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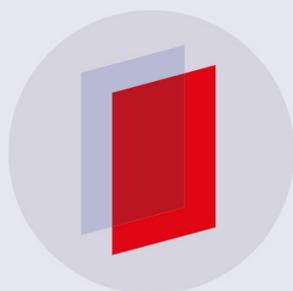
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**PAPER****Database-driven high-throughput study of coating materials for hybrid perovskites****OPEN ACCESS****RECEIVED**

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E-mail: azimatu.seidu@aalto.fi**Keywords:** perovskites, solar cells, coating materials, interlayer materials, databaseSupplementary material for this article is available [online](#)

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**Abstract**

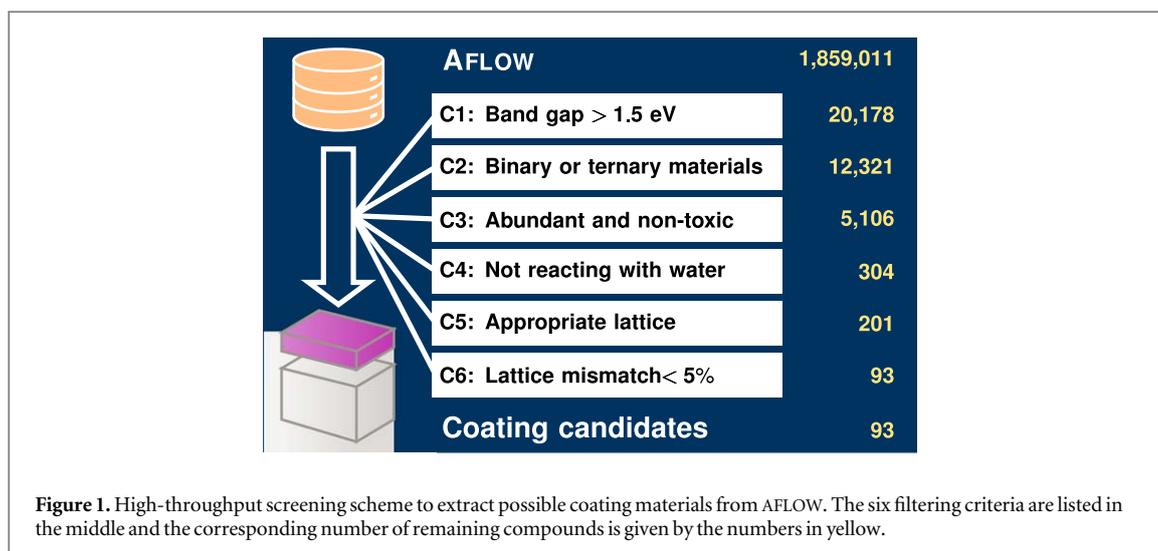
We developed a high-throughput screening scheme to acquire candidate coating materials for hybrid perovskites. From more than 1.8 million entries of an inorganic compound database, we collected 93 binary and ternary materials with promising properties for protectively coating halide-perovskite photoabsorbers in perovskite solar cells. These candidates fulfill a series of criteria, including wide band gaps, abundant and non-toxic elements, water-insoluble, and small lattice mismatch with surface models of halide perovskites.

1. Introduction

Perovskite solar cells (PSCs) [1–3] have recently reached a power-conversion efficiency (PCE) of >23% only six years after the invention of the state-of-the-art PSC architecture in 2012 (PCE~10%) [4, 5]. This has revived the hope for direct conversion of sustainable, affordable and environmentally friendly solar energy into electricity. The photoabsorbers in PSCs are hybrid (organic–inorganic) perovskites (denoted ABX₃ hereafter) especially methylammonium (MA) lead iodide (CH₃NH₃PbI₃ ≡ MAPbI₃). The salient properties of these materials in optoelectronic applications are optimal band gaps, excellent absorption in the visible range of the solar spectrum, good transport properties for both electrons and holes, flexibility of composition engineering, as well as low costs in both raw materials and fabrication [1, 2, 6–9].

