; Kohn and Sham, 1965). When it comes to specific practical problems, it is necessary to consider several choices of exchange-correlation functional, such as Local Density Approximation (LDA), Generalized Gradient Approximation (GGA) and hybrid density functional method (Jones and Gunnarsson, 1989; Parr Robert, 1989).

LDA is mainly aimed at uniform electron gas, meaning that the charge density needs to change slowly in the order of local Fermi wavelength. In the calculation of Raman spectrum and phonon spectrum, LDA tends to a good performance. GGA optimizes the exchange-correlation and adds the gradient of charge density change to the exchange-correlation functional, giving more reasonable simulation results for heterogeneous electronic systems (Richard, 2004; Jiang et al., 2010). The commonly used GGA functionals are Perdew-Burke-Ernzerhof (PBE) (Kresse and Joubert, 1999) and Perdew-Wang (PW91) (Blöchl, 1994). However, GGA ignores the nonlocality of exchange, which usually underestimates the band gap. Therefore, hybrid density functional method is developed, which can improve the calculation accuracy based on the exact exchange energy obtained by Hartree-Fock approximation and the partial exact exchange energy obtained by mixed density functional theory. The commonly used methods are Heyd-Scuseria-Ernzerhof (HSE), PBE0, etc. (Perdew et al., 1996; Heyd et al., 2003) In addition, there are not only correction methods for electronic correlation (Grimme et al., 2010; Cao et al., 2012), such as dispersion interaction correction (DFT +  $D$ ), self-interaction correction (DFT +  $U$ ), but also correction methods for magnetic materials such as Spin orbit coupling (SOC) (Afsari et al., 2017; Sehgal, 2017).

GW method provides a more rigorous theoretical framework for the theoretical description of the electronic energy band structure of materials, which can give high-precision theoretical predictions for physically simple semiconductor materials, such as  $G_0W_0$  method based on LDA/GGA self-consistent calculation (Aryasetiawan and Gunnarsson, 1998; Aulbur et al., 2000). However, there is still much room for improvement for physically more complex systems with stronger electronic correlation effects, because LDA/GGA often gives wrong description, which can lead to the wrong calculation of  $G_0W_0$  (Aryasetiawan and Gunnarsson, 1995; Jiang, 2010; Jiang and Zhang, 2020). Many new methods have been developed to choose an appropriate starting point to calculate the reference Hamiltonian, such as  $G_0W_0$  based on DFT +  $U$  or HSE (Miyake et al., 2006; Jiang et al., 2010), or quasi particle self-consistent GW, and fully self-consistent GW (van Schilfgaarde et al., 2006; Grumet et al., 2018). Among the above-mentioned methods, GGA-PBE in DFT calculation method is the most commonly used and inexpensive calculation method, because it does not cost so much computational power, while



**FIGURE 1** | Applications of first-principles atomistic modeling and simulation in halide perovskite-based photocatalysts.

