

Electrochemically stable lithium-ion and electron insulators (LEIs) for solid-state batteries

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ABSTRACT

Rechargeable solid-state Li metal batteries demand ordered flows of Li-ions and electrons in and out of solid structures, with repeated waxing and waning of Li_{BCC} phase near contact interfaces which gives rise to various electro-chemo-mechanical challenges. There have been approaches that adopt three-dimensional (3D) nanoporous architectures consisting of mixed ion-electron conductors (MIECs) to combat these challenges. However, there has remained an issue of Li_{BCC} nucleation at the interfaces between different solid components (e.g., solid electrolyte/MIEC interface), which could undermine the interfacial bonding, thereby leading to the evolution of mechanical instability and the loss of ionic/electronic percolation. In this regard, the present work shows that the Li-ion and electron insulators (LEIs) that are thermodynamically stable against Li_{BCC} could combat such challenges by blocking transportation of charge carriers on the interfaces, analogous to dielectric layers in transistors. We searched the *ab initio* database and have identified 48 crystalline compounds to be LEI candidates (46 experimentally reported compounds and 2 hypothetical compounds predicted to be stable) with a band gap greater than 3 eV and vanishing Li solubility. Among these compounds, those with good adhesion to solid electrolyte and mixed ion-electron conductor of interest, but are lithiophobic, are expected to be the most useful. We also extended the search to Na or K metal compatible alkali-ion and electron insulators, and identified some crystalline compounds with a property to resist corresponding alkali-ions and electrons.

KEYWORDS

electrochemical stability window, stress, fracture, adhesion, contact, lithium metal anode

1 Introduction

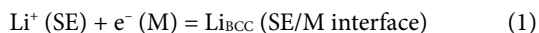
Alkali metals (Li, Na, K, etc.) have drawn great attention with the potential of realizing high-energy-density batteries. Pairing alkali metal anodes with advanced metal-oxide cathodes have been expected to make the energy density of the battery-electric motor combination competitive against the gasoline tank-internal engine system, without greenhouse gas emission [1, 2]. However, harnessing them for electrochemical energy conversion is a grand challenge in materials science. In rechargeable solid-state Li metal batteries (RSLB), for example, metallic Li in the body-centered cubic (BCC) phase can wax/wane during the charging/discharging process of the full cell [3]. This volume fluctuation generally increases/decreases the interfacial area with whatever solids that are in contact with Li_{BCC} , giving rise to associated stress and chemical/mechanical instabilities. Among these issues, the stress can be relieved given that there is an open volume for the inflow of Li_{BCC} . Being one of the softest metallic solids at $T = 0$ K [4] with a high homologous temperature ($T/T_M \sim 0.66$) at room temperature (RT), Li_{BCC} can carry out creep relaxation, flowing as if it is practically an “incompressible fluid” like water despite being bulk crystalline in diffraction. One may thus draw an analogy of Li_{BCC} in RSLB to working fluids in engines. That being said, there remain chemical/mechanical stability problems.

As a working fluid, Li_{BCC} is chemically very aggressive; many solids are thermodynamically unstable against Li_{BCC} , having a high propensity to react with Li_{BCC} . Hence, the engine with an open volume should be made of special solids. The only solid phases that would not react even in direct contact with Li_{BCC} are those with a direct tie-line to Li_{BCC} on the equilibrium phase diagram. For example, if there is no direct tie-line between an arbitrary compound A_2BC_3 and Li_{BCC} , $x\text{A}_2\text{BC}_3 + y\text{Li}_{\text{BCC}}$ has a thermodynamic driving force to react and decompose into the intervening phases on the Gibbs free-energy convex hull. Such reaction can be kinetically slowed down by a naturally formed passivation layer on A_2BC_3 ; nonetheless, thin passivation layers tend to be mechanically unstable against the waxing-waning volume change, which accompanies stress and adhesion (mechanical) problems. Simply put, if the “engine” architecture is made of solid phases without a direct tie-line to Li_{BCC} on the phase diagram, it inevitably encounters the problem of stress-corrosion cracking (SCC), where the dual aggressive forces of corrosion and stress make it immensely challenging to form a stable contact and passivation against waxing-waning Li_{BCC} .

Meanwhile, constructing the engine with solid phases that are thermodynamically stable against Li_{BCC} alone does not guarantee the engine’s mechanical stability. For a RSLB to power an external electrical load (e.g., an electrical motor) or be charged, Li-ions and electrons should travel separate ways. Thus, a

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RSLB needs at least two types of solids from the perspective of transport properties: a solid electrolyte (SE), which is a Li-ion conductor but electron insulator; and a metal (M), which is an electron conductor but Li-ion insulator. Assuming that a RSLB is constructed with only SE and M, Li_{BCC} can wax/wane at any SE/M interface that has kinetic access to both Li-ions and electrons through the following charge-transfer reaction



Upon waxing and waning of the Li_{BCC} , the relevant SE/M interface loses its capability of withstanding the accompanied stress. This waxing/waning behavior implies that the transport properties of constituent solids could inherently induce mechanical instability problems, even though the engine is constructed with solid phases with thermodynamic stability against Li_{BCC} .

While the adoption of SE (e.g., $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$, $\text{Li}_{10}\text{GeP}_2\text{S}_{12}$) and M (e.g., copper) in the construction of an RSLB is well-known, we herein show that the chemical and mechanical stabilities of the “engine” can be much enhanced by employing two additional types of solids: a mixed ion-electron conductor (MIEC) and a Li-ion and electron insulator (LEI). Thus, all four types of solids on the chart of Li-ion conducting/insulating and electron conducting/insulating solids (Fig. 1(a)) will find appropriate use in the proposed “engine”. A nanoporous three-dimensional (3D) structure shown in Fig. 1(b), which can accommodate the waxing-waning Li_{BCC} , is used as a model engine architecture. Such solids have been studied or proposed as constituent materials for nanoporous 3D structures, but here we aim at evaluating the necessity of these materials and understanding the requirements that these materials should meet to function properly. Based on these considerations, we identify candidate materials via a high-throughput screening in *ab initio* database of the Materials Project [5, 6]. This approach is then extended to other rechargeable solid-state batteries that adopt Na or K instead of Li, identifying ion and electron insulators for such alkali metals.

2 Results and discussion

2.1 The structure of 3D nanoporous engine: MIEC walls with LEI roots

The microstructural length scale of the MIEC beehive needs consideration to both areal capacity and creep relaxation of Li_{BCC} . In order to provide sufficient areal capacity, the height h

of tubules should be on the order of $10^1 \mu\text{m}$, and the wall thickness w should remain much smaller than the inter-wall thickness W . In addition, to offer sufficient Coble creep pathways ($\beta_1 + \beta_2$ in Fig. 1(b)) at room temperature, the W is recommended to be on the order of 100 nm or less—so that it can relax away the stress built up due to the insertion of Li atoms by the pathway α in Fig. 1(b). The pathways α and $\beta_1 + \beta_2$ both grow the Li_{BCC} phase in volume during electrochemical charging (of the full cell). The difference is as follows: $\beta_1 + \beta_2$ deposits Li atoms at the back end, where there is open space available, and does not generate stress but relieves the stress, while α deposits Li atoms at the front end by pushing out existing Li_{BCC} and engenders stress (namely, pressure) there. If there are too many α processes and insufficient $\beta_1 + \beta_2$ relaxation processes, the stress will build up at the front end, where the SE and the MIEC meet; once the stress in Li_{BCC} is large enough, the solid engine will fracture. If inert vapor instead of vacuum exists inside the nanopores, there will be additional stress generated due to gas compression, but the generated stress would be much gentler.

In such engine construct, MIEC walls serve as an electrochemical intermediary between the Li_{BCC} and the SE. Ceder et al. have surveyed many Li-containing solids and found that good SE candidates (defined as having a sufficient bulk Li-ion conductivity, while having a wide band gap to shut down electron conduction) that are also thermodynamically stable against Li_{BCC} are quite rare (see Fig. 2 in Ref. [7]). In contrast, there are many more MIEC choices that are thermodynamically absolutely stable against Li_{BCC} (e.g., LiC_6 , LiAl , $\text{Li}_{22}\text{Si}_4$), and since the final decomposition products of say $x\text{A}_2\text{BC}_3 + y\text{Li}_{\text{BCC}}$ are likely Li-containing and electronically conductive in the limit of large y . It should be noted that intermetallic Li compounds (e.g., LiAl) can be regarded essentially as a MIEC despite the fact that they conduct neutral Li atoms, not Li-ions as the reaction (1) can take place any intermetallic compound/SE interface once the necessary local electronic potential is met, provided that a medium’s electronic conductivity is fast enough. In our engine construct, most of the Li_{BCC} is in naked contact with the MIEC walls, instead of a SE or a M. Reaction (1) can cycle without the fear of losing interfacial contact, since no solid-electrolyte-interphase (SEI) layer can form between the MIEC walls and the Li_{BCC} , if we pick one of the many MIECs that are thermodynamically absolutely stable against Li_{BCC} . No SEI means that there are no side reactions to consume cyclable Li and no SEI debris, which may fall off and accumulate in the structure. The very limited direct contact area at the Li_{BCC} /SE interface (which could have SEI, if electrochemically unstable

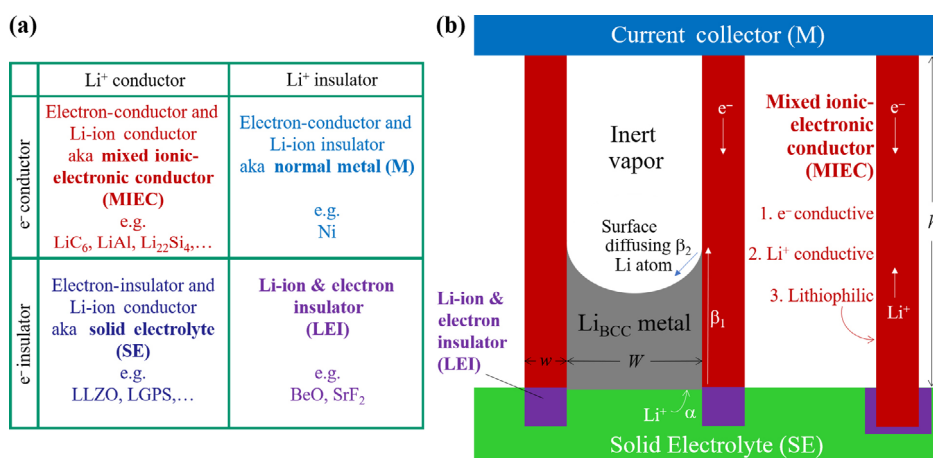


Figure 1 The components and architecture of the proposed Li_{BCC} cycling engine. (a) Four types of solid media in the engine, which regulate the transport of Li-ions and electrons. (b) Schematic diagram of the engine’s cross section; the MIEC has a beehive structure and the LEI is used as an interfacial binder between SE and MIEC to prevent waxing-waning Li_{BCC} crystals from pulling MIEC walls out from the SE.

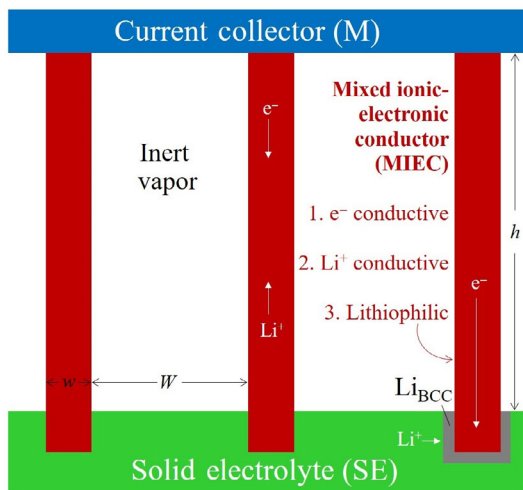


Figure 2 The situation without LEI mechanical binders. The Li_{BCC} nucleated at the SE/MIEC interface can make MIEC walls easily pulled out by waxing-waning Li_{BCC} .

SE like $\text{Li}_{10}\text{GeP}_2\text{S}_{12}$ [7] is used) should not be a problem, if one cycles the pore, say between 10% and 90% full of Li_{BCC} . In any case, most of the changing interfacial area with the waxing-waning Li_{BCC} is with MIEC, not with SE or M. As long as pressure at the front end is sufficiently relaxed by Coble creep pathways ($\beta_1 + \beta_2$ in Fig. 1(b)), which was demonstrated to be feasible by engineering W on the order of 100 nm or less [3] for room-temperature cycling, all should work.

In this engine construct, however, it may be hard to mechanically fix the MIEC walls. In order to provide a sufficient areal capacity (mAh/cm^2), h has to be on the order of 10 μm , and thus, the engine inevitably has a high aspect ratio ($h/w > h/W \sim 100$). Even though the MIEC/SE interface starts out mechanically strong and there is no adhesion problem before electrochemical cycling, a problem may occur when Li_{BCC} deposited during charging starts to wane upon discharging. Since MIEC conducts electrons, Li_{BCC} can nucleate anywhere that MIEC and SE touch and subsequently grow there like the rightmost pillar on Fig. 2, once the potential in the MIEC, $U(\text{MIEC})$, drops below 0 V versus Li^+/Li . As Li_{BCC} is extremely soft, this newly nucleated Li_{BCC} wedge or lubricant phase undermines the interfacial binding at the MIEC/SE interface and endangers the long-term mechanical stability of the engine. Although one designs the nanoporous engine to reduce stress in solid components as much as possible by Coble creep, still some parasitic stresses are unavoidable. They will be transmitted to the MIEC walls and concentrate at their interfaces. For example, because it is practically difficult to make the “open space” in Fig. 2 truly vacuum, we can imagine inert gases like Ar fill in the open spaces at the beginning. When the “working fluid” Li_{BCC} runs from 10% to 90% filled, we can have a factor of $9\times$ increase in the inert-gas pressure, from 1 to 9 atm. Such pressure change on the order of MPa will be transmitted to the MIEC walls and concentrate on its root with the SE, and if a soft Li_{BCC} wedge or lubricant phase nucleates and forms at the MIEC/SE interface, the MIEC walls could be pulled out from the SE in the long run, like a tooth from a bleeding gum in the case of gingivitis.

This problem calls for a material, which can electronically separate the SE from the MIEC walls to stop the “bleeding” (nucleation and growth of soft Li_{BCC} at the interface) and maintain the adhesion strength between them—like an inert dielectric layer in transistors, which regulates the transport of charge carriers (electrons and holes) in the gate region, or porcelain

suspension insulators for high-voltage power transmitters, which are necessary for holding the high-voltage metallic cables. To this end, the binder material must be a Li-ion and electron insulator. Otherwise, it is just another SE, which suffers from the same problem of “bleeding”. This LEI binder may either be a root (the left two pillars in Fig. 1(b)) or a conformal coating wrapping around the MIEC at the root (the rightmost pillar in Fig. 1(b)). The new interfaces (i.e., MIEC/LEI and SE/LEI), which replace the MIEC/SE interface, must both have strong adhesion strength at room temperature to be able to transmit at least tens of MPa tensile and shear stresses across the interfaces and make the MIEC “teeth” firmly attached onto the SE “gum”.

2.2 Identification of candidate materials for LEIs

The rest of the paper is dedicated to identifying candidate materials for LEI by data-mining in *ab initio* databases. As a first step, the requirements that they should meet to be a mechanical binder are investigated. First, they should be thermodynamically stable against Li_{BCC} . As illustrated in Fig. 1(b), LEI will be in naked contact with the “working fluid” Li_{BCC} phase, which carries out a corrosive attack. Furthermore, LEI has another interface with SE, and thus, it has to be stable at least within the range of the Li potential determined by given set of anode and cathode; otherwise, LEIs will decompose during cycling and produce phases with non-zero transference numbers for either Li-ions or electrons, thereby losing their function as an inert binder. Second, they should have vanishing Li solubility to ensure no Li-ion conductivity. While in principle Li-containing compounds like LiF , Li_3OCl , and Li_2O may have low enough Li-ion lattice conductivity to qualify as LEI (and not as SE), the effective Li-ion conductivity could be microstructure dependent as Li-ion can still conduct through the grain boundaries of these ceramics. Indeed, even though no one has claimed LiF and Li_2O to be good solid electrolytes, nanoscale LiF is a well-known SEI component [8], and Li_2O is often used as a solid electrolyte for *in situ* transmission electron microscopy experiments [9]. Thus, while LiF and Li_2O single crystals may theoretically have extremely low Li-ion diffusivity at room temperature, the mere fact that Li can exist inside the lattice (miscible) may disqualify them as realistic polycrystalline choices. Hence, vanishing Li solubility in the 3D LEI bulk is required. Generalizing this concept to interfaces, even the 2D surfaces/interfaces of LEI should not host Li atoms. Thus, it would be best if LEI is lithiophobic [10], to not only prevent the nucleation of Li_{BCC} phase there, but also to repel the encroachment of Li_{BCC} phase to any solid-LEI interfaces. Finally, LEI should have a large electronic band gap to block the electron transport, which is preferably greater than 3 eV, considering that the band gap values in the database are usually underestimated, as a result of the electronic structure calculations with Perdew–Burke–Ernzerhof (PBE) exchange-correlation functionals [11].

With these criteria, we performed a high-throughput screening for LEI candidates using the Materials Project database. The database provides density functional theory (DFT)-calculated properties of crystal structures in the Inorganic Crystal Structure Database (ICSD) [12], including ground-state stable and metastable crystal structures. It supports open access via application programming interfaces (API) [13] as well as user-friendly webpages. There are also many algorithms that have been implemented in a Python library called Python Materials Genomics (pymatgen) [14] to facilitate data-mining operations. Based on this set of DFT-calculated information and data-mining kits, we came up with our own Python code [15]

(<https://github.com/peikai/IEIs>) to construct *ab initio* lithium phase diagrams in batches and identified phases that are thermodynamically stable against Li_{BCC} at 0 K and to further screen LEI candidate phases according to the aforementioned LEI criteria.

2.2.1 Searching for phases thermodynamically stable against Li_{BCC}

Computational lithium phase diagrams can be constructed with crystal structures and their Gibbs free energies, which are determined by *ab initio* calculations. As LEI is supposed to be in a thermodynamically stable environment and has no reactive gas exchange in the battery engine, we can compare the relative thermodynamic stability of phases in a chemical system with their Gibbs free energies, which act as the thermodynamic potential for a closed system. According to the methodology proposed by S. P. Ong et al. [16, 17], an *ab initio* phase diagram can be constructed with a projected convex hull of a set of $\bar{E}(c)$ values, where $\bar{E}(c)$ is the normalized Gibbs free energy with respect to composition c at 0 K. Thus, we are able to construct lithium phase diagrams in a high-throughput way. Here we use the Li-Be- O_2 chemical system as an illustration of this process. First, we send a query to the database API to retrieve the internal energy per atom for all available phases belonging to the Li-Be- O_2 system and regard them as normalized Gibbs free energies because they can be simplified as the internal energies when we mainly compare thermodynamic stability of condensed phases in vacuum at 0 K. Then, the convex hull algorithm [18, 19] is utilized to locate the lowest Gibbs-free-energy surface in a geometric space that contains a set of points $\bar{E}(c)$. The surface is composed of several simplicial facets, and each of them is anchored with the phases in a thermodynamic equilibrium. In the end, those simplicial facets containing information of phase equilibria are projected onto the composition plane which forms the *ab initio* phase diagram in terms of the Li-Be- O_2 system, as shown in Fig. 3(a).

In the *ab initio* phase diagram, simplicial facets and corresponding phase regions embody the information of the phases in thermodynamic equilibrium. Now that the convex hull algorithm helps to locate the phases with the lowest Gibbs free energies in each phase region, a mixture of these ground-state stable phases must have a lower thermodynamic potential than metastable phases at the same composition. As a result, they will decompose spontaneously to the mixture of node phases that comprise the phase region with a fraction determined by the lever rule. Thus, we are able to find phase equilibria involving Li_{BCC} in the multi-component lithium phase diagrams,

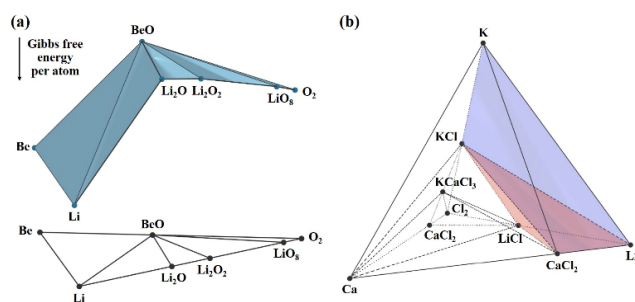


Figure 3 Phase equilibria in *ab initio* phase diagrams. (a) Generation of a Li-Be- O_2 *ab initio* phase diagram. Simplicial facets on the lowest Gibbs-free-energy surface are projected onto the composition plane to reveal phase equilibria with respect to compositions. The z -axis of this graph is reversed to present the projection intuitively. Phases beneath the lowest Gibbs-free-energy surface are not shown in the graph for brevity. (b) 3-Simplex (tetrahedral) phase regions involving Li_{BCC} (colored) in the Li-K-Ca- Cl_2 quaternary phase diagram.

not limited to two or three components but up to eight components in the LEI screening. A k -component *ab initio* phase diagram will consist of $(k - 1)$ -simplex phase regions, inside which k phases are in a thermodynamic equilibrium, as the example of Li-K-Ca- Cl_2 phase diagram shown in Fig. 3(b). With the help of the barycentric coordinate system algorithm implemented in pymatgen, we can determine whether Li_{BCC} is located in each simplicial phase region and find phase regions involving Li_{BCC} even from high-dimensional *ab initio* phase diagrams.

By searching for all available lithium phase diagrams in the database, the phases that are thermodynamically stable against Li_{BCC} can be obtained comprehensively. In addition to the methods to construct a lithium phase diagram and to find phase regions involving Li_{BCC} , the pipeline of the screening also needs Li-containing chemical systems as comprehensive as possible for the construction of a phase diagram, such as the chemical systems Li-Be- O_2 , Li-K-Ca- Cl_2 , etc. To this end, we retrieved all Li-containing chemical systems available in the database via database API, and eventually collected 4,840 unique simplicial phase regions involving Li_{BCC} with aforementioned methods. Inside those phase regions, we collected 1,186 phases that were connected to the Li_{BCC} by a direct tie-line, which were listed in Table S1 in the Electronic Supplementary Material (ESM). All of them have predicted thermodynamic stability against Li_{BCC} .

A sufficient approximation of the thermodynamic potential surface relies on the comprehensive discovery of thermodynamically stable crystal structures and the accuracy of calculated energies. There are more than 126,000 inorganic crystal structures with 19,000 Li-containing crystal structures in the Materials Project database (version 2020.09.08), which is comprehensive enough to take most chemical systems into account and to offer sufficient phases to find potential surfaces. However, upon updates in databases, some new phases may still come up, thereby reshaping convex hulls and corresponding phase diagrams. Nevertheless, the impact of new phases on screening results is limited, since the change would only occur when a new phase happens to be located in one of the Li-containing phase regions and besides be more thermodynamically stable than any of the other phases in that phase region. By comparison, the accuracy of energy calculations has a greater impact on the results. In the construction of phase diagrams, we have utilized the mixed generalized gradient approximation (GGA) and GGA + U scheme to improve both accuracy and comparability of calculated energies for phases at different electronic arrangements [20]; however, it should be noted that the calculations that involve heavy metal elements with f -electrons can still be less accurate. In terms of the impact of non-zero temperatures, some phase equilibria are expected to reform when the temperature grows above 0 K because the ground state energies used in phase diagram construction have ignored relevant excitations. However, in contrast with experimental phase diagrams, which are time-consuming and less comprehensive across chemical spaces, phase diagrams based on *ab initio* calculation properties have an obvious advantage in quickly providing candidate phases for further verification by experiments.

2.2.2 LEI candidates

In addition to being thermodynamically stable against Li_{BCC} , LEI candidates must have good insulation properties against Li-ions and electrons. Thus, we needed to further screen out the phases that we obtained above with the other two criteria (vanishing Li solubility and a band gap of $> \sim 3$ eV). First, we

excluded all lithium compounds to ensure that the rest have no dissolved Li species in their crystal structures. These phases that have a stable contact with Li_{BCC} phase but do not solute Li atoms are regarded as Li-ion insulators. Then, we set a band gap criterion, greater than 3 eV, to further screen electron insulators and ultimately got 48 LEI candidates (e.g., BeO, SrF_2) as tabulated in Table 1. They are expected to have a negligible electronic conductivity; BeO, for example, has an electronic conductivity smaller than 10^{-14} S/m [21]. There are 46 experimentally reported crystal compounds (with the “Experimental” tag in the “Structural type” column) having matched crystal structures in ICSD, and 2 hypothetical crystal compounds that are theoretically stable. Considering that experimentally reported phases with lower electronic conductivity are usually preferred, in the table we gave priority to the phases that are included in ICSD and have a wide band gap. In addition, we also listed the calculated density of the candidate materials for reference as those LEIs with a lower density are preferred when designing batteries with high gravimetric energy density and volumetric energy density [22].

As it turns out, in Table 1, only a small set of crystals (48 candidates from more than 126,000 crystals) can serve as a LEI binder between solid electrolyte and MIEC, fulfilling the aforementioned criteria. The valid LEI choices are few (much rarer than MIECs that are absolutely stable against Li_{BCC}) because typically, electron insulators with large band gaps are metal oxides, nitrides, fluorides, etc., or wide-bandgap semiconductor compounds made out of Si, Ge, C, Ga, etc., such as GaN, SiC, GeS_2 [21]. Since Li is one of the most electropositive elements, it generally would easily replace other M in $\text{M}_x(\text{O}, \text{N}, \text{F}, \dots)_y$ via replacement reactions. Moreover, Si, Ge, C, Ga, etc. individually form compounds with Li_{BCC} , so semiconductor compounds made out of these elements tend to be attacked by Li_{BCC} as well. Only oxides, nitrides, fluorides, etc., or semiconductor compounds with great thermodynamic stability can (a) be stable against Li_{BCC} on the equilibrium phase diagram, by having a tie-line to Li_{BCC} , (b) be immiscible to Li element, and (c) have a large electronic band gap to be able to qualify as a valid LEI choice.

By meeting the (a) and (b) criteria above, the electrochemical stability against varying Li potentials will be a built-in property of LEI. As a phase in contact with SE, in which the Li potential is constantly varying during cycling as the redox reactions take place in the anode and the cathode of interest, the stability of LEI in terms of the Li potential must be compatible with SE, i.e., remain stable in the range of the Li potential determined by the set of electrodes. It is well known that common SEs only have a partial stability range in terms of the Li potential [7], hence electrochemical stability of SEs can limit the working voltage of batteries if it is not compatible with the variation of the Li potential in electrodes. By contrast, LEIs are not sensitive to the variation of the Li potential and can remain stable at an entire range of the Li potential. As we mentioned above, LEIs are stable against Li_{BCC} ; this stability implies that LEI phases can endure a Li potential of 0 eV/atom vs. Li_{BCC} , which is the upper bound of the Li potential. Thus, even when SE holds the highest Li potential, which is the same as Li_{BCC} , LEI phases will not be reduced. In addition, if the Li potential in an anode decreases to that SE cannot withstand, a Li-deficient decomposition in SE will occur as a result of the excess loss of Li atoms, whereas LEI phases will not have the same problem as there are no Li atoms in their bulk phases to decompose with the drop of the Li potential. Considering that LEI phases can be stable at the highest Li potential and maintain stability with the drop of the Li potential, these phases will acquire

Table 1 Candidates of Li-ion & electron insulators (IEIs)

Material ID	Formula	Structural type	ICSD ID	Band gap (eV)	Density (g/cm ³)
mp-2542	BeO	Experimental	601160	7.463	2.967
mp-981	SrF_2	Experimental	41402	6.776	4.134
mp-568662	BaCl_2	Experimental	2191	5.612	3.394
mp-23193	KCl	Experimental	240508	5.045	1.904
mp-573697	CsCl	Experimental	52274	5.017	3.175
mp-23295	RbCl	Experimental	18016	5.016	2.672
mp-23251	KBr	Experimental	52243	4.515	2.624
mp-567744	SrBr_2	Experimental	15972	4.470	3.756
mp-643	ThO_2	Experimental	28778	4.464	9.884
mp-571222	CsBr	Experimental	61516	4.425	3.485
mp-23063	Ba_4OCl_6	Experimental	16026	4.373	3.778
mp-22867	RbBr	Experimental	44286	4.372	3.164
mp-27791	SrBe_3O_4	Experimental	26179	4.127	3.568
mp-2652	Y_2O_3	Experimental	193377	4.106	4.892
mp-22916	NaBr	Experimental	41440	4.090	3.121
mp-661	AlN	Experimental	608626	4.054	3.201
mp-22898	KI	Experimental	53843	4.043	2.972
mp-1427	Lu_2O_3	Experimental	193361	4.031	9.495
mp-1767	Tm_2O_3	Experimental	647578	3.991	8.919
mp-29909	Ba_4OI_6	Experimental	280584	3.988	4.813
mp-679	Er_2O_3	Experimental	39185	3.982	8.654
mp-812	Ho_2O_3	Experimental	184539	3.961	8.404
mp-22903	RbI	Experimental	53831	3.954	3.360
mp-2345	Dy_2O_3	Experimental	630047	3.936	8.144
mp-1056	Tb_2O_3	Experimental	33653	3.912	7.837
mp-218	Sm_2O_3	Experimental	96206	3.878	6.962
mp-614603	CsI	Experimental	61517	3.856	3.555
mp-553921	Pm_2O_3	Experimental	647284	3.775	6.605
mp-18337	Be_3N_2	Experimental	616348	3.717	2.703
mp-1045	Nd_2O_3	Experimental	191535	3.711	6.396
mp-2605	CaO	Experimental	60199	3.692	3.287
mp-16705	Pr_2O_3	Experimental	647301	3.659	6.090
mp-2292	La_2O_3	Experimental	641600	3.590	5.840
mp-23268	NaI	Experimental	61504	3.569	3.572
mp-11107	Ac_2O_3	Experimental	31750	3.562	8.975
mp-1216	YbO	Experimental	77710	3.531	11.723
mp-23260	BaI_2	Experimental	24366	3.436	4.899
mp-23713	CaH_2	Experimental	156881	3.186	1.959
mp-12671	$\text{Er}_2\text{O}_2\text{S}$	Experimental	109334	3.182	8.210
mp-12670	$\text{Ho}_2\text{O}_2\text{S}$	Experimental	109333	3.138	7.992
mp-12668	$\text{Tb}_2\text{O}_2\text{S}$	Experimental	109331	3.134	7.501
mp-12669	$\text{Dy}_2\text{O}_2\text{S}$	Experimental	109332	3.115	7.771
mp-4511	$\text{La}_2\text{O}_2\text{S}$	Experimental	31640	3.080	5.700
mp-5598	$\text{Sm}_2\text{O}_2\text{S}$	Experimental	191403	3.057	6.730
mp-3211	$\text{Nd}_2\text{O}_2\text{S}$	Experimental	645665	3.016	6.222
mp-3236	$\text{Pr}_2\text{O}_2\text{S}$	Experimental	109329	3.005	5.945
mp-865934	YbF_2	Theoretical	None	6.733	7.541
mp-865716	YbCl_2	Theoretical	None	5.400	4.773

stability over the entire range of the Li potential, namely from 0 eV/atom vs. Li_{BCC} to a neglectable Li potential (an environment without the reduction conditions contributed by Li atoms).

The electrochemical stability of LEIs over the entire range of the Li potential can also be understood in terms of phase

diagrams. As an intensive variable, the Li potential of the phases that are in a thermodynamic equilibrium must be the same, hence a lithium phase diagram is composed of several isopotential regions in terms of the Li potential. An isopotential region may comprise an individual or a combination of phase regions, as illustrated in Fig. 4(a). When we consider that the system is open to a Li reservoir, different Li potentials in the reservoir will induce a variation of the phase equilibrium, and some of the phases will decompose, only retaining those that are stable under the Li potential of the reservoir. As we can find in Fig. 4(a), phase equilibria may adopt and exist in different Li potentials. Nevertheless, we will find that LEI phases can always be one of the stable phases throughout the entire range of the Li potential. When the Li potential drops from 0 eV/atom vs. Li_{BCC} to the negative infinity, take BeO (one of the LEI candidates) as an example, we can find that it will not decompose during each transformation of phase equilibrium, as illustrated in Fig. 4(b). We can also validate this electrochemical stability property in several grand phase diagrams, which is essentially the same as our expression. In order to perform the verification process in a high-throughput way, we constructed grand phase diagrams by pymatgen library for the phases with vanishing Li solubility and the stability against Li_{BCC} and verified that 895 phases have the predicted stability over the entire range of the Li potential; these phases are listed in Table S2 in the ESM.

Except for the stability and transport properties of LEIs, we would also like to comment on the mechanical robustness of this concept. In making the engine, one can hardly have the SE in perfect alignment with the LEI or LEI-coated root, as the phase junctions in Fig. 1. We can only achieve either configuration of overhang and underhang, where the SE level is taller or shorter than the LEI, as illustrated in Figs. 5 and 6, respectively.

In the overhang case (Fig. 5), once electrochemical charging commences and $U(\text{MIEC})$ drops low enough, the MIEC/SE

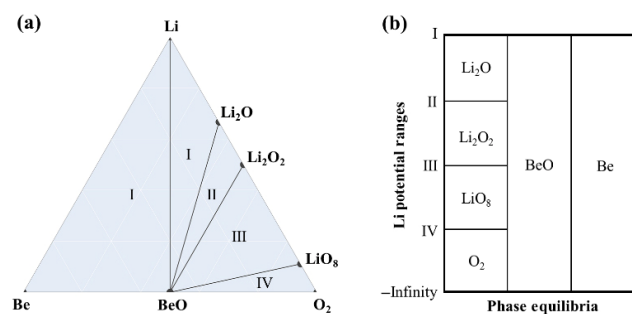


Figure 4 BeO is predicted to be stable over the entire range of the Li potential. (a) Li-Be-O₂ *ab initio* phase diagram, in which the Li potential of phase regions is labeled as I to IV, which is 0, -2.898 , -3.252 , -3.650 (eV/atom vs. Li_{BCC}), respectively. (b) Phase equilibria of the Li-Be-O₂ system when it is open to a Li reservoir.

