

High-throughput identification of one-dimensional atomic wires and first principles calculations of their electronic states

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DATA PAPER

High-throughput identification of one-dimensional atomic wires and first principles calculations of their electronic states*

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Low dimensional materials are suitable candidates applying in next-generation high-performance electronic, optoelectronic, and energy storage devices because of their uniquely physical and chemical properties. In particular, one-dimensional (1D) atomic wires (AWs) exfoliating from 1D van der Waals (vdW) bulks are more promising in next generation nanometer (nm) even sub-nm device applications owing to their width of few-atoms scale and free dandling bonds states. Although several 1D AWs have been experimentally prepared, few 1D AW candidates could be practically applied in devices owing to lack of enough suitable 1D AWs. Herein, 367 kinds of 1D AWs have been screened and the corresponding computational database including structures, electronic structures, magnetic states, and stabilities of these 1D AWs has been organized and established. Among these systems, unary and binary 1D AWs with relatively small exfoliation energy are thermodynamically stable and theoretically feasible to be exfoliated. More significantly, rich quantum states emerge, such as 1D semiconductors, 1D metals, 1D semimetals, and 1D magnetism. This database will offer an ideal platform to further explore exotic quantum states and exploit practical device applications using 1D materials. The database are openly available at http://www.dx.doi.org/10.11922/sciencedb.j00113.00004.

Keywords: high-throughput calculation, one-dimensional atomic wires, electronic structure, first principles calculation

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1. Introduction

Low dimensional van der Waals (vdW) materials are more flexible in designing electronic devices with high performance.[1,2] Since the discovery of graphene in 2004, the low dimensional materials[3–14] such as graphene and other two-dimensional (2D) materials,[3–12] one-dimensional (1D) materials like carbine[13] and metal trihydride MH_3[14] have attracted extensive attention. Different from three-dimensional (3D) bulks, the low dimensional systems possess a variety of unconventionally physical properties owing to unique band structures, charge screenings, and electron–phonon couplings modulated by the dimensionality.[15–18] For instance, 3D diamond, 2D graphene, and 1D carbine display completely distinguished properties owing to their different hybridization orbitals under different dimensions. Especially for 1D quantum materials, their potential applications in nanoelectronics, spintronic devices, and sensors are promising because they reach the physical limit scale of the electronic materials with periodic crystal structures. Thus, exploring realistic 1D quantum materials and unveiling their properties have been one of the central and significant topics in fields of condensed-matter physics and materials science.

Among 1D materials, one special kind of systems can be defined as 1D atomic wires (AWs) because their width is in few-atoms scale. In the past two decades, 1D AWs have demonstrated rich and unique properties, such as Peierls transition,[19,20] spin–charge separation,[21] Tomonaga–Luttinger liquids,[22] strongly quantum fluctuation,[23] and superconductivity.[24] Meanwhile, the electronic properties would change with the dimension reduction. For instance, the band gap type of 1D Sb_2S_3 and Nb_2Se_9 shows a transition from indirect to direct with the dimension reduction from 3D to 1D.[25,26] Moreover, the conducting property from metallic to semiconducting takes place in Mo_6Te_6 with the dimension reduction to 1D.[27] From the viewpoint of magnetic properties, 1D AW of CoH_3 is a half-metal with 100% spin-polarization.[14] 1D Mn/Fe-benzenetetramines are bipolar magnetic semiconductors, which could be modulated into half metals by carrier doping.[28] In addition, thermoelectric and catalytic performances of ultrafine 1D AWs would also be improved.[29–31] Therefore, 1D AW materials are more suitable to be applied in

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high-performance sensors, transistors, catalysts, etc.[30–33]

