On topological materials as photocatalysts for water splitting by visible light

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Keywords: topological materials, water splitting, photocatalyst

Abstract

We performed a virtual materials screening to identify promising topological materials for photocatalytic water splitting under visible light irradiation. Topological compounds were screened based on band gap, band edge energy, and thermodynamics stability criteria. In addition, topological types for our final candidates were computed based on electronic structures calculated using the hybrid density functional theory including exact Hartree–Fock exchange. Our final list contains materials which have band gaps between 1.0 and 2.7 eV in addition to band edge energies suitable for water oxidation and reduction. However, the topological types of these compounds calculated with the hybrid functional differ from those reported previously. To that end, we discuss the importance of computational methods for the calculation of atomic and electronic structures in materials screening processes.

1. Introduction

Hydrogen is widely regarded as the energy carrier of the future [1]. The methods for generating what is called green hydrogen [2] from sunlight resemble the natural process of photosynthesis by green leaves, where sunlight energy is used to convert water and carbon dioxide into oxygen and carbohydrates [3, 4]. Inspired by natural photosynthesis, solar water splitting devices for the dissociation of water into hydrogen and oxygen are now being designed [5]. Among the various techniques for the production of hydrogen based on water splitting [6, 7], photoelectrochemical (PEC) [8] water splitting is viewed as a promising solar-to-hydrogen pathway by which photons from sunlight can be converted into chemical energy. Depending on the PEC cell configuration, one electrode or both electrodes can act as a photoactive electrode [9].

Finding suitable materials as photoelectrodes for PEC water splitting is a challenge. Photoactive electrodes in PEC devices need to satisfy several requirements such as proper band gap size, correct band edge energies with respect to the water redox levels, long charge carrier lifetime, and fast charge carrier transport, as well as chemical and photo stability [10–16]. A large band gap (UV light-responsive) photocatalyst, such as TiO$_2$, guarantees the generation of high energy irradiation-excited charge carriers to drive the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) [17, 18]. However, the visible light absorption efficiency of a large band gap photoelectrode is low, limiting the solar-to-hydrogen conversion efficiency [7, 19]. It is worth mentioning that UV light (<400 nm) comprises a small fraction of solar radiation, while visible light accounts for more than 40% of solar radiation.

The surface electronic structure of the electrodes plays an important role in (photo)electrochemical water splitting reactions [20]. For example, surface contamination might alter surface states and lead to inactive electrodes. In this respect, the remarkable electronic structure of topological materials (TMs) are of great interest [21]. The topologically protected surface states of topological insulators (TIs) are robust against nonmagnetic impurities and disorders [22]. In addition, elastic backscattering is forbidden and electron transport is spin-momentum locked [23], which may improve charge transfer in (photo)electrochemical...
reactions. The use of TMs in catalytic reactions, either as substrates to enhance the activity of overlaying catalysts or directly as electrocatalysts and photocatalysts, has been shown to be promising [24–31].

Specifically, He et al [32] proposed topological metals to be utilized in the HER process to reduce the metal hydride effect. In addition, transition-metal dichalcogenide 1T*-MoTe2 single crystal was found to be an excellent candidate for the HER [33]. Recently, Qu et al [28] found that Bi2Te3 thin films exhibit high electrocatalytic activity in the HER. Through density functional theory (DFT) calculations, they showed that Bi2Te3 thin films with partially oxidized surfaces or Te vacancies have a higher HER activity compared to defect-free Bi2Te3 thin films [28]. It has also been shown that topological semimetals such as VAl and NbP are promising catalysts for the HER [25, 29, 34]. In addition, the photocatalytic HER has been demonstrated with Bi chalcogenide-based TIs such as Bi2Te3 [26]. It is noted that Bi2Te3 is a semiconductor with a band gap of about 0.35 eV, therefore its visible light absorption efficiency cannot be high.