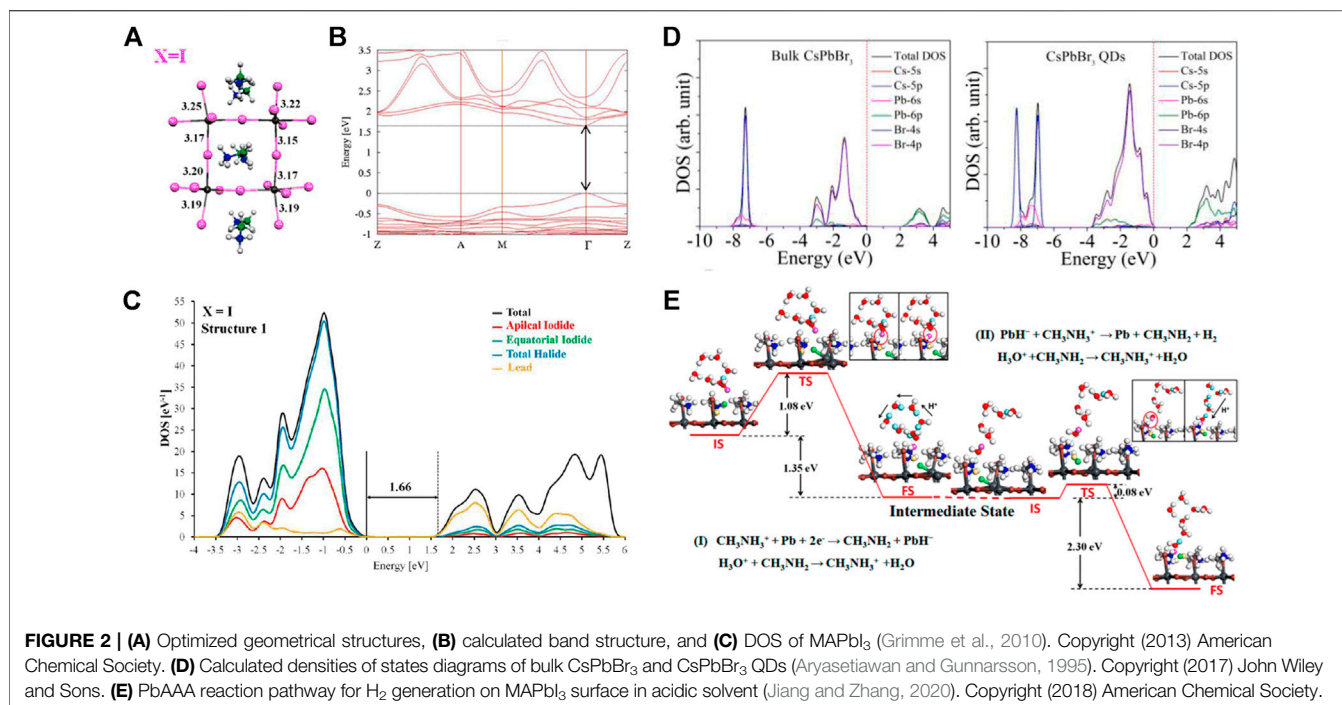
HSE and GW methods are more suitable for dealing with band gap calculation, and there are some problems such as complex program implementation and large amount of calculation.

First-principle methods can be used to explore the lattice constants, electronic structures, carrier mobility and diffusion lengths of photocatalyst, understand the reaction mechanism, and further predict new halide perovskite-based photocatalyst (Catlow et al., 2010; Luo and Daoud, 2015; Yu, 2019). The calculation of these properties is critical for optimizing the photocatalytic performance. Thus far, there has been limited research regarding the booming use of first-principles calculations to study halide perovskites as photocatalysts. Herein, we summarize the recent progress in the theoretical calculation study on halide perovskite-based photocatalysts (Figure 1), and focus on the link between calculated material properties and performance of photocatalysts, including 1) metal halide perovskites, 2) halide perovskite heterojunctions, and 3) other promising perovskite derivatives. Then, we discuss the challenges and future research directions of halide perovskite photocatalysis.

## THEORETICAL CALCULATION OF PROPERTIES OF HALIDE PEROVSKITE-BASED PHOTOCATALYSTS

### Metal Halide Perovskites

As is well known, for the  $ABX_3$  perovskites, the  $BX_6$  octahedra can be tilted and distorted at finite temperature or pressure (Glazer, 1972), and anharmonic effects are associated with the perovskite-phase transition (Buckeridge et al., 2013). Moreover, the bandgap of  $ABX_3$  perovskites can be tuned by chemical substitution (Sutton et al., 2016; Wang et al., 2019a). Several first-