Similar to exfoliating graphene from graphite, the 1D AWs could be exfoliated from the vdW bulks. Although preliminary classification on vdW bulk materials has been reported by Cheon *et al*. in 2017[34] and the progress on some 1D materials has been achieved, few excellent 1D AW candidates could be practically applied in devices due to lack of enough reliable 1D AWs. To solve this issue, the comprehensive database of 1D AWs is urgently required to be established based on 3D solid crystal database. Moreover, the stabilities, exfoliating feasibilities, and electronic properties of 1D AWs are demanded to be examined and provided. Without the direct connection between the reliable 1D AWs and their electronic properties, it severely limits the fundamental explorations on 1D AWs and their practical applications in devices. Herein, the detailed classifications on 367 kinds of potential 1D AW candidates and systematic investigations on their geometrical structures, electronic structures, possibly magnetic properties, and stabilities have been performed. At the meanwhile, all computational results are stored in the database with format of JavaScript Object Notation (JSON), which provides a comprehensive 1D AW candidate resource and a significant platform for the scientific community to further undertake theoretical analysis, experimental verification, and practical applications in devices using suitable 1D AW systems.

2. Computational methods and usage notes of the database

In this work, all the calculations were performed based on density functional theory (DFT) within Vienna *ab initio* simulation package (VASP).[35] The generalized gradient approximation (GGA) with Perdew–Burke–Ernzerhof (PBE) functional was adopted for the exchange–correlation potential.[36] Considering the weak vdW interactions between inter-wires in bulk materials, the Grimme's DFT-D3 approach was involved.[37] For 1D AWs, the vacuum thickness was set as 30 Å in order to minimize the interaction between periodic AWs. The plane-wave cutoff energy was set as 500 eV in all of the calculations. All the atomic positions were fully optimized to converge until the force on each atom was less than 0.02 eV/Å with the fixed bulk lattice constants along the wires. In the electronic structure calculations, the energy convergence was set as 10^{-5} eV. In order to investigate the structural stability of 1D AWs, phonon dispersions were studied by using Phonopy code based on the interface with VASP.[35,38,39]

All the computational results, including the structures, electronic structures, magnetic states, and stabilities of 367 1D AW candidates, are compiled in the supplementary materials (SM) in PDF format. To help researchers easily search some specific information from a large amount of data, these results are also stored in the database with format of JavaScript Object Notation (JSON). For the JSON format file, three nested layers of objects are included, where one can extract the required information according to the keys in each layer. The database are openly available at http://www.dx.doi.org/10.11922/sciencedb.j00113.00004.

3. Results and discussion

3.1. Screening and identification of 1D atomic wires

In order to obtain the potential 1D AWs, the possible 1D AW candidates can initially be explored by sweeping 3D crystal structure databases, such as Inorganic Crystal Structure Database (ICSD),[40,41] Materials Project (MP) database,[42] etc. The primary task is to discriminate the vdW bulk materials from the databases. In other words, how to distinguish the vdW interaction is the key issue. One of the common methods to identify the vdW interaction is through comparing the distance (d) of two atoms with the sum of their covalent bond radii, which effectively identifies 2D and 1D vdW solids and 2D/1D heterostructures materials by Cheon *et al*.[34] After tremendous screening of the possible vdW bulks list[34] combined with the latest MP database[42] (https://materialsproject.org) using data mining algorithm, the possible 1D AWs have been obtained. Meanwhile, it is required that the bond length along the 1D AW direction is smaller than the shortest distance between two nearest inter-wires in the parent bulk phase. Moreover, the f-electrons systems are not considered here since they could not be accurately described by GGA[36] or local density approximation (LDA)[43] based on DFT. Consequently, 367 1D AW candidates are obtained and considered in this work.

The structure, electronic structure, and stability information of 1D AWs are compiled in SM in PDF format. For facilitating the scientific researches to extract some specific information from a large amount of data in SM, an additional SM in JSON format is also provided. For the JSON format file, three nested layers of objects are included, where one can extract the required information according to the keys in each layer. Table 1 summarizes the keys corresponding to the objects in each layer. For example, one can get the structural information of 1D AW AuBr through the keys 'Binary 1D AWs' and 'AuBr'. It is worth noting that all the figures are encoded with Base64 format. Besides, a python code is also offered as an example to extract the data from the JSON file. To run the python code, the python relevant packages like json module and base64 module are required to be pre-installed.

