



Article High-Throughput Computational Search for Half-Metallic Oxides

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Abstract: Half metals are a peculiar class of ferromagnets that have a metallic density of states at the Fermi level in one spin channel and simultaneous semiconducting or insulating properties in the opposite one. Even though they are very desirable for spintronics applications, identification of robust half-metallic materials is by no means an easy task. Because their unusual electronic structures emerge from subtleties in the hybridization of the orbitals, there is no simple rule which permits to select a priori suitable candidate materials. Here, we have conducted a high-throughput computational search for half-metallic compounds. The analysis of calculated electronic properties of thousands of materials from the inorganic crystal structure database allowed us to identify potential half metals. Remarkably, we have found over two-hundred strong half-metallic oxides; several of them have never been reported before. Considering the fact that oxides represent an important class of prospective spintronics materials, we have discussed them in further detail. In particular, they have been classified in different families based on the number of elements, structural formula, and distribution of density of states in the spin channels. We are convinced that such a framework can help to design rules for the exploration of a vaster chemical space and enable the discovery of novel half-metallic oxides with properties on demand.

Keywords: half metals; transition metal oxides; high-throughput search; aflowlib; spintronics

1. Introduction

Spintronics attempts to employ electron's charge and spin degrees of freedom in novel computing and data storage applications, assumed to be faster and more energy efficient than their conventional counterparts [1,2]. Successful development of such devices strongly depends on the availability and integration of diverse materials which would enable harnessing of electrons spins. Among several obstacles on the route to the practical realization of both spin logic and memory elements is the lack of sufficiently spin-polarized magnetic electrodes that could act as spin current sources. The mixed spin current may not only impede the efficient spin injection, but also limit the performance of devices utilizing either giant (GMR) or tunneling magnetoresistance (TMR) [3]. In this regard, half-metals (HM), which are fully spin-polarized at the Fermi level [4–7] and only pass a spin-up or spin-down current, emerge as natural candidates to use as electrodes in such devices. The identification of half-metallic compounds integrable with mature architectures based on complementary metal oxide semiconductors (CMOS) would therefore represent an important step towards broader implementation of spintronics.

Regrettably, half metals are extremely rare in nature, and discovery of materials with suitable properties is challenging, either from experimental or theoretical side [8–11].

Most representative half-metallic compounds belong to either heusler/half-heusler alloys (e.g., NiMnSb and PtMnSb [12]) or transition metal oxides (TMO) in multiple structural forms, such as simple rutiles (CrO₂ [13]), spinels (Fe₃O₄ [14]), perovskites (La_{1-x}Sr_xMnO₃ [15]), pyrochlores $(Tl_2Mn_2O_7 [16])$, or double perovskites $(Sr_2FeMoO_6 [17])$. Interestingly, extensive studies of these and similar materials have clearly shown that half-metallicity, despite being quite peculiar, does not manifest in an obvious way in magnetic, electrical, or optical properties that could be measured. The simplest indicator is perhaps the integer magnetic moment per unit cell at absolute zero, which is a necessary condition for half-metallicity in a stoichiometric compound. However, it does not permit unambiguously distinguishing a half metal from a standard ferromagnet. Observation of conducting electrons of one spin direction could certainly provide a more direct proof, but experimental techniques such as spin-polarized photoemission or transport measurements in point contacts and tunnel junctions are flawed by uncertainty and full spin polarization is rarely confirmed. Electronic structure calculations are thus the most useful tool to identify half metals, even though the existence of a band gap for just one spin channel is by some means fortuitous and hard to predict. In fact, the design rules so far have strongly relied on investigations in specific crystal families based on a prototype.

Here, we have identified a large number of new candidates for half metals by performing a high-throughput (HT) screening of the electronic structure information from the AFLOWLIB database [18–20]. Currently, the repository contains over 3,000,000 different materials entries, among which 60,324 belong to the inorganic crystal structure database (ICSD) [21], representing fully determined and synthesized compounds. The data from this subset have been explored based on the analysis of their calculated density of states (DOS); the presence of a band gap in just one spin channel has been adapted as a major criterion for half-metallicity. The search revealed in total over one-thousand potential half metals, including most of the known examples. We have selected and described in detail a subgroup of oxides, among which 223 materials have been predicted to be strongly half-metallic. We have further classified them according to the number of elements and atomic structure, recognizing new crystal prototypes. Remarkably, the reported electronic structure parameters have shed more light on the mechanisms of hybridization and origin of half-metallicity. Figure 1 shows the schematic diagram of the full search procedure as well as the classification of the identified compounds.



Figure 1. Left: Scheme illustrating steps of the high-throughput (HT) search for half-metallic oxides starting with the AFLOWLIB database. Right: Diagram representing the distribution of different structural groups among the identified half-metal candidates.

2. Results

Before we start with an overview of the HT search, let us remark that materials repositories usually do not provide complete information on the magnetic ordering. Thus, some ferromagnetic compounds may be classified as paramagnetic and they cannot be included in this search. Conversely, several materials labeled as ferromagnetic may actually display different magnetic orders. As the ground state needs to be verified experimentally or theoretically via more realistic ab initio calculations, we will hereafter refer to potential half metals. In the screening procedure, we have first selected materials whose spin polarization at the Fermi level (E_F) is different from zero. This can be expressed as $P_0(E_F) = [N_{\uparrow} - N_{\downarrow})]/[N_{\uparrow} + N_{\downarrow}] \neq 0$, where $N_{\uparrow/\downarrow}$ denotes the density of states for spin majority/minority at E_F. Second, we have analyzed electronic states around the Fermi level, and classified the compounds as metals, half-metals, and semiconductors/insulators. We have further restricted the analysis to "half-metallic semiconductors" determined by conditions on the band gap ($E_g < 3.5 \text{ eV}$), valence band maximum (VBM > -1.5 eV), and conduction band minimum (CBM < 2.5 eV) of the insulating channel. Finally, in order to unveil materials that are strongly half-metallic, we have put a constraint on the spin polarization in the energy region limited by VBM and CBM, namely, $P_0(E_{gap}) > 0.8$. The spin-flip excitation energies of the transition from majority to minority spin, and vice versa, have been also constrained to ensure robustness of half-metallicity with respect to thermal fluctuations [4].

The high-throughput procedure revealed a total number of 223 candidates for strongly half-metallic oxides. They have been categorized according to the number of elements; we have classified 13 binary, 105 ternary, 101 quaternary, and four quinary compounds. Each of these categories has been further divided into families based on a crystalographic structure. The full list of the identified materials is provided in Tables A1–A4 in the Appendix A along with the descriptors and parameters essential for the analysis of the electronic structure phenomena behind half-metallicity. We have reported crystal lattice, saturation magnetization (M_s), spin polarization (P_0), energy gap (E_{gap}), as well as VBM and CBM of the insulating spin channel (either in spin majority or minority, as denoted by the arrows preceding the values). Finally, we have extracted quantities useful to determine the type of hybridization and strength of half-metallicity. The atom- and orbital-resolved spin magnetic moments are defined as fractions of the total magnetic moment per unit cell. We have also listed the overlaps of partial density of states functions projected on different orbitals, calculated as a percentage of a common area between each pair of functions in the metallic spin channel. These additional data are provided in the Supplementary Materials.