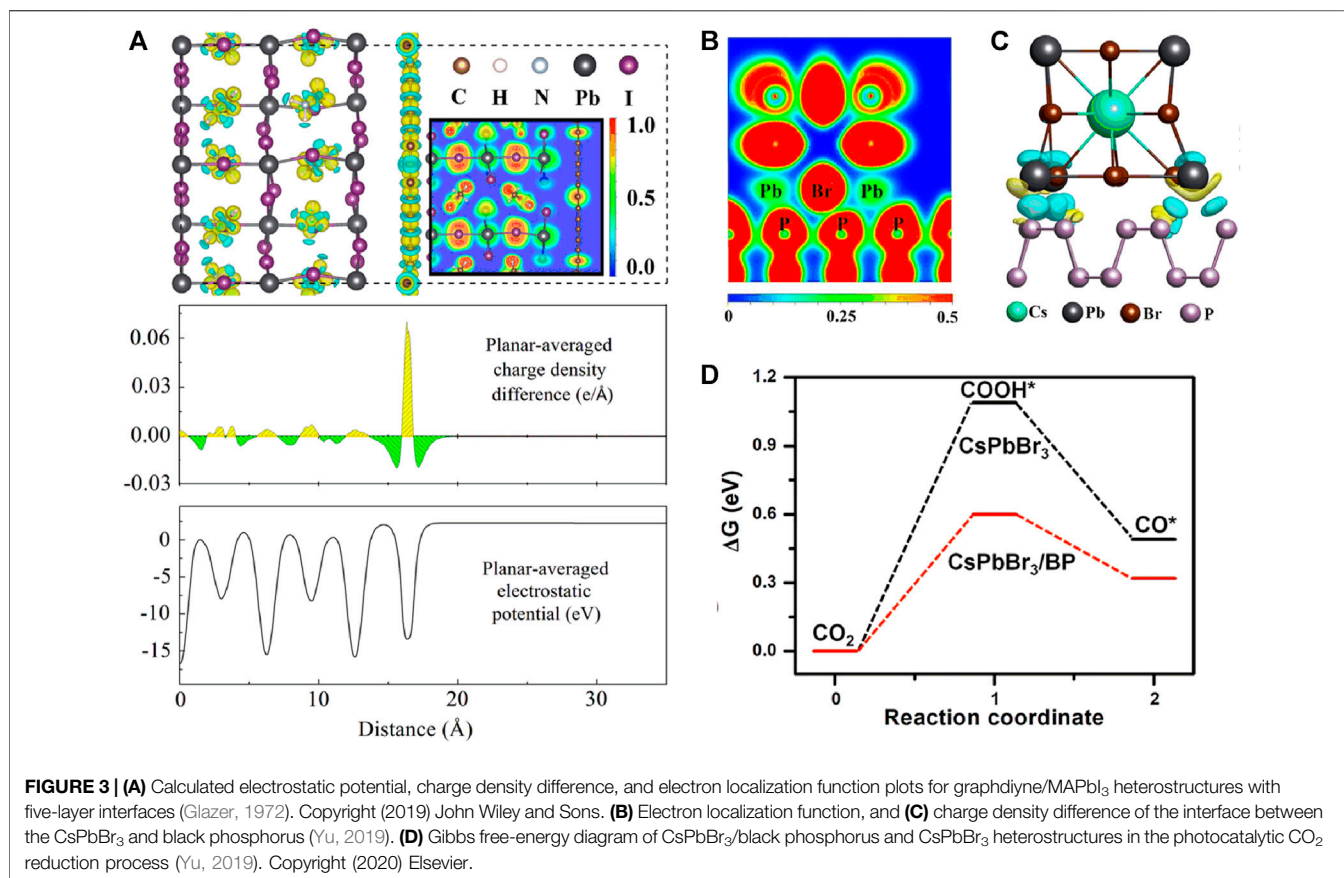
principles investigations into  $ABX_3$  structures have been conducted to explore their crystal structures, material stability properties, and defect physics. Most notably, the electronic and optical properties of  $ABX_3$  perovskite as light absorbers in photocatalysis are critical, and several theoretical calculation studies have focused on the electronic energy-band structure, corresponding density of states (DOS), carrier mobility, and other electronic properties of halide perovskite-based photocatalyst.