Based on the 1D vdW parent materials, a statistical classification and analysis is presented in Fig. 1. In terms of the

crystal structure classification in Fig. 1(a), it is found that the systems with monoclinic and orthorhombic symmetries hold $\sim 37\%$ and $\sim 39\%$, respectively. The system with triclinic symmetry is $\sim 10\%$, and other systems only hold smaller proportions with $\sim 5\%$ for tetragonal, $\sim 6\%$ for hexagonal, and $\sim 3\%$ for trigonal. Based on the point group distribution, it is found that the majority of $\sim 34\%$ is $2/m$, followed by *mmm* with $\sim 31\%$. A complete list of the crystal structure information among our predicted 367 1D AW materials is provided in SM. Figures 1(b) and 1(c) display the chemical formula types and composition species of these 1D AWs. Among them, halides, chalcogenides, and pnictides are partially overlapped. In details, 248 halides account for a large proportion of $\sim 68\%$ since their valence state of -1 is easier to be satisfied. Besides, 230 chalcogenides and 111 phosphides exist in Fig. 1(c).

Table 1. Description of keys in JSON file.

Layer number	Key	Description
1	Unary 1D AWs	structural information of unary 1D AWs without 3d transition metals
	Binary 1D AWs	structural information of binary 1D AWs without 3d transition metals
	Ternary 1D AWs	structural information of ternary 1D AWs without 3d transition metals
	Multi-element 1D AWs	structural information of multi-element 1D AWs without 3d transition metals
	Non-magnetic 1D AWs with 3d transition metals	structural information of non-magnetic 1D AWs with 3d transition metals
	Magnetic 1D AWs with 3d transition metals	structural information of magnetic 1D AWs with 3d transition metals
	Phonon spectra of typical 1D AWs	phonon spectra of some typical 1D AWs
	Exfoliation energies of unary and binary 1D AWs	exfoliation energies of 127 kinds of unary and binary 1D AWs
	Band structures of some systems using HSE functional	band structures of some 1D AWs using HSE functional
2	chemical formulas such as S, AuBr, AsSeI	information of one specific 1D AW
3	Formula	chemical formula of one specific 1D AW
	MP ID	ID of one specific 1D vdW parent material in MP database
	Bulk spacegroup	spacegroup of one specific 1D vdW parent material
	Bulk point group	point group of one specific 1D vdW parent material
	Bulk band gap	band gap of one specific 1D vdW parent material
	Magnetic state	magnetic state of one specific 1D AW
	Magnetic moment	magnetic moment of single transition metal element in one specific 1D AW
	1D band gap	band gap of one specific 1D AW
	Top view	top view of one specific 1D AW
	Side view	side view of one specific 1D AW
	Band-dos	electronic structure of one specific 1D AW
	Lattice constant	lattice constant of one specific 1D AW
	Crystal system	crystal system of one specific 1D vdW parent material
	Exfoliation energy	exfoliation energy of one specific 1D AW