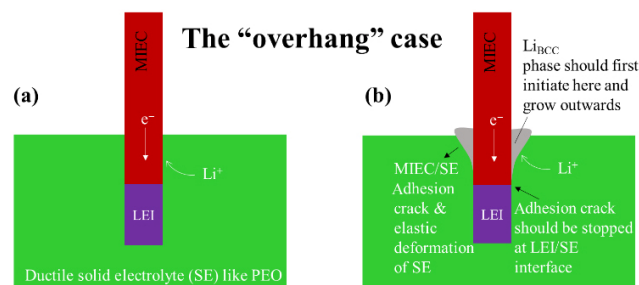


Figure 5 The case that LEI is anchored underneath the SE level. (a) LEI sinks into SE with part of the MIEC being in touch with SE. (b) LEI binds the MIEC and SE together, even if the Li_{BCC} nucleation grows along the MIEC/SE interface upon charging process.

interface may start to “bleed”, and new wedge-like Li_{BCC} phase may nucleate and start to grow, jacking open the MIEC/SE interface and separating them. According to the Nernst equation, a local overpotential of 0.135 V ($U(\text{MIEC}) = -0.135$ V versus Li^+/Li) can engender 1 GPa pressure locally [3]. To take a conservative approach here for the design, we will presume the original MIEC/SE interface cannot survive such GPa-level pressure and will be separated. This is not for certain in reality, depending on the MIEC/SE adhesion strength, size scale, and the actual local $U(\text{MIEC})$, however for conservative design we should presume the worst-case scenario. Effectively, we form an adhesion crack at the SE interface with the MIEC + LEI root as illustrated in Fig. 5(b). However, once this adhesion crack extends to the part where the LEI is, Li_{BCC} will no longer be injected locally into the interface. Then, according to fracture mechanics, as long as the separated MIEC/SE interface is not too long (the adhesion crack not too long), and the MIEC/LEI interface has strong enough adhesion, the adhesion crack can be stopped. There is some “bleeding”, and the SE “gum” will be pushed backward, but hopefully, the tooth may stay in the gum because of the LEI root that is buried deeper and stays inert. In this case of overhang, we would still prefer the SE to be somewhat ductile, so that it can survive the deformation and be displaced backward without fracturing. Then, upon electrochemical discharging, the Li_{BCC} will start to strip (reaction (1) goes from right to left), and the swollen gum will deform back. The detached MIEC/SE interface will not fully recover its original adhesion strength. During the subsequent cycles, there will be fresh bleeding and a new Li_{BCC} will nucleate and grow more easily.

In the underhang case (Fig. 6), when the SE is inadvertently shallower than the LEI height, we will have a problem in activating the electrochemical half-cell reaction (1). If there is no Li_{BCC} inventory initially in the anode, locally Li_{BCC} cannot nucleate when electrochemical charging commences in the full cell and $U(\text{MIEC})$ drops below 0 V (versus Li^+/Li) upon charging, due to lack of physical contact between the LEI and SE. We thus need an “ignition event” for the engine, which can be achieved if Li_{BCC} in other regions flows to this region, or if there is an extra MIEC branch touching the SE like a spark plug as shown in Fig. 6(b). Once a small Li_{BCC} crystal nucleates and physically connects the stranded MIEC walls with the SE, further growth of the Li_{BCC} will not be a problem, since the Li_{BCC} itself is a good electron conductor, and also supports rapid surface diffusion of charge-neutral Li atoms—thus, nanoscale Li_{BCC} can be classified as MIEC. Therefore, even an underhanging engine can cycle once the engine starts and is kept at least 10% filled at the bottom. Real batteries in electric vehicles are seldom fully charged (or fully discharged), and therefore we believe

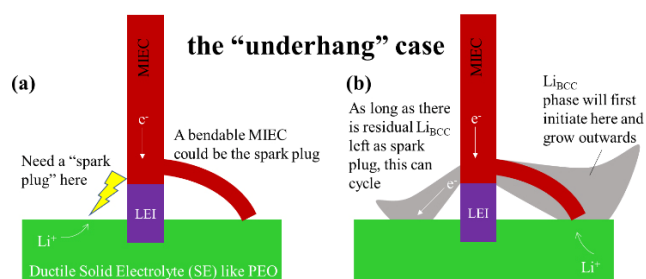


Figure 6 Routes to ignite the Li_{BCC} cycling engine in case LEI roots in a shallow SE. (a) Both a contacted bridge and an electronic spark can achieve the charge-transfer reaction happen between the electrons in MIEC and the Li-ions in SE at the first charge process. (b) Once MIEC physically connects with SE through one of the possible routes, the growth of a Li_{BCC} crystal can be promoted and the engine is supposed to cycle as the scenario.

some residual Li_{BCC} metal inventory on SE surface can always maintain the “ignition condition” once the ignition has been triggered once.

To avoid the interfaces being breached during cycling, the interfacial adhesion on the MIEC/LEI and SE/LEI interfaces should be capable of equilibrating the pressure from the Li_{BCC} crystals and the compressed vapors. Such strength of interfacial adhesion can be characterized by the work of adhesion (W_{Ad}) [23–27]. That of the LEI/MIEC interface, for example, is expressed as follows

$$W_{\text{Ad}} = \gamma_{\text{MIEC}} + \gamma_{\text{LEI}} - \gamma_{\text{MIEC/LEI}} \quad (2)$$

where γ_{MIEC} and γ_{LEI} are surface energies of MIEC and LEI, respectively, and $\gamma_{\text{MIEC/LEI}}$ is the interfacial energy of the MIEC/LEI interface. Equation (2) indicates that the interfacial adhesion would be relatively strong when having large γ_{LEI} and γ_{MIEC} but small $\gamma_{\text{MIEC/LEI}}$. Moreover, if the work of adhesion of the MIEC/LEI interface can be significantly larger than that of bulk phases (namely, W_{Ad} of the MIEC/MIEC interface), cracks tend to be initiated in bulk phases rather than at the interfaces [25, 26]. Thus, it is preferable to choose pairs of MIEC/LEI, and SE/LEI, that would give large surface energies but small interfacial energies, and thereby achieve a sufficient interfacial strength.

In case that the pairs of interest cannot provide sufficiently adhesive interfaces, strategies to promote interfacial adhesion are required. One commonly used approach is to contrive reactive wetting, for example, via the addition of metallic elements in the liquid phase to reduce ceramic substrates, which may not only decrease the interfacial energy [28], but also help to deoxidize and soften the interfaces [29]. Since interfacial energy $\gamma_{\text{MIEC/LEI}}$ generally decreases with formation enthalpy ΔH_f in spontaneous interfacial reactions [27], attempts at reactive wetting are effective in increasing W_{Ad} according to Eq. (2). In addition, kinetic conditions can also affect the interfacial adhesion. As in some reports, the porosity in substrates [10], impurities on interfaces [28], and phase transformation among allotropes of interfaces during deposition process [30] can reverse the wetting tendency and adhesiveness. For instance, chemical vapor deposition (CVD) diamond is hard to grow on Cu substrate because layers of its allotrope, graphite, primarily nucleate on the substrate and impede the subsequent adhesion of diamond [27, 30]. Another method to enhance adhesion is to manipulate the interfacial stoichiometry. For example, *ab initio* calculations show that nonstoichiometric O-terminated interfaces have significantly greater W_{Ad} than stoichiometric Al-terminated Ag/Al₂O₃ interfaces [25]. And one can try to tune the lattice configurations of interfaces by means of chemical potentials on interfaces [25], partial pressure of gases [25, 26], different experimental processing [31], etc. These approaches from the thermodynamic and kinetic perspectives should be helpful in improving the adhesion and wettability of MIEC/LEI and SE/LEI interfaces.

The lithiophobic property of LEI surfaces is beneficial to defend the interfacial adhesion. We have discussed about requirements for LEIs in terms of chemical/mechanical stability, i.e., should be stable against varying Li potentials and have enough interfacial adhesion to bind MIEC and SE. However, Li_{BCC} can still invade into cracks at SE/LEI and MIEC/LEI interfaces if the 2D surface of LEI has a tendency for segregation of Li atoms. Strong capillary effect [32] may happen at those nanoscale cracks since the tip of Li_{BCC} wedges can act like quasi-liquid, similar to the case that the surface of Ag nanoparticles (sub 10 nm) can reshape and diffuse like a liquid phase at room temperature [33], which will boost the degeneration

of interfacial adhesion. Hence, in contrast to common demand in Li metal encapsulation, which requires good interfacial wettability to Li_{BCC} [3, 34], LEI surfaces should ideally be very lithiophobic, being resistant against the wetting by Li_{BCC} to impede the penetration of Li_{BCC} into the 2D interfaces. This way, a small LEI coating or root can mechanically bind MIEC with SE without worry of stress-corrosion attack by Li_{BCC} .

2.2.3 Na-ion and electron insulators (NEIs) and K-ion and electron insulators (KEIs) candidates

We also identified the NEIs and KEIs from the phases that are thermodynamically stable against Na_{BCC} and K_{BCC} , respectively, based on the same principles as LEIs. Each of the candidate NEIs (or KEIs) has vanishing Na (or K) solubility and a band gap greater than 3 eV. They are also predicted to have intrinsic electrochemical stability against varying Na (or K) potentials. We collectively referred to LEIs, NEIs, and KEIs as “IEIs” and provided the statistics on identified candidates in Table 2 (see specific candidates in the ESM). It is worth mentioning that some phases meet all the criteria of LEIs, NEIs, and KEIs at the same time, and some phases are not IEIs but have certain properties such as the thermodynamic stability against alkali metals or the electrochemical stability against the Li/Na/K potentials. These phases were also listed in the ESM in case their stability is of interest against the corrosion of multiple alkali metals and varying chemical potentials from contacted phases in alkali-metal batteries.

Table 2 Statistics on Li/Na/K-ion & electron insulators

Type	Theoretical structures	Reported in ICSD	Unreported in ICSD
Li-ion and electron insulators	48	46	2
Na-ion and electron insulators	178	153	25
K-ion and electron insulators	137	120	17

3 Conclusions

We deduced that the Li-ion and electron insulators that are thermodynamically stable against Li_{BCC} can act as a buffer layer to block transport of charge carriers and as a mechanic binder for other solid media in the proposed prototype of the Li_{BCC} cycling engine. With the LEIs inserted into the SE with either the overhang or underhang situations in the Li engine, the structural stability of the engine can be preserved during Li_{BCC} reversible deposition and stripping along the MIEC/ Li_{BCC} interfaces. And the Li engine architecture can effectively relieve stress via the Coble creep interfacial diffusion and eliminate interfacial degradation. The LEIs are required to have negligible electron conductivity and Li-ions conductivity and preferably good interfacial adhesion to their solid counterparts. Furthermore, they should have thermodynamic stability against Li_{BCC} fuel and electrochemical stability against varying Li potentials of solid electrolytes, as well as being lithiophobic on its surface. By utilizing DFT-calculated properties in Materials Project database, we performed the high-throughput screening to identify LEIs candidates with three criteria: i) be thermodynamically stable against Li_{BCC} metal, ii) with vanishing Li solubility, iii) with a large band gap. In this process, we constructed lithium phase diagrams in batches and searched phases that have a tie-line with Li_{BCC} automatically via a set of python codes. Eventually, we identified 48 crystalline phases as candidates for Li-ion and electron insulators. With the same set of principles, we extended the search for solid-state Na/K metal batteries and found 178 candidates for Na-ion and electron insulators and 137

candidates for K-ion and electron insulators. These screening results will provide comprehensive choices of ion and electron insulators for alkali-metal creeping solid-state batteries.

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Electronic Supplementary Material

Electrochemically stable lithium-ion and electron insulators (LEIs) for solid-state batteries

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Table S1 Phases that are thermodynamically stable with LiBCC

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-867343	Li3Cd	mp-553921	Pm2O3	mp-1079399	V3Fe
mp-1018134	Li	mp-2290	NdRh2	mp-866134	VFe3
mp-862658	LiCu3	mp-999335	NdRh	mp-3236	Pr2SO2
mp-1197547	Li15Pd4	mp-1220520	Nd4Rh	mp-2495	PrS
mp-574275	Li17Pb4	mp-1104743	Nd3Rh2	mp-645	TbP
mp-864647	Hf2N	mp-1201296	Nd5Rh4	mp-569001	Sr2LiCoN2
mp-103	Hf	mp-18189	LiTmSn	mp-3503	Li6WN4
mp-1097065	Li2HfN2	mp-17706	Zr5Ge3	mp-1837	TbCu
mp-2828	HfN	mp-1203324	Zr3Ge	mp-1527	TbCu2
mp-1224388	Hf3N2	mp-1188062	Zr3Sc	mp-11363	TbCu5
mp-2251	Li3N	mp-1077791	ZrSc2	mp-1080443	YCu
mp-29210	Li2Ga	mp-1095690	Tm2Au	mp-994	YP
mp-1646	Li3Hg	mp-1358	DyIr2	mp-2698	YCu2
mp-19920	Ce3Ga	mp-1200226	Dy5Ir3	mp-2797	YCu5
mp-567332	Ce	mp-1105615	Dy3Ir	mp-1095352	LiEuAs
mp-1018276	CeGa	mp-861915	LiDy2Ir	mp-1975	TmN
mp-568417	PrAl	mp-861956	LiPm2Ir	mp-568793	Ca28Ga11
mp-38	Pr	mp-650	Be5Pd	mp-867805	LiCa2Ga
mp-1189	PrAl2	mp-862714	Be3Ir	mp-582055	La7Ni16
mp-1210753	Li2Al	mp-862377	LiBe2Ir	mp-1064719	LaNi
mp-30666	Sc3Ga2	mp-1102875	Er2Al	mp-2317	LaNi5
mp-67	Sc	mp-1208	ErAl2	mp-573855	La7Ni3
mp-1187073	Sr	mp-1188739	ErAl	mp-1679	La2Ni7
mp-1328	SrRh2	mp-862686	LiAc2Ru	mp-864614	LiMg2Pt
mp-600561	LiRh	mp-567750	ScRu2	mp-890	NdIr2
mp-1960	Li2O	mp-30867	ScRu	mp-30522	Nd5Ir3
mp-113	Tc	mp-1210377	Sc57Ru13	mp-1104605	Nd5Ir2
mp-44	U	mp-1194143	Sc11Ru4	mp-1189686	Nd3Ir
mp-976280	LiBr	mp-865795	LiSc2Ru	mp-679	Er2O3
mp-1189402	Ta2Be17	mp-1209947	Sc44Ru7	mp-10970	LiErO2
mp-1102049	TaBe3	mp-1438	ZrIr3	mp-24286	ZrH2
mp-1078957	Ta3Be2	mp-30749	Zr5Ir3	mp-864675	Yb3N2
mp-567842	TaBe12	mp-568992	ZrIr	mp-954	BaB6
mp-87	Be	mp-865925	LiZrIr2	mp-570007	SmOs2
mp-11278	Ta2Be	mp-30748	Zr3Ir	mp-1190029	Sm3Os

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(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-50	Ta	mp-866181	Li2NdIn	mp-866150	LiSm2Os
mp-861948	LiPm2Al	mp-866196	Li2PrIn	mp-1894	WC
mp-867200	Pm	mp-867148	LiHfRh2	mp-17751	Y5Ge3
mp-862980	PmAl3	mp-11457	HfRh	mp-14209	LiYGe
mp-862929	Li2PmAl	mp-1190626	Hf2Rh	mp-940	GdN
mp-1102133	Tm2Pt	mp-1101968	HoTc2	mp-24192	ErH2
mp-1018122	Tm	mp-571262	CaRh2	mp-1187696	VCr3
mp-867227	Li3Pt	mp-1214063	Ca5Rh	mp-1187695	V3Cr
mp-1025409	TmPt	mp-862764	LiCa2Rh	mp-1216394	VCr
mp-1199106	Tm5Pt4	mp-983444	LiPmZn2	mp-861894	Li2LaSn
mp-1198546	Er3Ga2	mp-1078961	LiTbGe	mp-11283	ZrBe5
mp-1184115	Er	mp-214	ZrRu	mp-30445	ZrBe13
mp-1018077	ErGa	mp-567258	LaZn2	mp-2544	Zr2Be17
mp-7396	Li3Tl	mp-2615	LaZn	mp-1169	ScCu
mp-11698	Tb	mp-1388	DyRh2	mp-1018149	ScCu2
mp-2322	YAl2	mp-232	DyRh	mp-7756	SrLiSb
mp-862555	LiY2Al	mp-1105786	Dy7Rh3	mp-646926	GdRu2
mp-1187739	Y	mp-1205201	Dy3Rh2	mp-866058	LiGd2Ru
mp-573471	Li17Sn4	mp-1107	Th7Rh3	mp-1974	CeB4
mp-10172	Na	mp-12755	ThRh	mp-30671	Ti2Ga
mp-2074	Li3Sb	mp-1185462	LiThRh2	mp-30672	Ti3Ga
mp-10659	Ho	mp-569074	Th7Pt3	mp-1232420	LiMg2Ir
mp-75	Nb	mp-12754	ThPt	mp-680653	Yb8In3
mp-2286	Li2Se	mp-862930	Li2PmIn	mp-1694	Yb2Ge
mp-1207777	Y3Pd	mp-14210	LiGdGe	mp-1937	YbCu
mp-1066136	YPd	mp-129	Mo	mp-1607	YbCu5
mp-570466	Li2Ca	mp-567412	Y5Sn3	mp-567538	YbCu2
mp-30367	Ca5Au2	mp-504790	LiYSn	mp-11219	LuB2
mp-567395	Li15Au4	mp-685209	Sc39N34	mp-571495	LuB4
mp-29720	Li21Si5	mp-2857	ScN	mp-1269	SmS
mp-210	BaLi4	mp-542435	Li3ScN2	mp-5598	Sm2SO2
mp-510430	Li13In3	mp-570670	YO2	mp-865912	LiZn2Rh
mp-865875	Li3Ag	mp-1188757	Y3Os	mp-1188656	Nd3Os
mp-1095265	LiYbBi	mp-862719	LiY2Os	mp-569630	NdOs2
mp-972364	Yb	mp-567612	ScOs2	mp-977391	LiNd2Os
mp-23222	Li3Bi	mp-568623	Sc44Os7	mp-1500	BaS
mp-865933	LiSiIr2	mp-12305	Sc11Os4	mp-22508	YMn12
mp-279	LiIr	mp-862887	LiSc2Os	mp-1077154	SmCu2
mp-1777	Li15Ge4	mp-863673	LiPm2Rh	mp-710	SmP
mp-1934	LiZn	mp-1095545	ZrTc2	mp-980769	SmCu
mp-867167	LiCa2Tl	mp-865893	LiZr2Tc	mp-227	SmCu5
mp-2474	YAg	mp-1102657	Y2Pt	mp-12670	Ho2SO2
mp-1187197	Ta3Os	mp-1025448	YPt	mp-1610	TbS
mp-1218177	Ta3Os2	mp-7343	Y3Pt	mp-12668	Tb2SO2
mp-1187243	TaOs3	mp-11564	TmRh	mp-1102	LuN
mp-49	Os	mp-867162	LiTm2Rh	mp-1949	TiMn2
mp-31441	Li2GaIr	mp-348	TmPd	mp-1202079	Ti21Mn25
mp-15822	LiSmGe	mp-16507	LuAl	mp-1514	UB2
mp-86	Sm	mp-1234	LuAl2	mp-619	UB4
mp-1102302	CeOs2	mp-16508	Lu3Al2	mp-2295	CaNi2
mp-2088	CeAl2	mp-568630	LuRu2	mp-774	CaNi5
mp-10740	Pa	mp-11495	LuRu	mp-193	Zr2Cu
mp-862690	Ac	mp-977393	LiLu2Ru	mp-1216441	Zr14Cu51
mp-865892	Li2CaPb	mp-984635	LiErSn	mp-1188077	Zr7Cu10

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-10658	Dy	mp-1079394	LiDyGe	mp-3201	Li2GaPd
mp-1102972	Er2Au	mp-2786	Ca5Zn3	mp-12684	LaAl
mp-865349	Li2GdTl	mp-1103570	Ca5Pt2	mp-2694	LaAl2
mp-155	Gd	mp-1294	YCo2	mp-1206996	La3AlO
mp-20353	GdGa	mp-865373	YCo	mp-8804	Li6MoN4
mp-1185394	LiGd2Ga	mp-1105598	Y3Co	mp-20689	Nb3B2
mp-861947	LiPm2Ga	mp-510184	GdOs2	mp-2580	NbB
mp-983460	Li2PmGa	mp-1185354	LiGd2Os	mp-10255	Nb3B4
mp-1192002	LiHoSn	mp-1742	GdRh	mp-1080021	Nb2B3
mp-1192210	LiDySn	mp-20084	GdRh2	mp-450	NbB2
mp-1106373	Sm5Si3	mp-3348	LiBIr	mp-9723	Sr4Li(BN2)3
mp-1025489	SmSi	mp-541365	LiEuH3	mp-23268	NaI
mp-23	Ni	mp-10622	PrAs	mp-3838	Li5ReN4
mp-1185319	LiCl	mp-862558	LiEr2Os	mp-305	TiFe
mp-1105989	Lu5Ge3	mp-864601	LiMg2Rh	mp-2605	CaO
mp-145	Lu	mp-1584	YbIr2	mp-568322	Sr3Li3(NiN)4
mp-1205878	LiLuGe	mp-864759	LiYb2Ir	mp-21009	EuSe
mp-570935	LiI	mp-632	TmCo2	mp-30816	Li2AlPd
mp-35	Mn	mp-1217007	Tm4Co3	mp-965	TbB2
mp-11854	Er5Ge3	mp-2762	YIr2	mp-568225	TbB4
mp-13474	LiErGe	mp-1198712	Y5Ir3	mp-1187198	SrMg2
mp-1192957	Li8Ce7Ge10	mp-1207785	Y3Ir	mp-3216	Li2ZrN2
mp-33	Ru	mp-867235	LiY2Ir	mp-1352	ZrN
mp-54	Co	mp-1185421	LiZnNi2	mp-1014265	Zr2N
mp-1001835	LiB	mp-867252	LiZn2Ni	mp-16264	LiCaSb
mp-30818	Li2AlPt	mp-2339	Ti3Pt	mp-2432	CaMg2
mp-30819	LiAl2Pt	mp-21246	Ba2Pb	mp-1198622	Li7La3Hf2O12
mp-518	Ti5Re24	mp-291	TiOs	mp-1409	TiNi3
mp-8	Re	mp-1072856	PrZn2	mp-1048	TiNi
mp-2179	TiRe	mp-460	PrZn	mp-1808	Ti2Ni
mp-1018125	Ti2Re	mp-544	Ti3Ir	mp-1774	ErB2
mp-72	Ti	mp-1235	TiIr	mp-2847	ErB4
mp-1102084	DyTc2	mp-864930	LiTiIr2	mp-24237	ScH2
mp-1762	ErRh2	mp-1129	ScIr	mp-2252	ScB2
mp-2381	ErRh	mp-861616	LiSc2Ir	mp-19830	ErN
mp-11437	Er3Rh	mp-1200708	Sc44Ir7	mp-2489	UC
mp-30612	Er7Rh3	mp-1103411	Dy2Au	mp-2486	UC2
mp-1198715	Er3Rh2	mp-567590	LuOs2	mp-2625	U2C3
mp-864772	LiSc2Au	mp-861963	LiLu2Os	mp-1095289	LiCaAs
mp-863697	LiPm2Si	mp-1102890	TmTc2	mp-23260	BaI2
mp-396	YbGa	mp-30385	Ho2Au	mp-29909	Ba4I6O
mp-1102309	Yb2Ga	mp-863675	LiPm2Ru	mp-2384	LaP
mp-2524	NdGa2	mp-865838	LiSiRu2	mp-8407	Li3LaP2
mp-1448	NdGa	mp-189	SiRu	mp-1202486	La7Ru3
mp-1203103	Nd3Ga2	mp-865936	LiSc2Tc	mp-1104417	La5Ru2
mp-123	Nd	mp-867262	ScTc3	mp-17193	Ca3GeO
mp-570684	ZrOs2	mp-1101953	HoOs2	mp-568636	TiCr2
mp-11541	ZrOs	mp-1190011	Ho3Os	mp-31205	Zr3Fe
mp-865870	LiZr2Os	mp-867269	LiHo2Os	mp-22447	Zr3P
mp-131	Zr	mp-1578	V3Rh	mp-1190681	ZrFe2
mp-865882	Li2SmIn	mp-867829	LiVRh2	mp-582924	Zr6Fe23
mp-866180	Li2YbPb	mp-867927	LiVIr2	mp-583740	Zr7P4
mp-866192	Li2YbSn	mp-2006	V3Ir	mp-1080525	FeB
mp-867253	LiZn2Ir	mp-1001613	LuGa	mp-10118	Mn3B4

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-867265	LiTm2Os	mp-1199315	Lu3Ga2	mp-20318	Mn2B
mp-607	CeRu2	mp-708	LaAs	mp-1915	Fe2B
mp-570629	Ce4Ru3	mp-1018766	Li3LaAs2	mp-2567	V3Si
mp-570369	Ce16Ru9	mp-542569	AlRu	mp-568671	V5Si3
mp-11534	Np	mp-1070580	Al3Ru2	mp-2090	FeCo
mp-1186374	Os3W	mp-10910	Al2Ru	mp-601842	Fe9Co7
mp-91	W	mp-11375	EuHg	mp-601848	Fe11Co5
mp-266	Zr2Pd	mp-2545	YbHg	mp-601820	Fe3Co
mp-253	ScCo2	mp-1211433	Li6Yb17Hg9	mp-1214417	BaC6
mp-2212	ScCo	mp-672286	Eu3Ga2	mp-568365	Li6Br3N
mp-27162	Sc3Co	mp-862318	LiAl2Ni	mp-28989	Li10BrN3
mp-1065995	ZrPt	mp-1487	AlNi	mp-31214	Ti3P
mp-8094	Ba2Hg	mp-2593	AlNi3	mp-22600	Sc3P2
mp-31172	Ca5Ag3	mp-867812	LiAlNi2	mp-1188800	Sc3P
mp-864735	Mn3Ir	mp-16514	Al3Ni5	mp-568643	RbC8
mp-1095380	LiEuBi	mp-862655	Ru3W	mp-28861	CsC8
mp-1057315	Eu	mp-861666	LiRu2W	mp-631	TiC
mp-1106357	Tb5Sn3	mp-867816	TaRu3	mp-27919	Ti8C5
mp-1857	YbCd	mp-977390	Ta3Ru	mp-10721	Ti2C
mp-1185270	LiNpRh2	mp-861954	LiTaRu2	mp-1000	BaTe
mp-865580	Li2DyIn	mp-1601	TaRu	mp-4547	La2TeO2
mp-865622	Li2HoIn	mp-1218044	Ta3Ru2	mp-1560	LaTe
mp-1102319	Lu2Pt	mp-862614	LiTm2Ru	mp-11649	Ca3SiO
mp-1025438	LuPt	mp-921	YRh2	mp-2517	Ca2Si
mp-1202267	Lu5Pt4	mp-191	YRh	mp-7084	SrCaSi
mp-30800	NdZn2	mp-1207780	Y3Rh	mp-12906	Sr3CrN3
mp-1053	NdZn	mp-1189474	Y7Rh3	mp-530262	Li15Cr2N9
mp-477	SmGa2	mp-1196999	Y3Rh2	mp-2542	BeO
mp-1195872	Sm3Ga2	mp-862842	LiPm2Pt	mp-1958	SrTe
mp-1188469	La5Ge3	mp-865959	LiHo2Ru	mp-542583	EuTe
mp-26	La	mp-2725	TbIr2	mp-7822	Sc5Si3
mp-1191159	LiPrSn	mp-1201266	Tb5Ir3	mp-1211088	LiCaP
mp-867474	Li2EuSn	mp-1106276	Tb3Ir	mp-24096	NdH2
mp-757	Li3As	mp-867285	LiTb2Ir	mp-1188283	V8N
mp-13	Fe	mp-16721	TmAl	mp-33090	V2N
mp-31442	Li2InRh	mp-858	TmAl2	mp-4604	Li7VN4
mp-23703	LiH	mp-982635	Tm3Al2	mp-1220316	NbW
mp-2602	NdAs	mp-1104	LaMg	mp-316	MnV
mp-8406	Li3NdAs2	mp-2292	La2O3	mp-1187702	VW3
mp-1761	LuIr2	mp-1094174	LaMg3	mp-1216231	VW
mp-1529	LuIr	mp-23193	KCl	mp-864984	MnV3
mp-861964	LiLu2Ir	mp-614603	CsI	mp-1192350	NbFe2
mp-862297	LiAlRh2	mp-1184151	Cs	mp-1221111	NbFe
mp-364	AlRh	mp-23295	RbCl	mp-1185970	Mn3Co
mp-30821	LiAl2Rh	mp-22903	RbI	mp-28731	V6C5
mp-569220	ErRu2	mp-2686	Ca2N	mp-20648	V2C
mp-862661	LiEr2Ru	mp-5515	Li7MnN4	mp-771082	Li4CrFe3O8
mp-568186	YRu2	mp-31468	LiCaN	mp-548	NbCr2
mp-1207781	Y3Ru	mp-1104937	Pr5Ru2	mp-1569	Be2C
mp-862673	LiY2Ru	mp-16705	Pr2O3	mp-30811	Ni4W
mp-862685	LiAc2Ir	mp-1197932	Pr7Ru3	mp-1216621	TiW
mp-570438	Yb8Ti3	mp-2665	PrRu2	mp-784631	CrNi2
mp-864769	LiYb2Ti	mp-1105741	Pr3Ru	mp-1585	V3Co
mp-37	Th	mp-1045	Nd2O3	mp-542614	VCo3

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-546	HoRh2	mp-3211	Nd2SO2	mp-771	MnAl
mp-2163	HoRh	mp-1748	NdS	mp-12659	Mn2Nb
mp-1106336	Ho7Rh3	mp-1427	Lu2O3	mp-977426	NbCo3
mp-1200753	Ho3Rh2	mp-754605	LiLuO2	mp-7250	Nb6Co7
mp-866200	Li2SmTl	mp-20874	EuB6	mp-1220522	NbVCo
mp-1095604	ErTc2	mp-21394	EuO	mp-1219177	Sm2C
mp-1197580	Li6Ca17Hg9	mp-504886	Gd2O3	mp-569335	Sm2C3
mp-867197	LiGaNi2	mp-1224869	Gd2C	mp-1216546	Tm2C
mp-1101816	Lu2Au	mp-1189998	Gd2C3	mp-7171	TmP
mp-928	HoIr2	mp-1021323	LiC12	mp-1205180	Tm3C4
mp-11476	HoIr	mp-21332	LiGdO2	mp-542830	Mn23C6
mp-1197997	Ho5Ir3	mp-863727	LiTiRh2	mp-20211	Mn3Si
mp-867913	LiHo2Ir	mp-554098	Ti6O	mp-21256	Mn7C3
mp-1095487	LuTc2	mp-1018124	Ti2Rh	mp-863690	Ti2MnCo
mp-977561	LiTaIr2	mp-2583	TiRh	mp-865537	TiMnCo2
mp-1187196	Ta3Ir	mp-1215377	Zr4O	mp-569424	Cr2B
mp-1458	Nb3Ir	mp-1102043	LaOs2	mp-1080664	CrB
mp-977563	LiNbIr2	mp-867813	LiLa2Os	mp-15617	Cr5B3
mp-1820	YbS	mp-284	AlCo	mp-20857	CoB
mp-1153	Li2S	mp-2652	Y2O3	mp-2091	V3B2
mp-1094591	Li3Mg	mp-7020	LiYO2	mp-9973	VB
mp-1188292	Y5Pb3	mp-16713	Pr2B5	mp-1491	VB2
mp-1204352	Y3Ga2	mp-12569	PrB4	mp-1206441	V5B6
mp-11420	YGa	mp-1542	YB2	mp-569270	V3B4
mp-1185233	Li2YIn	mp-637	YB4	mp-9208	V2B3
mp-736	Li3P	mp-568646	Ta3Si	mp-9546	Yb2C3
mp-90	Cr	mp-1989	Ta5Si3	mp-1103975	YbC6
mp-1222617	Li2ZnCu3	mp-569025	Ba19Na29Li13	mp-729	Cr3Si
mp-1885	AlIr	mp-1387	AlV3	mp-2157	Co3W
mp-11512	LiAl2Ir	mp-5840	LiScO2	mp-171	VNi3
mp-2206	LuCo2	mp-1183162	AlFe3	mp-11531	VNi2
mp-1222465	Lu4Co3	mp-2658	AlFe	mp-7226	V3Ni
mp-1185392	LiGd2Al	mp-978951	SmAl	mp-1216708	V3Ni2
mp-19923	GdAl2	mp-2358	SmAl2	mp-11501	MnNi3
mp-1078585	GdAl	mp-571222	CsBr	mp-1208170	TiVP
mp-1102354	ThTc2	mp-972256	Xe	mp-37906	LiMgN
mp-1190768	LiSmSn	mp-1014229	Ti2Zn	mp-29241	Ca3SnO
mp-1191015	LiNdSn	mp-608	TiCo3	mp-865964	Li2CaSn
mp-8481	LiPrGe	mp-823	TiCo	mp-865490	V2CrFe
mp-1865	UN	mp-1191331	Ti2Co	mp-865678	TiMn2V
mp-31066	LiUN2	mp-2057	DyB2	mp-1217201	Ti4Mn5V3
mp-1138	LiF	mp-2345	Dy2O3	mp-1451	NbNi3
mp-834	ThN	mp-2719	DyB4	mp-1220799	NbNi
mp-27487	Li2ThN2	mp-976726	LiDyO2	mp-1418	FeNi3
mp-605839	Li2B2Rh3	mp-749	SmN	mp-2213	FeNi
mp-861951	LiTaRh2	mp-218	Sm2O3	mp-567415	Nd2B5
mp-11452	HfOs	mp-2114	YN	mp-1632	NdB4
mp-862684	LiHf2Os	mp-1029592	Li3YN2	mp-2538	Y5Si3
mp-862934	Li2PmTl	mp-22898	KI	mp-14208	LiYSi
mp-2530	Li2Te	mp-1145	TiB2	mp-259	AlMo3
mp-2235	YbRh2	mp-7857	TiB	mp-19713	Sc3In
mp-567089	YbRh	mp-1025170	Ti3B4	mp-759	La2Sb
mp-864763	LiYb2Rh	mp-2675	MgNi2	mp-542503	La9(SbO)5
mp-865867	Li2YTl	mp-568151	Ti5Ge3	mp-8405	Li3LaSb2