One of the critical properties of a photocatalyst is its bandgap. Considering the utilization of visible light in the sunlight, the bandgap of  $\sim 2$  eV is desirable for photocatalytic reaction (Xiaobo et al., 2010). In addition, for CO<sub>2</sub> reduction, the position of conduction band minimum (CBM) should be lower than  $-0.52$  eV (vs. NHE PH = 0) (the energy barriers of reducing CO<sub>2</sub> to CO) (Kanhere and Chen, 2014; Schneider et al., 2012), that is more advantageous to the reduction reaction in thermodynamics. Angelis et al. first computationally investigated the MAPbX<sub>3</sub> hybrid halide perovskites in 2013 (Mosconi et al., 2013). They performed periodic DFT calculations within the GGA and found that the calculated bandgap values (MAPbI<sub>3</sub>:  $E_g = 1.57$  eV, MAPbBr<sub>3</sub>:  $E_g = 1.80$  eV, MAPbCl<sub>3</sub>:  $E_g = 2.34$  eV) agreed well with the experimental values. **Figures 2A–C** shows the optimized geometrical structures, calculated band structure, and DOS of MAPbI<sub>3</sub>. Afterward, Umari developed an effective GW method incorporating SOC to accurately model the electronic properties of MAPbI<sub>3</sub> and MASnI<sub>3</sub> (Umari et al., 2014). Furthermore, the HSE06 and PBE functionals, with and without SOC calculations, were used to compute the bandgap of  $ABX_3$  halide perovskites (Giorgi et al., 2013; Brivio et al., 2014; Melissen et al., 2015). By comparing the calculated values, it is proved that the strong electron-hole interaction should consider, and the SOC plays a

critical role in dominating the conduction band, although the computational requirements increase.

Moreover, the DOS can also be used to predict the performance of photocatalysts through the analysis of total and atomic-resolved DOS. The DOS can be obtained from a non-self-consistent-field (SCF) energy-band calculation, and from the analysis of the partial DOS, the contribution of each site to the valence band and conduction band can be revealed. For  $ABX_3$  halide perovskites, the CBM is usually dominated by B  $p$ -states, whereas the valence band maximum (VBM) consists of antibonding between B  $s$ -states and X  $p$ -states (Borriello et al., 2008; Chung et al., 2012; Mosconi et al., 2013; Umari et al., 2014). Furthermore, the photogenerated carrier transfer ability can be revealed by the calculated DOS. Sun et al. synthesized colloidal CsPbBr<sub>3</sub> quantum dots (QDs) as new photocatalytic material (Hou et al., 2017). To understand the advantages of the quantum size effect, they calculated the DOS of bulk CsPbBr<sub>3</sub> and atomic CsPbBr<sub>3</sub> QD slabs. Different from the bulk CsPbBr<sub>3</sub>, the conduction band of CsPbBr<sub>3</sub> QDs was primarily contributed by the coupling of Cs  $p$ -states, Br  $p$ -states, and Pb  $p$ -states, whereas the valence band was constructed by the coupling of Cs  $p$ -states, Pb  $s$ -states, and Br  $p$ -states (as shown in **Figure 2D**). Due to the increased DOS at CBM, more photogenerated carriers can reach CBM, resulting in more efficient photochemical conversion.

