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DATA PAPER

Databases of 2D material-substrate interfaces and 2D charged building blocks

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Discovery of materials using "bottom-up" or "top-down" approach is of great interest in materials science. Layered materials consisting of two-dimensional (2D) building blocks provide a good platform to explore new materials in this respect. In van der Waals (vdW) layered materials, these building blocks are charge neutral and can be isolated from their bulk phase (top-down), but usually grow on substrate. In ionic layered materials, they are charged and usually cannot exist independently but can serve as motifs to construct new materials (bottom-up). In this paper, we introduce our recently constructed databases for 2D material-substrate interface (2DMSI), and 2D charged building blocks. For 2DMSI database, we systematically build a workflow to predict appropriate substrates and their geometries at substrates, and construct the 2DMSI database. For the 2D charged building block database, 1208 entries from bulk material database are identified. Information of crystal structure, valence state, source, dimension and so on is provided for each entry with a json format. We also show its application in designing and searching for new functional layered materials. The 2DMSI database, building block database, and designed layered materials are available in Science Data Bank at https://doi.org/10.57760/sciencedb.j00113.00188.

Keywords: 2D material-substrate interfaces, charged building block database, functional-oriented materials design, layered materials, density functional theory

PACS: 61.50.Ah, 61.68.+n, 68.43.Bc, 68.43.Fg **DOI:** 10.1088/1674-1056/ad0626

1. Introduction

Layered materials, which are assemblies of two-dimensional building blocks with relatively strong internal bonds compared with those between adjacent layers, have ignited great enthusiasm in the materials science community due to their fruitful advantages. The weak interlayer coupling of layered materials provides unique degree of freedom to modulate their chemical and physical properties by exfoliation, intercalation, etc.[1] They also exhibit anisotropic electronic properties, which may facilitate their application in nonlinear optics,[2] mechanics,[3] etc. These layered materials can be classified into van der Waals (vdW) layered materials and ionic layered materials according to the interactions between layers.[3] In van der Waals (vdW) layered materials, the building blocks are charge neutral. While in ionic layered materials, the building blocks are charged and usually cannot exist independently.

Since 2017, plenty of vdW layered materials and their monolayer structures have been predicted. 2D databases containing stability, electronic, magnetic, and optical properties are constructed subsequently.[4–6] These monolayers can not only exist independently but also can be stacked or twisted to form heterojunctions with emergent phenomena.[7–9] Substrates usually are templates for the synthesis of two-dimensional (2D) materials, where the coupling between them could dramatically affect the intrinsic physical properties of the 2D materials.[10–12] The discovery of suitable substrates in experiment is however time-consuming and costly. Thus, it is quite demanding to predict configurations of 2D materials on substrates theoretically.

Ionic layered materials, in contrast to vdW layered materials, have stronger interlayer coupling. They are composed of 2D charged building blocks, and these 2D building blocks can be classified into different roles, i.e., functional layers that mostly determine the physical properties of the crystal, and charge compensating layers which provide carriers. Functional-oriented material design can be achieved by stacking different functional layers and charge compensating layers.[13,14] While, the accessible 2D charged building blocks are limited, which hinders the rational design of layered materials.

In this paper, we address the above issues and construct 2D material-substrate interface (2DMSI) database and a 2D charged building block database. We also show the application of 2D charged building block database in designing and searching for functional layered materials.

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2. Data acquisition

For the 2DMSI database, we choose materials in Materials Project[15] and Computational 2D Materials Database (C2DB)[6] as input for substrates and 2D materials. For substrates, we cleave their bulk phase along a Miller index to gain a surface, and then twist them with different angles. For 2D materials, we also make superlattice for them with different angles. Next, we put different twisted 2D materials on different twisted substrates with commensurate lattice, generating different twisted configurations. Finally, by high-throughput density functional calculations, we optimize the constructed superlattices to gain their binding energies. We also extend 2D materials-substrates to 2D–2D material heterojunctions [Fig. 1(a)]. Details can be found in Ref. [16].

For 2D charged building block database, we adopt a developed topological scaling algorithm (TSA)[5] to identify these 2D building blocks from Materials Project (MP) database.[15] There are three steps to map out them. The first step is data cleaning. We keep those structures in MP with ICSD codes and $E_{\text{hull}} = 0$ eV/atom to guarantee the high quality of the database. The second step is utilizing TSA to identify the bonded networks. We create an $n \times n \times n$ supercell for a structure, build the distance matrix $\boldsymbol{D}$ for the supercell and construct a bond matrix $\boldsymbol{B}$ according to $\boldsymbol{D}$. When the bond length between atom i and j $d_{ij} \leq k \times (r_i^{\text{cov}} + r_j^{\text{cov}})$, they are connected, where r_i^{cov} and r_j^{cov} are covalent radii for atoms i and j,[17] and k is a scaling parameter. Then we keep those bonded atoms as a network. The third step is identifying the dimension of the network. We build an $n \times n \times n$ supercell for the network and find the number of bonded networks N in the supercell. If $n^3/N = 1$, it is a zero-dimension (0D) cluster; if $n^3/N = n$, it is a one-dimension (1D) chain; if $n^3/N = n^2$, it is a two-dimension (2D) layer. Finally, we keep 2D layers with a different nominal elemental ratio with parent as 2D charged building blocks [Fig. 1(b)]. Here, we identify 1208 ones in total from the MP database.