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-865868	LiZrRh2	mp-2801	CeCu2	mp-903	ZrCr2
mp-669917	ZrRh	mp-2154	CeP	mp-1519	CaTe
mp-571664	Zr2Rh	mp-581942	CeCu6	mp-16032	Pr2TeO2
mp-1188413	Zr3Rh	mp-573697	CsCl	mp-5459	Nd2TeO2
mp-1374	Zr5Re24	mp-1188344	CsLiCl2	mp-4511	La2SO2
mp-12109	ZrRe2	mp-686129	Li5TiN3	mp-2350	LaS
mp-574458	Zr21Re25	mp-492	TiN	mp-1103990	EuC6
mp-866195	Li2LaTl	mp-8282	Ti2N	mp-675941	Li7IN2
mp-866669	Sr17(Li2Hg3)3	mp-865716	YbCl2	mp-1190061	Eu5Si3
mp-867111	LiDy2Ru	mp-2117	TbN	mp-2199	Fe3Si
mp-30622	Dy5Ru2	mp-1056	Tb2O3	mp-1800	Nd2C3
mp-1105841	Dy3Ru	mp-7137	LiTbO2	mp-1222310	Lu2C
mp-3726	Li2GaPt	mp-1183837	Co3Ni	mp-10192	LuP
mp-30743	TmIr2	mp-505002	Sc5As3	mp-1203767	Lu3C4
mp-11483	TmIr	mp-1095642	Eu2Ge	mp-15178	Lu4C7
mp-1198195	Tm5Ir3	mp-20587	EuS	mp-1216666	TiNbCr4
mp-867220	LiTm2Ir	mp-29149	Li4NCl	mp-640095	La3Co
mp-570436	CaIr2	mp-946	PrIr2	mp-30559	LaCo13
mp-570356	Ca5Ir	mp-1205021	Pr5Ir3	mp-20937	Cr3C2
mp-979911	Y2Au	mp-1104160	Pr5Ir2	mp-1196316	Cr7C3
mp-2205	LuPd	mp-1106395	Pr3Ir	mp-723	Cr23C6
mp-1087502	HoPd	mp-981	SrF2	mp-12894	Y2SO2
mp-1071848	Pr2Sb	mp-1101970	TbRu2	mp-1095443	ScFe2
mp-1095274	LiYbAs	mp-1189033	Tb3Ru	mp-22701	ScFeSi
mp-1095371	LiYbSb	mp-2267	HoB2	mp-505554	Sc(FeSi)2
mp-1095425	LiEuSb	mp-812	Ho2O3	mp-4755	Sc3Fe2Si3
mp-1187203	Ta3Re	mp-569281	HoB4	mp-3618	Sc2FeSi2
mp-1217894	TaRe	mp-12645	LiHoO2	mp-1018783	LiBeB
mp-866193	Li2LaIn	mp-10688	CeO	mp-2080	SrBe13
mp-971788	VRu3	mp-9610	Li2CN2	mp-27791	SrBe3O4
mp-1395	VRu	mp-1767	Tm2O3	mp-1220599	NbVNi
mp-865382	V3Ru	mp-754237	LiTmO2	mp-10961	La5Si3
mp-146	V	mp-1189863	Tm5Si3	mp-1202424	Li5La5(SiN3)4
mp-977434	Nb3Ru	mp-1066975	TmSi	mp-686208	Li5SiN3
mp-11517	NbRu3	mp-1216	YbO	mp-1104121	Li2La2Si3
mp-432	NbRu	mp-2643	Ti3Cu4	mp-22302	ZrVP
mp-1079796	Ti3Pd	mp-2078	TiCu	mp-571261	Pu
mp-1072399	Be5Pt	mp-742	Ti2Cu	mp-30428	BaCu
mp-1103421	Dy2Pt	mp-12546	TiCu3	mp-10181	LiSiNi2
mp-1078613	DyPt	mp-1245	Sr2N	mp-4495	KLiTe
mp-1105479	Dy3Pt	mp-15845	SrLi4N2	mp-15820	LiHoGe
mp-1205197	Dy3Ga2	mp-977380	LiMg2Pd	mp-683	Pr2C3
mp-30604	DyGa	mp-615	YMg	mp-30456	SrLiBi
mp-377	LuRh	mp-23251	KBr	mp-1018768	Li3LaBi2
mp-977405	LiLu2Rh	mp-643	ThO2	mp-1077063	La2Bi
mp-2529	PrRh2	mp-1779	YbTe	mp-24153	LaH2
mp-999305	PrRh	mp-11506	Ni3Mo	mp-28255	LaHO
mp-1104158	Pr3Rh2	mp-11507	Ni4Mo	mp-865656	TiMn2W
mp-570119	Yb7Au3	mp-1189967	Pr3Os	mp-1640	Ho2C
mp-570527	Yb5Au4	mp-567339	PrOs2	mp-744	HoP
mp-568944	Yb5Au3	mp-1105633	Y3Ni	mp-15238	Ho4C5
mp-1191877	LiGdSn	mp-582134	Y3Ni2	mp-1202754	Ho3C4
mp-1188310	Tm5Ge3	mp-1364	YNi	mp-1154	Ho4C7
mp-1205941	LiTmGe	mp-2152	YNi5	mp-867293	LiCo2Si

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1079937	Pr3Si2	mp-574339	Y2Ni7	mp-1038	MgCu2
mp-9968	PrSi	mp-1200338	Y15Ni32	mp-1216443	V6FeNi
mp-1210780	Li2Pr2Si3	mp-569196	YNi3	mp-567219	Li4Ca3(SiN3)2
mp-569501	LiCaBi	mp-772185	Li6Hf2O7	mp-1105563	GdB4
mp-1179656	Rb	mp-22916	NaBr	mp-28366	Gd2B5
mp-1102728	Dy2Al	mp-1253	BaSe	mp-29621	Ba5Bi3
mp-803	DyAl2	mp-510402	GdS	mp-973793	Li8SeN2
mp-433	DyAl	mp-4805	Gd2SO2	mp-12671	Er2SO2
mp-1212499	Hf5Ir3	mp-7283	LaB4	mp-23056	Sr2BrN
mp-1007786	HfIr	mp-2680	LaB6	mp-567744	SrBr2
mp-862610	LiHfIr2	mp-1184	La2C3	mp-1208630	SrC6
mp-862841	LiPm2Os	mp-2367	LaC2	mp-568662	BaCl2
mp-864631	LiNbRh2	mp-1410	DyN	mp-23063	Ba4Cl6O
mp-1545	Nb3Rh	mp-343	PrN	mp-866179	Li2NdTi
mp-1095658	Tb2Au	mp-862632	LiCa2Al	mp-12574	Dy2C
mp-865029	LiPaRu2	mp-1190809	Li8TeN2	mp-2014	DyP
mp-892	ScPt	mp-30228	Li4HN	mp-1212812	Dy4C5
mp-1196981	Sc57Pt13	mp-1078920	LaCu	mp-1213387	Dy3C4
mp-865444	LiSc2Pt	mp-2051	LaCu2	mp-10126	V5SiB2
mp-864637	NdAl	mp-2613	LaCu5	mp-570097	Sr(Li2P)2
mp-400	NdAl2	mp-969	YbAl2	mp-13276	SrLiP
mp-11454	Hf2Pd	mp-865934	YbF2	mp-1200894	Zr3As
mp-1197194	Ho3Ga2	mp-1097959	LiEu4(BN2)3	mp-27797	Li4H4Rh
mp-1018073	HoGa	mp-1212961	Eu2N	mp-1106011	Nd3Co
mp-30828	Sr2Pb	mp-5001	Li3BN2	mp-1104652	Nd5Co2
mp-867174	SrLi2Pb	mp-567290	LaN	mp-356	Nd2Co17
mp-1007691	HfPt	mp-2599	NdN	mp-1084826	Nd2Co3
mp-11460	HfTc	mp-2823	NdP	mp-21075	HfC
mp-1095669	HfTc2	mp-14712	Li7PN4	mp-504812	Hf3P
mp-7188	Al2Os	mp-12669	Dy2SO2	mp-29941	Sc2C
mp-861955	LiPm2Ge	mp-13322	LiGeRh2	mp-1219429	Sc2CO
mp-862259	Sc3Al	mp-1189298	YbB4	mp-15661	Sc4C3
mp-11220	Sc2Al	mp-419	YbB6	mp-28733	Sc3C4
mp-331	ScAl	mp-1079585	Nb2N	mp-1225044	Er2C
mp-813	ScAl2	mp-14827	Li7NbN4	mp-1144	ErP
mp-1102030	YTc2	mp-15821	LiNdGe	mp-1203719	Er3C4
mp-11566	ScZn	mp-1199558	Sm5Ir3	mp-1212833	Er4C7
mp-2031	Be2Cu	mp-7342	Sm3Ir	mp-20181	Ce2C3
mp-1227357	Be3Cu	mp-1104500	Sm5Ir2	mp-601	PrP
mp-11107	Ac2O3	mp-1025402	SrCu	mp-2058	Ni3B
mp-1385	CeZn2	mp-2116	ZrMn2	mp-2536	Ni2B
mp-668	PrGa2	mp-17190	Sc5Ge3	mp-1220374	NbVCr
mp-11404	PrGa	mp-242	SrB6	mp-864953	MnV2Cr
mp-1104052	Pr9Ga4	mp-1087	SrS	mp-775201	Cr3Fe(PO4)6
mp-669594	Pr5Ga3	mp-2576	Sr2Ge	mp-9244	LiBC
mp-1190862	Sc2Pd	mp-304	Ca2Ge	mp-1334	Y2C
mp-2781	ScPd	mp-867211	LiCa2In	mp-2795	ZrC
mp-1780	ScRh	mp-6799	LiCa4(BN2)3	mp-684623	Zr10C9
mp-30863	Sc57Rh13	mp-865	CaB6	mp-9459	Y4C5
mp-865793	LiSc2Rh	mp-1213975	CaB4	mp-1200885	Y4C7
mp-2988	Li2GaRh	mp-1570	YFe2	mp-1200613	Y3C4
mp-2748	CeAs	mp-11385	YFe5	mp-1193531	Ta2Al
mp-567490	Hf5Re24	mp-1104693	LiCa2HC3	mp-567735	Nd5Si3
mp-861875	LiHf2Re	mp-23713	CaH2	mp-355	Nd5Si4

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1203605	Hf21Re25	mp-1463	LaIr2	mp-9967	NdSi
mp-1689	HfRe2	mp-1199235	La5Ir3	mp-571109	Li2Nd2Si3
mp-1495	ErIr2	mp-1104396	La5Ir2	mp-866141	TiFe2Si
mp-2713	ErIr	mp-1104303	La3Ir2	mp-5529	MnFe2Si
mp-1201760	Er5Ir3	mp-23818	BaLiH3	mp-2108	Ti5Si3
mp-862554	LiEr2Ir	mp-570421	Sm2B5	mp-865652	TiMn2Si
mp-30843	Sr7Pt3	mp-8546	SmB4	mp-861983	Ti2MnFe
mp-862765	LiGd2Ir	mp-12614	Ca2Cu	mp-570175	Ce5Si3
mp-1104397	Yb5Pd2	mp-585949	CaCu	mp-555617	Ce10Si8O3
mp-2547	YbPd	mp-1882	CaCu5	mp-2493	CeN
mp-1184479	Gd3In	mp-979289	TaW3	mp-8181	Li2CeN2
mp-865483	Li2GdIn	mp-1187206	Ta3W	mp-1227650	BaSr4
mp-865715	Li2PrTl	mp-1217811	TaW	mp-862746	Sr2LiTl
mp-1207599	Yb2Si	mp-10485	BaLiSb	mp-13392	NdCu
mp-866191	Li2YbSi	mp-1079438	Ta2N	mp-11852	NdCu2
mp-1079180	HoPt	mp-14753	Li7TaN4	mp-1140	NdCu5
mp-1188476	Ho3Pt	mp-510401	GdP	mp-1216946	TiMnCr
mp-1102104	Ho2Pt	mp-625	Mg3Ru2	mp-1845	CaBe13
mp-1198999	Ho5Pt4	mp-1211143	LiEuP	mp-18337	Be3N2
mp-1102508	DyOs2	mp-13944	Li3AlN2	mp-29463	LiBeN
mp-1189887	Dy3Os	mp-1020031	LiCaAlN2	mp-13971	Nd2SeO2
mp-867776	LiDy2Os	mp-661	AlN	mp-4764	Pr2SeO2
mp-1184905	K	mp-22867	RbBr	mp-27869	Ba2PCL
mp-16502	Ho2Al	mp-1101989	SrLiAs	mp-864955	Mn2CrCo
mp-391	HoAl2	mp-614724	Cs3CrF7	mp-28930	KC8
mp-1188420	HoAl	mp-1188125	Sm3Ru	mp-1823	Ti3Al
mp-867902	LiSiRh2	mp-1104159	Sm5Ru2	mp-1953	TiAl
mp-1018166	AlTc2	mp-1102438	SmRu2	mp-9921	MgCr2O4
mp-1104669	Ca5Pd2	mp-800	TmB2	mp-1216850	TiCuNi
mp-1104661	Ca3Pd2	mp-568143	TmB4	mp-1217065	Ti8Cu3Ni
mp-1106061	Ca3Pd	mp-980757	Sm5Sb3	mp-865712	Ti2MnNi
mp-867171	SrLi2Sn	mp-867272	LiAlCu2	mp-1217247	Ti4CoNi
mp-2516	YZn	mp-623108	Eu4Ir	mp-1278	Zr2Si
mp-1199166	Be17Os3	mp-1185339	LiEu2Ir	mp-1207024	Zr3Si2
mp-1202141	Tm3Ga2	mp-1103979	Nd5Ru2	mp-893	ZrSi
mp-1065301	TmGa	mp-1106300	Nd3Ru		
mp-1185329	LiAcRh2	mp-1102217	NdRu2		

Table S2 Phases with stability in the entire range of Li potentials

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-864647	Hf2N	mp-1205201	Dy3Rh2	mp-1018149	ScCu2
mp-103	Hf	mp-1107	Th7Rh3	mp-646926	GdRu2
mp-2828	HfN	mp-12755	ThRh	mp-1974	CeB4
mp-1224388	Hf3N2	mp-569074	Th7Pt3	mp-30671	Ti2Ga
mp-19920	Ce3Ga	mp-12754	ThPt	mp-30672	Ti3Ga
mp-567332	Ce	mp-129	Mo	mp-680653	Yb8In3
mp-1018276	CeGa	mp-567412	Y5Sn3	mp-1694	Yb2Ge
mp-568417	PrAl	mp-685209	Sc39N34	mp-1937	YbCu
mp-38	Pr	mp-2857	ScN	mp-1607	YbCu5
mp-1189	PrAl2	mp-570670	YO2	mp-567538	YbCu2
mp-30666	Sc3Ga2	mp-1188757	Y3Os	mp-11219	LuB2
mp-67	Sc	mp-567612	ScOs2	mp-571495	LuB4
mp-1187073	Sr	mp-568623	Sc44Os7	mp-1269	SmS
mp-1328	SrRh2	mp-12305	Sc11Os4	mp-5598	Sm2SO2

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-113	Tc	mp-1095545	ZrTc2	mp-1188656	Nd3Os
mp-44	U	mp-1102657	Y2Pt	mp-569630	NdOs2
mp-1189402	Ta2Be17	mp-1025448	YPt	mp-1500	BaS
mp-1102049	TaBe3	mp-7343	Y3Pt	mp-22508	YMn12
mp-1078957	Ta3Be2	mp-11564	TmRh	mp-1077154	SmCu2
mp-567842	TaBe12	mp-348	TmPd	mp-710	SmP
mp-87	Be	mp-16507	LuAl	mp-980769	SmCu
mp-11278	Ta2Be	mp-1234	LuAl2	mp-227	SmCu5
mp-50	Ta	mp-16508	Lu3Al2	mp-12670	Ho2SO2
mp-867200	Pm	mp-568630	LuRu2	mp-1610	TbS
mp-862980	PmAl3	mp-11495	LuRu	mp-12668	Tb2SO2
mp-1102133	Tm2Pt	mp-2786	Ca5Zn3	mp-1102	LuN
mp-1018122	Tm	mp-1103570	Ca5Pt2	mp-1949	TiMn2
mp-1025409	TmPt	mp-1294	YCo2	mp-1202079	Ti21Mn25
mp-1199106	Tm5Pt4	mp-865373	YCo	mp-1514	UB2
mp-1198546	Er3Ga2	mp-1105598	Y3Co	mp-619	UB4
mp-1184115	Er	mp-510184	GdOs2	mp-2295	CaNi2
mp-1018077	ErGa	mp-1742	GdRh	mp-774	CaNi5
mp-11698	Tb	mp-20084	GdRh2	mp-193	Zr2Cu
mp-2322	YAl2	mp-10622	PrAs	mp-1216441	Zr14Cu51
mp-1187739	Y	mp-1584	YbIr2	mp-1188077	Zr7Cu10
mp-10172	Na	mp-632	TmCo2	mp-12684	LaAl
mp-10659	Ho	mp-1217007	Tm4Co3	mp-2694	LaAl2
mp-75	Nb	mp-2762	YIr2	mp-1206996	La3AlO
mp-1207777	Y3Pd	mp-1198712	Y5Ir3	mp-20689	Nb3B2
mp-1066136	YPd	mp-1207785	Y3Ir	mp-2580	NbB
mp-30367	Ca5Au2	mp-2339	Ti3Pt	mp-10255	Nb3B4
mp-972364	Yb	mp-21246	Ba2Pb	mp-1080021	Nb2B3
mp-2474	YAg	mp-291	TiOs	mp-450	NbB2
mp-1187197	Ta3Os	mp-1072856	PrZn2	mp-23268	NaI
mp-1218177	Ta3Os2	mp-460	PrZn	mp-305	TiFe
mp-1187243	TaOs3	mp-544	Ti3Ir	mp-2605	CaO
mp-49	Os	mp-1235	TiIr	mp-21009	EuSe
mp-86	Sm	mp-1129	ScIr	mp-965	TbB2
mp-1102302	CeOs2	mp-1200708	Sc44Ir7	mp-568225	TbB4
mp-2088	CeAl2	mp-1103411	Dy2Au	mp-1187198	SrMg2
mp-10740	Pa	mp-567590	LuOs2	mp-1352	ZrN
mp-862690	Ac	mp-1102890	TmTc2	mp-1014265	Zr2N
mp-10658	Dy	mp-30385	Ho2Au	mp-2432	CaMg2
mp-1102972	Er2Au	mp-189	SiRu	mp-1409	TiNi3
mp-155	Gd	mp-867262	ScTc3	mp-1048	TiNi
mp-20353	GdGa	mp-1101953	HoOs2	mp-1808	Ti2Ni
mp-1106373	Sm5Si3	mp-1190011	Ho3Os	mp-1774	ErB2
mp-1025489	SmSi	mp-1578	V3Rh	mp-2847	ErB4
mp-23	Ni	mp-2006	V3Ir	mp-24237	ScH2
mp-1105989	Lu5Ge3	mp-1001613	LuGa	mp-2252	ScB2
mp-145	Lu	mp-1199315	Lu3Ga2	mp-19830	ErN
mp-35	Mn	mp-708	LaAs	mp-2489	UC
mp-11854	Er5Ge3	mp-542569	AlRu	mp-2486	UC2
mp-33	Ru	mp-1070580	Al3Ru2	mp-2625	U2C3
mp-54	Co	mp-10910	Al2Ru	mp-23260	BaI2
mp-518	Ti5Re24	mp-11375	EuHg	mp-29909	Ba4I6O
mp-8	Re	mp-2545	YbHg	mp-2384	LaP
mp-2179	TiRe	mp-672286	Eu3Ga2	mp-1202486	La7Ru3

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Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1018125	Ti2Re	mp-1487	AlNi	mp-1104417	La5Ru2
mp-72	Ti	mp-2593	AlNi3	mp-17193	Ca3GeO
mp-1102084	DyTc2	mp-16514	Al3Ni5	mp-568636	TiCr2
mp-1762	ErRh2	mp-862655	Ru3W	mp-31205	Zr3Fe
mp-2381	ErRh	mp-867816	TaRu3	mp-22447	Zr3P
mp-11437	Er3Rh	mp-977390	Ta3Ru	mp-1190681	ZrFe2
mp-30612	Er7Rh3	mp-1601	TaRu	mp-582924	Zr6Fe23
mp-1198715	Er3Rh2	mp-1218044	Ta3Ru2	mp-583740	Zr7P4
mp-396	YbGa	mp-921	YRh2	mp-1080525	FeB
mp-1102309	Yb2Ga	mp-191	YRh	mp-10118	Mn3B4
mp-2524	NdGa2	mp-1207780	Y3Rh	mp-20318	Mn2B
mp-1448	NdGa	mp-1189474	Y7Rh3	mp-1915	Fe2B
mp-1203103	Nd3Ga2	mp-1196999	Y3Rh2	mp-2567	V3Si
mp-123	Nd	mp-2725	TbIr2	mp-568671	V5Si3
mp-570684	ZrOs2	mp-1201266	Tb5Ir3	mp-2090	FeCo
mp-11541	ZrOs	mp-1106276	Tb3Ir	mp-601842	Fe9Co7
mp-131	Zr	mp-16721	TmAl	mp-601848	Fe11Co5
mp-607	CeRu2	mp-858	TmAl2	mp-601820	Fe3Co
mp-570629	Ce4Ru3	mp-982635	Tm3Al2	mp-1214417	BaC6
mp-570369	Ce16Ru9	mp-1104	LaMg	mp-31214	Ti3P
mp-11534	Np	mp-2292	La2O3	mp-22600	Sc3P2
mp-1186374	Os3W	mp-1094174	LaMg3	mp-1188800	Sc3P
mp-91	W	mp-23193	KCl	mp-568643	RbC8
mp-266	Zr2Pd	mp-614603	CsI	mp-28861	CsC8
mp-253	ScCo2	mp-1184151	Cs	mp-631	TiC
mp-2212	ScCo	mp-23295	RbCl	mp-27919	Ti8C5
mp-27162	Sc3Co	mp-22903	RbI	mp-10721	Ti2C
mp-1065995	ZrPt	mp-2686	Ca2N	mp-1000	BaTe
mp-8094	Ba2Hg	mp-1104937	Pr5Ru2	mp-4547	La2TeO2
mp-31172	Ca5Ag3	mp-16705	Pr2O3	mp-1560	LaTe
mp-864735	Mn3Ir	mp-1197932	Pr7Ru3	mp-11649	Ca3SiO
mp-1057315	Eu	mp-2665	PrRu2	mp-2517	Ca2Si
mp-1106357	Tb5Sn3	mp-1105741	Pr3Ru	mp-7084	SrCaSi
mp-1857	YbCd	mp-1045	Nd2O3	mp-12906	Sr3CrN3
mp-1102319	Lu2Pt	mp-3211	Nd2SO2	mp-2542	BeO
mp-1025438	LuPt	mp-1748	NdS	mp-1958	SrTe
mp-1202267	Lu5Pt4	mp-1427	Lu2O3	mp-542583	EuTe
mp-30800	NdZn2	mp-20874	EuB6	mp-7822	Sc5Si3
mp-1053	NdZn	mp-21394	EuO	mp-24096	NdH2
mp-477	SmGa2	mp-504886	Gd2O3	mp-1188283	V8N
mp-1195872	Sm3Ga2	mp-1224869	Gd2C	mp-33090	V2N
mp-1188469	La5Ge3	mp-1189998	Gd2C3	mp-1220316	NbW
mp-26	La	mp-554098	Ti6O	mp-316	MnV
mp-13	Fe	mp-1018124	Ti2Rh	mp-1187702	VW3
mp-2602	NdAs	mp-2583	TiRh	mp-1216231	VW
mp-1761	LuIr2	mp-1215377	Zr4O	mp-864984	MnV3
mp-1529	LuIr	mp-1102043	LaOs2	mp-1192350	NbFe2
mp-364	AlRh	mp-284	AlCo	mp-1221111	NbFe
mp-569220	ErRu2	mp-2652	Y2O3	mp-1185970	Mn3Co
mp-568186	YRu2	mp-16713	Pr2B5	mp-28731	V6C5
mp-1207781	Y3Ru	mp-12569	PrB4	mp-20648	V2C
mp-570438	Yb8Ti3	mp-1542	YB2	mp-548	NbCr2
mp-37	Th	mp-637	YB4	mp-1569	Be2C
mp-546	HoRh2	mp-568646	Ta3Si	mp-30811	Ni4W

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-2163	HoRh	mp-1989	Ta5Si3	mp-1216621	TiW
mp-1106336	Ho7Rh3	mp-1387	AlV3	mp-784631	CrNi2
mp-1200753	Ho3Rh2	mp-1183162	AlFe3	mp-1585	V3Co
mp-1095604	ErTc2	mp-2658	AlFe	mp-542614	VCo3
mp-1101816	Lu2Au	mp-978951	SmAl	mp-771	MnAl
mp-928	HoIr2	mp-2358	SmAl2	mp-12659	Mn2Nb
mp-11476	HoIr	mp-571222	CsBr	mp-977426	NbCo3
mp-1197997	Ho5Ir3	mp-1014229	Ti2Zn	mp-7250	Nb6Co7
mp-1095487	LuTc2	mp-608	TiCo3	mp-1220522	NbVCo
mp-1187196	Ta3Ir	mp-823	TiCo	mp-1219177	Sm2C
mp-1458	Nb3Ir	mp-1191331	Ti2Co	mp-569335	Sm2C3
mp-1820	YbS	mp-2057	DyB2	mp-1216546	Tm2C
mp-1188292	Y5Pb3	mp-2345	Dy2O3	mp-7171	TmP
mp-1204352	Y3Ga2	mp-2719	DyB4	mp-1205180	Tm3C4
mp-11420	YGa	mp-749	SmN	mp-542830	Mn23C6
mp-90	Cr	mp-218	Sm2O3	mp-20211	Mn3Si
mp-1885	AlIr	mp-2114	YN	mp-21256	Mn7C3
mp-2206	LuCo2	mp-22898	KI	mp-863690	Ti2MnCo
mp-1222465	Lu4Co3	mp-1145	TiB2	mp-865537	TiMnCo2
mp-19923	GdAl2	mp-7857	TiB	mp-569424	Cr2B
mp-1078585	GdAl	mp-1025170	Ti3B4	mp-1080664	CrB
mp-1102354	ThTc2	mp-2675	MgNi2	mp-15617	Cr5B3
mp-1865	UN	mp-568151	Ti5Ge3	mp-20857	CoB
mp-834	ThN	mp-2801	CeCu2	mp-2091	V3B2
mp-11452	HfOs	mp-2154	CeP	mp-9973	VB
mp-2235	YbRh2	mp-581942	CeCu6	mp-1491	VB2
mp-567089	YbRh	mp-573697	CsCl	mp-1206441	V5B6
mp-669917	ZrRh	mp-492	TiN	mp-569270	V3B4
mp-571664	Zr2Rh	mp-8282	Ti2N	mp-9208	V2B3
mp-1188413	Zr3Rh	mp-865716	YbCl2	mp-9546	Yb2C3
mp-1374	Zr5Re24	mp-2117	TbN	mp-1103975	YbC6
mp-12109	ZrRe2	mp-1056	Tb2O3	mp-729	Cr3Si
mp-574458	Zr21Re25	mp-1183837	Co3Ni	mp-2157	Co3W
mp-30622	Dy5Ru2	mp-505002	Sc5As3	mp-171	VNi3
mp-1105841	Dy3Ru	mp-1095642	Eu2Ge	mp-11531	VNi2
mp-30743	TmIr2	mp-20587	EuS	mp-7226	V3Ni
mp-11483	TmIr	mp-946	PrIr2	mp-1216708	V3Ni2
mp-1198195	Tm5Ir3	mp-1205021	Pr5Ir3	mp-11501	MnNi3
mp-570436	CaIr2	mp-1104160	Pr5Ir2	mp-1208170	TiVP
mp-570356	Ca5Ir	mp-1106395	Pr3Ir	mp-29241	Ca3SnO
mp-979911	Y2Au	mp-981	SrF2	mp-865490	V2CrFe
mp-2205	LuPd	mp-1101970	TbRu2	mp-865678	TiMn2V
mp-1087502	HoPd	mp-1189033	Tb3Ru	mp-1217201	Ti4Mn5V3
mp-1071848	Pr2Sb	mp-2267	HoB2	mp-1451	NbNi3
mp-1187203	Ta3Re	mp-812	Ho2O3	mp-1220799	NbNi
mp-1217894	TaRe	mp-569281	HoB4	mp-1418	FeNi3
mp-971788	VRu3	mp-10688	CeO	mp-2213	FeNi
mp-1395	VRu	mp-1767	Tm2O3	mp-567415	Nd2B5
mp-865382	V3Ru	mp-1189863	Tm5Si3	mp-1632	NdB4
mp-146	V	mp-1066975	TmSi	mp-2538	Y5Si3
mp-977434	Nb3Ru	mp-1216	YbO	mp-259	AlMo3
mp-11517	NbRu3	mp-2643	Ti3Cu4	mp-19713	Sc3In
mp-432	NbRu	mp-2078	TiCu	mp-759	La2Sb
mp-1079796	Ti3Pd	mp-742	Ti2Cu	mp-542503	La9(SbO)5

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1072399	Be5Pt	mp-12546	TiCu3	mp-903	ZrCr2
mp-1103421	Dy2Pt	mp-1245	Sr2N	mp-1519	CaTe
mp-1078613	DyPt	mp-615	YMg	mp-16032	Pr2TeO2
mp-1105479	Dy3Pt	mp-23251	KBr	mp-5459	Nd2TeO2
mp-1205197	Dy3Ga2	mp-643	ThO2	mp-4511	La2SO2
mp-30604	DyGa	mp-1779	YbTe	mp-2350	LaS
mp-377	LuRh	mp-11506	Ni3Mo	mp-1103990	EuC6
mp-2529	PrRh2	mp-11507	Ni4Mo	mp-1190061	Eu5Si3
mp-999305	PrRh	mp-1189967	Pr3Os	mp-2199	Fe3Si
mp-1104158	Pr3Rh2	mp-567339	PrOs2	mp-1800	Nd2C3
mp-570119	Yb7Au3	mp-1105633	Y3Ni	mp-1222310	Lu2C
mp-570527	Yb5Au4	mp-582134	Y3Ni2	mp-10192	LuP
mp-568944	Yb5Au3	mp-1364	YNi	mp-1203767	Lu3C4
mp-1188310	Tm5Ge3	mp-2152	YNi5	mp-15178	Lu4C7
mp-1079937	Pr3Si2	mp-574339	Y2Ni7	mp-1216666	TiNbCr4
mp-9968	PrSi	mp-1200338	Y15Ni32	mp-640095	La3Co
mp-1179656	Rb	mp-569196	YNi3	mp-30559	LaCo13
mp-1102728	Dy2Al	mp-22916	NaBr	mp-20937	Cr3C2
mp-803	DyAl2	mp-1253	BaSe	mp-1196316	Cr7C3
mp-433	DyAl	mp-510402	GdS	mp-723	Cr23C6
mp-1212499	Hf5Ir3	mp-4805	Gd2SO2	mp-12894	Y2SO2
mp-1007786	HfIr	mp-7283	LaB4	mp-1095443	ScFe2
mp-1545	Nb3Rh	mp-2680	LaB6	mp-22701	ScFeSi
mp-1095658	Tb2Au	mp-1184	La2C3	mp-505554	Sc(FeSi)2
mp-892	ScPt	mp-2367	LaC2	mp-4755	Sc3Fe2Si3
mp-1196981	Sc57Pt13	mp-1410	DyN	mp-3618	Sc2FeSi2
mp-864637	NdAl	mp-343	PrN	mp-2080	SrBe13
mp-400	NdAl2	mp-1078920	LaCu	mp-27791	SrBe3O4
mp-11454	Hf2Pd	mp-2051	LaCu2	mp-1220599	NbVNi
mp-1197194	Ho3Ga2	mp-2613	LaCu5	mp-10961	La5Si3
mp-1018073	HoGa	mp-969	YbAl2	mp-22302	ZrVP
mp-30828	Sr2Pb	mp-865934	YbF2	mp-571261	Pu
mp-1007691	HfPt	mp-1212961	Eu2N	mp-30428	BaCu
mp-11460	HfTc	mp-567290	LaN	mp-683	Pr2C3
mp-1095669	HfTc2	mp-2599	NdN	mp-1077063	La2Bi
mp-7188	Al2Os	mp-2823	NdP	mp-24153	LaH2
mp-862259	Sc3Al	mp-12669	Dy2SO2	mp-28255	LaHO
mp-11220	Sc2Al	mp-1189298	YbB4	mp-865656	TiMn2W
mp-331	ScAl	mp-419	YbB6	mp-1640	Ho2C
mp-813	ScAl2	mp-1079585	Nb2N	mp-744	HoP
mp-1102030	YTc2	mp-1199558	Sm5Ir3	mp-15238	Ho4C5
mp-11566	ScZn	mp-7342	Sm3Ir	mp-1202754	Ho3C4
mp-2031	Be2Cu	mp-1104500	Sm5Ir2	mp-1154	Ho4C7
mp-1227357	Be3Cu	mp-1025402	SrCu	mp-1038	MgCu2
mp-11107	Ac2O3	mp-2116	ZrMn2	mp-1216443	V6FeNi
mp-1385	CeZn2	mp-17190	Sc5Ge3	mp-1105563	GdB4
mp-668	PrGa2	mp-242	SrB6	mp-28366	Gd2B5
mp-11404	PrGa	mp-1087	SrS	mp-29621	Ba5Bi3
mp-1104052	Pr9Ga4	mp-2576	Sr2Ge	mp-12671	Er2SO2
mp-669594	Pr5Ga3	mp-304	Ca2Ge	mp-23056	Sr2BrN
mp-1190862	Sc2Pd	mp-865	CaB6	mp-567744	SrBr2
mp-2781	ScPd	mp-1213975	CaB4	mp-1208630	SrC6
mp-1780	ScRh	mp-1570	YFe2	mp-568662	BaCl2
mp-30863	Sc57Rh13	mp-11385	YFe5	mp-23063	Ba4Cl6O