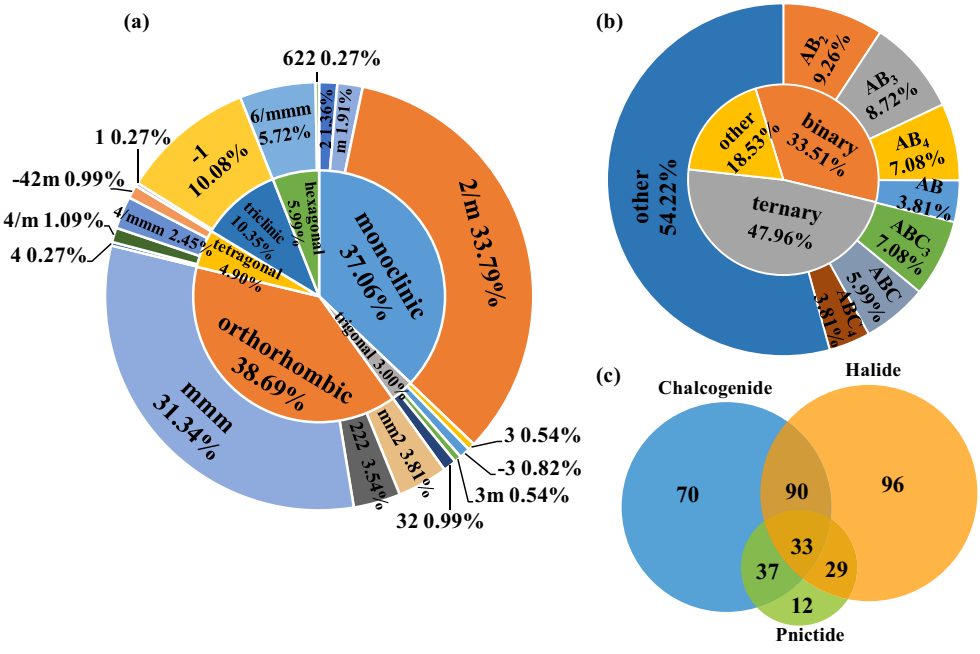


Fig. 1. Statistics on 1D vdW parent materials. Classification of 1D vdW bulk materials in terms of (a) crystal structures and point groups, (b) species of chemical elements and chemical formula prototypes, (c) chemical compositions.

Moreover, 123 binary and 176 ternary compounds are the major parts with ratios of 34% and 48% in Fig. 1(b). Furthermore, according to the chemical formula prototypes in Fig. 1(b), the major format is AB_2, which is followed by AB_3, ABC_3, AB_4, ABC, etc.

3.2. Electronic structures and magnetic properties of some specific 1D atomic wires

With the dimension reduction, the electronic properties of 1D AWs may demonstrate evident changes relative to 3D bulks. 1D $BeCl_2$and 1D $SnCl_2$ as typical 1D AWs show the band gap type transition and the band gap reduction compared with 3D bulks, respectively. In details, the bulk $BeCl_2$ is an indirect band gap semiconductor, but it turns into a direct band gap semiconductor for 1D AW in Fig. 2(a), implying that 1D $BeCl_2$ would be used in sub-nm optoelectronic devices. In general, 316 semiconductors and 51 metals are present among 367 kinds of 1D AWs, whose detailed band structures and density of states (DOS) are provided in the SM. Since the electronic correlation effect on the band structures could not be accurately described by GGA-PBE functional, the band gaps are usually underestimated. Thus, more accurate method such as Heyd–Scuseria–Ernzerhof (HSE) functional or GW correction is required to produce more accurate band structures and band gaps. As shown in Fig. S1 in SM, the band gap of the semiconducting 1D AW BPS_4 increases with HSE functional compared with those using GGA-PBE functional, and the metallic character of $ICl_2$and Ta_4SiTe_4 using HSE functional is maintained. Even for the transition metal compounds like $MoCl_3O$, the band gap is still absent and the metallic band structure is preserved after the HSE functional is considered. Thus, the qualitatively properties of most systems reported here may not change much in this work. In fact, the GW correction or dynamical mean field theory (DMFT) should be considered to obtain more accurate electronic states of transition metal compounds in further studies. From the vdW bulk materials to 1D AWs, several evident changes occur in the electronic structures owing to the bond length variation and the symmetry lowering, which deserves further thorough investigations. For most of 1D semiconducting AWs, the band gaps of most 1D AWs are enlarged compared with their bulks owing to the conventionally quantum confinement effect, which is basically induced by the reduced electronic interaction between the inter-wires. In contrast, some 1D AWs in the SM demonstrate decreased band gaps compared to the bulks. Taking $SnCl_2$ as an example in Fig. 2(b), the band gap of bulk $SnCl_2$ is 3.15 eV, but it shrinks to 2.95 eV for its 1D AW. The band gap reduction results from the bond length reduction of Sn–Cl from bulk to 1D AW.