The last, but the most important issue is the photocatalytic mechanism. Metal halide perovskites have been successfully confirmed as efficient photocatalysts. However, it is difficult to develop improved perovskite materials without a thorough analysis of reaction mechanisms. Wang et al. derived the photocatalytic hydrogen evolution reaction (HER) mechanism using PBE functional of DFT, including the D3 van der Waals



correction to account for London dispersion interactions (Zhang et al., 2018b). They constructed a supercell of the (010) surface of MAPbI<sub>3</sub> in HI aqueous solution, and by comparing the activation barriers and reaction energies of different reaction pathways, they found that the Pb atoms and surface organic molecules play critical roles in the HER reaction. Furthermore, a two-step Pb-activated amine-assisted (PbAAA) reaction mechanism was proposed (Figure 2E), which is widely accepted and approved. Tao et al. performed the DFT calculations with the PbAAA mechanism to explain the Br effect on the enhanced performance of the MAPb(I<sub>1-x</sub>Br<sub>x</sub>)<sub>3</sub> photocatalytic HER process (Zhao et al., 2019a). Due to the smaller Br ionic radius, the Br-Pb bonds can be easily broken, and more Pb defect sites were formed for lowering the H-Pb absorption energy, and thus MAPb(I<sub>1-x</sub>Br<sub>x</sub>)<sub>3</sub> shows a superb HER rate under visible light illumination.

### Halide Perovskite Heterojunctions

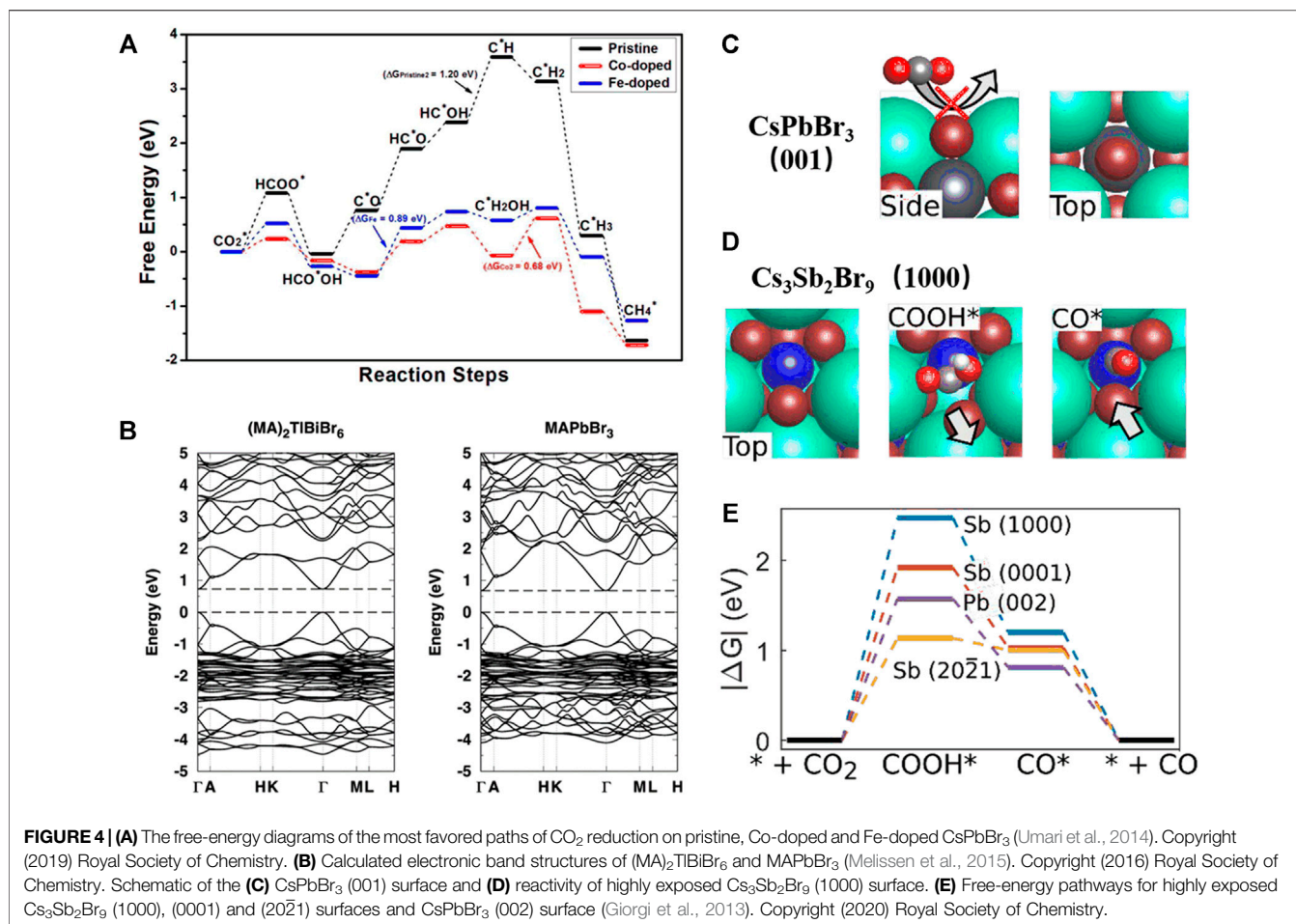
To enhance the photocatalytic performance, the construction of halide perovskite heterojunctions with two-dimensional (2D) materials such as graphene, g-C<sub>3</sub>N<sub>4</sub>, and black phosphorus has caused extensive concern due to improved stability, more efficient carrier mobility, and regulated bandwidth (Xu et al., 2017; Ou et al., 2018; Wu et al., 2018; Zhao et al., 2019b; Guo et al., 2019; Paul et al., 2019; Wang, 2020). For the heterojunction calculations, the main problem is the understanding of the