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-2748	CeAs	mp-23713	CaH2	mp-12574	Dy2C
mp-567490	Hf5Re24	mp-1463	LaIr2	mp-2014	DyP
mp-1203605	Hf21Re25	mp-1199235	La5Ir3	mp-1212812	Dy4C5
mp-1689	HfRe2	mp-1104396	La5Ir2	mp-1213387	Dy3C4
mp-1495	ErIr2	mp-1104303	La3Ir2	mp-10126	V5SiB2
mp-2713	ErIr	mp-570421	Sm2B5	mp-1200894	Zr3As
mp-1201760	Er5Ir3	mp-8546	SmB4	mp-1106011	Nd3Co
mp-30843	Sr7Pt3	mp-12614	Ca2Cu	mp-1104652	Nd5Co2
mp-1104397	Yb5Pd2	mp-585949	CaCu	mp-356	Nd2Co17
mp-2547	YbPd	mp-1882	CaCu5	mp-1084826	Nd2Co3
mp-1184479	Gd3In	mp-979289	TaW3	mp-21075	HfC
mp-1207599	Yb2Si	mp-1187206	Ta3W	mp-504812	Hf3P
mp-1079180	HoPt	mp-1217811	TaW	mp-29941	Sc2C
mp-1188476	Ho3Pt	mp-1079438	Ta2N	mp-1219429	Sc2CO
mp-1102104	Ho2Pt	mp-510401	GdP	mp-15661	Sc4C3
mp-1198999	Ho5Pt4	mp-625	Mg3Ru2	mp-28733	Sc3C4
mp-1102508	DyOs2	mp-661	AlN	mp-1225044	Er2C
mp-1189887	Dy3Os	mp-22867	RbBr	mp-1144	ErP
mp-1184905	K	mp-614724	Cs3CrF7	mp-1203719	Er3C4
mp-16502	Ho2Al	mp-1188125	Sm3Ru	mp-1212833	Er4C7
mp-391	HoAl2	mp-1104159	Sm5Ru2	mp-20181	Ce2C3
mp-1188420	HoAl	mp-1102438	SmRu2	mp-601	PrP
mp-1018166	AlTc2	mp-800	TmB2	mp-2058	Ni3B
mp-1104669	Ca5Pd2	mp-568143	TmB4	mp-2536	Ni2B
mp-1104661	Ca3Pd2	mp-980757	Sm5Sb3	mp-1220374	NbVCr
mp-1106061	Ca3Pd	mp-623108	Eu4Ir	mp-864953	MnV2Cr
mp-2516	YZn	mp-1103979	Nd5Ru2	mp-775201	Cr3Fe(PO4)6
mp-1199166	Be17Os3	mp-1106300	Nd3Ru	mp-1334	Y2C
mp-1202141	Tm3Ga2	mp-1102217	NdRu2	mp-2795	ZrC
mp-1065301	TmGa	mp-1079399	V3Fe	mp-684623	Zr10C9
mp-553921	Pm2O3	mp-866134	VFe3	mp-9459	Y4C5
mp-2290	NdRh2	mp-3236	Pr2SO2	mp-1200885	Y4C7
mp-999335	NdRh	mp-2495	PrS	mp-1200613	Y3C4
mp-1220520	Nd4Rh	mp-645	TbP	mp-1193531	Ta2Al
mp-1104743	Nd3Rh2	mp-1837	TbCu	mp-567735	Nd5Si3
mp-1201296	Nd5Rh4	mp-1527	TbCu2	mp-355	Nd5Si4
mp-17706	Zr5Ge3	mp-11363	TbCu5	mp-9967	NdSi
mp-1203324	Zr3Ge	mp-1080443	YCu	mp-866141	TiFe2Si
mp-1188062	Zr3Sc	mp-994	YP	mp-5529	MnFe2Si
mp-1077791	ZrSc2	mp-2698	YCu2	mp-2108	Ti5Si3
mp-1095690	Tm2Au	mp-2797	YCu5	mp-865652	TiMn2Si
mp-1358	DyIr2	mp-1975	TmN	mp-861983	Ti2MnFe
mp-1200226	Dy5Ir3	mp-568793	Ca28Ga11	mp-570175	Ce5Si3
mp-1105615	Dy3Ir	mp-582055	La7Ni16	mp-555617	Ce10Si8O3
mp-650	Be5Pd	mp-1064719	LaNi	mp-2493	CeN
mp-862714	Be3Ir	mp-2317	LaNi5	mp-1227650	BaSr4
mp-1102875	Er2Al	mp-573855	La7Ni3	mp-13392	NdCu
mp-1208	ErAl2	mp-1679	La2Ni7	mp-11852	NdCu2
mp-1188739	ErAl	mp-890	NdIr2	mp-1140	NdCu5
mp-567750	ScRu2	mp-30522	Nd5Ir3	mp-1216946	TiMnCr
mp-30867	ScRu	mp-1104605	Nd5Ir2	mp-1845	CaBe13
mp-1210377	Sc57Ru13	mp-1189686	Nd3Ir	mp-18337	Be3N2
mp-1194143	Sc11Ru4	mp-679	Er2O3	mp-13971	Nd2SeO2
mp-1209947	Sc44Ru7	mp-24286	ZrH2	mp-4764	Pr2SeO2

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Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1438	ZrIr3	mp-864675	Yb3N2	mp-27869	Ba2PbCl
mp-30749	Zr5Ir3	mp-954	BaB6	mp-864955	Mn2CrCo
mp-568992	ZrIr	mp-570007	SmOs2	mp-28930	KC8
mp-30748	Zr3Ir	mp-1190029	Sm3Os	mp-1823	Ti3Al
mp-11457	HfRh	mp-1894	WC	mp-1953	TiAl
mp-1190626	Hf2Rh	mp-17751	Y5Ge3	mpvc-9921	MgCr2O4
mp-1101968	HoTc2	mp-940	GdN	mp-1216850	TiCuNi
mp-571262	CaRh2	mp-24192	ErH2	mp-1217065	Ti8Cu3Ni
mp-1214063	Ca5Rh	mp-1187696	VCr3	mp-865712	Ti2MnNi
mp-214	ZrRu	mp-1187695	V3Cr	mp-1217247	Ti4CoNi
mp-567258	LaZn2	mp-1216394	VCr	mp-1278	Zr2Si
mp-2615	LaZn	mp-11283	ZrBe5	mp-1207024	Zr3Si2
mp-1388	DyRh2	mp-30445	ZrBe13	mp-893	ZrSi
mp-232	DyRh	mp-2544	Zr2Be17		
mp-1105786	Dy7Rh3	mp-1169	ScCu		

Table S3 Phases that are thermodynamically stable against Na_{BCC}

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-10419	Na4ReN3	mp-11247	Li3Au	mp-1314	Li12Si7
mp-10172	Na	mp-567395	Li15Au4	mp-1201871	Li7Si3
mp-8	Re	mp-600561	LiRh	mp-559904	NaLi3SiO4
mp-22003	NaN3	mp-1001787	LiRh3	mp-29720	Li21Si5
mp-1103252	ZnPd2	mp-1209185	RbPrF4	mp-672287	Li13Si4
mp-1652	ZnPd	mp-1220948	NaPrF4	mp-540945	Na2Li3GaO4
mp-1186074	Na3Pd	mp-1180133	NaCaH6Ir	mp-980757	Sm5Sb3
mp-950	NaZn13	mp-23713	CaH2	mp-770806	Sm2TiO5
mp-865357	Zn3Pd	mp-570436	CaIr2	mp-561233	Sm9(SbO)5
mp-1215714	Zn2Pd	mp-570356	Ca5Ir	mp-2281	SmSb
mp-1184905	K	mp-663	NdGe	mp-12049	Nd2Sb
mp-1179656	Rb	mp-1748	NdS	mp-1586	NdSb
mp-1363	Na2Au	mp-1464	Nd5Ge3	mp-530	Nd4Sb3
mp-1066254	YAu	mp-172	Nd5Ge4	mp-11284	CaGa2
mp-979911	Y2Au	mp-2015	Nd3Ge5	mp-11649	Ca3SiO
mp-1187739	Y	mp-510402	GdS	mp-568793	Ca28Ga11
mp-864675	Yb3N2	mp-8260	NaGdS2	mp-1227300	Ca2GaSi
mp-972364	Yb	mp-1463	LaIr2	mp-30473	Ca3Ga5
mp-864757	YbN2	mp-1104303	La3Ir2	mp-4481	Ca2SiO4
mp-571261	Pu	mp-1199235	La5Ir3	mp-6914	CaGa
mp-682	NaF	mp-1104396	La5Ir2	mp-31348	Sc2In
mp-542573	ThB4	mp-1562	ThBe13	mp-7822	Sc5Si3
mp-37	Th	mp-23818	BaLiH3	mp-1207100	ScIn
mp-1756	ThB6	mp-23703	LiH	mp-9969	ScSi
mp-1221215	Na3ThB24	mp-2747	TbPd3	mp-19713	Sc3In
mp-262	Na3B20	mp-1104088	Tb3Pd4	mp-1185970	Mn3Co
mp-2402	NaSi	mp-1080451	TbPd	mp-1109	Sr5Al9
mp-1199056	RbGe	mp-30667	Sr8Ga7	mp-2775	SrAl4
mp-29657	NaGe	mp-182	SrGa2	mp-3094	SrAl2O4
mp-573471	Li17Sn4	mp-1827	SrGa4	mp-3393	Sr3Al2O6
mp-1018134	Li	mp-797	DyPd3	mp-20273	Ca3PbO
mp-30767	Li7Sn2	mp-1104399	Dy3Pd4	mp-30478	Ca2Pb
mp-30794	Na15Sn4	mp-2345	Dy2O3	mp-551873	Ca4Bi2O
mp-31430	Na2In	mp-12543	Dy3Pd2	mp-569535	Ca2Bi
mp-862943	NaPmHg2	mp-2226	DyPd	mp-27145	Ca5Bi3
mp-541787	Na8Hg3	mp-752672	NaDyO2	mp-560767	KNaTiO3

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-867200	Pm	mp-1106373	Sm5Si3	mp-554346	KSr4(BO3)3
mp-865108	NaSmHg2	mp-1025489	SmSi	mp-504812	Hf3P
mp-86	Sm	mp-13955	SmSi2	mp-20672	Hf3P2
mp-20074	SrIn2	mp-2602	NdAs	mp-9953	HfP
mp-705522	Sr28In11	mp-1071422	CeAg2	mp-504659	Hf2P
mp-1187073	Sr	mp-4764	Pr2SeO2	mp-1211649	K4HfO4
mp-608072	SrIn	mp-1674	PrSe	mp-557753	K3PO4
mp-655	Na3As	mp-1183837	Co3Ni	mp-974482	K4Hf5O12
mp-87	Be	mp-20874	EuB6	mp-1201301	K2Hf2O5
mp-11807	LiPt	mp-505346	Eu3(BO3)2	mp-24136	Cs(BH)6
mp-2271	NaPt2	mp-335	BaGa4	mp-1225884	CsBH4
mp-2170	Li2Pt	mp-30429	Ba8Ga7	mp-9774	Ba4Sb2O
mp-867227	Li3Pt	mp-1219	BaGa2	mp-755293	Sr4Sb2O
mp-1029595	Na3OsN2	mp-9909	Ba5Sb3	mp-862620	IrRu3
mp-49	Os	mp-32635	Sr3P2	mp-974358	Ir3Ru
mp-30795	Na2Tl	mp-505528	Nb3P	mp-755558	BaLa2O4
mp-30434	BaTl2	mp-505064	Nb2P	mp-30666	Sc3Ga2
mp-11820	BaNa2	mp-13275	NaSrP	mp-6204	Cs2NaScF6
mp-21246	Ba2Pb	mp-9339	NbP	mp-11411	ScGa
mp-20136	BaPb	mp-648999	Nb5P3	mp-1200767	Sc3Ga5
mp-21895	Na15Pb4	mp-18254	Nb7P4	mp-932	ScGa3
mp-30352	NaAg2	mp-978	Sr2Sn	mp-1207024	Zr3Si2
mp-1185581	Mg149Cd	mp-1698	SrSn	mp-893	ZrSi
mp-30490	Mg3Cd	mp-17720	Sr5Sn3	mp-3834	BaZrO3
mp-1094909	Mg2Cd	mp-492	TiN	mp-1278	Zr2Si
mp-983509	Na3Cd	mp-8282	Ti2N	mp-1515	ZrSi2
mp-1186271	NaMg149	mp-23954	Na2H2Pd	mp-8335	Ba2ZrO4
mp-1188292	Y5Pb3	mp-697096	Na2H4Pt	mp-755895	Ba3Zr2O7
mp-1646	Li3Hg	mp-542583	EuTe	mp-23063	Ba4Cl6O
mp-1184151	Cs	mp-11534	Np	mp-568662	BaCl2
mp-27838	Na3Bi	mp-640095	La3Co	mp-14208	LiYSi
mp-21294	Y2In	mp-1205615	La2Co2I	mp-7020	LiYO2
mp-22704	YIn	mp-30559	LaCo13	mp-2379	CoSi2
mp-1105835	Y3In5	mp-1500	BaS	mp-7577	CoSi
mp-571262	CaRh2	mp-27335	NaAlSi	mp-19905	Co2Si
mp-74	Rh	mp-28726	KYF4	mp-20857	CoB
mp-1214063	Ca5Rh	mp-17077	K2YF5	mp-1777	Li15Ge4
mp-132	Ca	mp-13230	K3YF6	mp-27932	Li9Ge4
mp-1185579	Mg149Hg	mp-555932	RbEr3F10	mp-1202504	Rb7NaSi8
mp-11375	EuHg	mp-674459	NaErF4	mp-16836	RbNa2Si17
mp-1057315	Eu	mp-13815	Rb2NaErF6	mp-8780	Cr2N
mp-867164	Pm3Sn	mp-13816	Cs2NaErF6	mp-1183691	CrN
mp-7956	Na3Sb	mp-13925	Cs2NaYF6	mp-568643	RbC8
mp-1266	Na2Se	mp-2524	NdGa2	mp-1029828	RbCrN2
mp-10659	Ho	mp-1448	NdGa	mp-1029705	Na15Cr7N19
mp-22916	NaBr	mp-1203103	Nd3Ga2	mp-743	RbN3
mp-10658	Dy	mp-1201758	KGe	mp-1395	VRu
mp-2784	Na2Te	mp-1169	ScCu	mp-865382	V3Ru
mp-90	Cr	mp-1018149	ScCu2	mp-971788	VRu3
mp-1079438	Ta2N	mp-196	Al5Co2	mp-9172	Li4TiO4
mp-50	Ta	mp-284	AlCo	mp-38280	LiTiO2
mp-1279	TaN	mp-16488	Al9Co2	mp-2931	Li2TiO3
mp-5475	NaTaN2	mp-1104937	Pr5Ru2	mp-20831	Gd4Sb3
mp-134	Al	mp-1197932	Pr7Ru3	mp-510403	GdSb

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-22862	NaCl	mp-2665	PrRu2	mp-13042	NaSr3TaO6
mp-864803	NaAcAu2	mp-1105741	Pr3Ru	mp-22204	Co2P
mp-862690	Ac	mp-556	ZrNi	mp-28861	CsC8
mp-865090	NaAcTl2	mp-485	ZrNi3	mp-1804	Fe3N
mp-2541	SmTl	mp-2717	Zr2Ni7	mp-6988	FeN
mp-319	Sm2Tl	mp-328	Zr2Ni	mp-3972	Ce2SO2
mp-570469	Pr5Tl3	mp-11397	Ga3Ni2	mp-8300	Ba4As2O
mp-38	Pr	mp-815	GaNi3	mp-10004	Mo3P
mp-12599	PrTl	mp-11398	Ga3Ni5	mp-22447	Zr3P
mp-1079915	PrAu	mp-21589	Ga9Ni13	mp-11345	ZrP
mp-2714	Pr2Au	mp-570775	BaAu	mp-647729	Zr14P9
mp-11469	PrHg	mp-1104164	Ba3Au2	mp-583740	Zr7P4
mp-30422	Sr7Au3	mp-865934	YbF2	mp-1215204	ZrTi2O
mp-30420	SrAu	mp-1078265	Cs2YbCl4	mp-2795	ZrC
mp-30421	Sr3Au2	mp-1070599	CsYbCl3	mp-684623	Zr10C9
mp-867943	Na3H7Os	mp-865716	YbCl2	mp-1025402	SrCu
mp-23870	NaH	mp-28395	B6P	mp-1087	SrS
mp-648	Na2S	mp-2154	CeP	mp-2726	SrCu5
mp-976072	NaAc2Pb	mp-1205536	La2Os2I	mp-736	Li3P
mp-464	HoSe	mp-639805	Ta3Ge	mp-9488	SmOF
mp-999474	NaHoSe2	mp-17593	Ta5Ge3	mp-1192338	Na5Sm4Si4O16F
mp-510404	GdSe	mp-318	SrIr2	mp-31509	BaIn
mp-155	Gd	mp-1766	TmS	mp-1105101	Ba9In4
mp-2434	SrTl	mp-3556	Tm2SO2	mp-22141	BaIn2
mp-30828	Sr2Pb	mp-1767	Tm2O3	mp-605809	Ba11In6O3
mp-677	SrCd2	mp-754825	NaTmO2	mp-4511	La2SO2
mp-30496	SrCd	mp-9076	NaTmS2	mp-28255	LaHO
mp-542484	Sr5Cd3	mp-17190	Sc5Ge3	mp-24153	LaH2
mp-1078721	InPd3	mp-1198803	Sc5Ge4	mp-1104116	La2H5
mp-21215	InPd	mp-1196279	Sc11Ge10	mp-1103808	La4H9
mp-22146	In3Pd5	mp-2606	BaPd5	mp-1029851	Na2GeN2
mp-22646	InPd2	mp-1687	BaPd2	mp-2495	PrS
mp-2114	YN	mp-1193896	Ba2H4Pd	mp-3236	Pr2SO2
mp-2286	Li2Se	mp-1008505	BaPd	mp-12614	Ca2Cu
mp-28603	NaLiSe	mp-862693	BaNaH3Pd	mp-585949	CaCu
mp-5339	CsNaTe	mp-9068	K2NaAlP2	mp-1882	CaCu5
mp-1240	HoS	mp-5122	Na3AlP2	mp-2856	Mn4Al11
mp-5694	NaHoS2	mp-861910	Sc3Hg	mp-771	MnAl
mp-101	Ir	mp-11471	ScHg	mp-173	MnAl6
mp-570491	TaNi3	mp-12802	AlCu3	mp-15819	Mn3Al9Si
mp-23	Ni	mp-985806	Al2Cu	mp-568151	Ti5Ge3
mp-1867	Ta2Ni	mp-2500	AlCu	mp-17193	Ca3GeO
mp-23268	NaI	mp-593	Al4Cu9	mp-304	Ca2Ge
mp-862942	NaPmAu2	mp-1786	Ti3Au	mp-2360	CaGe
mp-867199	Pm3Tl	mp-11237	ScAg	mp-1198692	Ti5Ge4
mp-862949	NaPmTl2	mp-1018128	ScAg2	mp-1884	Ca5Ge3
mp-734	LaHg	mp-23222	Li3Bi	mp-2157	Co3W
mp-26	La	mp-865101	NaLi2Bi	mp-1139	Co3Mo
mp-1079811	SmAu	mp-2744	LiPd	mp-2786	Ca5Zn3
mp-1080709	NdAu	mp-728	Li2Pd	mp-30483	CaZn
mp-1102098	Nd2Au	mp-1197547	Li15Pd4	mp-1725	CaZn2
mp-123	Nd	mp-861936	LiPd3	mp-1734	CaZn5
mp-1105965	Er5Tl3	mp-2404	CaAl2	mp-18567	CaZn11
mp-1184115	Er	mp-1190736	Ca8Al3	mp-1227465	Ca4Zn51

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1079938	TlPd3	mp-13520	Na2ZnGe	mp-31205	Zr3Fe
mp-865126	NaTlPd2	mp-1213848	Ce4Ge7	mp-1190681	ZrFe2
mp-2861	CaTl	mp-1213824	Ce4Ge3	mp-540809	Zr2Fe12P7
mp-865051	NaCa2Tl	mp-1096	CeS	mp-20892	ZrFeP
mp-718	SnPd3	mp-675328	Ce4GeS3	mp-582924	Zr6Fe23
mp-1220866	NaSn2Pd3	mp-1200696	Ce5Ge4	mp-5380	Ca4P2O
mp-1610	TbS	mp-1226804	Ce3GeS2	mp-8937	CrSi2
mp-11698	Tb	mp-865782	Yb3SiO	mp-729	Cr3Si
mp-999126	NaTbS2	mp-10651	YbSi	mp-2058	Ni3B
mp-814	DySe	mp-1077404	YbSi2	mp-2536	Ni2B
mp-999488	NaDySe2	mp-1207599	Yb2Si	mp-640067	Ni4B3
mp-11266	BaCd2	mp-1542	YB2	mp-2199	Fe3Si
mp-527	BaCd	mp-24650	YH2	mp-871	FeSi
mp-8093	Ba2Cd	mp-637	YB4	mp-1714	FeSi2
mp-75	Nb	mp-20214	UGa3	mp-1078278	CrB4
mp-867318	Eu3Tl	mp-1185635	Mg149Tl	mp-1080664	CrB
mp-866047	NaEuTl2	mp-19839	LaGa2	mp-15617	Cr5B3
mp-19966	GdTl	mp-2350	LaS	mp-569424	Cr2B
mp-579628	Gd2Tl	mp-672217	La5Ga3	mp-1491	VB2
mp-13	Fe	mp-1002133	LaGa	mp-2091	V3B2
mp-1018122	Tm	mp-551203	Sr2I2O	mp-9973	VB
mp-286	YbSe	mp-29910	Sr4I6O	mp-9208	V2B3
mp-21199	Na3(GePt)4	mp-568284	SrI2	mp-569270	V3B4
mp-10740	Pa	mp-559	YPd3	mp-1206441	V5B6
mp-4276	NaSi2Pd3	mp-1104019	Y3Pd4	mp-292	V3As
mp-697068	SiPd2	mp-1066136	YPd	mp-861868	KNaLaTaO5
mp-20622	SiPd3	mp-1207777	Y3Pd	mp-13019	NaLa2TaO6
mp-28614	NaBPT3	mp-1078920	LaCu	mp-1620	Si2W
mp-505055	Na3B5Pt9	mp-2051	LaCu2	mp-568671	V5Si3
mp-582067	Hf3As	mp-2613	LaCu5	mp-10711	VSi2
mp-103	Hf	mp-1194443	LaCu13	mp-1187702	VW3
mp-1190267	Hf3As2	mp-1210006	NaLiTm2F8	mp-2567	V3Si
mp-865076	NaCd2Pt	mp-636253	GdCu5	mp-1216231	VW
mp-1025468	CeAu	mp-1077933	GdCu2	mp-1102914	Ba2Eu3Si7
mp-567332	Ce	mp-1221034	NaGdF4	mp-1949	TiMn2
mp-1540	HoTl	mp-614455	GdCu	mp-1202079	Ti21Mn25
mp-1181055	Ho5Tl3	mp-1198712	Y5Ir3	mp-20181	Ce2C3
mp-1002136	LaAu	mp-2762	YIr2	mp-556039	Na3Y(BO3)2
mp-1103395	La2Au	mp-1207785	Y3Ir	mp-1210775	LuOF
mp-371	La3Tl	mp-1472	ZrB2	mp-1222310	Lu2C
mp-11488	LaTl	mp-18337	Be3N2	mp-1203767	Lu3C4
mp-865102	NaLaTl2	mp-2147	SrGe	mp-17673	Lu3O2F5
mp-11374	DyTl	mp-30950	Sr3GeO	mp-15178	Lu4C7
mp-1181553	Dy5Tl3	mp-2576	Sr2Ge	mp-1178173	Ho2TeO2
mp-8658	CsNaSe	mp-408	Mg2Ge	mp-2267	HoB2
mp-1190038	Tm5Tl3	mp-35730	BaUO3	mp-569281	HoB4
mp-1199133	Y11Sn10	mp-583034	Ba2U2O7	mp-11219	LuB2
mp-567412	Y5Sn3	mp-976128	Hf5Sc	mp-571495	LuB4
mp-574275	Li17Pb4	mp-1220764	NaHfScO4	mp-24151	DyH2
mp-30761	Li7Pb2	mp-504502	Ta3P	mp-12669	Dy2SO2
mp-861939	Ac3Sn	mp-1067587	TaP	mp-2470	DyS
mp-976076	NaAc2Sn	mp-22477	Ta2P	mp-999490	NaDyS2
mp-20849	Pd3Pb	mp-4974	La2Zr2O7	mp-24192	ErH2
mp-1561	TbSe	mp-616559	Ti2S	mp-7224	ThC2

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-999127	NaTbSe2	mp-31214	Ti3P	mp-1189614	BaThO3
mp-1476	ScS	mp-30218	Ti2P	mp-1188514	Th2C3
mp-67	Sc	mp-739	TiP	mp-1164	ThC
mp-999460	NaScS2	mp-1191079	Ti7P4	mp-1217395	Th4C3
mp-1185570	Mg149Pb	mp-1960	Li2O	mp-1217298	Th5C
mp-11286	CaHg	mp-3924	LiNbO2	mp-708	LaAs
mp-1103139	Ca2Hg	mp-28030	Li8Nb2O9	mp-1017987	Tc3N
mp-11288	Ca3Hg2	mp-1213070	Eu2Sn	mp-113	Tc
mp-867297	AcIn3	mp-567833	EuSn	mp-30091	MgB9N
mp-985305	Ac3In	mp-1221229	Na4Eu2SiP4	mp-978275	MgB7
mp-1186111	NaAcIn2	mp-1409	TiNi3	mp-365	MgB4
mp-11422	GdHg	mp-1048	TiNi	mp-763	MgB2
mp-30878	TbTl	mp-1808	Ti2Ni	mp-556185	RbNaTiO3
mp-30879	Tb5Tl3	mp-1189501	La7Pt3	mp-1104652	Nd5Co2
mp-11575	YTl	mp-1002104	LaPt	mp-1106011	Nd3Co
mp-1188434	Y5Tl3	mp-912	LaPt2	mp-356	Nd2Co17
mp-11544	Yb2Pb	mp-1104856	La3Pt4	mp-1084826	Nd2Co3
mp-145	Lu	mp-2387	Th2Zn	mp-11824	Ca3PN
mp-570050	Yb2Sn	mp-7496	ThZn2	mp-8977	Ca2PN3
mp-569304	C	mp-536	ThZn4	mp-4387	SrZrO3
mp-571095	Na7Ga13	mp-540743	Th2Zn17	mp-1018104	Zr2Cd
mp-8584	NaErSe2	mp-316	MnV	mp-4547	La2TeO2
mp-864806	NaAcHg2	mp-864984	MnV3	mp-759	La2Sb
mp-21412	Ce3Tl	mp-1981	Ba2Sn	mp-1209044	Sc5Sb3
mp-1206755	CeTl	mp-872	BaSn	mp-1065	LaSb
mp-11467	NdHg	mp-1198302	Nb3Ge	mp-1076970	LaScSb
mp-1533	Nd3Tl	mp-16842	Nb5Ge3	mp-1223	La4Sb3
mp-571405	NdTl	mp-567339	PrOs2	mp-542503	La9(SbO)5
mp-1084808	YbAu	mp-1189967	Pr3Os	mp-7192	Sc2Sb
mp-570119	Yb7Au3	mp-2052	ScAs	mp-4500	ZrNbP
mp-570527	Yb5Au4	mp-505002	Sc5As3	mp-1079460	Ti3Sn
mp-568944	Yb5Au3	mp-1188926	Sc3As2	mp-1102980	NbFeP
mp-8094	Ba2Hg	mp-614724	Cs3CrF7	mp-1192350	NbFe2
mp-2197	BaHg	mp-784631	CrNi2	mp-1221111	NbFe
mp-656	LuS	mp-752658	Y2SeO2	mp-869	TaAl3
mp-9035	NaLuS2	mp-999448	NaYSe2	mp-1193531	Ta2Al
mp-1191538	Ca8In3	mp-2637	YSe	mp-1260	SrPd5
mp-20263	CaIn	mp-11239	ZrAg	mp-1558	SrPd2
mp-542	SrHg	mp-2221	Zr2Ag	mp-999143	SrPd
mp-13427	Sr3Hg2	mp-1000	BaTe	mp-23714	SrH2
mp-20711	Fe3Ge	mp-30428	BaCu	mp-1207079	SrH3Pd
mp-2970	Na4GeO4	mp-9212	NaAlO2	mp-1179173	Sr2H4Pd
mp-2352	Na2O	mp-1842	NbAl3	mp-30811	Ni4W
mp-601833	Fe13Ge3	mp-18427	Nb2Al	mp-2108	Ti5Si3
mp-984	BN	mp-31008	Na14Al4O13	mp-21289	TiZn3
mp-28630	Na3BN2	mp-556168	Na7Al3O8	mp-7092	TiSi
mp-827	KN3	mp-13998	Na5AlO4	mp-1077503	TiSi2
mp-985586	Na3BrO	mp-23850	NaH2N	mp-1014229	Ti2Zn
mp-551835	Ba2I2O	mp-1105989	Lu5Ge3	mp-1014230	TiZn
mp-1342	BaO	mp-1199467	Lu5Ge4	mp-505527	Ti5Si4
mp-22937	Na4I2O	mp-1104514	Lu3Ge4	mp-8418	ZrCoP
mp-29909	Ba4I6O	mp-1196590	Lu11Ge10	mp-18133	Zr2Co4P3
mp-23260	BaI2	mp-9972	YSi	mp-1215734	Zr5Co19P12
mp-1019519	Ba2NaO	mp-677445	Y4Si3	mp-972631	Zr2Co12P7

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-865985	CdPd3	mp-2538	Y5Si3	mp-29152	Zr2CoP
mp-1696	CdPd	mp-1106032	Ho5Ge3	mp-1207414	Zr9(CoP2)2
mp-636334	SnRh2	mp-812	Ho2O3	mp-9981	Mn2N
mp-317	SnRh	mp-9994	Ho11Ge10	mp-1009130	MnN
mp-6058	K2NaScF6	mp-1675	Ho3Ge4	mp-505622	Mn4N
mp-23251	KBr	mp-755617	NaHoO2	mp-4126	KUO3
mp-23193	KCl	mp-1097916	CsCaCl3	mp-2486	UC2
mp-129	Mo	mp-1025185	Cs2CaCl4	mp-2625	U2C3
mp-1225049	K18Na46Tl31	mp-1213703	Cs3Ca2Cl7	mp-2489	UC
mp-614603	CsI	mp-1428	Ni5Ge3	mp-558317	KNaPrNbO5
mp-571222	CsBr	mp-21008	Ni3Ge	mp-4495	KLiTe
mp-1080443	YCu	mp-1185597	Mg149Ga	mp-2530	Li2Te
mp-2698	YCu2	mp-1770	Mg5Ga2	mp-8754	NaLiTe
mp-2797	YCu5	mp-30650	Mg2Ga	mp-2800	USi3
mp-30	Cu	mp-242	SrB6	mp-956	U3Si
mp-1185319	LiCl	mp-10811	NaSr4(BN2)3	mp-505569	CeH2
mp-1018029	CuPd	mp-10564	SrN2	mp-1104579	Ce2H5
mp-580357	Cu3Pd	mp-29973	SrN	mp-8973	NaSi2N3
mp-22867	RbBr	mp-1245	Sr2N	mp-804	GaN
mp-2532	PrTe	mp-201	Yb5Sb3	mp-4571	CaZrO3
mp-1078589	EuAu	mp-1857	YbCd	mp-5977	Nd2Zr2O7
mp-1189094	Eu3Au	mp-1187653	YbCd3	mp-12724	SrZn
mp-1106137	Eu7Au3	mp-999544	YAg2	mp-569426	SrZn2
mp-1104457	Eu3Au2	mp-2474	YAg	mp-672707	SrZn13
mp-3744	NaNbO2	mp-18040	KPrF4	mp-1435	SrZn5
mp-5477	Na5NbO5	mp-29210	Li2Ga	mp-18026	SrZn11
mp-27247	Na3NbO4	mp-1205930	Li5Ga4	mp-683	Pr2C3
mp-981	SrF2	mp-9568	Li3Ga2	mp-601	PrP
mp-38725	NaBH4	mp-11363	TbCu5	mp-1591	Al4C3
mp-419	YbB6	mp-1527	TbCu2	mp-14266	Cu15Si4
mp-864603	YbH2	mp-1837	TbCu	mp-861607	KNaNdTaO5
mp-978278	Na(BH)6	mp-1213256	CsEuCl3	mp-31417	Nd3TaO7
mp-1189298	YbB4	mp-1079091	PrCu	mp-861944	KNaPrTaO5
mp-33	Ru	mp-1071904	PrCu2	mp-14964	Pr3TaO7
mp-1186974	Sc3Ti	mp-2462	PrCu5	mp-3564	BaSc2O4
mp-7806	Cr3P	mp-2675	MgNi2	mp-755950	Ba2Sc2O5
mp-1598	Na3P	mp-2137	Mg2Ni	mp-867889	KNaGdTaO5
mp-578604	NaCrO2	mp-1585	V3Co	mp-10942	KNaLaNbO5
mp-567415	Nd2B5	mp-542614	VCo3	mp-20049	LiFeP
mp-1045	Nd2O3	mp-503	ThS	mp-760680	Li2Fe12P7
mp-1632	NdB4	mp-1205021	Pr5Ir3	mp-643001	Na4H6Ru
mp-558805	Na3Nd(BO3)2	mp-946	PrIr2	mp-1195324	Pr2TiO5
mp-1929	NdB6	mp-1104160	Pr5Ir2	mp-570001	Al6Fe
mp-8128	NaNdO2	mp-1106395	Pr3Ir	mp-2658	AlFe
mp-30975	Na3BO3	mp-171	VNi3	mp-1183162	AlFe3
mp-10622	PrAs	mp-11531	VNi2	mp-570606	Pr4Ge3
mp-16705	Pr2O3	mp-7226	V3Ni	mp-511	PrGe
mp-8470	NaPrO2	mp-1216708	V3Ni2	mp-867190	Pr4Ge7
mp-19391	NaVO2	mp-582799	EuAl4	mp-1845	CaBe13
mp-146	V	mp-20111	EuAl2	mp-865	CaB6
mp-754829	Na4VO4	mp-1205409	Eu3(AlP2)2	mp-1213975	CaB4
mp-784	KZn13	mp-1193394	NaEu2AlP3	mp-3575	Ca3(BO3)2
mp-1534	YS	mp-21050	UFe2	mp-6632	Ca5B3O9F
mp-131	Zr	mp-7233	La2SeO2	mp-24747	Na3H6Rh