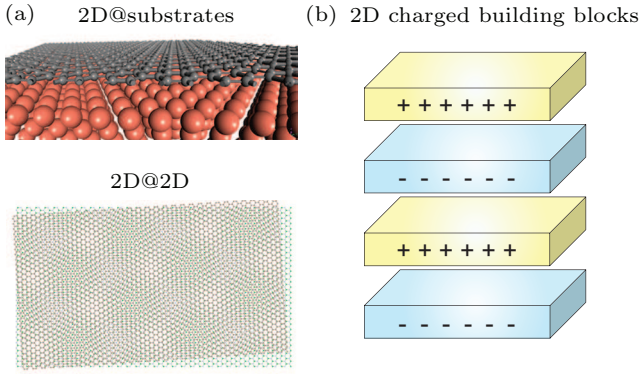


Fig. 1. Schematic diagram of (a) 2D materials-substrate interface (upper panel), twisted 2D–2D heterojunction (bottom panel), and (b) 2D charged building blocks.

We also build a workflow to construct layered materials by utilizing 2D charged building block database and identify 353 stable ones in terms of thermodynamics and lattice-dynamics by high-throughput calculations. In this work, we only consider 797 charged building blocks with tetragonal, trigonal and hexagonal symmetry as input. Then we stack them with commensurate lattice and charge neutrality. After constructing the layered structures, we resort to density functional calculations (DFT) to confirm their stability and investigate their physical properties. Details can be found in Ref. [18].

3. Data format and contents of the database

For the 2DMSI database, we provide an interactive webpage to exhibit our data as shown in Fig. 2, which can be accessed via http://n11.iphy.ac.cn/databases/2dinterface.html. The "shape" button defines the lattice type of substrate and 2D material, which can be "hexagonal" or "square". The "type" button can be "2D@substrate" or "2D@2D", which correspond to interface between a 2D material and a substrate or between a 2D material and a 2D material. Then specify the detailed adsorbate and substrate. Next, define mismatch, max size, and max perfect square number of the supercell (PSN). Clicking "query" button will generate configurations of the superlattice. The bottom table shows the

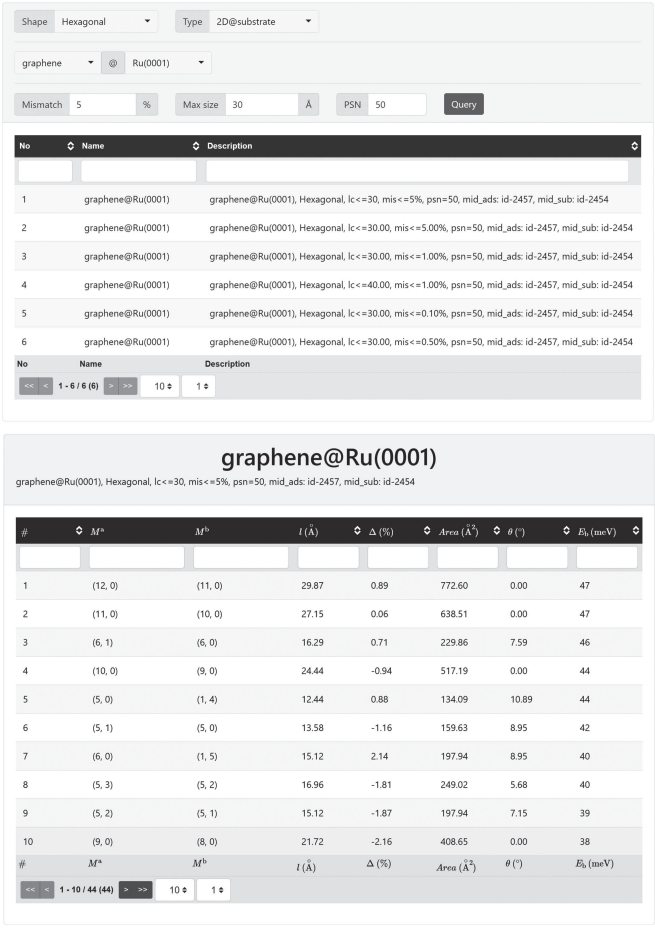


Fig. 2. Screenshot of interactive webpage for 2DMSI database.