charge density difference and charge transfer process at the contacting interface.

Guo et al. used density-functional first-principles calculations with empirical dispersion corrections to investigate the interfacial interactions and electronic properties of graphdiyne/MAPbI<sub>3</sub> heterostructures (Guo et al., 2019). By employing the projector-augmented wave (PAW) to describe the electron-core interaction, and GGA of PBE as the exchange-correlation functional, they found that the graphdiyne/MAPbI<sub>3</sub> heterostructure was formed by van der Waals interaction, and the PbI<sub>2</sub>-terminated surface showed high stability when contacting graphdiyne. Combining HSE06 with SOC, the electronic properties including charge density difference, electron localization field, Bader charge, and electrostatic potential were analyzed, as shown in Figure 3A. The electron-hole separation is obviously enhanced due to the built-in electric field at the interface.

In addition to the van der Waals interaction of the heterostructure interface, Zhu et al. found that a significant covalent bond between CsPbBr<sub>3</sub> and black phosphorus nanosheets was formed in the heterostructure by DFT calculation (Wang, 2020). Moreover, charge density difference analysis revealed that a directional electron transfer channel was generated reasonably between Pb and p elements, as shown in Figure 3B,C which was consistent with the experimental results. Furthermore, using *ab initio* atomistic thermodynamics





calculations, the possible mechanism of CO<sub>2</sub> reduction by CsPbBr<sub>3</sub> and black phosphorus nanosheet heterostructure was clarified. The black phosphorus nanosheets acted as the electron acceptor, which promoted the breaking of the C=O bonds and reduced the reaction barrier energy (Figure 3D).

### Other Promising Perovskite Derivatives

The exploration of new photocatalysts is an important way to achieve high photocatalytic performance. And the new promising halide perovskites offer distinct advantages over the traditional perovskite materials (Volonakis et al., 2016; Liu et al., 2018; Maughan et al., 2018; Yan et al., 2018; Tang et al., 2019; Yue et al., 2020), such as substitution or mixing, double perovskites, and other perovskite derivatives. Theoretical calculation is a powerful tool to predict new functional perovskite materials suitable for photocatalysis and optimize the stoichiometric ratio of mixed halide perovskites. Especially when introducing the Goldschmidt tolerance factor  $t = (r_A + r_X) / [\sqrt{2} (r_B + r_X)]$  (where  $r_A$ ,  $r_B$  and  $r_X$  refer to ionic radii for ions in A, B and X sites) (Goldschmidt, 1926), a useful parameter for basic formability prediction of any new materials with targeting perovskite structure, into the first-principle calculations, many studies have selected several promising perovskite

materials from hundreds of compounds (Bartel et al., 2020; Fedorovskiy et al., 2020).