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Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-10226	NaYS2	mp-1161	LaSe	mp-1199486	Gd5Si4
mp-1197374	Zr2S	mp-1937	YbCu	mp-601371	GdSi
mp-27191	Zr9S2	mp-567538	YbCu2	mp-21192	GdSi2
mp-864647	Hf2N	mp-1607	YbCu5	mp-17143	BaGd2O4
mp-776470	Hf3N4	mp-1979	HoPd3	mp-1779	YbTe
mp-2828	HfN	mp-1104206	Ho3Pd4	mp-1903	BaAl4
mp-1224388	Hf3N2	mp-1087502	HoPd	mp-4202	BaAl2O4
mp-1506	Sm5Ge4	mp-1201760	Er5Ir3	mp-567701	Ba21Al40
mp-1447	SmSe	mp-2713	ErIr	mp-560978	Ba4Al2O7
mp-972521	SmGe	mp-1495	ErIr2	mp-2631	Ba4Al5
mp-569320	Sm3Ge5	mp-1189478	Er3Ir	mp-570400	Ba7Al10
mp-1188469	La5Ge3	mp-530539	Sr4U2O9	mp-1199246	Ba5B3BrO9
mp-2292	La2O3	mp-2585	Sr5Sb3	mp-861957	KNaSmTaO5
mp-1211687	La5Ge3O	mp-570421	Sm2B5	mp-1198935	K2Na2Sm4Ta2O13
mp-1084830	LaGe	mp-8546	SmB4	mp-15237	Tb4C5
mp-1211472	La4Ge7	mp-6996	SmB6	mp-24724	TbH2
mp-755586	NaLaO2	mp-864941	MgSc2	mp-692	Tb2C
mp-8957	Na5TaO5	mp-1185790	Mg3Sc	mp-9858	Ba3Ge4
mp-1187206	Ta3W	mp-1185631	Mg149Sc	mp-2139	BaGe2
mp-979289	TaW3	mp-1202486	La7Ru3	mp-13922	Ba2Ge
mp-91	W	mp-1104417	La5Ru2	mp-1188954	Ba3Ge5
mp-1217811	TaW	mp-17695	Sc5Sn3	mp-24412	K2NaAlH6
mp-15698	Sr5As3	mp-867343	Li3Cd	mp-7704	Ca(AlSi)2
mp-9775	NaSrAs	mp-1437	LiCd	mp-570150	CaAlSi
mp-13660	Ca4Sb2O	mp-11393	Nb3Ga2	mp-721592	Ca6Al7O16
mp-2605	CaO	mp-1199558	Sm5Ir3	mp-1201345	Ba5B3ClO9
mp-9925	Ca2Sb	mp-7342	Sm3Ir	mp-30949	Sr3SiO
mp-1227708	Ca16Sb11	mp-1104500	Sm5Ir2	mp-18510	Sr2SiO4
mp-17564	Ca5Sb3	mp-1144	ErP	mp-1203324	Zr3Ge
mp-10688	CeO	mp-9939	Hf2Ge	mp-17706	Zr5Ge3
mp-542313	Ce2O3	mp-737	Hf5Ge4	mp-24286	ZrH2
mp-2629	Ce7O12	mp-976273	Hf3Ge2	mp-1200749	Zr5Ge4
mp-1173761	Na2CeO3	mp-570276	ZrZn	mp-1025513	ZrGe
mp-2517	Ca2Si	mp-1401	ZrZn2	mp-1865	UN
mp-1727	SrSi2	mp-864889	ZrZn3	mp-32590	U4N7
mp-2661	SrSi	mp-15318	Rb2NaHoF6	mp-32742	U16N25
mp-1563	CaSi	mp-2610	Tb5Ge3	mp-1776	UN2
mp-7084	SrCaSi	mp-1405	TbGe	mp-8961	Ba3NaTaO6
mp-2700	CaSi2	mp-1673	Tb5Ge4	mp-567276	TaV2
mp-793	Ca5Si3	mp-17751	Y5Ge3	mp-504554	Ba5Ta4O15
mp-1106	Sr2Si	mp-13360	Y5Ge4	mp-12659	Mn2Nb
mp-746	Sr5Si3	mp-17381	Y3Ge4	mp-12678	TaMn2
mp-10047	Ca5As3	mp-30569	Zr6Co23	mp-1185642	Mg149Zn
mp-961685	NaCaAs	mp-929	ZrCo2	mp-680671	Mg4Zn7
mp-685008	Ba20As13	mp-30619	Zr3Co	mp-978269	MgZn2
mp-2542	BeO	mp-628	Zr2Co	mp-6406	Na2MgSiO4
mp-28588	Na2BeO2	mp-2283	ZrCo	mp-22179	YTiSi
mp-28559	Na6Be8O11	mp-569630	NdOs2	mp-754225	YbTiO3
mp-679	Er2O3	mp-1188656	Nd3Os	mp-753192	Yb4Sb2O
mp-5586	NaErO2	mp-1200894	Zr3As	mp-1025200	Eu2TiO4
mp-504886	Gd2O3	mp-1191610	Zr7As4	mp-1079111	EuTiO3
mp-5088	NaGdO2	mp-972228	Zr3As2	mp-18167	Ca3Cd2
mp-35	Mn	mp-1203256	Zr14As9	mp-915	YCd
mp-2748	CeAs	mp-30671	Ti2Ga	mp-1073	CaCd

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-54	Co	mp-2767	TiGa	mp-1331	YCd2
mp-2251	Li3N	mp-30672	Ti3Ga	mp-1444	CaCd2
mp-1001	BaN2	mp-571342	TiGa2	mp-1105932	Li2MgSi
mp-569025	Ba19Na29Li13	mp-30673	Ti2Ga3	mp-1222798	Li14MgSi4
mp-567643	Ba12Na15Li8N6	mp-1218382	Sr4Bi2O	mp-866755	LiMg149
mp-645662	Ba14Na14LiN6	mp-29620	Sr5Bi3	mp-1094889	LiMg
mp-1892	Ba2N	mp-2090	FeCo	mp-973374	LiMg2
mp-8868	Ba3NaN	mp-601820	Fe3Co	mp-1094591	Li3Mg
mp-2686	Ca2N	mp-601848	Fe11Co5	mp-5962	NaMgAs
mp-1009657	CaN2	mp-601842	Fe9Co7	mp-5597	Ca(FeP)2
mp-844	Ca3N2	mp-567290	LaN	mp-1079146	Th3Si2
mp-6645	Ba14Na14CaN6	mp-645945	Na12SnGe8	mp-21238	ThSi
mp-541989	Na2CN2	mp-343	PrN	mp-17850	K3NaTh2O6
mp-1029375	BaCN2	mp-2493	CeN	mp-7497	ThSi2
mp-1214417	BaC6	mp-954	BaB6	mp-10961	La5Si3
mp-2209	CeGa2	mp-30905	Ba3(BN2)2	mp-567258	LaZn2
mp-2563	CeSe	mp-9705	Ba4Na(BN2)3	mp-7083	LaSi
mp-1018276	CeGa	mp-2741	CaF2	mp-2615	LaZn
mp-862696	CeGa3	mp-7104	CsCaF3	mp-9556	SrZnSi
mp-19920	Ce3Ga	mp-9732	BaNaP	mp-861620	LaZn4
mp-510430	Li13In3	mp-28164	Ba4P2O	mp-2062	LaSi2
mp-1138	LiF	mp-32606	Ba3P2	mp-30709	La2Zn17
mp-31324	Li2In	mp-1935	BaMg2	mp-1200584	La3Zn22
mp-21293	Li3In2	mp-568512	Ba6Mg23	mp-571191	LaZn11
mp-867226	Li3In	mp-8278	Ba(MgP)2	mp-1218375	Sr2Zn5Si3
mp-12723	CaAu	mp-2514	Mg3P2	mp-1218249	SrLa4Si3O13
mp-30367	Ca5Au2	mp-1813	Ba2Mg17	mp-1020648	NaLaSiO4
mp-30368	Ca5Au3	mp-1001835	LiB	mp-17833	Ba3GeO
mp-571264	Ca5Au4	mp-1222413	LiB3	mp-2892	BaNd2O4
mp-2364	PaO2	mp-6660	BaNaBO3	mp-8430	KLiS
mp-865120	NaPaO3	mp-6499	BaLiBO3	mp-505598	Zr(Ni2P)2
mp-2252	ScB2	mp-755417	Ba3(BO3)2	mp-14298	Zr6Ni20P13
mp-24237	ScH2	mp-27275	Li3BO3	mp-505278	Zr9(NiP2)2
mp-9069	K2NaAlAs2	mp-6575	Ba4Na(BO3)3	mp-1079999	Zr2NiP2
mp-22898	KI	mp-560189	NaLi2BO3	mp-29153	Zr2NiP
mp-1095642	Eu2Ge	mp-558455	Na4Li5(BO3)3	mp-17183	Na2BeSiO4
mp-21394	EuO	mp-8298	Sr4P2O	mp-551675	Li3UO4
mp-20712	EuGe	mp-972071	V3Mo	mp-8609	Li6UO6
mp-1188934	Eu5Ge3	mp-1220316	NbW	mp-3698	SrAlSi
mp-615	YMg	mp-1187695	V3Cr	mp-7068	Sr3(AlSi)2
mp-2652	Y2O3	mp-1216394	VCr	mp-15960	Li5AlO4
mp-865376	YMg3	mp-1187696	VCr3	mp-3427	LiAlO2
mp-1265	MgO	mp-985	TmCu	mp-9719	Na2LiAlP2
mp-30980	NaYO2	mp-1077209	TmCu2	mp-973391	LiSiB6
mp-1188082	YMg149	mp-30600	TmCu5	mp-41095	Na3Sr3AlP4
mp-1623	ErS	mp-30579	ErCu5	mp-24092	GdH2
mp-12671	Er2SO2	mp-1024991	ErCu2	mp-4805	Gd2SO2
mp-3613	NaErS2	mp-1955	ErCu	mp-3211	Nd2SO2
mp-573697	CsCl	mp-1211343	KNdF4	mp-1190994	NdHO
mp-1215	Ti2O	mp-1140	NdCu5	mp-24096	NdH2
mp-1071163	TiO	mp-11852	NdCu2	mp-2616	NpO2
mp-28017	Na8Ti5O14	mp-13392	NdCu	mp-754019	Na4NpO5
mp-554098	Ti6O	mp-1114456	Rb2NaScF6	mp-3210	Ca(CoP)2
mp-72	Ti	mp-21256	Mn7C3	mp-10923	Ca2Co12P7

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Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-2591	Ti3O	mp-542830	Mn23C6	mp-2384	LaP
mp-14726	Na4TiO4	mp-24123	Rb(BH)6	mp-29241	Ca3SnO
mp-865027	Mn3Ge	mp-1219553	RbBH4	mp-8789	Ca4As2O
mp-27569	Na14Mn2O9	mp-8755	KNaTe	mp-9564	Ca(MgAs)2
mp-1025122	LuCu2	mp-1747	K2Te	mp-1145	TiB2
mp-580136	LuCu5	mp-661	AlN	mp-1025170	Ti3B4
mp-34081	NaYF4	mp-504731	EuF2	mp-11750	Ti6Si2B
mp-2399	YHg	mp-554546	Eu2SiO4	mp-7857	TiB
mp-11256	ScAu	mp-14093	TbOF	mp-4056	CaSc2O4
mp-2647	Al2Au	mp-1924	TbSi	mp-11566	ScZn
mp-980769	SmCu	mp-11347	TbF3	mp-12137	Ca(ZnSi)2
mp-1077154	SmCu2	mp-206	Tb5Si3	mp-16266	CaZnSi
mp-227	SmCu5	mp-1077398	TbSi2	mp-13503	ScZn2
mp-1183995	GaCu3	mp-1207669	TmOF	mp-862260	ScZn3
mp-1087547	EuCu	mp-1066975	TmSi	mp-1219746	ScZn6
mp-2066	EuCu5	mp-1189863	Tm5Si3	mp-568646	Ta3Si
mp-1071732	EuCu2	mp-560114	Er3O2F5	mp-1989	Ta5Si3
mp-1018131	LuAg2	mp-31167	Er5Si3	mp-11192	TaSi2
mp-542681	Na3In2Ag	mp-378	ErSi	mp-18480	Na3Ca2TaO6
mp-279	LiIr	mp-1072193	ErOF	mp-9578	Ba3(AlSi)2
mp-30738	LiIr3	mp-1201519	K2Na2Nd4Nb2O13	mp-13149	BaAlSi
mp-12283	Li5Ti2	mp-1738	SmAs	mp-5506	Ba(AlSi)2
mp-7396	Li3Ti	mp-982	TmPd3	mp-2823	NdP
mp-18511	NdF3	mp-1104675	Tm3Pd4	mp-11580	TiCrP
mp-23295	RbCl	mp-348	TmPd	mp-568636	TiCr2
mp-22903	RbI	mp-33090	V2N	mp-1211138	Li5Ni9P7
mp-28602	Na3ClO	mp-1018027	VN	mp-685439	LiNi3P2
mp-1188441	TiCu4	mp-642644	V2H	mp-21075	HfC
mp-742	Ti2Cu	mp-1029711	NaVN2	mp-1225044	Er2C
mp-2078	TiCu	mp-1188283	V8N	mp-1203719	Er3C4
mp-2643	Ti3Cu4	mp-1209986	NaLiEr2F8	mp-1212833	Er4C7
mp-12546	TiCu3	mp-1787	NdMg3	mp-567705	TiAl2
mp-1182061	BaNaH6Ir	mp-1327	NdMg	mp-542915	TiAl3
mp-707836	Na3H6Ir	mp-31116	LaScO3	mp-1823	Ti3Al
mp-23715	BaH2	mp-18051	La2TiO5	mp-1953	TiAl
mp-643047	Ba3(H6Ir)2	mp-22432	Ti4Cu2O	mp-1849	Mn2P
mp-890	NdIr2	mp-21457	Ti3Cu3O	mp-4484	Ba(PRu)2
mp-30522	Nd5Ir3	mp-1349	SrPt2	mp-774749	RbNa3Li12Ti4O16
mp-1104605	Nd5Ir2	mp-30843	Sr7Pt3	mp-4156	Li2ZrO3
mp-1189686	Nd3Ir	mp-1104074	Sr3Pt2	mp-5418	Li6Zr2O7
mp-1753	ThAs	mp-556015	Dy9(SbO)5	mp-3949	K7LiSi8
mp-643	ThO2	mp-1927	Dy4Sb3	mp-2983	Ba(PN2)2
mp-4533	Na2SiO3	mp-1007	DySb	mp-1221737	MnFe3P2
mp-7500	Na4SiO4	mp-1185594	Mg149In	mp-23804	Mg2FeH6
mp-216	Sc2O3	mp-22735	Ca2Sn	mp-9921	MgCr2O4
mp-7914	NaScO2	mp-7400	NaAlGe	mp-5473	CaMgSi
mp-1709	U2Ti	mp-29566	CsNaGe2	mp-1672	CaS
mp-44	U	mp-1220826	NaLaF4	mp-29110	Al2(FeSi)3
mp-569744	UAl2	mp-13926	Rb2NaYF6	mp-1190708	Al3Fe2Si
mp-674332	U17O31	mp-28731	V6C5	mp-867878	AlFe2Si
mp-1597	UO2	mp-1195743	V18P9C2	mp-1229054	Al53Fe17Si12
mp-34842	Na3UO4	mp-684675	V12P7	mp-1229249	Al79(Fe13Si9)2
mp-5327	Na4UO5	mp-20648	V2C	mp-1227337	Ca6Al7O16F
mp-1079399	V3Fe	mp-20541	V2P	mp-15572	Na3Ca3AlAs4

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-866134	VFe3	mp-18350	V3P	mp-27791	SrBe3O4
mp-637224	Pu2O3	mp-30842	ZrPd3	mp-2080	SrBe13
mp-24720	PuH2	mp-266	Zr2Pd	mp-1800	Nd2C3
mp-1959	PuO2	mp-13495	ZrPd	mp-866691	La2PC
mp-27618	Na8Ga2O7	mp-1188310	Tm5Ge3	mp-1184	La2C3
mp-7656	Na5GaO4	mp-1203550	Tm11Ge10	mp-2367	LaC2
mp-494	GeMo3	mp-1104486	Tm3Ge4	mp-36111	LiMgP
mp-2857	ScN	mp-20685	Cr3Ge	mp-11507	Ni4Mo
mp-685209	Sc39N34	mp-568153	Al22Mo5	mp-4091	Ni2Mo3N
mp-2472	SrO	mp-2733	Al8Mo3	mp-11506	Ni3Mo
mp-1220915	NaSmF4	mp-259	AlMo3	mp-23432	BaClF
mp-1216	YbO	mp-1185596	Mg149Al	mp-1102496	EuH2
mp-2391	YbPd3	mp-1094116	MgAl2	mp-707218	Ba3AlHO4
mp-1104397	Yb5Pd2	mp-2151	Mg17Al12	mp-13686	Nb5Si3
mp-2547	YbPd	mp-9546	Yb2C3	mp-12104	NbSi2
mp-1105057	Yb3Pd4	mp-1103975	YbC6	mp-1334	Y2C
mp-561430	LiLuF4	mp-34763	NaAlB14	mp-9459	Y4C5
mp-1209991	NaLiLu2F8	mp-1103990	EuC6	mp-1200885	Y4C7
mp-675798	NaHoF4	mp-1104	LaMg	mp-1200613	Y3C4
mp-1210003	NaLiHo2F8	mp-1094174	LaMg3	mp-1216160	Y4Zr3O12
mp-1025059	LaAg2	mp-675	ZrW2	mp-1224869	Gd2C
mp-1560	LaTe	mp-28930	KC8	mp-510401	GdP
mp-1948	LaAg	mp-10408	K2CN2	mp-1189998	Gd2C3
mp-2825	ErPd3	mp-5532	Sr2TiO4	mp-569335	Sm2C3
mp-1104774	Er3Pd4	mp-6361	NaSr3NbO6	mp-24658	SmH2
mp-12545	Er3Pd2	mp-4651	SrTiO3	mp-1219177	Sm2C
mp-851	ErPd	mp-3349	Sr3Ti2O7	mp-1191829	Li2Co12P7
mp-581942	CeCu6	mp-5598	Sm2SO2	mp-753721	GdOF
mp-2801	CeCu2	mp-1218562	Sr4LaTi5O15	mp-12574	Dy2C
mp-1427	Lu2O3	mp-695042	Sr9LaTi10O30	mp-1212812	Dy4C5
mp-755311	NaLuO2	mp-17904	Nd2TiO5	mp-1213387	Dy3C4
mp-1056	Tb2O3	mp-28383	KNaS	mp-532160	Ca14MnP11
mp-6964	NaTbO2	mp-1039148	CaMg	mp-3637	YOF
mp-21009	EuSe	mp-2432	CaMg2	mp-3700	LiYF4
mp-13971	Nd2SeO2	mp-1184449	CaMg149	mp-1205337	Ca3(AlP2)2
mp-1453	NdSe	mp-3397	Ba2TiO4	mp-24726	TiH2
mp-1102143	ErRe2	mp-1228030	Ba4Bi2O	mp-866141	TiFe2Si
mp-754640	Ce2SeO2	mp-31235	BaNaBi	mp-8648	TiFeSi
mp-1187198	SrMg2	mp-29621	Ba5Bi3	mp-305	TiFe
mp-30782	Sr6Mg23	mp-631	TiC	mp-16253	BaCaSi
mp-1934	LiZn	mp-27919	Ti8C5	mp-21662	TiFeSi2
mp-1153	Li2S	mp-1217052	Ti6P2O	mp-5926	KCaF3
mp-975799	LiZn3	mp-10721	Ti2C	mp-1216621	TiW
mp-8452	NaLiS	mp-1205180	Tm3C4	mp-865656	TiMn2W
mp-1199934	Ti3As	mp-7171	TmP	mp-865652	TiMn2Si
mp-1201836	Ti5As3	mp-1216546	Tm2C	mp-21606	TiMnSi2
mp-1190061	Eu5Si3	mp-1640	Ho2C	mp-1217077	Ti2Si6W
mp-21279	EuSi	mp-744	HoP	mp-555617	Ce10Si8O3
mp-1072248	EuSi2	mp-15238	Ho4C5	mp-1898	CeSi2
mp-1345	CaP	mp-1154	Ho4C7	mp-1025450	CeFeSi2
mp-1214132	Ca4SiP4	mp-1202754	Ho3C4	mp-21115	CeSi
mp-1221207	Na4Ca2SiP4	mp-20318	Mn2B	mp-3187	BaCeO3
mp-20394	EuPb	mp-10118	Mn3B4	mp-3035	Ce(FeSi)2
mp-20300	EuP	mp-1106184	MnB4	mp-1196829	Ce5Si4

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1103985	Nd3Pt2	mp-680339	Mn4Si7	mp-570175	Ce5Si3
mp-1080485	NdPt	mp-568656	SiC	mp-11317	CeFe5
mp-2720	NdPt2	mp-20211	Mn3Si	mp-20245	CeFeSi
mp-20587	EuS	mp-1431	MnSi	mp-1018125	Ti2Re
mp-1102043	LaOs2	mp-1118	SiNi2	mp-2179	TiRe
mp-972256	Xe	mp-351	SiNi	mp-518	Ti5Re24
mp-2011	UP	mp-828	SiNi3	mp-1095145	TiReSi
mp-674333	Na3PO4	mp-2291	Si2Ni	mp-7948	ReSi
mp-11854	Er5Ge3	mp-27276	Si12Ni31	mp-568595	Re4Si7
mp-1203572	Er11Ge10	mp-1080525	FeB	mp-510522	Zr5Sn3
mp-1711	Er3Ge4	mp-1915	Fe2B	mp-1106020	Zr5SiSn3
mp-1198083	Gd5Ge4	mp-9905	Ba2Si	mp-543001	Zr5Sn4
mp-19918	GdGe	mp-1067235	BaSi	mp-2554	Al3V
mp-21237	CoGe	mp-1619	Ba3Si4	mp-1201511	Mg3(Al9V)2
mp-1418	FeNi3	mp-1477	BaSi2	mp-10126	V5SiB2
mp-2213	FeNi	mp-17612	Ba2SiO4	mp-1387	AlV3
mp-1001836	MnGa	mp-752573	Ba(NaSi2)2	mp-1216643	V10Si6B
mp-37722	KBH4	mp-560889	Ba6Na2Si4O15	mp-567224	Mg(SiB6)2
mp-24239	K(BH)6	mp-3952	BaY2O4	mp-1207086	MgAlB4
mp-1216441	Zr14Cu51	mp-17891	NaYSiO4	mp-1222150	Mg4AlB10
mp-193	Zr2Cu	mp-16432	Sr3(BO3)2	mp-1216481	V3Cr3Si2
mp-1188077	Zr7Cu10	mp-556695	NaSrBO3	mp-1216445	V9Cr3B8
mp-1224756	Hf14Cu51	mp-3933	Mg2PN3	mp-24288	LuH2
mp-30581	Hf2Cu	mp-10572	NaPN2	mp-640340	Ca4MgAl3
mp-1200988	Hf7Cu10	mp-1559	Mg3N2	mp-1215386	Zr3Ti2Si3
mp-7353	Hf3Cu8	mp-11501	MnNi3	mp-2116	ZrMn2
mp-1217	KSi	mp-1079891	Ba2Br2O	mp-31310	Zr3(Mn2Si3)2
mp-865834	Yb3GeO	mp-555218	Ba4Br6O	mp-865625	Na2MgSn
mp-1694	Yb2Ge	mp-27456	BaBr2	mp-11270	MnBe2
mp-21300	Yb5Ge4	mp-1021323	LiC12	mp-1185637	Mg149Sn
mp-767	Yb3Ge5	mp-541291	Na3MoN3	mp-1104792	MnBe12
mp-1106300	Nd3Ru	mp-1552	Mo2C	mp-1192960	Zr6Fe16Si7
mp-1103979	Nd5Ru2	mp-1079937	Pr3Si2	mp-1215517	Zr2MnFe3
mp-1102217	NdRu2	mp-769173	PrOF	mp-1102452	ZrFeSi
mp-1029	BaF2	mp-9968	PrSi	mp-1221619	MnFeSi2
mp-619	UB4	mp-27760	PrSi2	mp-5529	MnFe2Si
mp-1514	UB2	mp-1192370	Na5Pr4Si4O16F	mp-17435	Zr4Fe4Si7
mp-22319	UB12	mp-569851	Ho10Si17	mp-12894	Y2SO2
mp-1221	V3Ge	mp-12899	HoSi	mp-569989	Nb2C
mp-2363	HfMo2	mp-1072114	HoOF	mp-1079585	Nb2N
mp-352	HfO2	mp-13236	Ho5Si3	mp-2760	Nb6C5
mp-865500	Na2Hf2O5	mp-5634	NdOF	mp-2634	NbN
mp-931	ThP	mp-9967	NdSi	mp-1030657	NaNbN2
mp-13972	Sm2SeO2	mp-884	NdSi2	mp-3448	KMgF3
mp-218	Sm2O3	mp-567735	Nd5Si3	mp-31212	K2MgF4
mp-754027	NaSmO2	mp-355	Nd5Si4	mp-861983	Ti2MnFe
mp-7283	LaB4	mp-1192521	Na5Nd4Si4O16F	mp-23956	K2MgH4
mp-2680	LaB6	mp-13774	NaNSiO4	mp-1228149	Ba3Sr9Al4(O4F)4
mp-1210472	Na3La(BO3)2	mp-1072208	DyOF	mp-1199908	Cs7NaSi8
mp-1215377	Zr4O	mp-2620	DySi	mp-4877	CsNa2Si17
mp-2049	ZrMo2	mp-2836	Dy5Si3	mp-3161	LiAlSi
mp-561418	Zr3O	mp-1212889	DyF3	mp-1205813	Gd2MgSi2
mp-990440	Na2ZrO3	mp-569825	Dy10Si17	mp-2636	GdMg
mp-1269	SmS	mp-2057	DyB2	mp-20534	GdMg3

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-710	SmP	mp-2719	DyB4	mp-995201	Ti5Si3C
mp-1894	WC	mp-16037	Dy2TeO2	mp-5659	Ti3SiC2
mp-863707	KNa2Bi	mp-1774	ErB2	mp-1227232	Ca6Al7ClO16
mp-2599	NdN	mp-2847	ErB4	mp-11283	ZrBe5
mp-2593	AlNi3	mp-10192	LuP	mp-2544	Zr2Be17
mp-16514	Al3Ni5	mp-2014	DyP	mp-30445	ZrBe13
mp-1487	AlNi	mp-2296	Ni3P	mp-14324	K2Na4Be2O5
mp-622209	Al3Ni	mp-571370	Fe2NiP	mp-2807	ScP
mp-1057	Al3Ni2	mp-778	Fe2P	mp-1188062	Zr3Sc
mp-16515	Al4Ni3	mp-16594	K3TbSi2O7	mp-1077791	ZrSc2
mp-16839	Na3WN3	mp-645	TbP	mp-1188800	Sc3P
mp-28595	KNaSe	mp-11578	VZn3	mp-22600	Sc3P2
mp-510557	CsN3	mp-30883	V4Zn5	mp-1100806	Zr8Sc2O19
mp-28366	Gd2B5	mp-15743	Sr2CeO4	mp-974713	K2H4Pt
mp-1105563	GdB4	mp-30228	Li4HN	mp-777297	K5H(CN2)2
mp-22266	GdB6	mp-5001	Li3BN2	mp-28160	Ca3C3Cl2
mp-1158	LuPd3	mp-23702	LiH2N	mp-23859	CaHCl
mp-1103963	Lu3Pd4	mp-1201065	Li15H9N8	mp-984055	Ca7(H6Cl)2
mp-2205	LuPd	mp-1221143	NaLi4(H2N)5	mp-568987	Na2BeH4
mp-1210753	Li2Al	mp-1200910	Li7H5N4	mp-1219429	Sc2CO
mp-16506	Li3Al2	mp-1191288	Eu2Ta2O7	mp-15661	Sc4C3
mp-10890	LiAl3	mp-510374	GdAs	mp-28733	Sc3C4
mp-1067	LiAl	mp-7639	Na2CuP	mp-29941	Sc2C
mp-19879	PPd3	mp-27731	HfH2	mp-11908	Lu5Si3
mp-1039345	CeMg2	mp-31019	Al45Cr7	mp-1001612	LuSi
mp-1820	YbS	mp-867780	Al3Cr	mp-4883	Ba(FeP)2
mp-2390	YbP	mp-1699	AlCr2	mp-542995	Nb6Fe16Si7
mp-1187909	Yb3P	mp-1208630	SrC6	mp-1196167	NbFeSi2
mp-1367	Mg2Si	mp-576	B13C2	mp-1192618	Nb4Fe4Si7
mp-20995	Eu4As3	mp-20937	Cr3C2	mp-1209887	NbFeSi
mp-1106024	Eu5As3	mp-1196316	Cr7C3	mp-1101870	TiFeP
mp-757	Li3As	mp-723	Cr23C6	mp-1217193	Ti3Fe5P4
mp-1225307	DyCu5	mp-27757	Be4B	mp-1211088	LiCaP
mp-1071835	DyCu2	mp-30866	Rh3W	mp-570466	Li2Ca
mp-2334	DyCu	mp-994	YP	mp-13276	SrLiP
mp-2796	TmAg	mp-8960	Ba3NaNbO6	mp-570097	Sr(Li2P)2
mp-30359	TmAg2	mp-1014265	Zr2N	mp-695998	K2ZnH4
mp-979115	Ti2Ag	mp-1352	ZrN	mp-862658	LiCu3
mp-2074	Li3Sb	mp-277	Zr3N4	mp-1226479	CrH15N6Cl2O
mp-5077	NaLi2Sb	mp-1223129	Li4SiO4	mp-3805	Al(FeB)2

Table S4 Phases with stability in the entire range of Na potentials

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-8	Re	mp-542583	EuTe	mp-557753	K3PO4
mp-1103252	ZnPd2	mp-11534	Np	mp-974482	K4Hf5O12
mp-1652	ZnPd	mp-640095	La3Co	mp-1201301	K2Hf2O5
mp-865357	Zn3Pd	mp-1205615	La2Co2I	mp-24136	Cs(BH)6
mp-1215714	Zn2Pd	mp-30559	LaCo13	mp-1225884	CsBH4
mp-1184905	K	mp-1500	BaS	mp-9774	Ba4Sb2O
mp-1179656	Rb	mp-28726	KYF4	mp-755293	Sr4Sb2O
mp-1066254	YAu	mp-17077	K2YF5	mp-862620	IrRu3
mp-979911	Y2Au	mp-13230	K3YF6	mp-974358	Ir3Ru
mp-1187739	Y	mp-555932	RbEr3F10	mp-755558	BaLa2O4
mp-864675	Yb3N2	mp-2524	NdGa2	mp-30666	Sc3Ga2