In this work, we performed a systemic search to find photoelectrodes for photocatalytic water splitting. We asked ourselves whether virtual materials screening can identify TMs that have suitable characteristics for PCE water splitting. It is a relevant question considering the time and effort needed for the development of such materials based on trial and error [35]. With advances in computational techniques and the development of open databases, virtual materials screening is becoming a powerful approach for rapid materials development [36–52]. For example, search algorithms based on high-throughput (HT) calculations have been developed to identify TMs recently [53–56]. The results of these HT calculations are available in open databases [54–57] and can be used for virtual materials screening. Previously, we have performed computational materials screening to identify wide band gap semiconductors for optoelectronic applications [58–61]. Here, we performed materials screening for the compounds available in the TMs database (TMDB) [55, 57] to find appropriate TMs for use as photoactive electrodes for PEC water splitting under visible light.

2. Computational details

Electronic structure calculations were performed in the context of DFT using the projector augmented wave method as implemented in the Vienna Ab initio Simulation Package (VASP) [62, 63]. An energy cutoff of 520 eV and a k-point mesh of 500/number of atoms were used for all systems. The atomic positions and cell parameters of bulk structures were relaxed until the residual force on each atom was smaller than 1 meV Å−1. For accurate electronic structure calculations, the Heyd-Scuseria-Ernzerhof screened-exchange hybrid functional (HSE06) [64, 65] was used, which is a hybrid functional that includes 25% of exact Hartree–Fock exchange and has been shown to give good results for many systems [66].

To calculate band edge energies, the HSE06 band structures were processed by matminer [67] to compute the branch point energy [68]. Spin–orbit coupling (SOC) was taken into account self-consistently by the second variation method [69]. Job submission and result collection were done automatically using atomate [70], which is built on top of pymatgen [71], custodian, and FireWorks [72]. Details of all compounds were retrieved from the materials project database (MPDB) [73, 74], which makes its data available through the open materials application programming interface (API).

3. Results and discussion

We applied our screening criteria to TMs that are available in the TMDB [55, 57]. Although the TMDB has no API, each compound in the TMDB is linked to an entry in the MPDB. Hence, we were able to retrieve computed properties of compounds from the MPDB. All compounds that are labeled as SEBR for ‘split elementary band representations’ and NLC for ‘no linear combination of elementary band representations (LCEBR)’ were considered. In the first step of screening, which was based on the band gap, we selected topological compounds that have band gaps smaller than 3.0 eV. In addition, a criterion of $E_{\text{branch}} < 100$ meV atom$^{-1}$ was applied for thermodynamic stability. Out of 4076 TMs (retrieved in September 2020), 483 compounds satisfied our thermodynamic stability and band gap criteria. We note in passing that stability under working conditions was not considered here. Furthermore, compounds that contain magnetic elements and/or f-electron atoms were removed from the list following the pre-filtering procedure mentioned in reference [55]. In addition, we discarded compounds that contain hazardous elements like As, Pd, Cd, and Hg. Lastly, compound with more than one topological type in the TMDB were discarded.

In the second step of screening based on the band gap, only compounds with band gaps between 1.0 and 3.0 eV calculated with HSE06 + SOC were selected. To be able to perform electronic structure calculations with an hybrid functional including exact Hartree–Fock exchange, compounds containing more than 20 atoms in the primitive unit cell were discarded. The compounds that fulfilled the above-mentioned criteria are listed in table 1.
Table 1. List of final compounds and their band gaps calculated with the HSE06 hybrid functional including SOC. The atomic structures were retrieved from the MPDB and were fully relaxed. Topological types were retrieved from the TMDB, i.e. topological types were calculated with the semi-local PBE functional for the atomic structures retrieved from the ICSD.

| Compound       | MP ID     | Space group | Band gap (eV) | Topological type |
|----------------|-----------|-------------|---------------|------------------|
| CsGeBr$_3$     | mp-570223 | Pm3m        | 1.0           | SEBR             |
| ZnAg$_2$Sn$_4$I | mp-1079889| I42m        | 1.4           | SEBR             |
| Rb$_3$Sn$_4$Au | mp-17401  | Pmmn        | 1.0           | NLC              |
| CsTi$_2$Cl$_7$ | mp-505663 | P2$_1$/m    | 2.7           | NLC              |
| SrCuSeF        | mp-21228  | P4/nmm      | 2.4           | NLC              |

Figure 1. Band structures of (a) CsGeBr$_3$, (b) ZnAg$_2$Sn$_4$I, (c) Rb$_3$Sn$_4$Au, and (d) SrCuSeF calculated with the HSE06 hybrid functional.