Despite the excellent PSC-performance in the laboratory, stability problems limit the development and commercialization of this promising materials class. Hybrid perovskites degrade quickly in heat, oxygen and moisture [10–14]. With increasing exposure to any of these destabilizing factors, the structure of the hybrid perovskite degrades and the PCE reduces concomitantly after several days or even hours [15, 16]. Among the solutions that have been proposed to solve this stability and longevity problem are protective coating [17–19], the use of two-dimensional perovskites [20–25], and doping with small ions [14, 26–30]. Protective coating is particularly promising, as it can passivate the surface dangling bonds of the perovskite photoabsorber [31] and insulate the perovskite from heat and small molecules from the environment [17–19]. The use of inorganic semiconductors and insulators to enhance the stability of PSCs has been explored both experimentally and theoretically. The candidate coating materials in most of the previous work are common binary oxides such as ZnO [32, 33], SiO₂ [34], SnO₂ [35–37], TiO₂ [38], ZrO₂ [39], Al₂O₃ [10, 40] and NiO [26, 41]. Further possible coating candidates beyond these common oxides were rarely addressed so far. Considering the massive space of inorganic materials, we first need a database curation scheme that can screen the candidate which meet our requirements, as will be introduced in this work.

A good coating should have the following properties: (i) a wide band gap (>3 eV), (ii) little impact on the structure of the coated perovskite, (iii) good transport properties, and (iv) high stability in heat, air and water. It would be particularly attractive, if the coating material could also be used as a semiconducting interlayer, a key component in the modern perovskite-based device architectures. In this context, we are especially interested in cheap and efficient hole-transporting coatings, as *Spiro*-OMeTAD, the most common hole-transporting



material (HTM) in PSCs since the birth of this technology [4, 5], is expensive, has low charge-carrier mobilities and a negative impact on PSC stability [42].

We here present a database-driven high-throughput study that explores a wide range of possible candidates to find inorganic materials that have the potential to protectively coat perovskites in PSCs. We take the inorganic materials from the ‘Automatic Flow for Materials Discovery’ (AFLOW) database [43]. AFLOW contains nearly 2 million material entries that were computed with density-functional-theory (DFT) using the Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional [44].