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-972364	Yb	mp-1448	NdGa	mp-11411	ScGa
mp-864757	YbN ₂	mp-1203103	Nd ₃ Ga ₂	mp-1200767	Sc ₃ Ga ₅
mp-571261	Pu	mp-1201758	KGe	mp-932	ScGa ₃
mp-542573	ThB ₄	mp-1169	ScCu	mp-1207024	Zr ₃ Si ₂
mp-37	Th	mp-1018149	ScCu ₂	mp-893	ZrSi
mp-1756	ThB ₆	mp-196	Al ₅ Co ₂	mp-3834	BaZrO ₃
mp-1199056	RbGe	mp-284	AlCo	mp-1278	Zr ₂ Si
mp-573471	Li ₁₇ Sn ₄	mp-16488	Al ₉ Co ₂	mp-1515	ZrSi ₂
mp-1018134	Li	mp-1104937	Pr ₅ Ru ₂	mp-8335	Ba ₂ ZrO ₄
mp-30767	Li ₇ Sn ₂	mp-1197932	Pr ₇ Ru ₃	mp-755895	Ba ₃ Zr ₂ O ₇
mp-867200	Pm	mp-2665	PrRu ₂	mp-23063	Ba ₄ Cl ₆ O
mp-86	Sm	mp-1105741	Pr ₃ Ru	mp-568662	BaCl ₂
mp-20074	SrIn ₂	mp-556	ZrNi	mp-14208	LiYSi
mp-705522	Sr ₂₈ In ₁₁	mp-485	ZrNi ₃	mp-7020	LiYO ₂
mp-1187073	Sr	mp-2717	Zr ₂ Ni ₇	mp-2379	CoSi ₂
mp-608072	SrIn	mp-328	Zr ₂ Ni	mp-7577	CoSi
mp-87	Be	mp-11397	Ga ₃ Ni ₂	mp-19905	Co ₂ Si
mp-11807	LiPt	mp-815	GaNi ₃	mp-20857	CoB
mp-2170	Li ₂ Pt	mp-11398	Ga ₃ Ni ₅	mp-1777	Li ₁₅ Ge ₄
mp-867227	Li ₃ Pt	mp-21589	Ga ₉ Ni ₁₃	mp-27932	Li ₉ Ge ₄
mp-49	Os	mp-570775	BaAu	mp-8780	Cr ₂ N
mp-30434	BaTl ₂	mp-1104164	Ba ₃ Au ₂	mp-1183691	CrN
mp-21246	Ba ₂ Pb	mp-865934	YbF ₂	mp-568643	RbC ₈
mp-20136	BaPb	mp-1078265	Cs ₂ YbCl ₄	mp-1029828	RbCrN ₂
mp-1185581	Mg ₁₄₉ Cd	mp-1070599	CsYbCl ₃	mp-743	RbN ₃
mp-30490	Mg ₃ Cd	mp-865716	YbCl ₂	mp-1395	VRu
mp-1094909	Mg ₂ Cd	mp-28395	B ₆ P	mp-865382	V ₃ Ru
mp-1188292	Y ₅ Pb ₃	mp-2154	CeP	mp-971788	VRu ₃
mp-1646	Li ₃ Hg	mp-1205536	La ₂ O _s 2I	mp-9172	Li ₄ TiO ₄
mp-1184151	Cs	mp-639805	Ta ₃ Ge	mp-38280	LiTiO ₂
mp-21294	Y ₂ In	mp-17593	Ta ₅ Ge ₃	mp-2931	Li ₂ TiO ₃
mp-22704	YIn	mp-318	SrIr ₂	mp-20831	Gd ₄ Sb ₃
mp-1105835	Y ₃ In ₅	mp-1766	TmS	mp-510403	GdSb
mp-571262	CaRh ₂	mp-3556	Tm ₂ SO ₂	mp-22204	Co ₂ P
mp-74	Rh	mp-1767	Tm ₂ O ₃	mp-28861	CsC ₈
mp-1214063	Ca ₅ Rh	mp-17190	Sc ₅ Ge ₃	mp-1804	Fe ₃ N
mp-132	Ca	mp-1198803	Sc ₅ Ge ₄	mp-6988	FeN
mp-1185579	Mg ₁₄₉ Hg	mp-1196279	Sc ₁₁ Ge ₁₀	mp-3972	Ce ₂ SO ₂
mp-11375	EuHg	mp-2606	BaPd ₅	mp-8300	Ba ₄ As ₂ O
mp-1057315	Eu	mp-1687	BaPd ₂	mp-10004	Mo ₃ P
mp-867164	Pm ₃ Sn	mp-1193896	Ba ₂ H ₄ Pd	mp-22447	Zr ₃ P
mp-10659	Ho	mp-1008505	BaPd	mp-11345	ZrP
mp-10658	Dy	mp-861910	Sc ₃ Hg	mp-647729	Zr ₁₄ P ₉
mp-90	Cr	mp-11471	ScHg	mp-583740	Zr ₇ P ₄
mp-1079438	Ta ₂ N	mp-12802	AlCu ₃	mp-1215204	ZrTi ₂ O
mp-50	Ta	mp-985806	Al ₂ Cu	mp-2795	ZrC
mp-1279	TaN	mp-2500	AlCu	mp-684623	Zr ₁₀ C ₉
mp-134	Al	mp-593	Al ₄ Cu ₉	mp-1025402	SrCu
mp-862690	Ac	mp-1786	Ti ₃ Au	mp-1087	SrS
mp-2541	SmTl	mp-11237	ScAg	mp-2726	SrCu ₅
mp-319	Sm ₂ Tl	mp-1018128	ScAg ₂	mp-736	Li ₃ P
mp-570469	Pr ₅ Tl ₃	mp-23222	Li ₃ Bi	mp-9488	SmOF
mp-38	Pr	mp-2744	LiPd	mp-31509	BaIn
mp-12599	PrTl	mp-728	Li ₂ Pd	mp-1105101	Ba ₉ In ₄

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1079915	PrAu	mp-1197547	Li15Pd4	mp-22141	BaIn2
mp-2714	Pr2Au	mp-861936	LiPd3	mp-605809	Ba11In6O3
mp-11469	PrHg	mp-2404	CaAl2	mp-4511	La2SO2
mp-30422	Sr7Au3	mp-1190736	Ca8Al3	mp-28255	LaHO
mp-30420	SrAu	mp-1213848	Ce4Ge7	mp-24153	LaH2
mp-30421	Sr3Au2	mp-1213824	Ce4Ge3	mp-1104116	La2H5
mp-464	HoSe	mp-1096	CeS	mp-1103808	La4H9
mp-510404	GdSe	mp-675328	Ce4GeS3	mp-2495	PrS
mp-155	Gd	mp-1200696	Ce5Ge4	mp-3236	Pr2SO2
mp-2434	SrTl	mp-1226804	Ce3GeS2	mp-12614	Ca2Cu
mp-30828	Sr2Pb	mp-865782	Yb3SiO	mp-585949	CaCu
mp-677	SrCd2	mp-10651	YbSi	mp-1882	CaCu5
mp-30496	SrCd	mp-1077404	YbSi2	mp-2856	Mn4Al11
mp-542484	Sr5Cd3	mp-1207599	Yb2Si	mp-771	MnAl
mp-1078721	InPd3	mp-1542	YB2	mp-173	MnAl6
mp-21215	InPd	mp-24650	YH2	mp-15819	Mn3Al9Si
mp-22146	In3Pd5	mp-637	YB4	mp-568151	Ti5Ge3
mp-22646	InPd2	mp-20214	UGa3	mp-17193	Ca3GeO
mp-2114	YN	mp-1185635	Mg149Tl	mp-304	Ca2Ge
mp-2286	Li2Se	mp-19839	LaGa2	mp-2360	CaGe
mp-1240	HoS	mp-2350	LaS	mp-1198692	Ti5Ge4
mp-101	Ir	mp-672217	La5Ga3	mp-1884	Ca5Ge3
mp-570491	TaNi3	mp-1002133	LaGa	mp-2157	Co3W
mp-23	Ni	mp-551203	Sr2I2O	mp-1139	Co3Mo
mp-1867	Ta2Ni	mp-29910	Sr4I6O	mp-2786	Ca5Zn3
mp-867199	Pm3Tl	mp-568284	SrI2	mp-30483	CaZn
mp-734	LaHg	mp-559	YPd3	mp-1725	CaZn2
mp-26	La	mp-1104019	Y3Pd4	mp-1734	CaZn5
mp-1079811	SmAu	mp-1066136	YPd	mp-18567	CaZn11
mp-1080709	NdAu	mp-1207777	Y3Pd	mp-1227465	Ca4Zn51
mp-1102098	Nd2Au	mp-1078920	LaCu	mp-31205	Zr3Fe
mp-123	Nd	mp-2051	LaCu2	mp-1190681	ZrFe2
mp-1105965	Er5Tl3	mp-2613	LaCu5	mp-540809	Zr2Fe12P7
mp-1184115	Er	mp-1194443	LaCu13	mp-20892	ZrFeP
mp-1079938	TlPd3	mp-636253	GdCu5	mp-582924	Zr6Fe23
mp-2861	CaTl	mp-1077933	GdCu2	mp-5380	Ca4P2O
mp-718	SnPd3	mp-614455	GdCu	mp-8937	CrSi2
mp-1610	TbS	mp-1198712	Y5Ir3	mp-729	Cr3Si
mp-11698	Tb	mp-2762	YIr2	mp-2058	Ni3B
mp-814	DySe	mp-1207785	Y3Ir	mp-2536	Ni2B
mp-11266	BaCd2	mp-1472	ZrB2	mp-640067	Ni4B3
mp-527	BaCd	mp-18337	Be3N2	mp-2199	Fe3Si
mp-8093	Ba2Cd	mp-2147	SrGe	mp-871	FeSi
mp-75	Nb	mp-30950	Sr3GeO	mp-1714	FeSi2
mp-867318	Eu3Tl	mp-2576	Sr2Ge	mp-1078278	CrB4
mp-19966	GdTl	mp-408	Mg2Ge	mp-1080664	CrB
mp-579628	Gd2Tl	mp-35730	BaUO3	mp-15617	Cr5B3
mp-13	Fe	mp-583034	Ba2U2O7	mp-569424	Cr2B
mp-1018122	Tm	mp-976128	Hf5Sc	mp-1491	VB2
mp-286	YbSe	mp-504502	Ta3P	mp-2091	V3B2
mp-10740	Pa	mp-1067587	TaP	mp-9973	VB
mp-697068	SiPd2	mp-22477	Ta2P	mp-9208	V2B3
mp-20622	SiPd3	mp-4974	La2Zr2O7	mp-569270	V3B4
mp-582067	Hf3As	mp-616559	Ti2S	mp-1206441	V5B6

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-103	Hf	mp-31214	Ti3P	mp-292	V3As
mp-1190267	Hf3As2	mp-30218	Ti2P	mp-1620	Si2W
mp-1025468	CeAu	mp-739	TiP	mp-568671	V5Si3
mp-567332	Ce	mp-1191079	Ti7P4	mp-10711	VSi2
mp-1540	HoTl	mp-1960	Li2O	mp-1187702	VW3
mp-1181055	Ho5Tl3	mp-3924	LiNbO2	mp-2567	V3Si
mp-1002136	LaAu	mp-28030	Li8Nb2O9	mp-1216231	VW
mp-1103395	La2Au	mp-1213070	Eu2Sn	mp-1102914	Ba2Eu3Si7
mp-371	La3Tl	mp-567833	EuSn	mp-1949	TiMn2
mp-11488	LaTl	mp-1409	TiNi3	mp-1202079	Ti21Mn25
mp-11374	DyTl	mp-1048	TiNi	mp-20181	Ce2C3
mp-1181553	Dy5Tl3	mp-1808	Ti2Ni	mp-1210775	LuOF
mp-1190038	Tm5Tl3	mp-1189501	La7Pt3	mp-1222310	Lu2C
mp-1199133	Y11Sn10	mp-1002104	LaPt	mp-1203767	Lu3C4
mp-567412	Y5Sn3	mp-912	LaPt2	mp-17673	Lu3O2F5
mp-574275	Li17Pb4	mp-1104856	La3Pt4	mp-15178	Lu4C7
mp-30761	Li7Pb2	mp-2387	Th2Zn	mp-1178173	Ho2TeO2
mp-861939	Ac3Sn	mp-7496	ThZn2	mp-2267	HoB2
mp-20849	Pd3Pb	mp-536	ThZn4	mp-569281	HoB4
mp-1561	TbSe	mp-540743	Th2Zn17	mp-11219	LuB2
mp-1476	ScS	mp-316	MnV	mp-571495	LuB4
mp-67	Sc	mp-864984	MnV3	mp-24151	DyH2
mp-1185570	Mg149Pb	mp-1981	Ba2Sn	mp-12669	Dy2SO2
mp-11286	CaHg	mp-872	BaSn	mp-2470	DyS
mp-1103139	Ca2Hg	mp-1198302	Nb3Ge	mp-24192	ErH2
mp-11288	Ca3Hg2	mp-16842	Nb5Ge3	mp-7224	ThC2
mp-867297	AcIn3	mp-567339	PrOs2	mp-1189614	BaThO3
mp-985305	Ac3In	mp-1189967	Pr3Os	mp-1188514	Th2C3
mp-11422	GdHg	mp-2052	ScAs	mp-1164	ThC
mp-30878	TbTl	mp-505002	Sc5As3	mp-1217395	Th4C3
mp-30879	Tb5Tl3	mp-1188926	Sc3As2	mp-1217298	Th5C
mp-11575	YTl	mp-614724	Cs3CrF7	mp-708	LaAs
mp-1188434	Y5Tl3	mp-784631	CrNi2	mp-1017987	Tc3N
mp-11544	Yb2Pb	mp-752658	Y2SeO2	mp-113	Tc
mp-145	Lu	mp-2637	YSe	mp-30091	MgB9N
mp-570050	Yb2Sn	mp-11239	ZrAg	mp-978275	MgB7
mp-569304	C	mp-2221	Zr2Ag	mp-365	MgB4
mp-21412	Ce3Tl	mp-1000	BaTe	mp-763	MgB2
mp-1206755	CeTl	mp-30428	BaCu	mp-1104652	Nd5Co2
mp-11467	NdHg	mp-1842	NbAl3	mp-1106011	Nd3Co
mp-1533	Nd3Tl	mp-18427	Nb2Al	mp-356	Nd2Co17
mp-571405	NdTl	mp-1105989	Lu5Ge3	mp-1084826	Nd2Co3
mp-1084808	YbAu	mp-1199467	Lu5Ge4	mp-11824	Ca3PN
mp-570119	Yb7Au3	mp-1104514	Lu3Ge4	mp-8977	Ca2PN3
mp-570527	Yb5Au4	mp-1196590	Lu11Ge10	mp-4387	SrZrO3
mp-568944	Yb5Au3	mp-9972	YSi	mp-1018104	Zr2Cd
mp-8094	Ba2Hg	mp-677445	Y4Si3	mp-4547	La2TeO2
mp-2197	BaHg	mp-2538	Y5Si3	mp-759	La2Sb
mp-656	LuS	mp-1106032	Ho5Ge3	mp-1209044	Sc5Sb3
mp-1191538	Ca8In3	mp-812	Ho2O3	mp-1065	LaSb
mp-20263	CaIn	mp-9994	Ho11Ge10	mp-1076970	LaScSb
mp-542	SrHg	mp-1675	Ho3Ge4	mp-1223	La4Sb3
mp-13427	Sr3Hg2	mp-1097916	CsCaCl3	mp-542503	La9(SbO)5
mp-20711	Fe3Ge	mp-1025185	Cs2CaCl4	mp-7192	Sc2Sb

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-601833	Fe13Ge3	mp-1213703	Cs3Ca2Cl7	mp-4500	ZrNbP
mp-984	BN	mp-1428	Ni5Ge3	mp-1079460	Ti3Sn
mp-827	KN3	mp-21008	Ni3Ge	mp-1102980	NbFeP
mp-551835	Ba2I2O	mp-1185597	Mg149Ga	mp-1192350	NbFe2
mp-1342	BaO	mp-1770	Mg5Ga2	mp-1221111	NbFe
mp-29909	Ba4I6O	mp-30650	Mg2Ga	mp-869	TaAl3
mp-23260	BaI2	mp-242	SrB6	mp-1193531	Ta2Al
mp-865985	CdPd3	mp-10564	SrN2	mp-1260	SrPd5
mp-1696	CdPd	mp-29973	SrN	mp-1558	SrPd2
mp-636334	SnRh2	mp-1245	Sr2N	mp-999143	SrPd
mp-317	SnRh	mp-201	Yb5Sb3	mp-23714	SrH2
mp-23251	KBr	mp-1857	YbCd	mp-1207079	SrH3Pd
mp-23193	KCl	mp-1187653	YbCd3	mp-1179173	Sr2H4Pd
mp-129	Mo	mp-999544	YAg2	mp-30811	Ni4W
mp-614603	CsI	mp-2474	YAg	mp-2108	Ti5Si3
mp-571222	CsBr	mp-18040	KPrF4	mp-21289	TiZn3
mp-1080443	YCu	mp-29210	Li2Ga	mp-7092	TiSi
mp-2698	YCu2	mp-1205930	Li5Ga4	mp-1077503	TiSi2
mp-2797	YCu5	mp-9568	Li3Ga2	mp-1014229	Ti2Zn
mp-30	Cu	mp-11363	TbCu5	mp-1014230	TiZn
mp-1185319	LiCl	mp-1527	TbCu2	mp-505527	Ti5Si4
mp-1018029	CuPd	mp-1837	TbCu	mp-8418	ZrCoP
mp-580357	Cu3Pd	mp-1213256	CsEuCl3	mp-18133	Zr2Co4P3
mp-22867	RbBr	mp-1079091	PrCu	mp-1215734	Zr5Co19P12
mp-2532	PrTe	mp-1071904	PrCu2	mp-972631	Zr2Co12P7
mp-1078589	EuAu	mp-2462	PrCu5	mp-29152	Zr2CoP
mp-1189094	Eu3Au	mp-2675	MgNi2	mp-1207414	Zr9(CoP2)2
mp-1106137	Eu7Au3	mp-2137	Mg2Ni	mp-9981	Mn2N
mp-1104457	Eu3Au2	mp-1585	V3Co	mp-1009130	MnN
mp-981	SrF2	mp-542614	VCo3	mp-505622	Mn4N
mp-419	YbB6	mp-503	ThS	mp-4126	KUO3
mp-864603	YbH2	mp-1205021	Pr5Ir3	mp-2486	UC2
mp-1189298	YbB4	mp-946	PrIr2	mp-2625	U2C3
mp-33	Ru	mp-1104160	Pr5Ir2	mp-2489	UC
mp-1186974	Sc3Ti	mp-1106395	Pr3Ir	mp-4495	KLiTe
mp-7806	Cr3P	mp-171	VNi3	mp-2530	Li2Te
mp-567415	Nd2B5	mp-11531	VNi2	mp-2800	USi3
mp-1045	Nd2O3	mp-7226	V3Ni	mp-956	U3Si
mp-1632	NdB4	mp-1216708	V3Ni2	mp-505569	CeH2
mp-1929	NdB6	mp-582799	EuAl4	mp-1104579	Ce2H5
mp-10622	PrAs	mp-20111	EuAl2	mp-804	GaN
mp-16705	Pr2O3	mp-1205409	Eu3(AlP2)2	mp-4571	CaZrO3
mp-146	V	mp-21050	UFe2	mp-5977	Nd2Zr2O7
mp-784	KZn13	mp-7233	La2SeO2	mp-12724	SrZn
mp-1534	YS	mp-1161	LaSe	mp-569426	SrZn2
mp-131	Zr	mp-1937	YbCu	mp-672707	SrZn13
mp-1197374	Zr2S	mp-567538	YbCu2	mp-1435	SrZn5
mp-27191	Zr9S2	mp-1607	YbCu5	mp-18026	SrZn11
mp-864647	Hf2N	mp-1979	HoPd3	mp-683	Pr2C3
mp-776470	Hf3N4	mp-1104206	Ho3Pd4	mp-601	PrP
mp-2828	HfN	mp-1087502	HoPd	mp-1591	Al4C3
mp-1224388	Hf3N2	mp-1201760	Er5Ir3	mp-14266	Cu15Si4
mp-1506	Sm5Ge4	mp-2713	ErIr	mp-31417	Nd3TaO7
mp-1447	SmSe	mp-1495	ErIr2	mp-14964	Pr3TaO7

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-972521	SmGe	mp-1189478	Er3Ir	mp-3564	BaSc2O4
mp-569320	Sm3Ge5	mp-530539	Sr4U2O9	mp-755950	Ba2Sc2O5
mp-1188469	La5Ge3	mp-2585	Sr5Sb3	mp-20049	LiFeP
mp-2292	La2O3	mp-570421	Sm2B5	mp-760680	Li2Fe12P7
mp-1211687	La5Ge3O	mp-8546	SmB4	mp-1195324	Pr2TiO5
mp-1084830	LaGe	mp-6996	SmB6	mp-570001	Al6Fe
mp-1211472	La4Ge7	mp-864941	MgSc2	mp-2658	AlFe
mp-1187206	Ta3W	mp-1185790	Mg3Sc	mp-1183162	AlFe3
mp-979289	TaW3	mp-1185631	Mg149Sc	mp-570606	Pr4Ge3
mp-91	W	mp-1202486	La7Ru3	mp-511	PrGe
mp-1217811	TaW	mp-1104417	La5Ru2	mp-867190	Pr4Ge7
mp-15698	Sr5As3	mp-17695	Sc5Sn3	mp-1845	CaBe13
mp-13660	Ca4Sb2O	mp-867343	Li3Cd	mp-865	CaB6
mp-2605	CaO	mp-1437	LiCd	mp-1213975	CaB4
mp-9925	Ca2Sb	mp-11393	Nb3Ga2	mp-3575	Ca3(BO3)2
mp-1227708	Ca16Sb11	mp-1199558	Sm5Ir3	mp-6632	Ca5B3O9F
mp-17564	Ca5Sb3	mp-7342	Sm3Ir	mp-1199486	Gd5Si4
mp-10688	CeO	mp-1104500	Sm5Ir2	mp-601371	GdSi
mp-542313	Ce2O3	mp-1144	ErP	mp-21192	GdSi2
mp-2629	Ce7O12	mp-9939	Hf2Ge	mp-17143	BaGd2O4
mp-2517	Ca2Si	mp-737	Hf5Ge4	mp-1779	YbTe
mp-1727	SrSi2	mp-976273	Hf3Ge2	mp-1903	BaAl4
mp-2661	SrSi	mp-570276	ZrZn	mp-4202	BaAl2O4
mp-1563	CaSi	mp-1401	ZrZn2	mp-567701	Ba21Al40
mp-7084	SrCaSi	mp-864889	ZrZn3	mp-560978	Ba4Al2O7
mp-2700	CaSi2	mp-2610	Tb5Ge3	mp-2631	Ba4Al5
mp-793	Ca5Si3	mp-1405	TbGe	mp-570400	Ba7Al10
mp-1106	Sr2Si	mp-1673	Tb5Ge4	mp-1199246	Ba5B3BrO9
mp-746	Sr5Si3	mp-17751	Y5Ge3	mp-15237	Tb4C5
mp-10047	Ca5As3	mp-13360	Y5Ge4	mp-24724	TbH2
mp-685008	Ba20As13	mp-17381	Y3Ge4	mp-692	Tb2C
mp-2542	BeO	mp-30569	Zr6Co23	mp-9858	Ba3Ge4
mp-679	Er2O3	mp-929	ZrCo2	mp-2139	BaGe2
mp-504886	Gd2O3	mp-30619	Zr3Co	mp-13922	Ba2Ge
mp-35	Mn	mp-628	Zr2Co	mp-1188954	Ba3Ge5
mp-2748	CeAs	mp-2283	ZrCo	mp-7704	Ca(AlSi)2
mp-54	Co	mp-569630	NdOs2	mp-570150	CaAlSi
mp-2251	Li3N	mp-1188656	Nd3Os	mp-721592	Ca6Al7O16
mp-1001	BaN2	mp-1200894	Zr3As	mp-1201345	Ba5B3ClO9
mp-1892	Ba2N	mp-1191610	Zr7As4	mp-30949	Sr3SiO
mp-2686	Ca2N	mp-972228	Zr3As2	mp-18510	Sr2SiO4
mp-1009657	CaN2	mp-1203256	Zr14As9	mp-1203324	Zr3Ge
mp-844	Ca3N2	mp-30671	Ti2Ga	mp-17706	Zr5Ge3
mp-1029375	BaCN2	mp-2767	TiGa	mp-24286	ZrH2
mp-1214417	BaC6	mp-30672	Ti3Ga	mp-1200749	Zr5Ge4
mp-2209	CeGa2	mp-571342	TiGa2	mp-1025513	ZrGe
mp-2563	CeSe	mp-30673	Ti2Ga3	mp-1865	UN
mp-1018276	CeGa	mp-1218382	Sr4Bi2O	mp-32590	U4N7
mp-862696	CeGa3	mp-29620	Sr5Bi3	mp-32742	U16N25
mp-19920	Ce3Ga	mp-2090	FeCo	mp-1776	UN2
mp-510430	Li13In3	mp-601820	Fe3Co	mp-567276	TaV2
mp-1138	LiF	mp-601848	Fe11Co5	mp-504554	Ba5Ta4O15
mp-31324	Li2In	mp-601842	Fe9Co7	mp-12659	Mn2Nb
mp-21293	Li3In2	mp-567290	LaN	mp-12678	TaMn2

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-867226	Li3In	mp-343	PrN	mp-1185642	Mg149Zn
mp-12723	CaAu	mp-2493	CeN	mp-680671	Mg4Zn7
mp-30367	Ca5Au2	mp-954	BaB6	mp-978269	MgZn2
mp-30368	Ca5Au3	mp-30905	Ba3(BN2)2	mp-22179	YTiSi
mp-571264	Ca5Au4	mp-2741	CaF2	mp-754225	YbTiO3
mp-2364	PaO2	mp-7104	CsCaF3	mp-753192	Yb4Sb2O
mp-2252	ScB2	mp-28164	Ba4P2O	mp-1025200	Eu2TiO4
mp-24237	ScH2	mp-32606	Ba3P2	mp-1079111	EuTiO3
mp-22898	KI	mp-1935	BaMg2	mp-18167	Ca3Cd2
mp-1095642	Eu2Ge	mp-568512	Ba6Mg23	mp-915	YCd
mp-21394	EuO	mp-8278	Ba(MgP)2	mp-1073	CaCd
mp-20712	EuGe	mp-2514	Mg3P2	mp-1331	YCd2
mp-1188934	Eu5Ge3	mp-1813	Ba2Mg17	mp-1444	CaCd2
mp-615	YMg	mp-1001835	LiB	mp-1105932	Li2MgSi
mp-2652	Y2O3	mp-1222413	LiB3	mp-1222798	Li14MgSi4
mp-865376	YMg3	mp-6499	BaLiBO3	mp-866755	LiMg149
mp-1265	MgO	mp-755417	Ba3(BO3)2	mp-1094889	LiMg
mp-1188082	YMg149	mp-27275	Li3BO3	mp-973374	LiMg2
mp-1623	ErS	mp-8298	Sr4P2O	mp-1094591	Li3Mg
mp-12671	Er2SO2	mp-972071	V3Mo	mp-5597	Ca(FeP)2
mp-573697	CsCl	mp-1220316	NbW	mp-1079146	Th3Si2
mp-1215	Ti2O	mp-1187695	V3Cr	mp-21238	ThSi
mp-1071163	TiO	mp-1216394	VCr	mp-7497	ThSi2
mp-554098	Ti6O	mp-1187696	VCr3	mp-10961	La5Si3
mp-72	Ti	mp-985	TmCu	mp-567258	LaZn2
mp-2591	Ti3O	mp-1077209	TmCu2	mp-7083	LaSi
mp-865027	Mn3Ge	mp-30600	TmCu5	mp-2615	LaZn
mp-1025122	LuCu2	mp-30579	ErCu5	mp-9556	SrZnSi
mp-580136	LuCu5	mp-1024991	ErCu2	mp-861620	LaZn4
mp-2399	YHg	mp-1955	ErCu	mp-2062	LaSi2
mp-11256	ScAu	mp-1211343	KNdF4	mp-30709	La2Zn17
mp-2647	Al2Au	mp-1140	NdCu5	mp-1200584	La3Zn22
mp-980769	SmCu	mp-11852	NdCu2	mp-571191	LaZn11
mp-1077154	SmCu2	mp-13392	NdCu	mp-1218375	Sr2Zn5Si3
mp-227	SmCu5	mp-21256	Mn7C3	mp-1218249	SrLa4Si3O13
mp-1183995	GaCu3	mp-542830	Mn23C6	mp-17833	Ba3GeO
mp-1087547	EuCu	mp-24123	Rb(BH)6	mp-2892	BaNd2O4
mp-2066	EuCu5	mp-1219553	RbBH4	mp-8430	KLiS
mp-1071732	EuCu2	mp-1747	K2Te	mp-505598	Zr(Ni2P)2
mp-1018131	LuAg2	mp-661	AlN	mp-14298	Zr6Ni20P13
mp-279	LiIr	mp-504731	EuF2	mp-505278	Zr9(NiP2)2
mp-30738	LiIr3	mp-554546	Eu2SiO4	mp-1079999	Zr2NiP2
mp-12283	Li5Ti2	mp-14093	TbOF	mp-29153	Zr2NiP
mp-7396	Li3Ti	mp-1924	TbSi	mp-551675	Li3UO4
mp-18511	NdF3	mp-11347	TbF3	mp-8609	Li6UO6
mp-23295	RbCl	mp-206	Tb5Si3	mp-3698	SrAlSi
mp-22903	RbI	mp-1077398	TbSi2	mp-7068	Sr3(AlSi)2
mp-1188441	TiCu4	mp-1207669	TmOF	mp-15960	Li5AlO4
mp-742	Ti2Cu	mp-1066975	TmSi	mp-3427	LiAlO2
mp-2078	TiCu	mp-1189863	Tm5Si3	mp-973391	LiSiB6
mp-2643	Ti3Cu4	mp-560114	Er3O2F5	mp-24092	GdH2
mp-12546	TiCu3	mp-31167	Er5Si3	mp-4805	Gd2SO2
mp-23715	BaH2	mp-378	ErSi	mp-3211	Nd2SO2
mp-643047	Ba3(H6Ir)2	mp-1072193	ErOF	mp-1190994	NdHO

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-890	NdIr2	mp-1738	SmAs	mp-24096	NdH2
mp-30522	Nd5Ir3	mp-982	TmPd3	mp-2616	NpO2
mp-1104605	Nd5Ir2	mp-1104675	Tm3Pd4	mp-3210	Ca(CoP)2
mp-1189686	Nd3Ir	mp-348	TmPd	mp-10923	Ca2Co12P7
mp-1753	ThAs	mp-33090	V2N	mp-2384	LaP
mp-643	ThO2	mp-1018027	VN	mp-29241	Ca3SnO
mp-216	Sc2O3	mp-642644	V2H	mp-8789	Ca4As2O
mp-1709	U2Ti	mp-1188283	V8N	mp-9564	Ca(MgAs)2
mp-44	U	mp-1787	NdMg3	mp-1145	TiB2
mp-569744	UAl2	mp-1327	NdMg	mp-1025170	Ti3B4
mp-674332	U17O31	mp-31116	LaScO3	mp-11750	Ti6Si2B
mp-1597	UO2	mp-18051	La2TiO5	mp-7857	TiB
mp-1079399	V3Fe	mp-22432	Ti4Cu2O	mp-4056	CaSc2O4
mp-866134	VFe3	mp-21457	Ti3Cu3O	mp-11566	ScZn
mp-637224	Pu2O3	mp-1349	SrPt2	mp-12137	Ca(ZnSi)2
mp-24720	PuH2	mp-30843	Sr7Pt3	mp-16266	CaZnSi
mp-1959	PuO2	mp-1104074	Sr3Pt2	mp-13503	ScZn2
mp-494	GeMo3	mp-556015	Dy9(SbO)5	mp-862260	ScZn3
mp-2857	ScN	mp-1927	Dy4Sb3	mp-1219746	ScZn6
mp-685209	Sc39N34	mp-1007	DySb	mp-568646	Ta3Si
mp-2472	SrO	mp-1185594	Mg149In	mp-1989	Ta5Si3
mp-1216	YbO	mp-22735	Ca2Sn	mp-11192	TaSi2
mp-2391	YbPd3	mp-28731	V6C5	mp-9578	Ba3(AlSi)2
mp-1104397	Yb5Pd2	mp-1195743	V18P9C2	mp-13149	BaAlSi
mp-2547	YbPd	mp-684675	V12P7	mp-5506	Ba(AlSi)2
mp-1105057	Yb3Pd4	mp-20648	V2C	mp-2823	NdP
mp-561430	LiLuF4	mp-20541	V2P	mp-11580	TiCrP
mp-1025059	LaAg2	mp-18350	V3P	mp-568636	TiCr2
mp-1560	LaTe	mp-30842	ZrPd3	mp-1211138	Li5Ni9P7
mp-1948	LaAg	mp-266	Zr2Pd	mp-685439	LiNi3P2
mp-2825	ErPd3	mp-13495	ZrPd	mp-21075	HfC
mp-1104774	Er3Pd4	mp-1188310	Tm5Ge3	mp-1225044	Er2C
mp-12545	Er3Pd2	mp-1203550	Tm11Ge10	mp-1203719	Er3C4
mp-851	ErPd	mp-1104486	Tm3Ge4	mp-1212833	Er4C7
mp-581942	CeCu6	mp-20685	Cr3Ge	mp-567705	TiAl2
mp-2801	CeCu2	mp-568153	Al22Mo5	mp-542915	TiAl3
mp-1427	Lu2O3	mp-2733	Al8Mo3	mp-1823	Ti3Al
mp-1056	Tb2O3	mp-259	AlMo3	mp-1953	TiAl
mp-21009	EuSe	mp-1185596	Mg149Al	mp-1849	Mn2P
mp-13971	Nd2SeO2	mp-1094116	MgAl2	mp-4484	Ba(PRu)2
mp-1453	NdSe	mp-2151	Mg17Al12	mp-4156	Li2ZrO3
mp-1102143	ErRe2	mp-9546	Yb2C3	mp-5418	Li6Zr2O7
mp-754640	Ce2SeO2	mp-1103975	YbC6	mp-3949	K7LiSi8
mp-1187198	SrMg2	mp-1103990	EuC6	mp-2983	Ba(PN2)2
mp-30782	Sr6Mg23	mp-1104	LaMg	mp-1221737	MnFe3P2
mp-1934	LiZn	mp-1094174	LaMg3	mp-23804	Mg2FeH6
mp-1153	Li2S	mp-675	ZrW2	mp-9921	MgCr2O4
mp-975799	LiZn3	mp-28930	KC8	mp-5473	CaMgSi
mp-1199934	Ti3As	mp-10408	K2CN2	mp-1672	CaS
mp-1201836	Ti5As3	mp-5532	Sr2TiO4	mp-29110	Al2(FeSi)3
mp-1190061	Eu5Si3	mp-4651	SrTiO3	mp-1190708	Al3Fe2Si
mp-21279	EuSi	mp-3349	Sr3Ti2O7	mp-867878	AlFe2Si
mp-1072248	EuSi2	mp-5598	Sm2SO2	mp-1229054	Al53Fe17Si12
mp-1345	CaP	mp-1218562	Sr4LaTi5O15	mp-1229249	Al79(Fe13Si9)2