Table 1. Contents for the json files.

Content	Type	Comment
cluster_id	str	Unique id of the building block
ads_id	str	Source id (cluster_id) of building block1 to construct structure
sub_id	str	Source id (cluster_id) of building block2 to construct structure
band	dict	Contains band gap, high symmetry points etc., which can be read by "plot_band.py" script
crys_sys	str	Crystal system
e_above_hull	float	Energy above hull (eV/atom)
efermi	float	Fermi energy (eV)
elements	dict	Contains elements of the crystal/building block
etot	float	Total energy (eV)
lattice	dict	lattice parameters a, b, c, α, β, γ
phonon	dict	Contains phonon dispersions and datasets that can be read by Phonopy. The dispersion data can be read by "plot_phonon.py"
point_group	str	Point group
prototype	str	Structural prototype
spg	str	Space group
structure	dict	Structure information that can be read by pymatgen.core.structure module.
structure_id	str	Unique id of the structure in the database
vdw	bool	A boolean telling if the structure is a van der Waals material or not
dimension	list	Tell the periodicity of the building block along a, b, c direction and its dimension
parent	dict	Information of parent compound for a cluster
functionality	str	Functionality of the cluster
reference	str	Reference for the functionality
type	str	Type of the cluster, "ionic" or "vdw"
valence	list	Possible valence state of the cluster

detailed information for each configuration, containing their superlattice matrix M, lattice constant l, mismatch Δ, area S, twisted degree θ (°), and binding energy E_b. Here, E_b is defined as $E_\mathrm{b} = (E^\mathrm{a} + E^\mathrm{s} - E^\mathrm{c})/S$, where E^a is the total energy of adsorbate, E^s is the total energy of substrate, and E^c is the total energy of the composite superlattice.

For both 2D charged building block database and the designed layered materials, we provide a json format file for each entry, which is free to be read by multiple languages, e.g., python. For 2D charged building block database, each entry contains the basic lattice information, crystal structure, valence state, and its parent information. For the designed layered structures, each entry contains its energy, energy above hull, lattice information, crystal structure, band structure and phonon dispersions. Detailed information of the json file can be found in Table 1. We also provide python scripts to export the crystal structures, plot phonon dispersions and band structures, which are included in the database files.

4. Statistics of data properties

For the 2DMSI database, it contains data of 34 interfaces at present, including 6 2D@substrate entries, and 28 2D@2D entries. For each interface, there are usually 40–100 twisted configurations.

For the 2D charged building blocks, they are classified into 59 space groups (Fig. 3). The most common one is *P*-3*m*1, which contains 287 entries in this subset. We also label functionality for part of building blocks based on the physical property of their parent compounds.

For the constructed 353 layered structures, they are classified into 30 space groups [Fig. 4(a)]. For their electronic structures, there are 52.1% non-magnetic (NM) metals, 35.1% NM semiconductors, 6.8% magnetic metals and 5.9% magnetic semiconductors [Fig. 4(b)]. For semiconductors, their band gaps spread from 0–6 eV [Fig. 4(c)]. As a benchmark of utility of our databases for screening functional 2D materials, we present the discovery of 2D semiconductors with high carrier mobilities. According to the Drude model, the mobility μ of carrier can be expressed as $\mu = e\tau/m^*$, where e, τ, m^* are the electron charge, scattering rate, and effective mass, respectively. Thus, the carrier mobility is inversely related to the effective mass. We firstly screen out those semiconductors with both low electron and hole mobility ($|m^*| \leq 0.2m_0$) as candidates, which yields 26 ones. Then those nonmagnetic semiconductors with direct bandgaps are considered for further processing. Then, we calculate their mobilities according to the deformation potential (DP) theory,[19,20] $\mu = \frac{2(2\pi)^{1/2} e\hbar^4 C}{3E_l^2 (k_\mathrm{B}T)^{3/2} m^{*5/2}}$, where $\hbar$ is the reduced Planck's constant, C the elastic constant, E_l the DP constant, k_B the Boltzmann constant, T temperature, and m^* the effective mass, which can

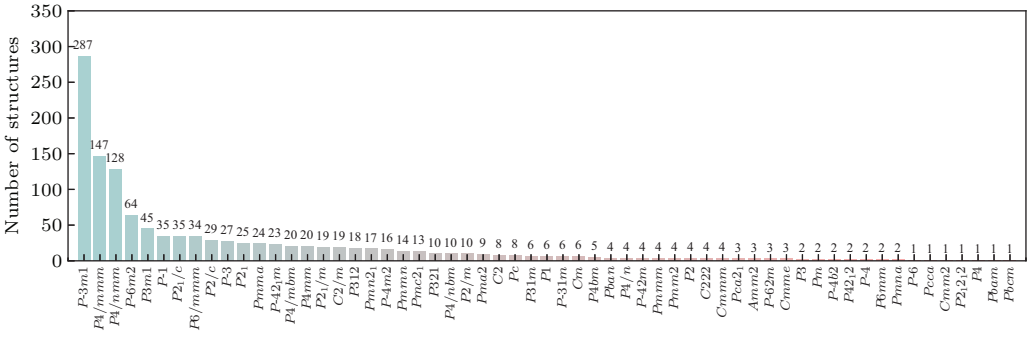


Fig. 3. Statistics of space group for 2D charged building blocks.