The 1D magnetism is also a significant topic in the low dimensional materials, especially among 3d transition metal compounds. As listed in Table 2, the stable magnetic configurations of 1D AWs with 3d transition metal elements have been explored through comparing the energies of nonmagnetic, ferromagnetic (FM), and Néel antiferromagnetic (AFM) states. Generally, 61 kinds of 1D AWs show stable magnetic ground states, including 39 antiferromagnets and 22 ferromagnets. The magnetic configurations and magnetic moments of these 1D AWs are listed in Section VI of the SM.

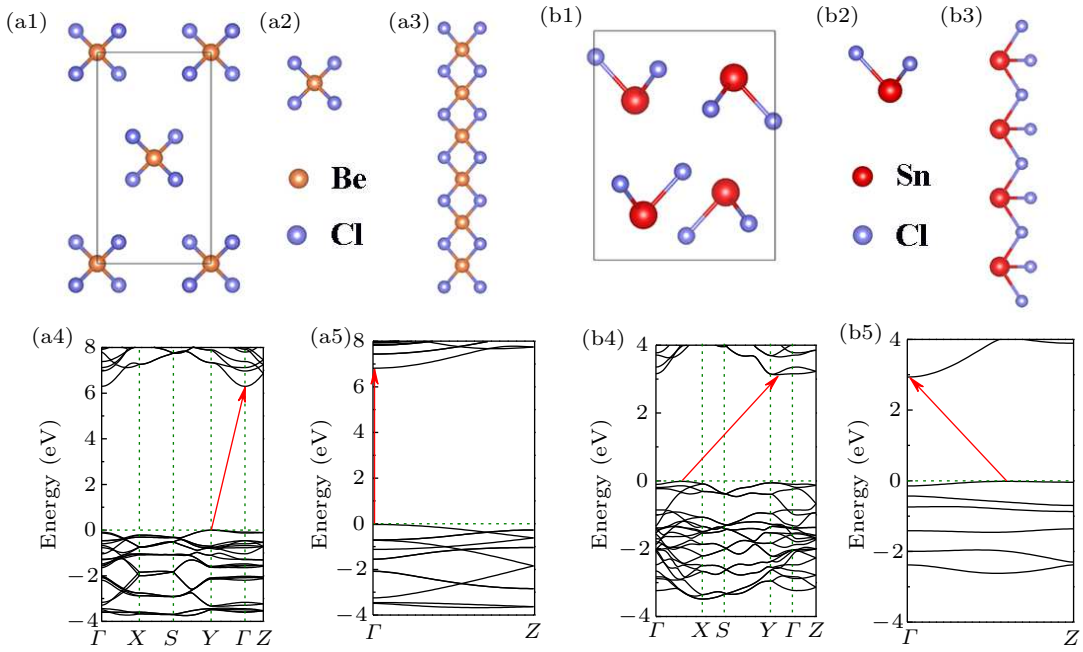


Fig. 2. Crystal and electronic structures of two typical 1D vdW bulks and their 1D AWs. (a1) Side view of bulk $BeCl_2$. (a2) Top and (a3) side views for 1D AW of $BeCl_2$. The band structures of bulk $BeCl_2$ (a4) and 1D AW of $BeCl_2$ (a5). (b1) Side view of bulk $SnCl_2$. (b2) Top and (b3) side views for 1D AW of $SnCl_2$. The band structures of bulk $SnCl_2$ (b4) and 1D AW of $SnCl_2$ (b5).

Table 2. Detailed list of 61 kinds of 1D magnetic AWs based on FM/AFM ground states and electrical properties of metal/semiconductors. Detailed magnetic and electronic properties are presented in Section VI of the SM.