2.1. Binary Oxides

Binary compounds are the simplest half-metallic structures; yet no element can be a half metal. However, few binary oxides beyond the representative CrO_2 are known to exhibit half-metallicity. The high-throughput search has not greatly improved this status, as binaries account for only a small fraction of revealed materials. Moreover, among the 13 compounds listed in Table A1, several are polytypes or almost identical structures. One example is the well-studied rutile CrO_2 (ORC) whose half-metallic properties are a consequence of the exchange splitting larger than the occupied bandwidth. The same mechanism leads to full spin polarization in CrO_2 (TET), which can be considered a strained variant of the former; note nearly identical parameters in Table A1. Similarly, most of the Fe₃O₄ phases can be associated with the cubic magnetite structure (FCC) above the Verwey transition, which is ferrimagnetic due to the presence of two different ions Fe(3+) and Fe(2+); Fe₃O₄ is a well known half metal with the highest reported $T_C > 800$ K. Last, stoichiometrically different Fe₂O₃ was previously found to be antiferromagnetic and insulating, thus the crystal ground state is not a half metal.

Table A1 contains several materials that have never been proposed as potential half metals. However, a detailed consideration of their properties indicates that the half-metallicity might be unfeasible in most of them. Both reported phases of CoO are antiferromagnetic [22]. Moreover, the vanadates do not manifest ferromagnetic ground states. The simpler VO₂ is non-magnetic and shows a strong metal-to-insulator (MIT) transition at 340 K, accompanied by a structural change from tetragonal to monoclinic. The latter was previously suggested to be metallic, but we emphasize that its electronic structure is still under debate. V_6O_{13} with its mixed-valence state V(4+) and V(5+) is again a MIT system, shown to be antiferromagnetic below 50 K and ferrimagnetic at higher temperatures; half-metallicity of the ferrimagnetic phase has never been reported. Finally, we conclude that the only binary compound that indeed seems to be half-metallic is Ce₇O₁₂, one of few rare-earth oxides revealed in this study. The crystal structure is rather complex, whereby inequivalent Ce sites are likely to cause a ferrimagnetic ordering.

2.2. Ternary Oxides

The diversity of the revealed ternaries is reflected in complex chemical formulas that can be found in Table A2. Although most of the structures belong to one of three main crystal families, including (i) spinels (AB_2O_4), (ii) perovskites (ABO_3), and (iii) pyrochlores ($A_2B_2O_7$), there are materials containing more than seven and up to 20 oxygen atoms in the unit cell; many of them have not been considered as candidates for half metals and can be thus regarded as new prototypes. Below, we have briefly characterized the known structural families in which we have found several new HM.

2.2.1. Spinels

Spinels are cubic lattice structures characterized by a general formula AB_2O_4 [23,24]. Multiple degrees of freedom present in these complex crystals can be used to engineer their physical properties. In particular, they exhibit complex magnetic properties ranging from ferrimagnetism and ferromagnetism, to strong-magnetostructural coupling which is often related to the occupation of the magnetic ions in two different sublattices. According to their cation distributions, spinels can be categorized as "normal" and "inverted" spinel structures [25]. In the normal spinel structures, one-eighth of the tetrahedral interstices in oxygen sublattice are occupied by the *A* atoms and one-half of the octahedral interstices are occupied by the *B* atoms. In the inverted spinel structures, tetahedral interstices are occupied by *B* atoms and the octahedral interstices are occupied by both *A* and *B* atoms. The HT search revealed in total 18 spinels; most of them were never proposed as HM candidates.

2.2.2. Perovskites

Half-metallic ternary perovskite oxides are very rare. The crystals sharing the general formula ABO₃ contain BO₆ octahedra whereby B cations are surrounded by oxygen atoms. Such a configuration causes a superexchange mechanism mediated by dominating oxygen atoms, which makes the magnetic state more likely to be antiferromagnetic than ferromagnetic. Thus, the electronic structure is usually semiconducting and insulating. It has been though proven that the half-metallic state could emerge upon doping, strain, or intrinsic defects. The most known example is a non-stoichiometric La_xSr_{1-x}MnO₃, based on antiferromagnetic and insulating LaMnO₃ in which the sufficient Sr doping may yield half-metallicity [15]. The HT search revealed 23 potentially half-metallic perovskites that could be interesting for similar non-stoichiometric-doped configurations. Indeed, we have identified BaFeO₃ recently reported to be ferromagnetic and half-metallic below $T_C \sim 180$ K [26]. We have also listed BaRuO₃, which was shown to be ferromagnetic [27], while the previous prediction of half-metallicity still awaits experimental verification [28]. Finally, we have revealed stoichiometric SrRuO₃, which was theoretically predicted to be half-metallic under doping with Sn or Ti [29,30].

2.2.3. Pyrochlores

The most representative example of a half-metallic pyrochlore is $Tl_2Mn_2O_7$ [16]. However, it has not been listed in Table A2, as the electronic structure from the AFLOWLIB database does not comply with the criteria for robust half-metallicity adapted in the HT search. In particular, the stringent condition imposed on the density of states eliminates the materials that would have more than 0.005 states/eV at energies within the band gap of the insulating channel. The closer inspection of the calculated electronic structure confirms that $Tl_2Mn_2O_7$ indeed does not fit in this regime; this compound could only be included upon increasing the threshold. Nevertheless, we have found 11 different pyrochlores with the half-metallic electronic structure.

2.3. Quaternary Oxides

The majority of the quaternary oxides reported in Table A3 belongs to the crystal family group of the double perovskites with the general formula $A_2BB'O_6$, consisting of two different perovskites—ABO₃ and AB'O₃—arranged in a three-dimensional checkerboard pattern. The possibility of choosing two different transition metal ions opens up a wide range of possibilities to tailor the magnetic properties in this class of materials. The most known compound from this family is Sr₂MoFeO₆ with a large magnetic moment and Curie temperature of more than 420 K [17,31]. The HT search revealed over 30 double perovskites, including a similar Sr₂MoCoO₆ structure. The mechanism that determines half-metallicity in these compounds is quite complex and related to a combination of superexchange interaction in the B-O-B' chains and the hybridization of transition metal orbitals with O *2p* states. The magnetic properties of double perovskites are, however, quite well known [32]. In addition, Table A1 contains previously unrecognized prototypes, many of which seem to be good candidates for half metals.

2.4. Quinary Oxides

Finally, we note that the search revealed only four quinary compounds. Such a result does not mean that quinary half-metallic oxides would not occur in nature. The reason is mostly related to a currently limited number of quinary materials in the AFLOWLIB repository. In particular, we have noticed that a known half-metallic quadruple perovskite $CaCu_3Fe_2Re_2O_{12}$ has not been found because it is yet absent in the database [33]. The materials listed in Table A4 are rather difficult to analyze without performing additonal calculations. Although the radioactive $CH_2P_2PuO_6$ is useless for spintronics, $CuH_{12}Mn_2N_4O_8$, $H_4K_2N_4PdO_{10}$, and $La_3MnS_3WO_6$ indeed seem to be robust half metals. The latter can be considered a quasi-1D spin chain and would probably reveal short range magnetic ordering below 4 K. The ground states still need to be verified but these structures are clearly new prototypes of half metals (see Figure 2).