Xu et al. compared the catalytic efficiency of bulk CsPbBr<sub>3</sub> doped with different metals (Co, Fe, Ni, Cu, Ag, Mg, Mn, and Bi) and concluded that Co- and Fe doping could be ideal for CO<sub>2</sub> reduction (Tang et al., 2019). They specifically analyzed the adsorption-free energy using GGA of PBE functional with the PAW method. As shown in Figure 4A the *ab initio* molecular dynamics calculations indicated that Co- and Fe-doped systems showed stronger CO<sub>2</sub>\* adsorption energy (\* refers to the adsorption site), which is the most important factor to determine the catalytic efficiency. Furthermore, using HSE06 with DFT + U correction to calculate the Hirshfeld charges and DOS of the strongly correlated effect of Co atoms, they further illustrated the proposed reaction mechanism and confirmed that Co-doped CsPbBr<sub>3</sub> could be a great candidate for CO<sub>2</sub> reduction.

The toxicity of lead limits the wide commercialization of metal halide perovskite, and thus lead-free alternatives have recently attracted great attention, such as double perovskites (A<sub>2</sub>BX<sub>6</sub> or A<sub>2</sub>B<sup>+1</sup>B<sup>+3</sup>X<sub>6</sub>) and other perovskite derivatives (A<sub>3</sub>B<sub>2</sub>X<sub>9</sub>, A<sub>3</sub>BX<sub>5</sub>, A<sub>4</sub>BX<sub>6</sub>, etc.), where Pb<sup>2+</sup> cations are replaced using other metal cations, e.g., Na<sup>+</sup>, Ag<sup>+</sup>, Bi<sup>3+</sup>, and Sb<sup>3+</sup>. It is relatively difficult to experimentally synthesize thin films of these materials for

photovoltaic and photocatalysis applications. However, the theoretical calculation is extremely useful because of its predicting power. For example, Cheetham et al. have used DFT calculations to compare the bandgaps and electronic structures of  $(MA)_2B^{+1}BiX_6$  ( $B^{+1} = e.g., K^{+1}, Ag^{+1}, Cu^{+1}, TI^{+1}$ ) and  $MAPbX_3$ , and found that the new double perovskite  $(MA)_2TL^{+1}BiBr_6$ , had strikingly isoelectronic properties with  $MAPbBr_3$ , as shown in **Figure 4 2**) (Deng et al., 2016). This study provided an intriguing alternative to the lead-containing  $MAPbX_3$  for photoelectronic applications.

For the all-inorganic halide double perovskites, Giustino et al. (Volonakis et al., 2017) proposed a new promising halide double perovskites,  $Cs_2InAgX_6$ , with the direct band gaps between the visible and the ultraviolet as computed by the HSE06 and PBE0. Recently, Bartel et al. (Bartel et al., 2020) predicted 47 likely synthesizable compounds containing non toxic elements and with direct or nearly direct band gaps among the 311 cesium chloride double perovskites ( $Cs_2BB'Cl_6$ ) compounds by computing with HSE06, and identified that the triple-alkali perovskites (where  $B$  refers to a group 1 alkali, and  $B'$  refers to a transition-metal cation) showed remarkable optical properties as computed by the  $GW$ -Bethe-Salpeter equation method. These studies are helpful to realize the future studies aim and synthesize more efficient photocatalyst with unique optoelectronic properties.