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1214132	Ca4SiP4	mp-695042	Sr9LaTi10O30	mp-1227337	Ca6Al7O16F
mp-20394	EuPb	mp-17904	Nd2TiO5	mp-27791	SrBe3O4
mp-20300	EuP	mp-1039148	CaMg	mp-2080	SrBe13
mp-1103985	Nd3Pt2	mp-2432	CaMg2	mp-1800	Nd2C3
mp-1080485	NdPt	mp-1184449	CaMg149	mp-866691	La2PC
mp-2720	NdPt2	mp-3397	Ba2TiO4	mp-1184	La2C3
mp-20587	EuS	mp-1228030	Ba4Bi2O	mp-2367	LaC2
mp-1102043	LaOs2	mp-29621	Ba5Bi3	mp-36111	LiMgP
mp-2011	UP	mp-631	TiC	mp-11507	Ni4Mo
mp-11854	Er5Ge3	mp-27919	Ti8C5	mp-4091	Ni2Mo3N
mp-1203572	Er11Ge10	mp-1217052	Ti6P2O	mp-11506	Ni3Mo
mp-1711	Er3Ge4	mp-10721	Ti2C	mp-23432	BaClF
mp-1198083	Gd5Ge4	mp-1205180	Tm3C4	mp-1102496	EuH2
mp-19918	GdGe	mp-7171	TmP	mp-707218	Ba3AlHO4
mp-21237	CoGe	mp-1216546	Tm2C	mp-13686	Nb5Si3
mp-1418	FeNi3	mp-1640	Ho2C	mp-12104	NbSi2
mp-2213	FeNi	mp-744	HoP	mp-1334	Y2C
mp-1001836	MnGa	mp-15238	Ho4C5	mp-9459	Y4C5
mp-37722	KBH4	mp-1154	Ho4C7	mp-1200885	Y4C7
mp-24239	K(BH)6	mp-1202754	Ho3C4	mp-1200613	Y3C4
mp-1216441	Zr14Cu51	mp-20318	Mn2B	mp-1216160	Y4Zr3O12
mp-193	Zr2Cu	mp-10118	Mn3B4	mp-1224869	Gd2C
mp-1188077	Zr7Cu10	mp-1106184	MnB4	mp-510401	GdP
mp-1224756	Hf14Cu51	mp-680339	Mn4Si7	mp-1189998	Gd2C3
mp-30581	Hf2Cu	mp-568656	SiC	mp-569335	Sm2C3
mp-1200988	Hf7Cu10	mp-20211	Mn3Si	mp-24658	SmH2
mp-7353	Hf3Cu8	mp-1431	MnSi	mp-1219177	Sm2C
mp-1217	KSi	mp-1118	SiNi2	mp-1191829	Li2Co12P7
mp-865834	Yb3GeO	mp-351	SiNi	mp-753721	GdOF
mp-1694	Yb2Ge	mp-828	SiNi3	mp-12574	Dy2C
mp-21300	Yb5Ge4	mp-2291	Si2Ni	mp-1212812	Dy4C5
mp-767	Yb3Ge5	mp-27276	Si12Ni31	mp-1213387	Dy3C4
mp-1106300	Nd3Ru	mp-1080525	FeB	mp-532160	Ca14MnP11
mp-1103979	Nd5Ru2	mp-1915	Fe2B	mp-3637	YOF
mp-1102217	NdRu2	mp-9905	Ba2Si	mp-3700	LiYF4
mp-1029	BaF2	mp-1067235	BaSi	mp-1205337	Ca3(ALP2)2
mp-619	UB4	mp-1619	Ba3Si4	mp-24726	TiH2
mp-1514	UB2	mp-1477	BaSi2	mp-866141	TiFe2Si
mp-22319	UB12	mp-17612	Ba2SiO4	mp-8648	TiFeSi
mp-1221	V3Ge	mp-3952	BaY2O4	mp-305	TiFe
mp-2363	HfMo2	mp-16432	Sr3(BO3)2	mp-16253	BaCaSi
mp-352	HfO2	mp-3933	Mg2PN3	mp-21662	TiFeSi2
mp-931	ThP	mp-1559	Mg3N2	mp-5926	KCaF3
mp-13972	Sm2SeO2	mp-11501	MnNi3	mp-1216621	TiW
mp-218	Sm2O3	mp-1079891	Ba2Br2O	mp-865656	TiMn2W
mp-7283	LaB4	mp-555218	Ba4Br6O	mp-865652	TiMn2Si
mp-2680	LaB6	mp-27456	BaBr2	mp-21606	TiMnSi2
mp-1215377	Zr4O	mp-1021323	LiC12	mp-1217077	Ti2Si6W
mp-2049	ZrMo2	mp-1552	Mo2C	mp-555617	Ce10Si8O3
mp-561418	Zr3O	mp-1079937	Pr3Si2	mp-1898	CeSi2
mp-1269	SmS	mp-769173	PrOF	mp-1025450	CeFeSi2
mp-710	SmP	mp-9968	PrSi	mp-21115	CeSi
mp-1894	WC	mp-27760	PrSi2	mp-3187	BaCeO3
mp-2599	NdN	mp-569851	Ho10Si17	mp-3035	Ce(FeSi)2

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-2593	AlNi3	mp-12899	HoSi	mp-1196829	Ce5Si4
mp-16514	Al3Ni5	mp-1072114	HoOF	mp-570175	Ce5Si3
mp-1487	AlNi	mp-13236	Ho5Si3	mp-11317	CeFe5
mp-622209	Al3Ni	mp-5634	NdOF	mp-20245	CeFeSi
mp-1057	Al3Ni2	mp-9967	NdSi	mp-1018125	Ti2Re
mp-16515	Al4Ni3	mp-884	NdSi2	mp-2179	TiRe
mp-510557	CsN3	mp-567735	Nd5Si3	mp-518	Ti5Re24
mp-28366	Gd2B5	mp-355	Nd5Si4	mp-1095145	TiReSi
mp-1105563	GdB4	mp-1072208	DyOF	mp-7948	ReSi
mp-22266	GdB6	mp-2620	DySi	mp-568595	Re4Si7
mp-1158	LuPd3	mp-2836	Dy5Si3	mp-510522	Zr5Sn3
mp-1103963	Lu3Pd4	mp-1212889	DyF3	mp-1106020	Zr5SiSn3
mp-2205	LuPd	mp-569825	Dy10Si17	mp-543001	Zr5Sn4
mp-1210753	Li2Al	mp-2057	DyB2	mp-2554	Al3V
mp-16506	Li3Al2	mp-2719	DyB4	mp-1201511	Mg3(Al9V)2
mp-10890	LiAl3	mp-16037	Dy2TeO2	mp-10126	V5SiB2
mp-1067	LiAl	mp-1774	ErB2	mp-1387	AlV3
mp-19879	PPd3	mp-2847	ErB4	mp-1216643	V10Si6B
mp-1039345	CeMg2	mp-10192	LuP	mp-567224	Mg(SiB6)2
mp-1820	YbS	mp-2014	DyP	mp-1207086	MgAlB4
mp-2390	YbP	mp-2296	Ni3P	mp-1222150	Mg4AlB10
mp-1187909	Yb3P	mp-571370	Fe2NiP	mp-1216481	V3Cr3Si2
mp-1367	Mg2Si	mp-778	Fe2P	mp-1216445	V9Cr3B8
mp-20995	Eu4As3	mp-16594	K3TbSi2O7	mp-24288	LuH2
mp-1106024	Eu5As3	mp-645	TbP	mp-640340	Ca4MgAl3
mp-757	Li3As	mp-11578	VZn3	mp-1215386	Zr3Ti2Si3
mp-1225307	DyCu5	mp-30883	V4Zn5	mp-2116	ZrMn2
mp-1071835	DyCu2	mp-15743	Sr2CeO4	mp-31310	Zr3(Mn2Si3)2
mp-2334	DyCu	mp-30228	Li4HN	mp-11270	MnBe2
mp-2796	TmAg	mp-5001	Li3BN2	mp-1185637	Mg149Sn
mp-30359	TmAg2	mp-23702	LiH2N	mp-1104792	MnBe12
mp-979115	Ti2Ag	mp-1201065	Li15H9N8	mp-1192960	Zr6Fe16Si7
mp-2074	Li3Sb	mp-1200910	Li7H5N4	mp-1215517	Zr2MnFe3
mp-11247	Li3Au	mp-1191288	Eu2Ta2O7	mp-1102452	ZrFeSi
mp-567395	Li15Au4	mp-510374	GdAs	mp-1221619	MnFeSi2
mp-600561	LiRh	mp-27731	HfH2	mp-5529	MnFe2Si
mp-1001787	LiRh3	mp-31019	Al45Cr7	mp-17435	Zr4Fe4Si7
mp-1209185	RbPrF4	mp-867780	Al3Cr	mp-12894	Y2SO2
mp-23713	CaH2	mp-1699	AlCr2	mp-569989	Nb2C
mp-570436	CaIr2	mp-1208630	SrC6	mp-1079585	Nb2N
mp-570356	Ca5Ir	mp-576	B13C2	mp-2760	Nb6C5
mp-663	NdGe	mp-20937	Cr3C2	mp-2634	NbN
mp-1748	NdS	mp-1196316	Cr7C3	mp-3448	KMgF3
mp-1464	Nd5Ge3	mp-723	Cr23C6	mp-31212	K2MgF4
mp-172	Nd5Ge4	mp-27757	Be4B	mp-861983	Ti2MnFe
mp-2015	Nd3Ge5	mp-30866	Rh3W	mp-23956	K2MgH4
mp-510402	GdS	mp-994	YP	mp-1228149	Ba3Sr9Al4(O4F)4
mp-1463	LaIr2	mp-1014265	Zr2N	mp-3161	LiAlSi
mp-1104303	La3Ir2	mp-1352	ZrN	mp-1205813	Gd2MgSi2
mp-1199235	La5Ir3	mp-277	Zr3N4	mp-2636	GdMg
mp-1104396	La5Ir2	mp-1223129	Li4SiO4	mp-20534	GdMg3
mp-1562	ThBe13	mp-1314	Li12Si7	mp-995201	Ti5Si3C
mp-23818	BaLiH3	mp-1201871	Li7Si3	mp-5659	Ti3SiC2
mp-23703	LiH	mp-29720	Li21Si5	mp-1227232	Ca6Al7ClO16

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-2747	TbPd3	mp-672287	Li13Si4	mp-11283	ZrBe5
mp-1104088	Tb3Pd4	mp-980757	Sm5Sb3	mp-2544	Zr2Be17
mp-1080451	TbPd	mp-770806	Sm2TiO5	mp-30445	ZrBe13
mp-30667	Sr8Ga7	mp-561233	Sm9(SbO)5	mp-2807	ScP
mp-182	SrGa2	mp-2281	SmSb	mp-1188062	Zr3Sc
mp-1827	SrGa4	mp-12049	Nd2Sb	mp-1077791	ZrSc2
mp-797	DyPd3	mp-1586	NdSb	mp-1188800	Sc3P
mp-1104399	Dy3Pd4	mp-530	Nd4Sb3	mp-22600	Sc3P2
mp-2345	Dy2O3	mp-11284	CaGa2	mp-1100806	Zr8Sc2O19
mp-12543	Dy3Pd2	mp-11649	Ca3SiO	mp-974713	K2H4Pt
mp-2226	DyPd	mp-568793	Ca28Ga11	mp-777297	K5H(CN)2
mp-1106373	Sm5Si3	mp-1227300	Ca2GaSi	mp-28160	Ca3C3Cl2
mp-1025489	SmSi	mp-30473	Ca3Ga5	mp-23859	CaHCl
mp-13955	SmSi2	mp-4481	Ca2SiO4	mp-984055	Ca7(H6Cl)2
mp-2602	NdAs	mp-6914	CaGa	mp-1219429	Sc2CO
mp-1071422	CeAg2	mp-31348	Sc2In	mp-15661	Sc4C3
mp-4764	Pr2SeO2	mp-7822	Sc5Si3	mp-28733	Sc3C4
mp-1674	PrSe	mp-1207100	ScIn	mp-29941	Sc2C
mp-1183837	Co3Ni	mp-9969	ScSi	mp-11908	Lu5Si3
mp-20874	EuB6	mp-19713	Sc3In	mp-1001612	LuSi
mp-505346	Eu3(BO3)2	mp-1185970	Mn3Co	mp-4883	Ba(FeP)2
mp-335	BaGa4	mp-1109	Sr5Al9	mp-542995	Nb6Fe16Si7
mp-30429	Ba8Ga7	mp-2775	SrAl4	mp-1196167	NbFeSi2
mp-1219	BaGa2	mp-3094	SrAl2O4	mp-1192618	Nb4Fe4Si7
mp-9909	Ba5Sb3	mp-3393	Sr3Al2O6	mp-1209887	NbFeSi
mp-32635	Sr3P2	mp-20273	Ca3PbO	mp-1101870	TiFeP
mp-505528	Nb3P	mp-30478	Ca2Pb	mp-1217193	Ti3Fe5P4
mp-505064	Nb2P	mp-551873	Ca4Bi2O	mp-1211088	LiCaP
mp-9339	NbP	mp-569535	Ca2Bi	mp-570466	Li2Ca
mp-648999	Nb5P3	mp-27145	Ca5Bi3	mp-13276	SrLiP
mp-18254	Nb7P4	mp-554346	KSr4(BO3)3	mp-570097	Sr(Li2P)2
mp-978	Sr2Sn	mp-504812	Hf3P	mp-695998	K2ZnH4
mp-1698	SrSn	mp-20672	Hf3P2	mp-862658	LiCu3
mp-17720	Sr5Sn3	mp-9953	HfP	mp-1226479	CrH15N6Cl2O
mp-492	TiN	mp-504659	Hf2P	mp-3805	Al(FeB)2
mp-8282	Ti2N	mp-1211649	K4HfO4		

Table S5 Phases that are thermodynamically stable against K_{BCC}

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-2675	MgNi2	mp-972521	SmGe	mp-24237	ScH2
mp-1184905	K	mp-1506	Sm5Ge4	mp-29941	Sc2C
mp-23	Ni	mp-1447	SmSe	mp-15661	Sc4C3
mp-2137	Mg2Ni	mp-1006891	KSmSe2	mp-28733	Sc3C4
mp-1185599	Mg149Ni	mp-9339	NbP	mp-1173761	Na2CeO3
mp-1094122	Mg	mp-505528	Nb3P	mp-28383	KNaS
mp-1179656	Rb	mp-505064	Nb2P	mp-3972	Ce2SO2
mp-10172	Na	mp-648999	Nb5P3	mp-510522	Zr5Sn3
mp-1184151	Cs	mp-18254	Nb7P4	mp-543001	Zr5Sn4
mp-286	YbSe	mp-13743	K3GaO3	mp-559426	Pr2Zr2O7
mp-972364	Yb	mp-983509	Na3Cd	mp-1842	NbAl3
mp-8426	K2Se	mp-1197369	K16Na9(Tl6Cd)3	mp-18427	Nb2Al
mp-90	Cr	mp-1217395	Th4C3	mp-1104164	Ba3Au2
mp-867200	Pm	mp-1164	ThC	mp-1214417	BaC6
mp-1202753	KTmF4	mp-643	ThO2	mp-570775	BaAu

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1018122	Tm	mp-1217298	Th5C	mp-30363	BaAu2
mp-1211645	K3TmF6	mp-1188514	Th2C3	mp-9488	SmOF
mp-463	KF	mp-7224	ThC2	mp-1025489	SmSi
mp-1211536	K2TmF5	mp-1211547	K2ThO3	mp-1106373	Sm5Si3
mp-1223845	K(SiPd)4	mp-20711	Fe3Ge	mp-17697	KSmF4
mp-1217	KSi	mp-601833	Fe13Ge3	mp-17434	K2SmF5
mp-697068	SiPd2	mp-1363	Na2Au	mp-1195475	K3SmSi2O7
mp-20622	SiPd3	mp-1205574	Cs2KScF6	mp-8298	Sr4P2O
mp-505071	Si2Pd9	mp-2744	LiPd	mp-32635	Sr3P2
mp-2	Pd	mp-728	Li2Pd	mp-7931	SrP
mp-1747	K2Te	mp-1079855	LiPd7	mp-777297	K5H(CN2)2
mp-23251	KBr	mp-1197547	Li15Pd4	mp-1029347	KPtN
mp-14017	K3Sb	mp-861936	LiPd3	mp-976876	K2PtC2
mp-35	Mn	mp-1560	LaTe	mp-505622	Mn4N
mp-1202778	K3Cd16	mp-1103990	EuC6	mp-9981	Mn2N
mp-1203760	Si7Tc4	mp-17904	Nd2TiO5	mp-28861	CsC8
mp-1079910	SiTc	mp-1211538	KNdTiO4	mp-1246385	K2MnN2
mp-113	Tc	mp-1025059	LaAg2	mp-2157	Co3W
mp-1072399	Be5Pt	mp-1948	LaAg	mp-1222825	Lu4Zr3O12
mp-126	Pt	mp-11283	ZrBe5	mp-29792	CaNb2O4
mp-87	Be	mp-30445	ZrBe13	mp-1228030	Ba4Bi2O
mp-1201758	KGe	mp-2544	Zr2Be17	mp-567280	Yb5Bi3
mp-13	Fe	mp-541787	Na8Hg3	mp-23171	PrBi
mp-542374	KSn	mp-31205	Zr3Fe	mp-1105548	Pr5Bi3
mp-22898	KI	mp-1190681	ZrFe2	mp-17412	BaPr2O4
mp-2197	BaHg	mp-582924	Zr6Fe23	mp-5977	Nd2Zr2O7
mp-11462	KHg	mp-2823	NdP	mp-988	Si3N4
mp-8094	Ba2Hg	mp-2116	ZrMn2	mp-1029418	KSi2N3
mp-122	Ba	mp-12662	Re24Mo5	mp-1029584	KSi5N7
mp-38	Pr	mp-1981	Ba2Sn	mp-3949	K7LiSi8
mp-1185570	Mg149Pb	mp-872	BaSn	mp-1223129	Li4SiO4
mp-21526	KPb	mp-567276	TaV2	mp-1201871	Li7Si3
mp-1087476	K2Mg5Sn3	mp-10408	K2CN2	mp-1105932	Li2MgSi
mp-1185637	Mg149Sn	mp-637224	Pu2O3	mp-1222798	Li14MgSi4
mp-2364	PaO2	mp-24720	PuH2	mp-1367	Mg2Si
mp-10740	Pa	mp-1959	PuO2	mp-866755	LiMg149
mp-1206970	KPaO3	mp-626785	KHO	mp-29720	Li21Si5
mp-971	K2O	mp-862794	K2Pu2O5	mp-1094889	LiMg
mp-1187073	Sr	mp-1025158	K2PuO4	mp-672287	Li13Si4
mp-1212010	K2DyF5	mp-639805	Ta3Ge	mp-973374	LiMg2
mp-10658	Dy	mp-17593	Ta5Ge3	mp-1185634	Mg149Si
mp-1211654	K3DyF6	mp-21511	K2NaInP2	mp-1094591	Li3Mg
mp-1211691	K2TbF5	mp-1210753	Li2Al	mp-15171	K2MgSiO4
mp-11698	Tb	mp-23703	LiH	mp-11189	Li2MgSiO4
mp-865934	YbF2	mp-16506	Li3Al2	mp-561474	K3LiSiO4
mp-1958	SrTe	mp-10890	LiAl3	mp-1220327	NbMo
mp-134	Al	mp-1067	LiAl	mp-22141	BaIn2
mp-155	Gd	mp-18337	Be3N2	mp-1105101	Ba9In4
mp-23193	KCl	mp-24428	KH2N	mp-31509	BaIn
mp-44	U	mp-24355	KBe(H2N)3	mp-605809	Ba11In6O3
mp-14018	K3As	mp-15684	K2CuAs	mp-28685	Ba8Ni6N7
mp-571261	Pu	mp-14623	K5CuAs2	mp-21653	BaNiN
mp-1022	K2S	mp-11427	GdPd	mp-560924	K2NaFeO3
mp-72	Ti	mp-21427	GdPd3	mp-1205067	KNa4FeO4

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-19876	InNi	mp-1190736	Ca8Al3	mp-823	TiCo
mp-582929	K8In11	mp-2741	CaF2	mp-1102138	TiCoP
mp-54	Co	mp-2404	CaAl2	mp-867373	Ti2Co12P7
mp-12174	HfNi3	mp-5926	KCaF3	mp-1191331	Ti2Co
mp-1018056	HfNi	mp-9774	Ba4Sb2O	mp-608	TiCo3
mp-103	Hf	mp-1500	BaS	mp-5380	Ca4P2O
mp-30849	TaPt2	mp-2602	NdAs	mp-1345	CaP
mp-50	Ta	mp-7439	K3Cu3P2	mp-1225044	Er2C
mp-567638	TaPt3	mp-8446	K2CuP	mp-24192	ErH2
mp-131	Zr	mp-999291	PrPd	mp-1203719	Er3C4
mp-75	Nb	mp-16705	Pr2O3	mp-13236	Ho5Si3
mp-253	ScCo2	mp-1104184	Pr3Pd4	mp-12899	HoSi
mp-2212	ScCo	mp-1571	PrPd3	mp-5835	Ho(CoSi)2
mp-27162	Sc3Co	mp-4519	KPrO2	mp-977345	Ho2Co3Si5
mp-67	Sc	mp-11239	ZrAg	mp-1203317	Ho5(Co2Si7)2
mp-8	Re	mp-2221	Zr2Ag	mp-7577	CoSi
mp-569535	Ca2Bi	mp-28395	B6P	mp-2435	HoCo5
mp-132	Ca	mp-9664	K3BP2	mp-2396	HoCo2
mp-27145	Ca5Bi3	mp-1189967	Pr3Os	mp-622565	Ho3Co
mp-773137	KCaBi	mp-567339	PrOs2	mp-19905	Co2Si
mp-31286	K3Bi	mp-510401	GdP	mp-2379	CoSi2
mp-2512	AsPd5	mp-931	ThP	mp-569851	Ho10Si17
mp-1212012	K10Tl7	mp-6500	KRb2ScF6	mp-510688	HoCoSi
mp-123	Nd	mp-778	Fe2P	mp-30969	Ho12Co7
mp-1201270	KErF4	mp-1206409	K(FeP)2	mp-16596	K3HoSi2O7
mp-1184115	Er	mp-20587	EuS	mp-1185589	Mg149Nb
mp-1211695	K3ErF6	mp-24650	YH2	mp-4883	Ba(FeP)2
mp-17371	K2ErF5	mp-2114	YN	mp-631	TiC
mp-101	Ir	mp-1849	Mn2P	mp-27919	Ti8C5
mp-2732	PRh2	mp-20422	KMnP	mp-10721	Ti2C
mp-74	Rh	mp-17751	Y5Ge3	mp-1102496	EuH2
mp-12098	K(PRh)2	mp-17381	Y3Ge4	mp-1640	Ho2C
mp-28424	K4P3	mp-13360	Y5Ge4	mp-744	HoP
mp-1211665	K3LuF6	mp-2637	YSe	mp-15238	Ho4C5
mp-145	Lu	mp-29210	Li2Ga	mp-1154	Ho4C7
mp-34232	K(AsRh)2	mp-9568	Li3Ga2	mp-1202754	Ho3C4
mp-1299	SiPt2	mp-1205930	Li5Ga4	mp-1246246	Ca5(CuN2)2
mp-1223832	K(SiPt)4	mp-9703	K2LiGaAs2	mp-844	Ca3N2
mp-864675	Yb3N2	mp-1225940	K30Ga9As19	mp-1882	CaCu5
mp-864757	YbN2	mp-9546	Yb2C3	mp-585949	CaCu
mp-827	KN3	mp-1103975	YbC6	mp-2686	Ca2N
mp-91	W	mp-1185628	Mg149Sb	mp-12614	Ca2Cu
mp-29584	K4BeAs2	mp-7089	KMgSb	mp-1208630	SrC6
mp-1057315	Eu	mp-600561	LiRh	mp-20181	Ce2C3
mp-504498	K2CdPb	mp-1001787	LiRh3	mp-1199934	Ti3As
mp-33	Ru	mp-510430	Li13In3	mp-1201836	Ti5As3
mp-49	Os	mp-31324	Li2In	mp-9172	Li4TiO4
mp-784	KZn13	mp-21293	Li3In2	mp-38280	LiTiO2
mp-705522	Sr28In11	mp-867226	Li3In	mp-762240	K2Li2TiO4
mp-20074	SrIn2	mp-557798	K5Li2NdF10	mp-2931	Li2TiO3
mp-608072	SrIn	mp-1184658	HgPd3	mp-692	Tb2C
mp-2286	Li2Se	mp-1077442	CeAu2	mp-645	TbP
mp-1018134	Li	mp-1025468	CeAu	mp-15237	Tb4C5
mp-8756	KLiSe	mp-1095658	Tb2Au	mp-1585	V3Co

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1187198	SrMg2	mp-999141	TbAu	mp-542614	VCo3
mp-30782	Sr6Mg23	mp-570179	TbAu2	mp-555617	Ce10Si8O3
mp-86	Sm	mp-1071422	CeAg2	mp-2088	CeAl2
mp-1519	CaTe	mp-1080709	NdAu	mp-567305	CeAl3
mp-37	Th	mp-12788	Nd3Au4	mp-1206597	CeAlSi
mp-8700	K2Au3	mp-567586	Nd17Au36	mp-1213865	Ce3Al11
mp-1079438	Ta2N	mp-1102098	Nd2Au	mp-866134	VFe3
mp-1279	TaN	mp-1217874	Tb14Ag51	mp-1079399	V3Fe
mp-570755	KTaN2	mp-30358	TbAg2	mp-20937	Cr3C2
mp-975834	MoRu3	mp-2268	TbAg	mp-1196316	Cr7C3
mp-129	Mo	mp-1223451	KCeF4	mp-723	Cr23C6
mp-1076	KB6	mp-13392	NdCu	mp-866691	La2PC
mp-1183252	BIr	mp-11852	NdCu2	mp-730	P2Pt
mp-1185513	HfMg149	mp-1140	NdCu5	mp-13871	P2Pt5
mp-1265	MgO	mp-30841	UPd3	mp-769173	PrOF
mp-352	HfO2	mp-1326	Nb3Sn	mp-1192490	K5Pr4Si4O16F
mp-974482	K4Hf5O12	mp-1196988	K5Li2PrF10	mp-1223421	KPr9(Si3O13)2
mp-12171	K6MgO4	mp-1542	YB2	mp-11649	Ca3SiO
mp-1211649	K4HfO4	mp-637	YB4	mp-2517	Ca2Si
mp-1201301	K2Hf2O5	mp-419	YbB6	mp-956	U3Si
mp-755802	K2MgO2	mp-864603	YbH2	mp-2800	USi3
mp-615	YMg	mp-1189298	YbB4	mp-1563	CaSi
mp-2652	Y2O3	mp-1186271	NaMg149	mp-793	Ca5Si3
mp-1187739	Y	mp-1185635	Mg149Tl	mp-4481	Ca2SiO4
mp-865376	YMg3	mp-20831	Gd4Sb3	mp-2090	FeCo
mp-1188082	YMg149	mp-510403	GdSb	mp-601848	Fe11Co5
mp-8409	KYO2	mp-570606	Pr4Ge3	mp-601820	Fe3Co
mp-769176	K5YO4	mp-1674	PrSe	mp-601842	Fe9Co7
mp-1185557	Mg149Bi	mp-511	PrGe	mp-12108	VPt2
mp-11534	Np	mp-867190	Pr4Ge7	mp-2678	VPt
mp-6058	K2NaScF6	mp-504731	EuF2	mp-2211	V3Pt
mp-682	NaF	mp-201	Yb5Sb3	mp-1079997	VPt8
mp-1111079	K3ScF6	mp-1857	YbCd	mp-2705	VPt3
mp-1184119	CuPd3	mp-1187653	YbCd3	mp-316	MnV
mp-1018029	CuPd	mp-770806	Sm2TiO5	mp-28731	V6C5
mp-580357	Cu3Pd	mp-753192	Yb4Sb2O	mp-20648	V2C
mp-30	Cu	mp-601	PrP	mp-864984	MnV3
mp-568052	K2Ga3	mp-13971	Nd2SeO2	mp-1195556	K5Y2Si4O13F
mp-1138	LiF	mp-1453	NdSe	mp-3637	YOF
mp-11471	ScHg	mp-7233	La2SeO2	mp-4511	La2SO2
mp-861910	Sc3Hg	mp-22266	GdB6	mp-28255	LaHO
mp-19713	Sc3In	mp-1105563	GdB4	mp-24153	LaH2
mp-31348	Sc2In	mp-1211764	K3Gd(BO3)2	mp-1104116	La2H5
mp-1207100	ScIn	mp-28366	Gd2B5	mp-1103808	La4H9
mp-571222	CsBr	mp-2748	CeAs	mp-568656	SiC
mp-614603	CsI	mp-18051	La2TiO5	mp-861957	KNaSmTaO5
mp-1200207	Cs8Ga11	mp-1211901	KLaTiO4	mp-1198935	K2Na2Sm4Ta2O13
mp-1837	TbCu	mp-1766	TmS	mp-23715	BaH2
mp-1610	TbS	mp-3556	Tm2SO2	mp-2091	V3B2
mp-1527	TbCu2	mp-1767	Tm2O3	mp-9973	VB
mp-999129	KTbS2	mp-753774	KTmO2	mp-1206441	V5B6
mp-11363	TbCu5	mp-467	Th3N4	mp-569270	V3B4
mp-1971	HoCu	mp-834	ThN	mp-9208	V2B3
mp-1240	HoS	mp-1464	Nd5Ge3	mp-1491	VB2

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-10659	Ho	mp-172	Nd5Ge4	mp-8780	Cr2N
mp-30584	HoCu2	mp-663	NdGe	mp-1183691	CrN
mp-15786	KHoS2	mp-2015	Nd3Ge5	mp-1029673	KCrN2
mp-30585	HoCu5	mp-865834	Yb3GeO	mp-1029850	K15Cr7N19
mp-28382	K4ZnO3	mp-1694	Yb2Ge	mp-24092	GdH2
mp-674332	U17O31	mp-21300	Yb5Ge4	mp-1191288	Eu2Ta2O7
mp-2104	UAs	mp-13973	Gd2SeO2	mp-1101654	NaEuO2
mp-1597	UO2	mp-1216020	Zn35Cu17	mp-2489	UC
mp-8794	K4UO5	mp-987	ZnCu	mp-2486	UC2
mp-4126	KUO3	mp-1368	Zn8Cu5	mp-2625	U2C3
mp-1206920	K(PIr)2	mp-1065	LaSb	mp-10970	LiErO2
mp-768368	K4I2O	mp-759	La2Sb	mp-12645	LiHoO2
mp-554146	K14In4O13	mp-1223	La4Sb3	mp-1672	CaS
mp-28171	K3IO	mp-32606	Ba3P2	mp-17785	KNa2GaO3
mp-667326	K5InO4	mp-1223894	K5BaTaP4	mp-14428	KNa4GaO4
mp-18073	K7TaAs4	mp-17566	Ba5P4	mp-7656	Na5GaO4
mp-30794	Na15Sn4	mp-28823	Ba4P3	mp-27618	Na8Ga2O7
mp-1211956	K2Na4ZnSn2	mp-9968	PrSi	mp-568151	Ti5Ge3
mp-1014265	Zr2N	mp-1079937	Pr3Si2	mp-1198692	Ti5Ge4
mp-1352	ZrN	mp-27760	PrSi2	mp-1699	AlCr2
mp-277	Zr3N4	mp-1185586	Mg149Be	mp-867780	Al3Cr
mp-1183425	Be3Co	mp-855	MgBe13	mp-31019	Al45Cr7
mp-2773	BeCo	mp-14429	CsK4GaO4	mp-754237	LiTmO2
mp-1071690	Be5Co	mp-30842	ZrPd3	mp-21332	LiGdO2
mp-554098	Ti6O	mp-266	Zr2Pd	mp-540809	Zr2Fe12P7
mp-2591	Ti3O	mp-13495	ZrPd	mp-20892	ZrFeP
mp-1215	Ti2O	mp-1623	ErS	mp-31415	La3TaO7
mp-1071163	TiO	mp-12671	Er2SO2	mp-30337	Al5W
mp-13133	K2TiO3	mp-679	Er2O3	mp-1620	Si2W
mp-756510	K4TiO4	mp-4326	KErS2	mp-1227997	AlSi3W2
mp-7375	KNbO3	mp-7959	KErO2	mp-11227	Al12W
mp-5455	K6Ti2O7	mp-1213824	Ce4Ge3	mp-1018178	Ba2Zn
mp-1195947	K23(Sn3Au4)3	mp-2563	CeSe	mp-303	BaZn5
mp-685008	Ba20As13	mp-1200696	Ce5Ge4	mp-30435	BaZn2
mp-12735	KAg2	mp-1213848	Ce4Ge7	mp-210	BaLi4
mp-504425	Nb3As	mp-2154	CeP	mp-672225	BaZn13
mp-1223953	K5BaNbAs4	mp-1144	ErP	mp-1192350	NbFe2
mp-18361	K7NbAs4	mp-13415	Ta3B2	mp-1221111	NbFe
mp-492	TiN	mp-1097	TaB	mp-768342	SrNb2O4
mp-8282	Ti2N	mp-1108	TaB2	mp-28940	Sr4Nb2O9
mp-1225049	K18Na46Ti131	mp-10142	Ta3B4	mp-729	Cr3Si
mp-28627	K4Br2O	mp-1269	SmS	mp-8937	CrSi2
mp-28166	K3BrO	mp-710	SmP	mp-784631	CrNi2
mp-926	PuP	mp-15783	KSmS2	mp-19096	Ba2VO4
mp-999336	NdPd	mp-31380	SmPd	mp-18892	KBaVO4
mp-1045	Nd2O3	mp-1104311	Sm3Pd4	mp-1185655	Mg149Zr
mp-1104199	Nd3Pd4	mp-662804	Sm10Pd21	mp-11317	CeFe5
mp-2333	NdPd3	mp-357	SmPd3	mp-259	AlMo3
mp-754158	KNdO2	mp-19830	ErN	mp-568153	Al22Mo5
mp-7806	Cr3P	mp-551675	Li3UO4	mp-2733	Al8Mo3
mp-21048	CrP	mp-8609	Li6UO6	mp-1219908	PdPt
mp-570421	Sm2B5	mp-1072248	EuSi2	mp-754225	YbTiO3
mp-218	Sm2O3	mp-21279	EuSi	mp-23714	SrH2
mp-8546	SmB4	mp-1190061	Eu5Si3	mp-541294	SrNi9P5