Figure 2. Crystal structures of quinary prototypes of half metals revealed in the HT search.

3. Discussion

The presented search based on the HT screening suggests that several new half-metallic oxides could be discovered. In fact, the choice of oxides as target materials for the above analysis was deliberate in a larger perspective of rapidly evolving oxide spintronics [34]. TMO often host a large variety of physical phenomena that emerge due to the complex interplay of the electronic charge, spin, and orbital degrees of freedom. Beyond magnetic properties, more exotic effects have been extensively studied, including multiferroicity, superconductivity, or magnetocaloric behavior [35–37]. Thus, the role of half-metallic oxides does not need to be limited solely to the generation of spin-polarized

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currents; being highly multifunctional, they could be capable to perform multiple tasks within one spin-based device [38]. The interplay of diverse phenomena in realistic half-metallic systems is therefore an interesting direction to explore in more specific studies.

Importantly, realization of either novel or conventional spintronics devices operating at room temperature requires robust half-metallicity. One could therefore raise a question, how many of the identified compounds will be still half-metallic at 300 K? Our search and analysis based primarily on the electronic structure information from the AFLOWLIB cannot give a precise answer at the present stage. As we have previously explained, most of the magnetic compounds in materials databases are in a ferromagnetic configuration, whereas, in reality, oxides often exhibit antiferromagnetic or more complex magnetic ground states. Although a large number of the identified materials may indeed be ferromagnetic and several are confirmed half metals, a complete verification of the magnetic phase along with the transition temperature would be desirable [39–41]. Multi-step calculations of numerous hypothetical magnetic configurations for each compound are though a great challenge. In a short-term perspective, exploring particular oxide-based interfaces could be more appropriate than the verification of the whole dataset ground states.

4. Methods

The high-throughput screening has been performed utilizing the AFLUX search engine, which helps to extract the electronic structure data from the AFLOWLIB database [42]. In particular, we have analyzed the output files of density functional calculations performed within the AFLOW framework [43–45], which leverages the Vienna Ab initio Simulation Package (VASP) [46,47]. Projector-augmented-wave pseudopotentials were used to treat electron–ion interactions [48]; kinetic energy cut-offs were set to highest recommended value among corresponding pseudopotentials. The exchange–correlation interaction was treated in the generalized gradient approximation in the parametrization of Perdew, Burke, and Ernzerhof (PBE) [49]. LSDA+U approach in formulation of Dudarev [50] was used to account for electronic correlations of transition metal ions (U parameters are listed in [19]). Spin–orbit interaction was not included in the calculations.

The search procedure has been described in Results; we hereby give technical details which determine the exact output of each phase, necessary to reproduce the list of compounds extracted from AFLOWLIB. In the first step, based on the condition $P_0(E_F) = \neq 0$, we select thousands of magnetic materials with spin imbalance at the Fermi level. Certainly, such a descriptor cannot provide sufficient information about the half-metallic state. Several materials that satisfy this criterion may not have a robust band gap. For instance, binary compound CuO (ICSD-628616) switches the conductance between two spin channels just around $E_{F_{\ell}}$ and reveals semi-metallic rather than half-metallic properties. The essential phase of screening relies on the analysis of DOS. Materials with more (less) than 0.005 states/eV at energies within the band gap in the insulating (conducting) channel around E_F are screened out as not half-metallic (note that this criterion eliminates a known half metal $Tl_2Mn_2O_7$, see Section 2.2.3). As an outcome of this phase, we have revealed 1061 compounds, among which 494 are oxides. Finally, we have selected materials referred to as strong half metals potentially useful for spintronics, whose spin imbalance is sufficiently large within the energy window of the band gap and robust against thermal fluctuations. Screening based on the set of constraints $(P_0(E_{gap}) > 0.8; E_g < 3.5 \text{ eV}; -0.01 > \text{VBM} > -1.5 \text{ eV}; 0.1 < \text{CBM} < 2.5 \text{ eV})$ revealed 223 oxides reported in Tables A1–A4.

5. Conclusions

In summary, we have explored the AFLOWLIB repository containing electronic structure data of thousands of materials, and identified over one hundred potentially half-metallic oxides. A large number of these compounds were not previously recognized as half metals. Remarkably, we have revealed new crystal prototypes, suggesting a way to design additional half-metallic oxides sharing the same structure. Finally, we have also indicated numerous crystals belonging to the same families as some

of the known half-metallic compounds. These include newly identified spinels, perovskites, pyrochlores, and double perovskites. The quantitative analysis of the electronic structure has indicated a strong p-d hybridization as a common mechanism behind half-metallicity in a vast majority of the considered compounds. We believe that this study will stimulate further exploration of a larger chemical space as well as an ultimate confirmation of half-metallicity in selected structures.

Supplementary Materials: The following are available online, Data File S1.

Author Contributions: L.S.I.L. performed the high-throughput search. L.S.I.L., J.S., and P.G. analyzed and validated the data. L.S.I.L. and J.S. wrote the manuscript. S.C., M.F., and M.B.N. conceptualized and supervised the project. All authors have read and agreed to the published version of the manuscript.

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Abbreviations

The following abbreviations are used in this manuscript:

HM	half metal
HT	high-throughput
AFLOW	automatic flow for materials discovery
ICSD	inorganic crystal structure database
DOS	density of states
VBM	valence band maximum
CBM	conduction band minimum

Appendix A

Table A1. Binary half-metallic oxides. $P_0(E_F)$ and $P_0(E_{gap})$ denote spin polarization at the Fermi level and within the band gap, respectively. E_{gap} , VBM, and CBM are calculated for the insulating channel either in spin majority or minority (identified by \uparrow and \downarrow). M_S refers to the saturation magnetization.

Name	ICSD	Lattice	$P_0(E_F)$	$P_0(E_{gap})$	Egap	VBM	CBM	\mathbf{M}_S
Fe ₃ O ₄	92356	RHL	1.0	1.000	↑ 2.90	$\uparrow -1.08$	↑ 1.82	28.00
Ce_7O_{12}	88754	RHL	1.0	0.978	↓ 3.09	$\downarrow -0.99$	$\downarrow 2.10$	4.00
Fe ₃ O ₄	31156	ORCI	1.0	1.000	↑ 2.6 7	$\uparrow -1.08$	$\uparrow 1.59$	28.00
CoO	53059	BCT	1.0	1.000	† 2.22	$\uparrow -0.78$	$\uparrow 1.44$	3.00
Fe ₃ O ₄	77589	FCC	1.0	1.000	† 2.7 3	$\uparrow -1.20$	$\uparrow 1.53$	27.99
CoO	245320	FCC	1.0	0.999	† 2 .31	$\uparrow -0.27$	$\uparrow 2.04$	3.00
Fe ₃ O ₄	98086	MCL	1.0	0.999	↑ 2.76	$\uparrow -0.88$	$\uparrow 1.88$	52.00
CrO ₂	155832	ORC	1.0	1.000	$\downarrow 3.03$	$\downarrow -0.63$	$\downarrow 2.40$	4.00
Fe ₃ O ₄	164813	ORC	1.0	1.000	† 2.6 1	$\uparrow -0.72$	$\uparrow 1.89$	95.97
V ₆ O ₁₃	16779	MCLC	1.0	0.997	$\downarrow 2.34$	$\downarrow -1.48$	$\downarrow 0.86$	4.00
VO ₂	34417	MCLC	1.0	1.000	↓ 2.13	$\downarrow -1.05$	$\downarrow 1.08$	4.00
CrO ₂	166023	TET	1.0	1.000	$\downarrow 3.03$	$\downarrow -0.65$	↓ 2.39	4.00
Fe ₂ O ₃	108905	BCC	1.0	0.999	$\downarrow 1.60$	$\downarrow -1.35$	$\downarrow 0.25$	55.99