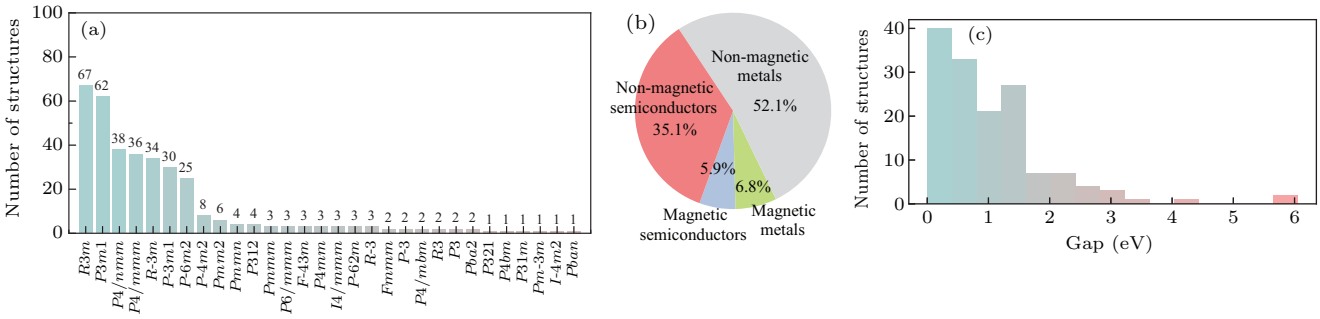


Fig. 4. Statistics of (a) space groups, and (b) electronic structures for 353 layered structures. (c) Band gaps distribution for semiconductors.

Table 2. Computed carrier mobility of 8 non-magnetic semiconductors.

Formula	ID	Carrier	E_l (eV)	C (GPa)	$m^*(m_0)$	μ (10^3 cm^2/V·s)
YZnPO	s-618	electron	18.84	188.31	0.43	5.0
		light hole	12.27		0.15	100.6
		heavy hole			63.14	0.00003
BaCdBiF	s-941	electron	10.46	74.12	0.14	62.5
		light hole	11.39		0.09	145.6
		heavy hole			2.20	0.054
CaZnPF	s-2166	electron	10.58	146.56	0.23	34.2
		light hole	11.97		0.16	71.5
		heavy hole			12.65	0.001
$CuBiTe_2$	s-3500	electron	13.63	88.72	0.13	60.1
		light hole	12.42		0.21	22.7
		heavy hole			0.30	9.0
CuPbSeI	s-4315	electron	13.86	76.59	0.12	74.2
		light hole	13.86		0.17	26.6
		heavy hole			0.49	2.1
Ca_2MgAsP	s-4651	electron	10.59	91.70	0.16	55.5
		hole	3.90		1.65	0.4
Ca_2MgAs_2	s-4715	electron	9.96	86.01	0.14	70.4
		hole	3.73		1.87	0.3
AgBiTeSe	s-5385	electron	12.09	77.31	0.10	128.2
		light hole	10.47		0.09	191.8
		heavy hole			0.80	0.8

be extracted by DFT calculations. We find that 8 non-magnetic direct-bandgap semiconductors own high electron or hole mobility as shown in Table 2, which are potential candidates for application in high-speed electronic devices.

We also explore functionality of these materials. We find ferromagnetic semiconductor Na_2CuIO_6 with valley Hall effect, superconductors CaAlSiF/Ba_2F_2PtAs, and topological material LaRhGeO, which is discussed in Ref. [18].

5. Conclusion

In this paper, we show detailed procedures to build the 2DMSI database and 2D charged building block database. For the 2DMSI database, we systematically study the possible configurations 2D materials at substrates or 2D materials, and provide an interactive webpage to exhibit our database. For the 2D charged building blocks, we have done its searching, classification and show its applications in designing and searching layered functional materials. This database and related layered structures are provided with json format, which can be extracted by python scripts that we provide. These databases provide a valuable resource to explore suitable substrate for 2D materials or 2D material heterojunctions and will serve as a valuable resource to construct functional layered materials. We will continuously expand the contents of the databases.

Data availability statement

The data that support the findings of this study are openly available in Science Data Bank at https://doi.org/10.57760/sciencedb.j00113.00188.

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