Besides the analyses of the structural, electronic and optical properties, first-principles calculations can also be used to predict phase transition temperatures, which have instructive significance on the exploration of new materials. Kye et al. calculated the bandgaps and optical properties of  $K_2SnX_6$  ( $X = I, Br, Cl$ ) in cubic, tetragonal, and monoclinic phases, and concluded that the cubic  $K_2SnBr_6$  and monoclinic  $K_2SnI_6$  can be promising candidates for light absorber materials (Jong et al., 2020). Moreover, they calculated the Helmholtz-free-energy differences among the above three phases, and gave the phase transition temperatures of  $K_2SnX_6$ , respectively.

As mentioned above, it is difficult to experimentally synthesize uniform thin films of double perovskites or other perovskite derivatives; however, nanocrystals or other nanostructures of these materials can be synthesized more easily. Furthermore, they are proved to be promising candidates because of their highly exposed surface. Geyer et al. developed  $Cs_3Sb_2Br_9$  nanocrystals with significantly improved photocatalytic CO production efficiency (Lu et al., 2020). Moreover, the analogous mechanism was observed using DFT calculations, as shown in **Figures 4C–E**. They calculated the surface energies and adsorption free energies of the (0,001) (1,000), and (20 $\bar{2}$ 1) surfaces of  $Cs_3Sb_2Br_9$ , as well as the (001) and (002) surfaces of  $CsPbBr_3$ , and found that the surfaces of  $Cs_3Sb_2Br_9$  had a lower free-energy for the adsorption of  $COOH^*$  and  $CO^*$  intermediates because of the predominant defects, which suggested the enhanced catalysis activity.

As mentioned above, perovskite heterojunctions are usually endowed with optimized charge carrier dynamics for improved photocatalytic performance, and perovskite derivative heterojunctions are no exception (Feng et al., 2017; Guo et al., 2017; Wang et al., 2019b). By employing the DFT calculation,

Kuang et al. (Wang et al., 2019b) investigated the electronic structures and interfacial properties in the  $Cs_2SnI_6/SnS_2$  hybrid heterojunctions. Then, they revealed that a typical type II band alignment formed in the heterojunction, which was in accordance with the experimental values. Due to the facilitated charge separation between  $Cs_2SnI_6$  and  $SnS_2$  (i.e., holes from  $SnS_2$  to  $Cs_2SnI_6$  and electrons from  $Cs_2SnI_6$  to  $SnS_2$ ), the  $CO_2$  photocatalytic reduction activity was unquestionably boosted.

We believed that the theoretical calculation of perovskite derivatives and heterojunction can help predict more direct or nearly direct band-gap materials and choose some more matching materials forming heterojunction with promoted the charge carrier mobility and reduced charge carrier recombination.

## CONCLUSION AND OUTLOOK

Herein, we summarized current computational work on the halide perovskite-based photocatalyst. To reveal the underlying photocatalytic mechanisms, first-principles calculations were used to investigate the crystal structures, electronic properties, defect physics, and surface and interface interaction of perovskites. Furthermore, the promising potential of the first-principles material design for predicting new halide perovskites such as substitution or mixing, double perovskites, or other perovskite derivatives has also been demonstrated.

From our perspective, several critical issues and challenges still need to be overcome. First, several unique properties of halide perovskites, such as piezoelectric, and ferroelectric properties due to the anharmonicity in lattice dynamics should be illustrated and explored to promote the photocatalytic reaction efficiency. Second, the influence of structure on the photocatalytic performance of halide perovskite-based heterojunctions, such as the types of ligands, defects, dopants, and crystalline phases, needs to be further researched to improve the activity of the heterostructures. Third, theoretical analytical models of perovskite derivatives can be helpful to promote the charge carrier mobility and reduce charge carrier recombination.

## AUTHOR CONTRIBUTIONS

XL proposed the research idea and manuscript; JF and CH performed check collection, collation and analysis; All authors reviewed the manuscript, have given approval to the final version of the manuscript, and confirmed the authorship to this work.

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**Conflict of Interest:** The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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