Name	ICSD	Lattice	P ₀ (E _{F})	P ₀ (E _{gap})	Egap	VBM	CBM	\mathbf{M}_S
FeNaO ₂	167376	RHL	1.0	0.996	↑ 2.52	$\uparrow -1.41$	↑ 1.11	1.00
$CoLaO_3$	180176	RHL	1.0	0.997	↓ 2.42	$\downarrow -0.51$	↓ 1.91	4.00
$Ca_3Co_2O_6$	82175	RHL	1.0	0.995	↓ 1.32	$\downarrow -0.83$	$\downarrow 0.49$	12.00
LaNiO ₃	173477	RHL	1.0	0.999	↓ 2.28	$\downarrow -0.64$	↓ 1.64	2.00
BaRuO ₃	91075	RHL	1.0	0.999	$\uparrow 1.84$	$\uparrow -0.55$	† 1.29	6.00
CuNdO ₂	18104	RHL	1.0	1.000	↓ 3.02	$\downarrow -0.92$	↓ 2.10	3.00
PuSrO ₄	31974	RHL	1.0	1.000	↓ 2.25	$\downarrow -0.98$	$\downarrow 1.27$	2.00
Ba ₂ Co ₉ O ₁₄	161771	RHL	1.0	0.999	$\downarrow 1.58$	$\downarrow -0.53$	$\downarrow 1.05$	25.00
SrV ₁₃ O ₁₈	97949	RHL	1.0	0.993	$\downarrow 1.41$	$\downarrow -0.72$	$\downarrow 0.69$	25.00
$RhSr_4O_6$	109297	RHL	1.0	0.999	↑ 2.62	$\uparrow -0.20$	$\uparrow 2.43$	2.00
FeLiO ₂	51207	RHL	1.0	0.994	↑ 2.62	$\uparrow -1.39$	↑ 1. 2 3	1.00
AgNiO ₂	73974	RHL	1.0	0.999	↓ 2.39	$\downarrow -0.89$	$\downarrow 1.50$	1.00
Cu_2PO_4	80181	TRI	1.0	0.992	$\uparrow 1.98$	$\uparrow -0.33$	$\uparrow 1.65$	4.00
CaIrO ₃	159027	ORCC	1.0	0.999	$\uparrow 2.55$	$\uparrow -0.31$	$\uparrow 2.24$	2.00
Fe ₄ Sr ₄ O ₁₁	249009	ORCC	1.0	0.999	$\downarrow 1.14$	$\downarrow -0.15$	↓ 0.99	18.00
UYO ₄	16492	ORCC	1.0	1.000	↓ 3.06	$\downarrow -1.02$	$\downarrow 2.04$	1.00
Bi ₃ Mn ₂ O ₇	184382	ORCC	1.0	1.000	↓ 2.46	$\downarrow -0.84$	↓ 1.62	18.00
$K_3Pd_2O_4$	245610	ORCC	1.0	0.998	$\uparrow 2.54$	$\uparrow -0.22$	† 2. 31	1.99
CaRhO ₃	164774	ORCC	1.0	0.999	$\uparrow 2.08$	$\uparrow -0.20$	† 1.89	2.00
Eu ₃ OsO ₇	170874	ORCC	1.0	1.000	↓ 1.61	$\downarrow -0.81$	$\downarrow 0.79$	42.77
MgVO ₃	15927	ORCC	1.0	0.997	↓ 0.95	$\downarrow -0.15$	$\downarrow 0.80$	2.00
$Cl_5U_2O_2$	23084	ORCC	1.0	1.000	↓ 3.05	$\downarrow -1.04$	↓ 2.01	3.00
$RuSr_2O_4$	73394	BCT	1.0	0.995	↑ 0.69	$\uparrow -0.65$	$\uparrow 0.04$	2.00
Nd ₄ Ni ₃ O ₈	51097	BCT	1.0	0.962	↓ 1.41	↓ v0.52	↓ 0.88	14.00
NdVO ₄	15610	BCT	1.0	1.000	↓ 3.12	$\downarrow -1.47$	↓ 1.65	6.00
FeSr ₂ O ₄	74419	BCT	1.0	0.998	↓ 1.34	$\downarrow -0.42$	↓ 0.92	4.00
KRu ₄ O ₈	1562	BCT	1.0	0.988	↑ 2. 01	↑ v0.66	↑ 1.35	7.00
La ₃ Ni ₂ O ₆	249209	BCT	1.0	0.942	↓ 1.85	$\downarrow -0.39$	$\downarrow 1.46$	1.00
$IrSr_2O_4$	45974	BCT	1.0	0.994	$\uparrow 0.34$	$\uparrow -0.19$	$\uparrow 0.15$	1.00
$K_2Ru_8O_{16}$	61378	BCT	1.0	0.989	↑ 2. 01	$\uparrow -0.64$	↑ 1.37	7.00
$CoSr_2O_4$	246483	BCT	1.0	0.997	↓ 0.98	$\downarrow -0.21$	$\downarrow 0.77$	3.00
Pr ₂ TeO ₂	89559	BCT	1.0	1.000	↓ 2.04	$\downarrow -0.54$	$\downarrow 1.50$	4.02
$CrSr_2O_4$	245595	BCT	1.0	0.999	$\downarrow 1.56$	$\downarrow -0.11$	$\downarrow 1.46$	2.00
BaFeO ₃	50869	HEX	1.0	1.000	↓ 1.22	$\downarrow -0.14$	$\downarrow 1.08$	23.99
BaRhO ₃	15520	HEX	1.0	1.000	$\uparrow 1.48$	$\uparrow -0.19$	† 1.29	4.00
BaRuO ₃	84652	HEX	1.0	0.999	$\uparrow 1.68$	$\uparrow -0.42$	$\uparrow 1.26$	8.00
AgNiO ₂	415451	HEX	1.0	0.999	$\downarrow 2.40$	$\downarrow -0.89$	$\downarrow 1.52$	2.00
InMnO ₃	186856	HEX	1.0	1.000	↓ 2.52	$\downarrow -1.49$	$\downarrow 1.03$	24.01
BaCrO ₃	35029	HEX	1.0	1.000	↓ 2.32	$\downarrow -0.42$	$\downarrow 1.90$	8.00
HNiO ₂	169980	HEX	1.0	0.994	↓ 3.38	$\downarrow -0.93$	$\downarrow 2.44$	1.00
Fe ₂ NaO ₃	200009	HEX	1.0	1.000	$\uparrow 2.77$	$\uparrow -1.02$	$\uparrow 1.75$	9.00
Fe ₁₂ SrO ₁₉	16158	HEX	1.0	0.994	$\downarrow 0.86$	$\downarrow -0.31$	$\downarrow 0.54$	77.92
CuMn ₂ O ₄	174000	FCC	1.0	1.000	↓ 2.97	$\downarrow -1.01$	↓ 1.96	14.01
$Ir_2Pr_2O_7$	156436	FCC	1.0	0.998	$\uparrow 2.07$	$\uparrow -0.24$	$\uparrow 1.83$	12.00
Co ₂ GeO ₄	21115	FCC	1.0	1.000	$\uparrow 2.04$	$\uparrow -1.40$	$\uparrow 0.64$	12.00
Mn ₂ Sb ₂ O ₇	247301	FCC	1.0	0.941	↓ 1.26	$\downarrow -1.25$	↓ 0.02	20.00
Ni ₂ Sb ₂ O ₇	247303	FCC	1.0	0.997	$\uparrow 0.97$	$\uparrow -0.53$	$\uparrow 0.45$	8.00
$Eu_2Mo_2O_7$	173946	FCC	1.0	0.999	$\downarrow 1.42$	$\downarrow -0.88$	$\downarrow 0.54$	32.00
Pr ₂ Te ₂ O ₇	92444	FCC	1.0	0.998	$\downarrow 1.61$	$\downarrow -0.41$	↓ 1.20	7.99
Cd ₂ Tc ₂ O ₇	180008	FCC	1.0	0.999	$\downarrow 1.86$	$\downarrow -1.20$	$\downarrow 0.66$	8.00
$Ru_2Tl_2O_7$	51158	FCC	1.0	0.998	$\uparrow 0.88$	$\uparrow -0.72$	$\uparrow 0.17$	8.00
CuRh ₂ O ₄	88962	FCC	1.0	0.980	↑ 2.13	$\uparrow -0.25$	$\uparrow 1.87$	1.99
$Ir_2Y_2O_7$	187534	FCC	1.0	1.000	↑ 2.29	$\uparrow -0.17$	↑ 2.13	4.00
AlFe ₂ O ₄	76977	FCC	1.0	1.000	† 3.36	$\uparrow -1.38$	$\uparrow 1.98$	18.00