In the next step of our materials screening, band edge energies were considered. The primary requirement to realize photocatalytic water splitting is that the water redox levels must lie between the band edges of a photocatalyst. That is, the conduction band minimum should be higher than the energy level for the HER and the valence band maximum should be lower than the OER energy level. The band edge energies for our compounds were calculated with the HSE06 hybrid functional (see figure 1) and compared with those of anatase TiO$_2$ (mp-390) [75–77] (see figure 2). It can be concluded from figure 2 that while all compounds have favorable band alignment for water oxidation, only the band edge energies of CsTi$_2$Cl$_7$ are good for the overall water splitting process. Moreover, the conduction band minimum of SrCuSeF is sufficiently close to the energy level for the HER to be considered as a photocatalyst for water reduction. It should be noted that narrow band gap semiconductors (<2 eV) are usually only suitable for either the HER or the OER and they can be used in tandem PCE water splitting devices [9, 75, 78].

In the next step, the topological types for the compounds listed in table 1 were computed, as described by Vergniory et al [79]. It is noted that the topological analysis of compounds available in the TMDB is based on electronic structures calculated with the semi-local Perdew–Burke–Ernzerhof (PBE) functional [80]. It is likely that computing electronic structures with a different exchange and correlation (XC) functional changes the energies of states and consequently the band topology of the occupied bands. Therefore, we recalculated the topological types of our compounds with the ‘check topological magnetic mat’ script [81, 82] available on the Bilbao Crystallographic Server [83, 84]. For band structures calculated with the HSE06 hybrid functional, we employed vasp2trace version 1.1 [55, 85]. We note in passing that we did not calculate the topological type if the ground state of a compound converged to a magnetic state (indicated by ‘—’ in tables).
First, we calculated the topological types for the atomic structures that were retrieved from the TMDB. As can be seen from the tabulated results in table 2, the topological types computed based on the semi-local DFT employing the PBE functional are in quantitative agreement with TMBD data. The topological types based on the more accurate HSE06 hybrid functional, however, differ qualitatively from TMBD data. In particular, the topological types of CsGeBr$_3$ and ZnAg$_2$SnS$_4$ turned into LCEBR when computed at the HSE06-based hybrid DFT level. Furthermore, our hybrid DFT calculations predicted the ground states of CsTi$_2$Cl$_7$ and SrCuSeF to be magnetic with non-negligible magnetic moments, whereas the semi-local PBE-computed ground states of all compounds listed in table 2 are nonmagnetic. It is well known that generalized gradient approximations to the XC potential cannot accurately describe the electronic and magnetic properties of semiconductors [86, 87]. Therefore, we believe that the true topological nature of these compounds cannot be predicted with semi-local XC functionals and at least hybrid DFT including exact Hartree–Fock exchange, or even more accurate electronic structure methods must be employed.

Moreover, we observed that the calculated residual forces on individual atoms were high for some structures retrieved from the TMDB, suggesting that those atoms are not at their respective nuclear ground state. For example, the residual forces on the Rb atoms of Rb$_3$Sn$_4$Au before geometry optimization were about 26 eV Å$^{-1}$. Therefore, we did not calculate the topological type for the atomic structure of Rb$_3$Sn$_4$Au retrieved from the TMDB (indicated by ** in table 2). Instead, we computed the topological types for atomic structures after geometry optimization. Specifically, two types of optimization calculations were performed: either all atomic positions were optimized (geometry optimization) while the cell volume and shape were kept constant or all atomic positions as well as the cell volume and shape were concurrently optimized (geometry and cell optimization). The computed topological types for the optimized structures are summarized in tables 3 and 4. It should be mentioned that after geometry optimization the magnetic ground states calculated via semi-local PBE-DFT remained the same, i.e. nonmagnetic. The corresponding ground states of optimized structures calculated with the HSE06 hybrid functional converged to nonmagnetic states except for CsTi$_2$Cl$_7$ after geometry and cell optimization.
Table 3. List of final compounds and their calculated topological types. The atomic structures were retrieved from the TMDB, and the atomic positions were relaxed with the semi-local PBE functional.