	FM ground states	AFM ground states
Metals	CrF_4, CrP_4, $CuBr_2$, CuO_2, NiO_2, Sc_7CBr_{12}, Sc_7CI_{12}, $CuSb_2(XeF_8)_2$	CrF_5, $TiCl_3$,TiI_3, VBr_3,VI_3
Semiconductors	$CuCl_2$, CrN_2, MnF_4, Al_2CoCl_8, Al_2NiCl_8, $CrSbF_{10}$, $CrSbS_3$, $CuClF_{10}$, $Sc_6C_2I_{11}$, CuH_6SO_7, $CoSb_2S_2(OF_3)_4$, $SiCuH_8(O_2F_3)_2$, $ZrCuH_8(O_2F_3)_2$, $CuH_{12}C_3SN_6O_7$	Mn_2F_7, V_3O_7, VP_4, VS_2, Al_2VCl_8, $Co(IO_3)_2$, $CrSbSe_3$, $Mn(IO_3)_2$, $Mn(SbS_2)_2$, $Na_3(CuO_2)_2$, $Na_8(CuO_2)_5$, $Ni(IO_3)_2$, $Ti(AlBr_4)_2$, $Ti(AlCl_4)_2$, V_2OF_7, VSb_2O_5, $CoH_4(CO_3)_2$, $CoH_6(NCl)_2$, $CoP_4(H_5O_8)_2$, $MnInBr_3$, $Cu_2BH_5O_6$, $CuH_4(OF)_2$, $FeH_4(SO_5)_2$, $FeSb_6(Pb_2S_7)_2$, $MnH_4(ClO)_2$, $MnH_4(CO_3)_2$, $MnH_4(SO_5)_2$, MnH_5SO_7, $MnH_6(SO_4)_4$, MnH_6SO_6, $MnSb_6(Pb_2S_7)_2$, $CrH_{10}S_2(NO_2)_4$, $FeH_8C_4(S_2N_3)_2$, $MnH_{10}S_2(NO_2)_4$