Table A2. Ternary half-metallic oxides. Parameters are the same as in Table A1.

Table	A2.	Cont.
		001111

Name	ICSD	Lattice	P ₀ (E _{F})	P ₀ (E _{gap})	Egap	VBM	CBM	\mathbf{M}_S
FeNi ₂ O ₄	109150	FCC	1.0	0.998	$\downarrow 1.52$	$\downarrow -0.27$	$\downarrow 1.25$	4.00
Ca ₂ Ru ₂ O ₇	156409	FCC	1.0	0.997	$\uparrow 1.56$	$\uparrow -0.12$	$\uparrow 1.44$	12.00
$Mn_3P_2O_8$	415107	MCL	1.0	0.996	$\downarrow 3.03$	$\downarrow -0.87$	↓ 2.16	22.00
$Ru_3Sr_4O_{10}$	96729	MCL	1.0	0.999	$\uparrow 1.11$	$\uparrow -0.70$	$\uparrow 0.41$	12.03
Co ₃ La ₃ O ₈	86176	MCL	1.0	0.994	$\downarrow 1.11$	$\downarrow -0.66$	$\downarrow 0.45$	18.04
$Co_3La_4O_{10}$	51177	MCL	1.0	0.982	↓ 1.26	$\downarrow -0.60$	$\downarrow 0.66$	18.00
$Co_3P_2O_8$	9850	MCL	1.0	0.995	$\downarrow 1.44$	$\downarrow -0.66$	$\downarrow 0.78$	14.00
CoSrO ₃	108896	MCL	1.0	0.999	↓ 2.06	$\downarrow -0.38$	↓ 1.68	0.00
BFe ₃ O ₅	25101	MCL	1.0	1.000	[↑] 2.97	$\uparrow -1.14$	↑ 1.83	26.00
Cr ₃ HO ₈	156386	MCL	1.0	0.998	↓ 2.67	$\downarrow -1.28$	$\downarrow 1.40$	6.00
CaRhO ₃	183583	MCL	1.0	0.998	↑ 2.02	↑ -0.23	$\uparrow 1.80$	6.00
As ₂ Co ₃ O ₈	59000	MCL	1.0	0.996	⁺ 2.24	+ -1.26	$\uparrow 0.97$	36.01
$Bi_3Ru_3O_{11}$	74382	CUB	1.0	0.998	$^{+}1.65$	$\uparrow -0.36$	↑ 1.29	28.00
CaSnO ₂	27777	CUB	1.0	1.000	↑ 2.49	$^{+}-0.57$	↑1.92	2.01
PhVO ₂	187637	CUB	1.0	1.000	2.13	-1.31	0.83	1.00
$CrSrO_2$	245834	CUB	1.0	0.998	2.61	-0.36	1225	2.00
Fe5LiO _o	35769	CUB	1.0	0.946	12.01	1 - 0.62	1 42	76.00
Na ₁₁ U-O ₁	15 137	CUB	1.0	0.981	12.01	$\downarrow -0.41$	1.12	18.00
$LaR_{110}O_{11}$	100517	CUB	1.0	1 000	↓ <u>2</u> .00 ↑ 2 36	$^{+}_{-0.44}$	↓ <u>2.10</u> ↑ 1.92	28.00
$C_{2}R_{1}O_{2}$	99451	ORC	1.0	1.000	+ 2.00	$\uparrow -0.11$	↑ 1.7 <u>2</u> ↑ 1.12	8.00
NaRhaO.	170598	ORC	1.0	0.996	$\uparrow 1.11$ $\uparrow 1.46$	$^+$ -0.24	↑ 1.1 <u>2</u> ↑ 1.22	3.00
RuSrOa	56697	ORC	1.0	1,000	1. 1 0	1 - 0.24 1 - 0.50	1.22	8.00
NiVhO-	1510/0	ORC	1.0	0.000	2 13	-0.50	1 63	0.00
LiPuO-	191949	OPC	1.0	0.999	+ 2.13 + 1.52	+ 0.30	+1.03	2.00
$N_2 R_{11} O$	172608	ORC	1.0	0.999	1.55 ↑ 1.60	−0.30 ↑ 0.55	1.17 ↑ 1.05	12.00
CaEoO	02240	ORC	1.0	1.000	1.00	-0.55	1.05	12.00
CareO ₃	92349	ORC	1.0	1.000	\downarrow 1.09	$\downarrow -0.43$	$\downarrow 1.14$ $\downarrow 1.64$	22.02
$R_1 = R_2 O_5$	1/44/4	ORC	1.0	1.000	+2.50	$\downarrow -0.72$	$\downarrow 1.04$	32.02
DagreU5	201029	ORC	1.0	0.998	$\downarrow 2.00$	$\downarrow -0.55$	↓ 2.27	16.00
$Fer U_3$	23822 ((E00	MCLC	1.0	0.999	↓ 1.00	$\downarrow -0.59$	$\downarrow 1.09$	16.00
$Cu_2Li_3O_4$	414129	MCLC	1.0	1.000	↓ 1.55	$\downarrow -0.79$	$\downarrow 0.75$ $\uparrow 1.12$	14.00
$Co_2Na_7O_6$	414128	MCLC	1.0	0.987	1.95	-0.82	1.15	14.00
$MoYb_2O_6$	99574	MCLC	1.0	0.998	↑ 2.45	↑ -0.19	↑ 2.25	8.00
$Ba_2Mn_8O_{16}$	62096	MCLC	1.0	1.000	$\downarrow 2.73$	$\downarrow -0.80$	$\downarrow 1.94$	14.00
$BaMn_3O_6$	93226	MCLC	1.0	0.998	$\downarrow 2.44$	$\downarrow -0.27$	$\downarrow 2.17$	22.00
$IrNa_2O_3$	187130	MCLC	1.0	0.999	↑ 2.34 L 2.34	$\uparrow -0.33$	↑ 2.01	2.00
HgV_4O_{10}	418029	MCLC	1.0	0.995	↓ 2.22	$\downarrow -1.38$	$\downarrow 0.84$	2.00
MnPbO ₃	246351	MCLC	1.0	1.000	↓ 2.49	$\downarrow -0.10$	↓ 2.38	18.04
Fe ₂ K ₉ O ₈	174307	MCLC	1.0	0.897	↓ 2.94	$\downarrow -0.70$	↓ 2.24	36.01
Eu_2ReO_5	88686	TET	1.0	0.998	$\downarrow 0.89$	$\downarrow -0.10$	$\downarrow 0.78$	48.27
FeSrO ₂	418603	TET	1.0	0.974	↓ 1.25	$\downarrow -1.23$	↓ 0.02	4.00
CaFeO ₂	173438	TET	1.0	0.970	$\downarrow 1.09$	$\downarrow -1.00$	$\downarrow 0.09$	4.00
Fe5Y ₃ O ₁₂	23855	BCC	1.0	1.000	† 2.35	$\uparrow -1.38$	$\uparrow 0.97$	68.00
La ₄ Ru ₆ O ₁₉	100098	BCC	1.0	0.975	$\uparrow 2.47$	$\uparrow -1.00$	$\uparrow 1.47$	14.00
$La_4Os_6O_{19}$	100099	BCC	1.0	0.986	† 1.23	$\uparrow -0.61$	$\uparrow 0.62$	8.00
Fe5Pr ₃ O ₁₂	248013	BCC	1.0	0.993	$\uparrow 2.42$	$\uparrow -1.37$	$\uparrow 1.05$	92.00
Mn ₇ NaO ₁₂	151587	BCC	1.0	1.000	$\downarrow 3.32$	$\downarrow -0.98$	$\downarrow 2.34$	26.00
Bi ₁₂ MnO ₂₀	75079	BCC	1.0	0.999	$\downarrow 2.47$	$\downarrow -1.23$	$\downarrow 1.25$	3.00
Ba ₂ Ir ₃ O ₉	54725	BCC	1.0	0.988	$\uparrow 2.50$	$\uparrow -0.21$	† 2.29	10.00
Bi ₁₂ MnO ₂₀	75390	BCC	1.0	1.000	$\downarrow 2.37$	$\downarrow -1.14$	↓ 1.23	3.00
Cs ₁₈ Tl ₈ O ₆	421376	BCC	1.0	0.984	$\downarrow 0.27$	$\downarrow -0.18$	$\downarrow 0.09$	1.99
			1.0	0.040	1 1 00	A 0.45		20.00