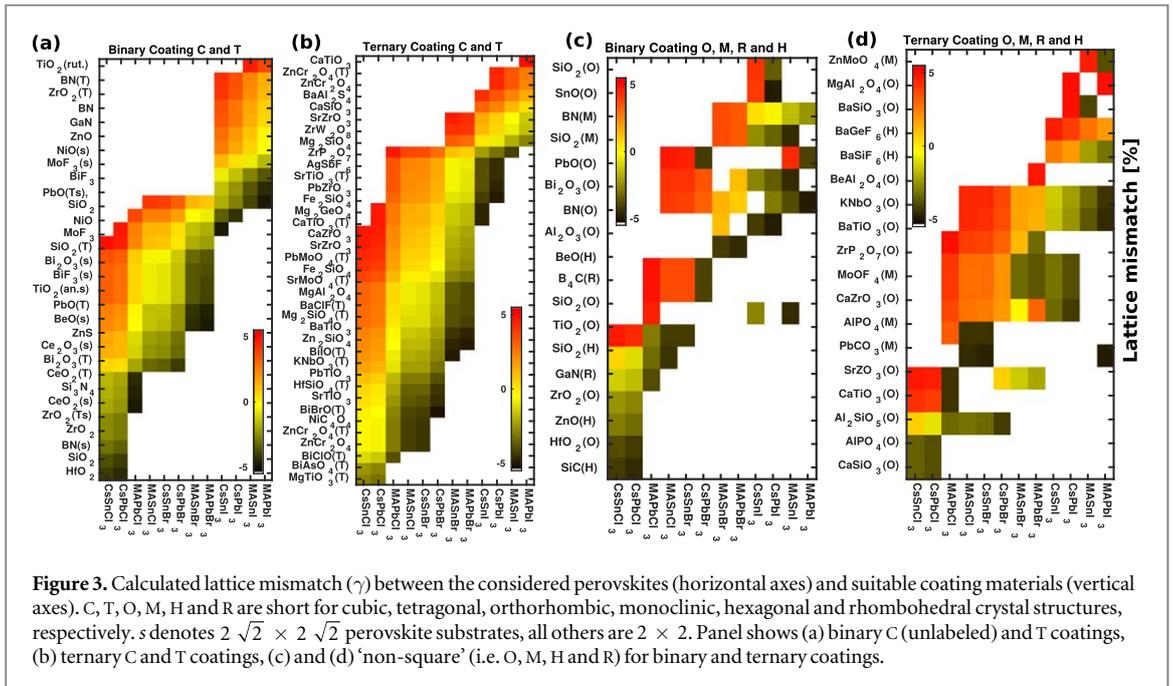
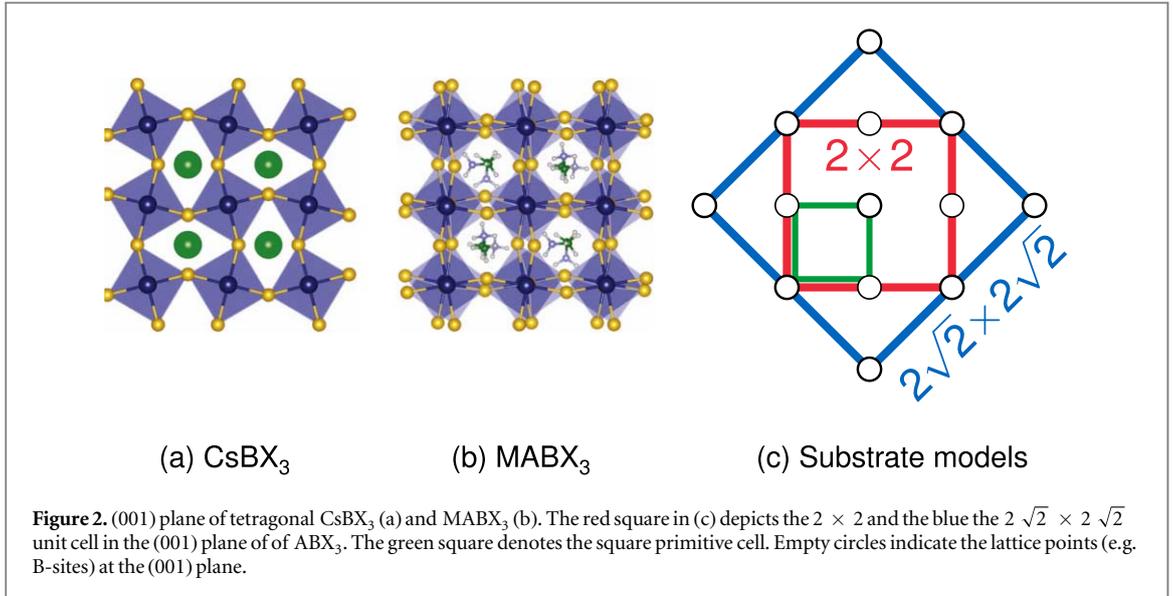
2. Database curation

In the following, we will describe our filtering scheme with which we reduced the large number of database entries to only those material candidates with promising coating properties. The workflow is illustrated in figure 1. Since PBE generally underestimates band gaps by $\sim 50\%$ [45], we set our first criterion (C1) to screen materials with ‘PBE band gap > 1.5 eV’. Considering the technical difficulties of coating with quaternary or even more complicated compounds [41, 46], we limited our target materials to binary and ternary compounds in this work (C2). In C3 we excluded all compounds that contain toxic or rare elements, and in C4 we discarded the compounds that are unstable in contact with water. Details of how we implemented C3 and C4 are available in the supplementary material (SM), available online at stacks.iop.org/NJP/21/083018/mmedia. In C5, we selected candidates with appropriate lattices, meaning candidates with at least two perpendicular lattice vectors in the conventional cell. In the final step (C6), we calculated the lattice mismatch between selected perovskite substrates and the coating materials that survived from C5. This last step produced some coating materials with several phases. In such cases, we prioritized the phase with the least lattice mismatch to MAPbI_3 . The other crystal phases are presented in the SM.

2.1. Computational details

As substrates, we chose 12 ABX_3 perovskites ($A = \text{Cs/MA}$, $B = \text{Sn/Pb}$, and $X = \text{Cl/Br/I}$) that are commonly used in halide-perovskite-based devices. We optimized the structure of the tetragonal $\text{P4}/\text{mbm}$ phase of CsBX_3 and the tetragonal (quasi) $\text{I4}/\text{mcm}$ phase of MABX_3 using PBE [44] (to stay consistent with AFLOW data [47]) and the analytic stress tensor [48] implemented in the all-electron numeric-atom-centered orbital code FHI-AIMS [49–51]. Details of the DFT calculations are given in the SM. Upon a test calculation, we selected the (001) crystal planes of the perovskites (figures 2(a) and (b)) since they are the most stable surface of these materials. We determined the lattice mismatch based on the lattice constants alone and did not carry out any interface calculations with DFT. Figure 2(c) shows the two ‘virtual surface models’ considered in this work. We did not consider larger surface models, since they would make further computational modeling intractable.