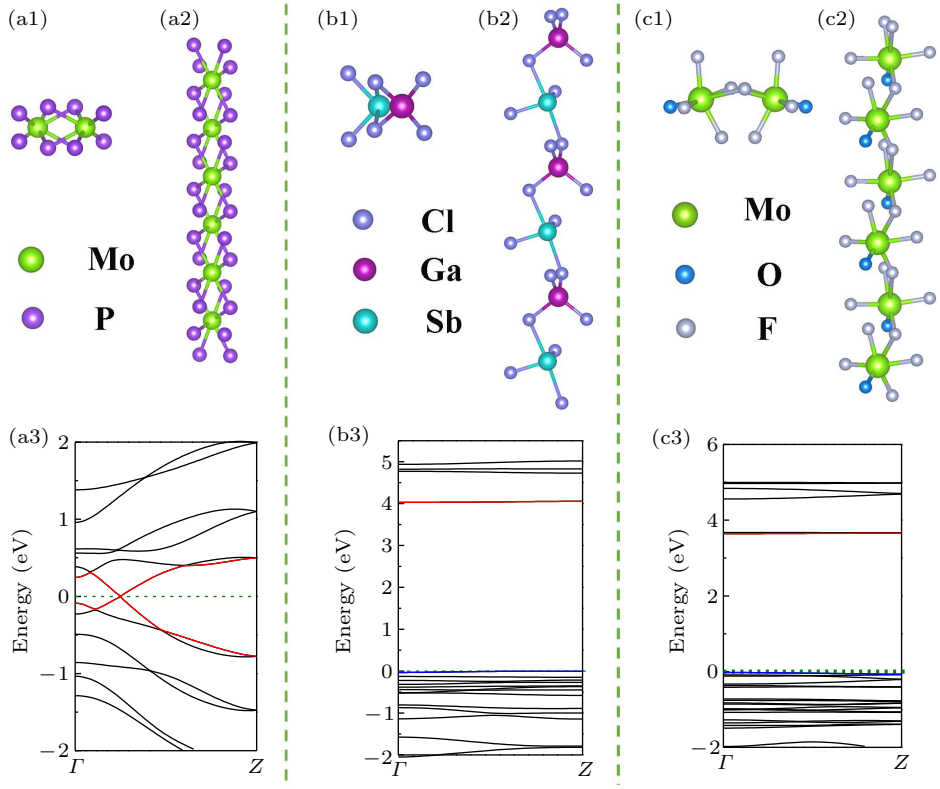


Fig. 3. Crystal and band structures of three representative 1D AW materials. (a1) Top and (a2) side views for 1D AW of MoP_4. (a3) The band structures for 1D AW of MoP_4. (b1) Top and (b2) side views for 1D AW of $GaSbCl_6$. (b3) The band structures for 1D AW of $GaSbCl_6$. (c1) Top and (c2) side views for 1D AW of $MoOF_4$. (c3) The band structures for 1D AW of $MoOF_4$.

Among the metallic 1D AWs, some behave like semimetals. As shown in Fig. 3(a3), MoP_4 displays a linear dispersion character near Fermi level (E_F). The similar linear dispersions are also present in 1D AWs of InI, NiO_2, CuO_2, TiI_3, $TcCl_4$, CrP_4, Ta_4SiTe_4, $CuSb_2(XeF_8)_2$, which are all listed in the SM. It implies the ultrafast carrier motilities and promising applications of these 1D AWs in high-speed electronic devices.[44,45]

In addition, the discovery of Mott insulators and superconductors in magic-angle graphene superlattices has stimulated extensive interest in the community to look for the systems with flat-bands structures.[46,47] From the theoretical results in SM, it is found that 123 kinds of 1D AWs demonstrate the flat-bands characters. Compared with the binary 1D AWs, the flat-bands prefer to occur in ternary and multi-element composed 1D AWs. For instance, the electron (hole) effective masses of 1D $GaSbCl_6$ and $MoOF_4$ are 132.7 m (14.5 m) and 77.4 m (26.5 m), respectively, where m is the mass of a free electron. The bandwidths of the conduction (valence) bands for 1D $GaSbCl_6$ and $MoOF_4$ are only 13.7 (28.5) meV and 23.4 (45.2) meV. The obvious difference between $GaSbCl_6$ in Fig. 3(b3) and $MoOF_4$ in Fig. 3(c3) originates from the valence band components near E_F, which is completely contributed by Cl-3p orbitals in $GaSbCl_6$ and by the hybridized O-2p and F-2p orbitals in $MoOF_4$. It also indicates that the flat bands show complex orbital dependencies in different 1D AWs. It is noted that the flat band physics here is

nontrivial since the flat band occurs along the wire direction rather than the quantum confinement direction. Further considering the correlation effect between electrons in these flat bands systems, the 1D AWs may display various exotic quantum states, such as Hubbard insulators and superconductors. Thus, the flat-bands characters make these 1D AWs in particular the multi-element composed 1D AWs be ideal low dimensional systems to explore the correlated effect and exotic quantum phases.

4. Stability and exfoliation energy

To further examine the structural stability of these 1D AW materials, the phonon spectra of typical materials with different crystal structures are examined, as shown in Section VII of the SM. The 1D AWs without imaginary frequencies in their phonon spectra are dynamically stable and would be reasonably acquired in experiments. Beside the dynamical stability of these 1D AWs, it is essential to evaluate the exfoliating possibility from the 3D bulks. Here the exfoliation energies of 1D unary and binary AWs are calculated based on the formula of $E_{\rm exf} = \frac{E_{\rm 1D}}{N_{\rm 1D}} - \frac{E_{\rm bulk}}{N_{\rm bulk}}$, which is utilized to validate the inter-wires interactions between the nearest neighboring 1D vdW wires in the bulks.[48] Here, $E_{\rm 1D}$ and $E_{\rm bulk}$ are the total energies of the 1D and 3D unit cells, and $N_{\rm 1D}$ and $N_{\rm bulk}$ are the number of the atoms in the 1D and 3D unit cells, respectively. It is also noted that the exfoliation energy less than 200 meV/atom is usually set as the criterion to judge the feasibility of cleaving 1D materials.[48] Based on this criterion, it is concluded that $\sim 72\%$ unary and binary 1D AWs are relatively easier to be exfoliated in Fig. 4. Meanwhile, the systems with relatively small exfoliation energy tend to be dynamically stable. In fact, two steps of exfoliating 2D monolayer from 3D bulk and exfoliating 1D AW from 2D monolayer are relatively reasonable and feasible during practically exfoliating process. In addition, the 1D AWs with larger exfoliation energies could be still prepared through other techniques, such as ionic scissoring preparation technique.[49]