Name	ICSD	Lattice	P ₀ (E _{F})	P ₀ (E _{gap})	Egap	VBM	CBM	\mathbf{M}_S
Ba ₄ Ru ₃ ZrO ₁₂	47132	RHL	1.0	0.998	↑ 2.78	$\uparrow -0.75$	↑ 2.03	6.00
Ba ₇ Cl ₂ Ru ₄ O ₁₅	71755	RHL	1.0	0.993	↑ 2 .15	$\uparrow -0.72$	$\uparrow 1.42$	10.03
Ba ₄ Ru ₃ TbO ₁₂	160870	RHL	1.0	0.982	↑ 2.98	$\uparrow -1.03$	↑ 1.95	7.00
B ₄ Fe ₃ NdO ₁₂	83507	RHL	1.0	0.998	↓ 2.30	$\downarrow -0.72$	↓ 1.58	18.00
CoPb ₂ TeO ₆	169195	RHL	1.0	0.998	↑ 1.60	↑ <i>−</i> 1.20	$\uparrow 0.41$	3.00
Ca ₃ CoMnO6	93775	RHL	1.0	0.994	[↑] 2.08	↑ −1.29	⁺ 0.79	12.00
Ba7Br2Ru4O15	73,069	RHL	1.0	0.996	⁺ 2.15	$\uparrow -0.72$	$\uparrow 1.42$	10.07
InNiSr ₃ O ₆	81660	RHL	1.0	0.945	J 3.20	$\downarrow -0.81$	2.39	2.00
BaEu2NiO5	68086	ORCI	1.0	1.000	2.46	$\downarrow -0.45$	1 2.01	14.00
Ca ₂ GaMnO ₅	51466	ORCI	1.0	1.000	J. 3.15	1 - 0.84	1 2.31	8.00
BaCoEu ₂ O ₅	78173	ORCI	1.0	0.999	1.3.00	-0.56	. 2.44	15.00
Ba2GdMoO6	236363	TRI	1.0	0.982	↑ 0.95	$^{+}_{-0.20}$	$\uparrow 0.75$	8.00
$Ag_2Co_2P_4O_{14}$	93591	TRI	1.0	0.997	↑ 2.6 0	↑ −1.35	↑ 1.24	18.03
NiOsSr ₂ O ₄	152442	BCT	1.0	0.999	1.36			4.00
ClaFeaSraO4	174532	BCT	1.0	0 999	↑ 1 11	$\uparrow -0.72$	↑ 0.39	8.00
Feal aaSeaOa	183143	BCT	1.0	0.992	↑ 2 91	$\uparrow -1.26$	↑ 0.0 <i>j</i> ↑ 1.65	8.00
Fe2Pr2Se2O2	183145	BCT	1.0	0.999	↑ 2.64	↑ –1.25	↑ 1.39	12.00
BaFe ₄ YO ₇	262842	BCT	1.0	0.996	↑ <u>2</u> .01 ↑ 2 27	↑ _1. <u>-</u> 0 ↑ _1.19	↑ 1.09 ↑ 1.08	12.00 17.00
FeaPraSaOa	181168	BCT	1.0	0.991	$\uparrow 2.2.7$	$\uparrow -1.33$	1.00	11 99
$Cl_{10}Cs_2Re_2O$	231	BCT	1.0	0.999	↑ <u>1</u> 23	$\uparrow -0.89$	↑ 0.35	2 99
AsaBaaMnaOa	32011	BCT	1.0	0.989	0.77	-0.54	0.00	10.99
CoMoSroO	153546	BCT	1.0	0.999	↓ 0.77 ↑ 2 30	$1.04 \\ 1.04 \\ 1.03 $	↓ 0.25 ↑ 0.87	3.00
AINdaNOa	201358	BCT	1.0	1 000	1 97	-0.32	1 65	6.00
BaalraMaOa	201000	HEY	1.0	1.000	+ 1.57 ↑ 2.50	↓ 0.52 ↑ _0.19	↓ 1.00 ↑ 2.40	8.01
BaaNaOsaOa	243232	HEY	1.0	0.984	1 2.55	$ -0.1 \rangle$	1 1 1 1	6.00
Bas LiOss Os	201240	HEY	1.0	1 000	+ 1.23 + 2.12	$\downarrow -0.10$	+ 0.84	10.00
$B_{2a}B_{11a}ZrO_{2}$	172754	HEY	1.0	1.000	+ 2.12 + 2.61	1.20 1.20	↓ 0.0 1 ↑ 1.05	8.05
Bas NiOcO	16406	HEY	1.0	0.998	1 60	1 00	1.55	11 00
BacCoRua	50830	HEY	1.0	0.990	+ 1.00 $+ 2.46$	+ -1.00 $+ -0.19$	↓ 0.00 ↑ 2 27	18.00
BaaCoRu2Og	94024	HEY	1.0	0.998	↑ 2. 1 0 ↑ 2.17	$\uparrow -0.17$ $\uparrow -0.76$	↑ 2.27 ↑ 1.41	8.02
BasClaC11=Ora	9678	HEY	1.0	1 000	0.51	_0.70	0.23	5.02
EaMos RbOs	245666	HEY	1.0	0.000	+ 2.68	+ 1.42	↓ 0.25 ↑ 1.26	1.00
BaalraNiOa	245000	HEY	1.0	1,000	↑ 2.00 ↑ 2.35	+ 0.24	↑ 1.20 ↑ 2.11	12.00
KaNaOsaOa	423654	HEY	1.0	0.999	1 51	-0.24	0.36	12.00
R31VaO52O9	281126	HEY	1.0	1,000	+ 1.51 + 1.47	$\downarrow -0.48$	↓ 0.50 ↓ 0.90	10.01
Baa Rua VbOa	400598	HEY	1.0	1.000	+ 1. 1 / ↑ 2.07	+ -0.40 $+ -0.81$	+ 0.77	12.00
Baa Na Rua Oa	281127	HEY	1.0	1.000	1 58	0.51	1 07	10.02
BaaCalraOa	201127	HEY	1.0	0.999	+ 1.00 $+ 2.12$	+ 0.31	+1.07 $+1.65$	10.02
Ba-ClCo-O	03657	HEY	1.0	0.999	1 1 10	-0.40	1.05	24.00
CrEnToO	164040	HEY	1.0	0.995	+3.30	$\downarrow -0.23$	$\downarrow 0.90$	18.00
Bar CoWO	27425	FCC	1.0	0.995	↓ 3.30 ↑ 2.00	+ 0.00	↓ 2. 1 5 ↑ 2.11	2.00
Ba ₂ CowO ₆	27423 410142	FCC	1.0	0.992	5.00	-0.69	2.11	5.00 1.00
Da2INaOSO6	412145	FCC	1.0	1.000	$\downarrow 1.55$	$\downarrow -1.11$	$\downarrow 0.24$	1.00
NiPuSr O	20407 101752	FCC	1.0	0.996	$\downarrow 1.22$ $\downarrow 1.20$	$\downarrow -0.79$	$\downarrow 0.42$ $\downarrow 1.07$	1.00
R_{1}	101755	FCC	1.0	0.997	$\downarrow 1.20$	$\downarrow -0.13$	$\downarrow 1.07$	4.00
$Da_2 ND N dO_6$	109152	FCC	1.0	0.995	↓ 3.32	$\downarrow -1.12$	↓ 2.19	3.00
$COPD_2 IeO_6$	169196	FCC	1.0	0.992	↑ 1.97 ★ 0 .10	↑ -1.19	↑ 0.78 ↑ 1.79	3.00
$Ba_2 BirO_6$	174289	FCC	1.0	1.000	↑ 2.18	↑ -0.56	1.62	2.00
Ba_2COMOO_6	184910	FCC	1.0	0.999	7 2.19	η -0.79	1.40	3.00
Ba_2MnReO_6	109256	FCC	1.0	0.986	$\downarrow 0.54$	$\downarrow -0.38$	$\downarrow 0.17$	2.02
Ba_2KuTmO_6	55713	FCC	1.0	0.997	↑ 3.03	$\uparrow -0.60$	↑ 2.43	20.00
Ba_2CaOsO_6	171988	FCC	1.0	0.997	$\downarrow 1.77$	$\downarrow -1.01$	↓ 0.77	2.00
Ba_2LiOsO_6	412142	FCC	1.0	1.000	↓ 1.28	$\downarrow -1.08$	$\downarrow 0.19$	1.00
CICu ₆ YO ₈	188351	FCC	1.0	0.989	↓ 1.32	$\downarrow -0.86$	$\downarrow 0.47$	4.00
ClCu ₆ InO ₈	69612	FCC	1.0	1.000	↓ 1.23	$\downarrow -0.87$	↓ 0.36	4.00
CoMoSr ₂ O ₆	181517	FCC	1.0	0.992	↑ 2.06	$\uparrow -0.85$	$\uparrow 1.20$	3.00