| Compound   | Space group | Lattice parameters (Å) | Topological type |
|------------|-------------|------------------------|------------------|
| CsGeBr₃    | Pm3m        | 5.360, 5.360, 5.360    | SEBR             |
| ZnAg₂SnS₄ | I42m        | 6.786, 6.786, 6.786    | LCEBR            |
| Rb₃Sn₄Au  | Pmmn        | 6.558, 7.147, 13.081   | LCEBR            |
| CsTi₂Cl₇  | P2₁/m       | 6.354, 11.630, 7.280   | LCEBR            |
| SrCuSeF    | P4/nmm      | 4.063, 4.063, 8.842    | LCEBR            |

Table 4. List of final compounds and their calculated topological types. The atomic structures were retrieved from the TMDB and followed by a geometry and cell optimization by means of semi-local PBE-DFT. ‘—’ means that the ground state of the compound is magnetic.

| Compound   | Space group | Lattice parameters (Å) | Topological type |
|------------|-------------|------------------------|------------------|
| CsGeBr₃    | Pm3m        | 5.360, 5.360, 5.360    | SEBR             |
| ZnAg₂SnS₄ | I42m        | 7.276, 7.276, 7.276    | LCEBR            |
| Rb₃Sn₄Au  | Pmmn        | 6.718, 7.166, 13.464   | LCEBR            |
| CsTi₂Cl₇  | P2₁/m       | 6.847, 11.310, 7.767   | LCEBR            |
| SrCuSeF    | P4/nmm      | 4.095, 4.095, 8.907    | LCEBR            |

One notices from the results listed in tables 3 and 4 that the topological types of the compounds varied after geometry or geometry and cell optimization, except for CsGeBr₃, whose atomic structure did not change upon optimization. Specifically, the topological types of the initially determined TMs listed in table 1 turned into LCEBR after geometry or geometry and cell optimization. This observation, which is independent of the particular XC functional we have employed here, immediately suggests that the calculated topological types depend rather sensitive on the atomic structure [88]. In addition, as already alluded to above, a material that is predicted by the semi-local PBE functional to be topological might turn into a different topological type when its electronic structure is computed with hybrid DFT. In fact, since XC functionals within the generalized gradient approximation typically underestimate the band gap, they have the tendency to artificially favor band inversion that is a necessary condition for a TM. This is to say that the usage of conventional semi-local DFT overestimates the abundance of materials that are topological [55], which is consistent with the present findings.

4. Conclusions

In this work, we screened compounds that are labeled as TMs in the TMDB for application in photocatalytic water splitting. Our screening criteria were band gap, band edge energies, and thermodynamic stability. Based on hybrid DFT calculations we determined five materials to be potential photocatalysts. It turned out that CsTi₂Cl₇ is the most promising candidate for overall photocatalytic water splitting, whereas the conduction band minimum of SrCuSeF is sufficiently close to the energy level for the HER to be considered as a photocatalyst for photocatalytic water splitting. The remaining materials, i.e. CsGeBr₃, Rb₃Sn₄Au, and ZnAg₂nS₄ are suitable photocatalysts for water oxidation. In addition, we computed the topological types for the final candidates at the hybrid DFT level. Interestingly, all of the initially labeled TMs tuned into LCEBR, clearly highlighting the importance of accurate electronic structure calculations to determine atomic and electronic structures and eventually the topological type. Our results immediately suggest that TMs are rarer than previously suggested.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

Acknowledgments

The authors would like to acknowledge the Paderborn Center for Parallel Computing (PC²) for computing time on OCUUS and the FPGA-based supercomputer NOCTUA. H M is grateful for helpful comments.
from Zhijun Wang (Beijing National Laboratory for Condensed Matter Physics) and M G Vergniory (Donostia International Physics Center).

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