From the PBE-optimized lattice constants, we calculated the lattice mismatch at each coating-perovskite interface. To avoid large strain, we required that the coatings should have rectangular lattice planes with small miller indices, e.g. the (100) plane of the cubic lattice or the (11 $\bar{2}$ 0) plane of the hexagonal lattice. More details of this selection is given in the SM. If the lattice constant of the coating and the perovskite are a_c and a_p along one direction, then the lattice mismatch is



$$\gamma \triangleq \frac{ma_c - a_p}{ma_c} \times 100\%, \quad m \in \mathbb{N}. \quad (1)$$

m is the integer that minimizes $|\gamma|$. We set the criterion $\gamma \in (-5, +5)\%$ as shown in figure 1.

With the high-throughput screening scheme in figure 1, we extracted 93 inorganic semiconductor coating candidates (39 binaries and 54 ternaries) from AFLOW. In addition, there are ~ 1000 suitable ternary compounds, for which we could not find any data on their solubility in water. These remaining compounds will be investigated further in the future.

Figure 3 shows the calculated lattice mismatch between the candidates and the 12 ABX₃ perovskite substrates. Panels 3(a) and (b) reveal that several materials with cubic or tetragonal lattices can be used to coat most of the investigated perovskites: ZnS, BN, some fluorides (BiF₃, MoF₃ and AgSbF₆), some binary oxides (Bi₂O₃ in both cubic and tetragonal phases, Ce₂O₃, BeO, PbO, TiO₂-anatase, NiO and tetragonal SiO₂) and a large range of ternary oxides. In contrast, figures 3(c) and (d) show that most of the materials that are neither the cubic nor the tetragonal phase can only cover a small range of perovskite substrates. This is because the $|\gamma| < 5\%$ criterion must be satisfied by two lattice constants, which makes the coating less ‘versatile’ in these phases.

Table 1. Selected candidate coating materials for MAPbI₃. Listed are their space groups, band gaps (in eV, data from AFLOW[43]) and dominant charge carriers (n- or p-type conductivity) with corresponding references. Intrinsic n- and p-type materials, and n- and p-type dopable materials, are labeled by N, P, n and p, respectively.

	Space group	Band gap	Major carrier	References
PbO	P4/nmm	1.57	P	[53, 54]
ZnO	F $\bar{4}3$ m	1.69	N	[61]
MoF ₃	Pm $\bar{3}$ m	1.74		
GaN	F $\bar{4}3$ m	1.75	n, p	[62]
BaTiO ₃	Pm $\bar{3}$ m	2.14	n	[63]
NiO	Fm $\bar{3}$ m	2.22	P	[61]
PbZrO ₃	Pm $\bar{3}$ m	2.28	n, p	[64]
CaTiO ₃	Pm $\bar{3}$ m	2.36	n, p	[65]
CaZrO ₃	Pm $\bar{3}$ m	3.21	n, p	[66, 67]
Si ₃ N ₄	Fd $\bar{3}$ m	3.33		
BaAl ₂ S ₄	Pa $\bar{3}$	3.65		
CaSiO ₃	Pm $\bar{3}$ m	3.67		
ZrO ₂	P4 ₂ /nmc	3.86	N	[68]
BiF ₃	Fm $\bar{3}$ m	3.95	P	[59]
BN	F $\bar{4}3$ m	4.46	n, p	[69]
HfO ₂	P4 ₂ /nmc	4.67	p	[60]
BN	P6 ₃ mc	5.22	n, p	[69]
HfSiO ₄	I4 ₁ /amd	5.31		
BeO	Fm $\bar{3}$ m	8.17		

3. Results and discussion

From figures 3(a) and (b), one can immediately deduce that the lattice mismatch increases from -5% to 5% as the lattice constant of the substrates increases. The yellow spots show the most promising candidates with mismatch $<1\%$. Only a few coating candidates with ‘non-square’ planes survived our screening criteria. This is because in such materials, at least two lattice constants must have lattice mismatch between -5% and 5% . For instance, the γ values for the interface between the hexagonal phase of Bi₂O₃ at MAPbBr₃ interface are -6.5% and 0.73% along the a - and c -axis, respectively. Thus we do not consider Bi₂O₃ as a suitable candidate to coat MAPbBr₃.