 Table A3. Quaternary half-metallic oxides. Parameters are the same as in Table A1.

Table A3. (Cont.
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Name	ICSD	Lattice	P ₀ (E _{F})	P ₀ (E _{gap})	Egap	VBM	СВМ	\mathbf{M}_S
Ba ₂ CoUO ₆	245141	FCC	1.0	0.980	$\uparrow 2.58$	$\uparrow -0.77$	$\uparrow 1.81$	3.00
Ba ₂ NdRuO ₆	155551	FCC	1.0	0.997	$\downarrow 1.41$	$\downarrow -1.05$	$\downarrow 0.36$	5.99
MnNbSr ₂ O ₆	181751	FCC	1.0	0.997	↓ 2.92	$\downarrow -1.27$	$\downarrow 1.65$	3.98
Ba ₂ ReYbO ₆	25399	FCC	1.0	0.994	$\downarrow 1.64$	$\downarrow -1.21$	$\downarrow 0.42$	0.73
Ba ₂ PrPtO ₆	80636	FCC	1.0	0.992	↓ 2.64	$\downarrow -0.33$	↓ 2.31	1.00
CoSr ₂ WO ₆	28598	FCC	1.0	0.995	† 2.82	$^{\uparrow}-0.96$	$\uparrow 1.86$	3.00
BaMn ₂ TbO ₆	154009	MCL	1.0	1.000	↓ 3.12	$\downarrow -0.66$	$\downarrow 2.46$	14.00
CdCsN ₃ O ₆	28649	CUB	1.0	1.000	$\downarrow 1.67$	$\downarrow -0.69$	$\downarrow 0.97$	4.00
CdN ₃ TlO ₆	28650	CUB	1.0	1.000	↓ 1.31	$\downarrow -0.77$	$\downarrow 0.54$	4.00
CdKN ₃ O ₆	28647	CUB	1.0	1.000	$\downarrow 1.70$	$\downarrow -0.84$	$\downarrow 0.86$	4.00
CdN ₃ RbO ₆	28648	CUB	1.0	1.000	$\downarrow 1.79$	$\downarrow -0.94$	$\downarrow 0.84$	4.00
BaCo ₂ YO ₅	171435	ORC	1.0	0.999	$\downarrow 1.54$	$\downarrow -0.15$	$\downarrow 1.40$	10.00
CKLaO ₄	90735	ORC	1.0	0.998	$\uparrow 1.44$	$\uparrow -0.75$	↑ 0.69	8.00
BaEuFe ₂ O ₅	416716	ORC	1.0	0.946	$\uparrow 0.95$	$\uparrow -0.10$	$\uparrow 0.84$	33.15
Ca ₂ FeMnO ₅	85125	ORC	1.0	0.998	↓ 2.46	$\downarrow -1.14$	↓ 1.32	35.96
Ca ₂ GaMnO ₅	51464	ORC	1.0	0.996	↓ 3.33	$\downarrow -0.93$	↓ 2.40	16.04
MnPb ₂ ReO ₆	182002	MCLC	1.0	0.975	$\uparrow 0.45$	$\uparrow -0.15$	$\uparrow 0.30$	13.99
Ag ₄ CuTeO ₆	416931	MCLC	1.0	0.999	↓ 0.26	$\downarrow -0.20$	↓ 0.06	2.01
BaMn ₂ NdO ₆	158890	TET	1.0	1.000	↓ 2.81	$\downarrow -0.31$	↓ 2.49	10.00
BaErMn ₂ O ₅	188495	TET	1.0	1.000	↓ 2.70	$\downarrow -1.42$	↓ 1.28	18.01
BaMn ₂ PrO ₅	158885	TET	1.0	0.998	J 2.62	$\downarrow -1.47$	↓ 1.16	11.00
$BaMn_2PrO_6$	150704	TET	1.0	0.997	↓ 2.96	$\downarrow -0.51$	↓ 2.45	9.00
CuPrSO	92,494	TET	1.0	0.998	↓ 2.16	$\downarrow -0.76$	$\downarrow 1.40$	4.00
ClCoSr ₂ O ₃	90122	TET	1.0	0.996	↓ 2.15	$\downarrow -0.10$	↓ 2.04	4.00
BaLaMn ₂ O ₆	150703	TET	1.0	0.998	↓ 2.94	$\downarrow -0.45$	↓ 2.49	7.00