Through analyzing the electronic structures, phonon spectra, and exfoliation energies of 1D AWs, the most promising and possibly synthesizable 1D AWs in experiments are proposed as follows. In terms of the thermodynamical stabilities and relatively lower exfoliation energies in SM, 1D AWs of CuO_2 and MnF_4 are FM metal and FM semiconductor, respectively. Besides, 1D AWs of VBr_3 and VS_2 display AFM metal and AFM semiconductor characters, respectively. Moreover, 1D AWs of $TeBr_2$, $SiCl_2$, and $BeCl_2$ demonstrate semiconducting properties with direct band gaps, which are in the range of ~ 0.66 eV–6.84 eV. Thus, these typical 1D AWs are highly expected to be prepared and applied in versatile electronic and optoelectronic devices with smaller scale. In this work, the undistorted 1D AWs have been systematically explored. In fact, due to the strong electronphonon coupling, these 1D AWs may undergo interesting Peierls distortions. For example, 1D carbon chain will form a dimerization configuration along the chain direction to minimize the total energy, resulting in the transition of 1D carbon chain from the metallic to insulating. For 1D AWs with more complex structures, the atoms would move and twist within 3D space, inducing more complex and interesting Peierls distortions. It is deserved to exploit in further work.

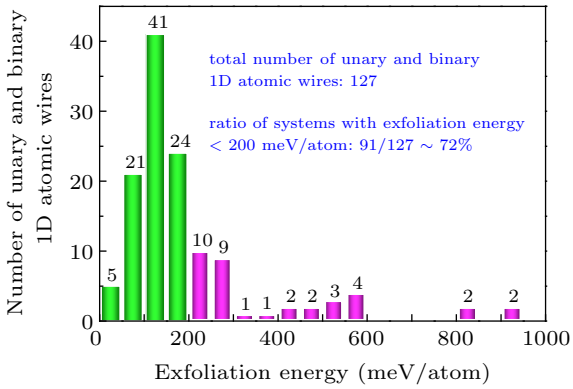


Fig. 4. Distribution of the exfoliation energies of unary and binary 1D AWs. The exfoliation energies of most 1D AWs are in the range of 50–200 meV/atom. The specific values of the exfoliation energies for all 1D AWs are listed in Table S1 in the SM.

5. Conclusion and perspectives

In this work, a database of 367 types of 1D AWs has been established, where the crystal structures, electronic properties, and stabilities are included based on DFT calculations. It is found that $\sim 81\%$ of 1D AWs are binary and ternary compounds. Furthermore, the unary and binary 1D AWs with relatively small exfoliation energy tend to be thermodynamically stable and 72% unary and binary 1D AWs are suitable to be mechanically exfoliated from their bulks. More significantly, the rich physical properties and quantum phases, such as 1D semiconductors, 1D metals/semimetals, 1D magnetism, shed light on potential applications of these 1D AWs in next-generation sub-nm electronic, spintronic, and energy relevant devices, etc. In addition, some 1D AWs possessing flat bands characters would provide an exciting and ideal platform to explore strongly correlated phenomena. Therefore, this database will offer a valuable resource for the scientific community to further explore 1D exotic quantum states and exploit practical 1D device applications based on 1D AW systems.

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