As a first consistency check, we compared the material candidates in figures 3(a) and b to materials that have already been used as transport or mesoporous scaffold layers in PSCs. We found that our search is consistent with common materials such as: NiO [25, 52] and PbO [53, 54] as intrinsic HTMs in PSCs, as well as ZnO [52] and TiO₂ [38] as electron-transporting materials (ETMs). Similarly, our candidate materials included ZrO₂ [39] and Al₂O₃ [55] which are used as mesoporous scaffolds in PSCs.

Aside from the commonly known metal oxides used in PSCs, we discovered some surprising binary candidates (MoF₃, GaN, BiF₃, Si₃N₄ and BN) that have properties suitable to coat the photovoltaic-active halide perovskites (figure 3(a)). Similarly, for ternaries we found BaAl₂S₄, AgSbF₆, BaSiF₆ and BaGeF₆. These materials came as surprise since they are usually not considered in PSCs due to their high melting temperatures. However, with new coating techniques such as radio-frequency sputtering [40], pulsed laser deposition [56], vapor-deposition [57] and modified hybrid methods such as spin-coating/vapor-deposition [33], these materials become contenders as effective coating materials for future PSC devices.

Of particular interest are the potential coating materials for MAPbI₃, the most common photoabsorber in PSCs. Interestingly, our screening procedure reveals that Al₂O₃ (figure 3(c)), which is the most common mesoporous material in today’s PSC architectures [5], does not have the minimum lattice mismatch for coating MAPbI₃. ZnO, NiO, CaSiO₃, SiO₂, SrZrO₃, BaAl₂S₄, GaN, MoF₃, BN, Si₃N₄ and ZrO₂ lead to better lattice match. The actual strain values for MAPbI₃ can be found in the far right column of each panel in figure 3.

Next we briefly address the charge-carrier properties of the potential candidates. Table 1 lists the PBE band gaps of the found candidate coatings for MAPbI₃ provided by AFLOW [43], together with some data about their dominant charge-carrier type (n- or p-type) provided by other resources. Here, we observe that intrinsic p-type semiconductors such as NiO and PbO, will not only protect PSCs against ambient conditions, but could also serve as efficient HTMs to replace the inefficient *Spiro*-OMeTAD.

We also found insulators such as ZrO₂, Si₃N₄, and BeO (table 1). Due to the large band gap of these materials and their insolubility in water, they can be used as efficient mesoporous scaffolds to passivate PSCs against

degradation. Beside photovoltaic applications, insulators play an important role in a recently developed perovskite-based light-emitting-diodes architecture as they can significantly facilitate the hole injection [58]. Additionally, BN could be used as a p- or n-type semiconductor with different doping mechanisms (table 1). It was recently reported that BiF₃ has a high-lying valence band [59] thus potentially being a good HTM. Also HfO₂ could be engineered into a p-type material by controlling the oxygen vacancy content [60].

Lastly, we briefly comment on realistic coating interfaces. The actual phase of the coating material and the structure of the interface depend on many factors such as the perovskite surface structure and properties, the deposition method, the deposition conditions, as well as the coating thickness. These factors are not included in our database study. An atomistic description of coating-perovskite interfaces requires further computational (e.g. DFT) and experimental work. Results from such future work, such as the stability of the coating materials, could then be incorporated as additional criteria in our screening procedure.

4. Conclusion

In summary, we have developed a systematic and efficient screening scheme for perovskite coating materials. Our scheme reduces the ~1.8 million materials entries in AFLOW to 93 possible coating candidates for a series of perovskite photoabsorbers in PSCs. We have identified inexpensive HTMs (NiO and PbO) that can replace the inefficient and expensive *Spiro*-OMeTAD, as well as several efficient ETMs (e.g. ZnO) for PSCs. Our results feature new materials beyond metal oxides that will not only enhance the stability of PSCs but also serve as a starting point in the search of novel device materials for emergent PSC technologies.

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