Cu ₃ NdRu ₄ O ₁₂	202061	BCC	1.0	0.993	↑ 1.63	$\uparrow -0.39$	↑ 1.25	13.00
Cu ₃ LaRu ₄ O ₁₂	51897	BCC	1.0	0.998	↑ 1.61	$\uparrow -0.39$	↑ 1. 2 1	10.00
Cu ₃ HoMn ₄ O ₁₂	153872	BCC	1.0	0.999	↓ 2.58	$\downarrow -0.45$	↓ 2.13	10.00
Cu ₃ Ru ₄ SrO ₁₂	51895	BCC	1.0	0.997	$\uparrow 1.44$	$\uparrow -0.32$	† 1.12	11.00
Cu ₃ Fe ₄ SrO ₁₂	262855	BCC	1.0	0.999	↓ 0.63	$\downarrow -0.45$	$\downarrow 0.18$	19.00
CeCu ₃ Mn ₄ O ₁₂	169043	BCC	1.0	0.999	$\downarrow 1.68$	$\downarrow -0.58$	↓ 1.09	11.00
Cu ₃ Mn ₄ YO ₁ 2	38418	BCC	1.0	0.999	↓ 2.59	$\downarrow -0.43$	↓ 2.16	10.00
CaCu ₃ Ru ₄ O ₁₂	95715	BCC	1.0	0.998	$\uparrow 1.47$	$\uparrow -0.30$	$\uparrow 1.17$	11.00
Cu ₃ Mn ₄ YbO ₁₂	153874	BCC	1.0	0.999	↓ 2.37	$\downarrow -0.27$	↓ 2.10	9.00
Cu ₃ NaRu ₄ O ₁₂	95716	BCC	1.0	0.998	↑ 1.33	$\uparrow -0.27$	$\uparrow 1.07$	12.00
$CaCo_4Cu_3O_{12}$	169095	BCC	1.0	0.988	↓ 1.28	$\downarrow -0.24$	↓ 1.04	7.00
Cu ₃ Mn ₄ ThO ₁₂	34316	BCC	1.0	0.999	↓ 2.82	$\downarrow -0.49$	↓ 2.33	11.00
Cu ₃ DyMn ₄ O ₁₂	153871	BCC	1.0	0.999	↓ 2.60	$\downarrow -0.44$	↓ 2.16	10.00
Fe ₂ Mn ₃ Si ₃ O ₁₂	27381	BCC	1.0	0.999	$\uparrow 2.47$	$\uparrow -0.92$	$\uparrow 1.56$	68.00
$Mn_3Si_3V_2O_{12}$	27380	BCC	1.0	1.000	↑ 2 .16	$\uparrow -0.83$	$\uparrow 1.33$	59.99
CaCu ₃ V ₄ O ₁₂	250094	BCC	1.0	0.999	$\downarrow 1.53$	$\downarrow -0.88$	$\downarrow 0.65$	1.00
FeMoSr ₂ O ₆	150701	BCT	1.0	0.999	↑ 2.6 7	↑ -1.80	$\uparrow 0.87$	4.00
FeMoSr ₂ O ₆	157603	FCC	1.0	0.988	† 2 .70	↑ -1.81	$\uparrow 0.88$	4.00
$GdReSr_2O_6$	25400	FCC	1.0	0.996	$\uparrow 2.87$	↑ -2.00	$\uparrow 0.87$	5.00
Ba ₂ ReYO ₆	94215	FCC	1.0	0.998	↓ 2.87	↓ -1.92	$\downarrow 0.95$	2.00
DyReSr ₂ O ₆	25402	FCC	1.0	0.997	↓ 2.91	↓ -1.98	$\downarrow 0.93$	2.00

 Table A4. Quinary half-metallic oxides. Parameters are the same as in Table A1.

Name	ICSD	Lattice	$P_0(E_F)$	P ₀ (E _{gap})	Egap	VBM	CBM	\mathbf{M}_S
H ₄ K ₂ N ₄ PdO ₁₀	164218	TRI	1.0	0.996	↓ 0.60	$\downarrow -0.39$	$\downarrow 0.21$	0.00
La ₃ MnS ₃ WO ₆	380406	HEX	1.0	1.000	$\downarrow 1.55$	$\downarrow -0.25$	↓ 1.29	8.00
CuH ₁₂ Mn ₂ N ₄ O ₈	61243	MCL	1.0	0.980	$\downarrow 0.74$	$\downarrow -0.68$	$\downarrow 0.06$	17.99
CH ₂ P ₂ PuO ₆	262902	MCLC	1.0	0.998	$\downarrow 3.42$	$\downarrow -1.40$	$\downarrow 2.02$	8.00

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