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Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-559574	K3Sm(BO3)2	mp-1751	ThSb	mp-18632	SrNi5P3
mp-3919	KBO2	mp-736	Li3P	mp-1418	FeNi3
mp-6996	SmB6	mp-6450	K2LiAlP2	mp-2213	FeNi
mp-1346	B6O	mp-541684	K3AlP2	mp-29634	V4P2C
mp-1178133	KSmO2	mp-11270	MnBe2	mp-1195743	V18P9C2
mp-17015	K4GeO4	mp-1104792	MnBe12	mp-1029457	Ba(CoN)2
mp-1960	Li2O	mp-1153	Li2S	mp-505765	BaCoN
mp-28825	K3CoO2	mp-8430	KLiS	mp-20737	KNaEuNbO5
mp-7083	LaSi	mp-1934	LiZn	mp-28645	CaNiN
mp-1161	LaSe	mp-975799	LiZn3	mp-2295	CaNi2
mp-10961	La5Si3	mp-1077209	TmCu2	mp-774	CaNi5
mp-26	La	mp-985	TmCu	mp-9921	MgCr2O4
mp-2062	LaSi2	mp-2822	TmSe	mp-1185585	Mg149Cr
mp-862690	Ac	mp-30600	TmCu5	mp-1216160	Y4Zr3O12
mp-9069	K2NaAlAs2	mp-677	SrCd2	mp-27731	HfH2
mp-655	Na3As	mp-2585	Sr5Sb3	mp-763	MgB2
mp-541682	K3AlAs2	mp-30496	SrCd	mp-365	MgB4
mp-34127	K2NaAs	mp-542484	Sr5Cd3	mp-978275	MgB7
mp-146	V	mp-20995	Eu4As3	mp-1191101	KMgBO3
mp-20300	EuP	mp-1106024	Eu5As3	mp-24095	PrH2
mp-21394	EuO	mp-9068	K2NaAlP2	mp-343	PrN
mp-1105092	Eu3P4	mp-9666	K2NaGaP2	mp-532160	Ca14MnP11
mp-557753	K3PO4	mp-15417	K2GaP2	mp-30980	NaYO2
mp-768949	KEuO2	mp-7642	K2AgAs	mp-17891	NaYSiO4
mp-2292	La2O3	mp-1169	ScCu	mp-30811	Ni4W
mp-7283	LaB4	mp-1018149	ScCu2	mp-5327	Na4UO5
mp-2680	LaB6	mp-1025122	LuCu2	mp-34842	Na3UO4
mp-1019777	K2La2B2O7	mp-580136	LuCu5	mp-1229032	AgPt4
mp-7958	KLaO2	mp-1017985	TiAg	mp-1229015	AgPt
mp-262	Na3B20	mp-979115	Ti2Ag	mp-8470	NaPrO2
mp-984	BN	mp-980769	SmCu	mp-558317	KNaPrNbO5
mp-1019888	KNa2BN2	mp-1077154	SmCu2	mp-1477	BaSi2
mp-2315	NaB15	mp-227	SmCu5	mp-1619	Ba3Si4
mp-28630	Na3BN2	mp-1018737	KMgP	mp-1067235	BaSi
mp-1187343	RbMg149	mp-1185593	Mg149P	mp-9905	Ba2Si
mp-1104	LaMg	mp-1185632	Mg149Se	mp-17612	Ba2SiO4
mp-1094174	LaMg3	mp-1077788	BPt2	mp-755363	Ba3SiO
mp-1104815	LaMg12	mp-2807	ScP	mp-559670	KBaYSi2O7
mp-1079679	K2CdSn	mp-22600	Sc3P2	mp-4495	KLiTe
mp-2616	NpO2	mp-1188800	Sc3P	mp-10923	Ca2Co12P7
mp-28930	KC8	mp-9778	K2AgP	mp-3210	Ca(CoP)2
mp-1025162	K2NpO4	mp-1186074	Na3Pd	mp-567290	LaN
mp-3963	K2CO3	mp-862658	LiCu3	mp-1019893	La3Si6N11
mp-1185015	KNpO3	mp-742	Ti2Cu	mp-1019967	LaSi3N5
mp-1183995	GaCu3	mp-1188441	TiCu4	mp-569576	La5(SiN3)3
mp-1197621	Ga4Cu9	mp-2078	TiCu	mp-7400	NaAlGe
mp-1185639	Mg149Ti	mp-2643	Ti3Cu4	mp-2970	Na4GeO4
mp-21949	K4PbO3	mp-12546	TiCu3	mp-31008	Na14Al4O13
mp-2334	DyCu	mp-1079111	EuTiO3	mp-556168	Na7Al3O8
mp-2470	DyS	mp-1025200	Eu2TiO4	mp-9212	NaAlO2
mp-1071835	DyCu2	mp-12670	Ho2SO2	mp-13998	Na5AlO4
mp-15785	KDyS2	mp-1029	BaF2	mp-14266	Cu15Si4
mp-1225307	DyCu5	mp-2080	SrBe13	mp-571056	CsSn
mp-1226185	K6InAs3	mp-981	SrF2	mp-2363	HfMo2

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-11247	Li3Au	mp-4764	Pr2SeO2	mp-22907	DyBi
mp-1206794	LiAu	mp-16847	K3Na2SnP3	mp-31464	Dy5Bi3
mp-567395	Li15Au4	mp-12802	AlCu3	mp-568646	Ta3Si
mp-21294	Y2In	mp-985806	Al2Cu	mp-1989	Ta5Si3
mp-28726	KYF4	mp-2500	AlCu	mp-1192906	Ba4Ta2O9
mp-17077	K2YF5	mp-593	Al4Cu9	mp-11192	TaSi2
mp-22704	YIn	mp-20712	EuGe	mp-504554	Ba5Ta4O15
mp-1105835	Y3In5	mp-1095642	Eu2Ge	mp-2631	Ba4Al5
mp-13230	K3YF6	mp-1188934	Eu5Ge3	mp-4202	BaAl2O4
mp-20131	YIn3	mp-530539	Sr4U2O9	mp-13149	BaAlSi
mp-571095	Na7Ga13	mp-3956	Sr3UO6	mp-1903	BaAl4
mp-2074	Li3Sb	mp-1898	CeSi2	mp-567701	Ba21Al40
mp-22903	RbI	mp-570175	Ce5Si3	mp-9578	Ba3(AlSi)2
mp-7956	Na3Sb	mp-21115	CeSi	mp-570400	Ba7Al10
mp-15724	KNa2Sb	mp-1196829	Ce5Si4	mp-5506	Ba(AlSi)2
mp-757	Li3As	mp-972256	Xe	mp-560978	Ba4Al2O7
mp-28994	KLi2As	mp-11506	Ni3Mo	mp-11651	Yb3SnO
mp-1220249	Pr14Ag51	mp-11507	Ni4Mo	mp-570050	Yb2Sn
mp-1072619	PrAg2	mp-890	NdIr2	mp-2806	YbSn
mp-18040	KPrF4	mp-30522	Nd5Ir3	mp-542915	TiAl3
mp-2525	PrAg	mp-1104605	Nd5Ir2	mp-567705	TiAl2
mp-985805	AlAg2	mp-1189686	Nd3Ir	mp-1823	Ti3Al
mp-1228988	AlAg3	mp-1777	Li15Ge4	mp-1953	TiAl
mp-1018131	LuAg2	mp-27932	Li9Ge4	mp-12894	Y2SO2
mp-568953	LuAg4	mp-1188469	La5Ge3	mp-30352	NaAg2
mp-2647	Al2Au	mp-1084830	LaGe	mp-2493	CeN
mp-29484	K4HgAs2	mp-1211472	La4Ge7	mp-1212001	K3Si6H6N11
mp-979911	Y2Au	mp-1738	SmAs	mp-1409	TiNi3
mp-1066254	YAu	mp-19891	Pu2C3	mp-1048	TiNi
mp-1018113	YAu2	mp-980757	Sm5Sb3	mp-1808	Ti2Ni
mp-1079811	SmAu	mp-2281	SmSb	mp-1018104	Zr2Cd
mp-2474	YAg	mp-1029504	KNbN2	mp-8299	Sr4As2O
mp-1216365	Y14Ag51	mp-2634	NbN	mp-24338	Sr5As3H
mp-999544	YAg2	mp-1079585	Nb2N	mp-21188	CeNi
mp-2399	YHg	mp-2760	Nb6C5	mp-580354	CeNi3
mp-1103395	La2Au	mp-569989	Nb2C	mp-1654	CeNi2
mp-1002136	LaAu	mp-12659	Mn2Nb	mp-1204381	Ce2Ni7
mp-1072087	LaAu2	mp-542583	EuTe	mp-1910	CeNi5
mp-11237	ScAg	mp-11345	ZrP	mp-1229288	Ce15Ni32
mp-30354	ScAg4	mp-22447	Zr3P	mp-24119	Ca2HN
mp-1018128	ScAg2	mp-647729	Zr14P9	mp-720856	KCa(H2N)3
mp-1236	NdAg	mp-583740	Zr7P4	mp-644307	Ca(H2N)2
mp-18511	NdF3	mp-2296	Ni3P	mp-34932	CaHN
mp-1220721	Nd14Ag51	mp-9672	K2NiP2	mp-867264	Re3Os
mp-1072737	NdAg2	mp-2790	Ni12P5	mp-1219509	ReOs
mp-1211343	KNdF4	mp-17833	Ba3GeO	mp-867141	ReOs3
mp-1211860	K2NdF5	mp-13922	Ba2Ge	mp-24589	K2HBrO
mp-2621	ErAg	mp-9858	Ba3Ge4	mp-13975	Er2SeO2
mp-30339	ErAg2	mp-1188954	Ba3Ge5	mp-28302	K4CdP2
mp-1225453	Er14Ag51	mp-2627	DyAs	mp-1334	Y2C
mp-2667	CsAu	mp-510557	CsN3	mp-9459	Y4C5
mp-567332	Ce	mp-1079938	TlPd3	mp-1200613	Y3C4
mp-28273	K3CuO2	mp-1063174	GdAu2	mp-1200885	Y4C7
mp-9200	K3AuO	mp-635426	GdAu	mp-1894	WC

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-20857	CoB	mp-2475	SmAg	mp-31167	Er5Si3
mp-1019608	Cs3BO3	mp-1219378	Sm14Ag51	mp-378	ErSi
mp-1056	Tb2O3	mp-2167	DyAg	mp-16597	K3ErSi2O7
mp-504840	K4WO5	mp-1225847	Dy14Ag51	mp-749	SmN
mp-1253	BaSe	mp-2618	DyAg2	mp-24724	TbH2
mp-31212	K2MgF4	mp-464	HoSe	mp-1591	Al4C3
mp-1019089	KMgAs	mp-8300	Ba4As2O	mp-1216546	Tm2C
mp-865782	Yb3SiO	mp-1221	V3Ge	mp-7171	TmP
mp-1216	YbO	mp-752658	Y2SeO2	mp-1205180	Tm3C4
mp-10651	YbSi	mp-1753	ThAs	mp-1219177	Sm2C
mp-1207599	Yb2Si	mp-1405	TbGe	mp-569335	Sm2C3
mp-1077404	YbSi2	mp-2610	Tb5Ge3	mp-3151	Li3TaO4
mp-15379	K2SiO3	mp-1673	Tb5Ge4	mp-755013	Li5TaO5
mp-30990	K6Si2O7	mp-1193534	YBe13	mp-9059	KLi6TaO6
mp-18700	K4SiO4	mp-965	TbB2	mp-861607	KNaNdTmO5
mp-567735	Nd5Si3	mp-568225	TbB4	mp-31417	Nd3TaO7
mp-884	NdSi2	mp-1211631	K3Tb(BO3)2	mp-755586	NaLaO2
mp-9967	NdSi	mp-13972	Sm2SeO2	mp-861868	KNaLaTaO5
mp-355	Nd5Si4	mp-558482	K17Fe5O16	mp-861944	KNaPrTaO5
mp-8614	K3NdSi2O7	mp-12040	K5FeO4	mp-14964	Pr3TaO7
mp-1224505	K6InP3	mp-21075	HfC	mp-867889	KNaGdTaO5
mp-540914	K3MnO3	mp-12960	Er5Sb3	mp-1222413	LiB3
mp-19148	K2Mn2O3	mp-2191	ErSb	mp-27275	Li3BO3
mp-19879	PPd3	mp-2593	AlNi3	mp-1001835	LiB
mp-7505	K2P2Pd	mp-622209	Al3Ni	mp-557632	K2LiBO3
mp-1618	PPd6	mp-1057	Al3Ni2	mp-558628	KLi2BO3
mp-3614	KTaO3	mp-16515	Al4Ni3	mp-1078191	Ba2TeO
mp-1820	YbS	mp-1487	AlNi	mp-10942	KNaLaNbO5
mp-1007636	KLuS2	mp-16514	Al3Ni5	mp-554034	KLa2NbO6
mp-12673	Lu2SO2	mp-29585	K4CdAs2	mp-2117	TbN
mp-1427	Lu2O3	mp-1224114	K4Ba2SnP4	mp-1189033	Tb3Ru
mp-1178135	KLuO2	mp-29621	Ba5Bi3	mp-1101970	TbRu2
mp-11266	BaCd2	mp-1189863	Tm5Si3	mp-866641	K2Na(H2N)3
mp-9909	Ba5Sb3	mp-1066975	TmSi	mp-23850	NaH2N
mp-527	BaCd	mp-16598	K3TmSi2O7	mp-30883	V4Zn5
mp-8093	Ba2Cd	mp-1203324	Zr3Ge	mp-505040	Cs2K4Fe2O5
mp-2801	CeCu2	mp-17706	Zr5Ge3	mp-972422	U3Ge
mp-1096	CeS	mp-1025513	ZrGe	mp-571370	Fe2NiP
mp-581942	CeCu6	mp-1200749	Zr5Ge4	mp-6499	BaLiBO3
mp-570001	Al6Fe	mp-865166	HfPd5	mp-8204	LiAlB14
mp-2658	AlFe	mp-11453	HfPd3	mp-530274	Al23B50
mp-1183162	AlFe3	mp-11454	Hf2Pd	mp-557268	KLi4AlO4
mp-13155	Hf2Ag	mp-1007692	HfPd	mp-15960	Li5AlO4
mp-13156	HfAg	mp-17774	K2Li3GaO4	mp-3427	LiAlO2
mp-21289	TiZn3	mp-4657	Li5GaO4	mp-567415	Nd2B5
mp-1014229	Ti2Zn	mp-8253	Na5ReO6	mp-1632	NdB4
mp-1014230	TiZn	mp-1199558	Sm5Ir3	mp-1929	NdB6
mp-543051	Lu5Sb3	mp-7342	Sm3Ir	mp-1195894	K9Li3Nd3(BO3)7
mp-516	LuSb	mp-1104500	Sm5Ir2	mp-1211700	K3Nd(BO3)2
mp-2681	Ho5Sb3	mp-1104610	Eu5Pd2	mp-1380	Zn3Ru
mp-812	Ho2O3	mp-1854	EuPd2	mp-1205290	Zn6Ru
mp-2050	HoSb	mp-1018147	EuPd	mp-27335	NaAlSi
mp-754883	KHoO2	mp-1105286	Eu3Pd2	mp-24412	K2NaAlH6
mp-2147	SrGe	mp-1002115	LaPd	mp-477	SmGa2

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-2472	SrO	mp-1104435	La3Pd4	mp-1195872	Sm3Ga2
mp-30950	Sr3GeO	mp-674	LaPd3	mp-1776	UN2
mp-2576	Sr2Ge	mp-1105925	La7Pd3	mp-32590	U4N7
mp-1218382	Sr4Bi2O	mp-30753	LaPd5	mp-32742	U16N25
mp-29620	Sr5Bi3	mp-567412	Y5Sn3	mp-1865	UN
mp-979289	TaW3	mp-1199133	Y11Sn10	mp-1216828	U2CN
mp-1187206	Ta3W	mp-994	YP	mp-12668	Tb2SO2
mp-1217811	TaW	mp-1219144	Sm2AsSe	mp-485	ZrNi3
mp-683	Pr2C3	mp-661	AlN	mp-556	ZrNi
mp-2384	LaP	mp-1472	ZrB2	mp-328	Zr2Ni
mp-571461	K4ZnAs2	mp-27191	Zr9S2	mp-2717	Zr2Ni7
mp-1038	MgCu2	mp-1197374	Zr2S	mp-2271	NaPt2
mp-2481	Mg2Cu	mp-708	LaAs	mp-1018129	Pt2W
mp-1342	BaO	mp-30975	Na3BO3	mp-5598	Sm2SO2
mp-3020	BaNbO3	mp-8263	KNa2BO3	mp-1139	Co3Mo
mp-542201	Ba3Nb2O8	mp-7664	Na6ZnO4	mp-3161	LiAlSi
mp-1223493	KBa2Nb3O9	mp-19334	Na4WO5	mp-976726	LiDyO2
mp-1224039	K4BaNb5O15	mp-1220316	NbW	mp-754605	LiLuO2
mp-4651	SrTiO3	mp-3744	NaNbO2	mp-1185578	Mg149S
mp-5532	Sr2TiO4	mp-27247	Na3NbO4	mp-24726	TiH2
mp-3349	Sr3Ti2O7	mp-5477	Na5NbO5	mp-4805	Gd2SO2
mp-2011	UP	mp-972071	V3Mo	mp-24727	TmH2
mp-787	U3P4	mp-19391	NaVO2	mp-1975	TmN
mp-1377	ThCu2	mp-754829	Na4VO4	mp-14565	K3P6N11
mp-503	ThS	mp-8957	Na5TaO5	mp-10572	NaPN2
mp-1217740	Th14Cu51	mp-1187695	V3Cr	mp-7639	Na2CuP
mp-12834	ThCu6	mp-1216394	VCr	mp-1019519	Ba2NaO
mp-279	LiIr	mp-1187696	VCr3	mp-866141	TiFe2Si
mp-30738	LiIr3	mp-578604	NaCrO2	mp-2199	Fe3Si
mp-8753	K4HgP2	mp-2542	BeO	mp-1247744	BaNa
mp-30579	ErCu5	mp-27757	Be4B	mp-11820	BaNa2
mp-1024991	ErCu2	mp-28158	K4Be3O5	mp-8648	TiFeSi
mp-1955	ErCu	mp-27915	K2BeO2	mp-2108	Ti5Si3
mp-2491	ErSe	mp-1111110	K2LiScF6	mp-505527	Ti5Si4
mp-1203025	Np2N3	mp-1188434	Y5Ti3	mp-305	TiFe
mp-2596	NpN	mp-11575	YTi	mp-16253	BaCaSi
mp-560869	K3VO4	mp-1101816	Lu2Au	mp-21662	TiFeSi2
mp-10688	CeO	mp-11249	LuAu	mp-1714	FeSi2
mp-542313	Ce2O3	mp-1018152	LuAu2	mp-7092	TiSi
mp-2629	Ce7O12	mp-6245	K5Nb4O12F	mp-871	FeSi
mp-760323	Ce5O9	mp-695998	K2ZnH4	mp-1077503	TiSi2
mp-23222	Li3Bi	mp-11219	LuB2	mp-560889	Ba6Na2Si4O15
mp-37722	KBH4	mp-10192	LuP	mp-10247	U2CrN3
mp-23870	NaH	mp-571495	LuB4	mp-865652	TiMn2Si
mp-24239	K(BH)6	mp-1104289	LuB12	mp-27569	Na14Mn2O9
mp-24084	KH	mp-1211659	K3Lu(BO3)2	mp-1216621	TiW
mp-504886	Gd2O3	mp-23956	K2MgH4	mp-1202079	Ti21Mn25
mp-757021	KGdO2	mp-1185565	Mg149Mo	mp-865656	TiMn2W
mp-1215377	Zr4O	mp-1185556	Mg149H	mp-1949	TiMn2
mp-1200894	Zr3As	mp-21256	Mn7C3	mp-21606	TiMnSi2
mp-561418	Zr3O	mp-542830	Mn23C6	mp-559242	KNaMnO2
mp-1211624	K4ZrO4	mp-1188076	ThMg149	mp-1217077	Ti2Si6W
mp-27377	K4Zr5O12	mp-642644	V2H	mp-2726	SrCu5
mp-1682	ZrAs	mp-554546	Eu2SiO4	mp-21609	SrCuN

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Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-972228	Zr3As2	mp-206	Tb5Si3	mp-29136	Sr6Cu3N5
mp-1191610	Zr7As4	mp-1924	TbSi	mp-1025402	SrCu
mp-18449	K2ZrO3	mp-6964	NaTbO2	mp-6406	Na2MgSiO4
mp-1203256	Zr14As9	mp-7500	Na4SiO4	mp-5473	CaMgSi
mp-1198302	Nb3Ge	mp-16594	K3TbSi2O7	mp-9702	Sr3BPO3
mp-16842	Nb5Ge3	mp-4533	Na2SiO3	mp-555495	K3Y(BO3)2
mp-1598	Na3P	mp-754027	NaSmO2	mp-1079146	Th3Si2
mp-541694	K2Na3SiP3	mp-1200960	K2Na2Sm4Nb2O13	mp-21238	ThSi
mp-8235	K2SiP2	mp-556438	KNaSmNbO5	mp-17850	K3NaTh2O6
mp-31430	Na2In	mp-8128	NaNdO2	mp-7497	ThSi2
mp-2352	Na2O	mp-1201519	K2Na2Nd4Nb2O13	mp-3536	MgAl2O4
mp-504962	K2Na3InO4	mp-558212	KNaNdNbO5	mp-1185596	Mg149Al
mp-553975	K3Na2InO4	mp-558128	KNd2NbO6	mp-1094116	MgAl2
mp-5525	KAlO2	mp-1569	Be2C	mp-2151	Mg17Al12
mp-9157	K3AlO3	mp-2390	YbP	mp-1185597	Mg149Ga
mp-769284	Dy2SeO2	mp-1187909	Yb3P	mp-1770	Mg5Ga2
mp-814	DySe	mp-19340	LiVO2	mp-30650	Mg2Ga
mp-2345	Dy2O3	mp-9872	K4BeP2	mp-23063	Ba4Cl6O
mp-1178141	KDyO2	mp-551835	Ba2I2O	mp-17143	BaGd2O4
mp-18350	V3P	mp-1196393	Y3Sb	mp-173	MnAl6
mp-684675	V12P7	mp-568320	Y4Sb3	mp-408	Mg2Ge
mp-1192783	V4P3	mp-215	YSb	mp-2856	Mn4Al11
mp-20541	V2P	mp-7020	LiYO2	mp-771	MnAl
mp-20689	Nb3B2	mp-7137	LiTbO2	mp-865027	Mn3Ge
mp-2580	NbB	mp-10004	Mo3P	mp-1185627	Mg149Mn
mp-450	NbB2	mp-219	MoP	mp-570150	CaAlSi
mp-10255	Nb3B4	mp-1029869	K15Mo7N19	mp-7704	Ca(AlSi)2
mp-1080021	Nb2B3	mp-1552	Mo2C	mp-721592	Ca6Al7O16
mp-1211821	K4MoO5	mp-7822	Sc5Si3	mp-640340	Ca4MgAl3
mp-3211	Nd2SO2	mp-216	Sc2O3	mp-867878	AlFe2Si
mp-1006885	KNdS2	mp-1727	SrSi2	mp-29110	Al2(FeSi)3
mp-1748	NdS	mp-9969	ScSi	mp-1190708	Al3Fe2Si
mp-1193889	HoBe13	mp-2661	SrSi	mp-1229054	Al53Fe17Si12
mp-1202279	KHoF4	mp-18510	Sr2SiO4	mp-1229249	Al79(Fe13Si9)2
mp-1212022	K2HoF5	mp-557577	K3ScSi2O7	mp-351	SiNi
mp-1211714	K3HoF6	mp-770771	SrSc2O4	mp-1118	SiNi2
mp-546552	KCrO2	mp-30949	Sr3SiO	mp-828	SiNi3
mp-1211715	K4CrO4	mp-746	Sr5Si3	mp-27276	Si12Ni31
mp-576	B13C2	mp-8188	KScO2	mp-1214980	Al11(CoSi)6
mp-574275	Li17Pb4	mp-560535	K4Sr(SiO3)3	mp-1214851	Al3Co3Si4
mp-30761	Li7Pb2	mp-1106	Sr2Si	mp-10010	Al(CoSi)2
mp-30760	Li3Pb	mp-505002	Sc5As3	mp-1185642	Mg149Zn
mp-561202	K6NbAs3O	mp-17695	Sc5Sn3	mp-680671	Mg4Zn7
mp-2350	LaS	mp-1188926	Sc3As2	mp-978269	MgZn2
mp-15781	KLaS2	mp-2052	ScAs	mp-5529	MnFe2Si
mp-614724	Cs3CrF7	mp-865168	Be3Ni	mp-861983	Ti2MnFe
mp-739	TiP	mp-1033	BeNi	mp-559904	NaLi3SiO4
mp-1191079	Ti7P4	mp-1892	Ba2N	mp-549671	KLiMnO2
mp-30218	Ti2P	mp-29199	BaCuN	mp-1221619	MnFeSi2
mp-31214	Ti3P	mp-1001	BaN2	mp-1079460	Ti3Sn
mp-616559	Ti2S	mp-30428	BaCu	mp-30875	Ti2Sn
mp-1224756	Hf14Cu51	mp-10736	Ba3N	mp-676653	Lu4Hf3O12
mp-30581	Hf2Cu	mp-568643	RbC8	mp-1559	Mg3N2
mp-1200988	Hf7Cu10	mp-14726	Na4TiO4	mp-759183	K2Mg(H2N)4

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-7353	Hf3Cu8	mp-560767	KNaTiO3	mp-1106020	Zr5SiSn3
mp-1102043	LaOs2	mp-242	SrB6	mp-20318	Mn2B
mp-1207022	K(PRu)2	mp-556695	NaSrBO3	mp-10118	Mn3B4
mp-863707	KNa2Bi	mp-554346	KSr4(BO3)3	mp-1106184	MnB4
mp-28595	KNaSe	mp-16432	Sr3(BO3)2	mp-1185549	Mg149Br
mp-16839	Na3WN3	mp-1241	BaAg2	mp-1185584	Mg149Cl
mp-1030950	K15W7N19	mp-1000	BaTe	mp-18793	LiCrO2
mp-1223632	KNa2WN3	mp-11840	BaAg	mp-1199908	Cs7NaSi8
mp-978	Sr2Sn	mp-1814	BaAg5	mp-2252	ScB2
mp-15698	Sr5As3	mp-12612	Ba3Ag2	mp-1226479	CrH15N6Cl2O
mp-17720	Sr5Sn3	mp-504812	Hf3P	mp-24152	HoH2
mp-1698	SrSn	mp-20672	Hf3P2	mp-1206820	HoRu3C
mp-29424	Sr4As3	mp-9953	HfP	mp-883	HoN
mp-570240	La14C14Cl9	mp-504659	Hf2P	mp-977585	Zr3Ti
mp-2367	LaC2	mp-7226	V3Ni	mp-505569	CeH2
mp-567694	La2C2Cl	mp-171	VNi3	mp-1104579	Ce2H5
mp-1184	La2C3	mp-11531	VNi2	mp-1080525	FeB
mp-14988	K4SnO3	mp-1216708	V3Ni2	mp-1915	Fe2B
mp-7258	K4SnO4	mp-9712	Ba3BPO3	mp-1194531	Fe2B7
mp-2795	ZrC	mp-954	BaB6	mp-1121	GaCo
mp-684623	Zr10C9	mp-755417	Ba3(BO3)2	mp-20559	Ga3Co
mp-21009	EuSe	mp-28164	Ba4P2O	mp-24151	DyH2
mp-2599	NdN	mp-6812	KBaPO4	mp-12669	Dy2SO2
mp-11908	Lu5Si3	mp-30429	Ba8Ga7	mp-12574	Dy2C
mp-1001612	LuSi	mp-1219	BaGa2	mp-1212812	Dy4C5
mp-557543	K3LuSi2O7	mp-335	BaGa4	mp-1213387	Dy3C4
mp-504502	Ta3P	mp-1105598	Y3Co	mp-570466	Li2Ca
mp-22477	Ta2P	mp-865373	YCo	mp-865965	Li2CaSi
mp-1067587	TaP	mp-1294	YCo2	mp-13916	LiCaSi2
mp-769271	Sr4Ta2O9	mp-3952	BaY2O4	mp-20150	LiCa2Si3
mp-7148	K2SrTa2O7	mp-19870	GaFe3	mp-30766	Li5Sn2
mp-1077933	GdCu2	mp-636368	Ga3Fe	mp-573471	Li7Sn4
mp-510404	GdSe	mp-804	GaN	mp-30767	Li7Sn2
mp-614455	GdCu	mp-1804	Fe3N	mp-1185265	Li3Sn
mp-636253	GdCu5	mp-6988	FeN	mp-990440	Na2ZrO3
mp-9687	K2PAu	mp-1185592	Mg149Fe	mp-28559	Na6Be8O11
mp-14624	K5P2Au	mp-22204	Co2P	mp-28588	Na2BeO2
mp-9972	YSi	mp-1206349	K(CoP)2	mp-14324	K2Na4Be2O5
mp-677445	Y4Si53	mp-1185590	Mg149I	mp-1105633	Y3Ni
mp-1534	YS	mp-1039148	CaMg	mp-582134	Y3Ni2
mp-2538	Y5Si3	mp-2432	CaMg2	mp-1364	YNi
mp-1006888	KYS2	mp-1184449	CaMg149	mp-2152	YNi5
mp-1216441	Zr14Cu51	mp-1185641	Mg149V	mp-574339	Y2Ni7
mp-193	Zr2Cu	mp-21895	Na15Pb4	mp-1200338	Y15Ni32
mp-1188077	Zr7Cu10	mp-568636	TiCr2	mp-569196	YNi3
mp-1039345	CeMg2	mp-11580	TiCrP	mp-35730	BaUO3
mp-1038976	CeMg5	mp-1217052	Ti6P2O	mp-583034	Ba2U2O7
mp-19918	GdGe	mp-1102537	NbVP	mp-557448	Ba2CaUO6
mp-1198083	Gd5Ge4	mp-3397	Ba2TiO4	mp-1845	CaBe13
mp-510402	GdS	mp-292	V3As	mp-707337	K3H3Pd
mp-15784	KGdS2	mp-680437	K3GdSi2O7	mp-643257	K2H4Pd
mp-1186974	Sc3Ti	mp-1199486	Gd5Si4	mp-11449	HfMn2
mp-7396	Li3Ti	mp-601371	GdSi	mp-1212189	HfMnP
mp-12283	Li5Ti2	mp-21192	GdSi2	mp-33090	V2N

(Continued)

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1786	Ti3Au	mp-952	MoPt2	mp-1018027	VN
mp-1087547	EuCu	mp-999502	MoPt	mp-1080848	KVN2
mp-2066	EuCu5	mp-974713	K2H4Pt	mp-1188283	V8N
mp-1071732	EuCu2	mp-1278	Zr2Si	mp-1215471	Zr2HC
mp-1018148	ScAu2	mp-893	ZrSi	mp-1185594	Mg149In
mp-11256	ScAu	mp-1207024	Zr3Si2	mp-30228	Li4HN
mp-2462	PrCu5	mp-8789	Ca4As2O	mp-2251	Li3N
mp-1071904	PrCu2	mp-23713	CaH2	mp-1201065	Li15H9N8
mp-1079091	PrCu	mp-10047	Ca5As3	mp-1198663	K2Li(H2N)3
mp-1095690	Tm2Au	mp-1194887	Ca4As3	mp-23702	LiH2N
mp-1017507	TmAu	mp-680339	Mn4Si7	mp-1200910	Li7H5N4
mp-560	TmAu2	mp-1431	MnSi	mp-20147	ZrMnP
mp-1102972	Er2Au	mp-20211	Mn3Si	mp-1112	CeCo2
mp-11243	ErAu	mp-5088	NaGdO2	mp-864889	ZrZn3
mp-2466	ErAu2	mp-13170	KNaGdNbO5	mp-1401	ZrZn2
mp-1103411	Dy2Au	mp-680381	K2Na2Gd4Nb2O13	mp-570276	ZrZn
mp-1007918	DyAu	mp-13686	Nb5Si3	mp-3236	Pr2SO2
mp-11241	DyAu2	mp-12104	NbSi2	mp-2495	PrS
mp-1080443	YCu	mp-2836	Dy5Si3	mp-15782	KPrS2
mp-2698	YCu2	mp-2620	DySi	mp-1213975	CaB4
mp-2797	YCu5	mp-569825	Dy10Si17	mp-865	CaB6
mp-2714	Pr2Au	mp-16595	K3DySi2O7	mp-555023	KCa4(BO3)3
mp-1079915	PrAu	mp-21524	SrNiN	mp-1102980	NbFeP
mp-30415	PrAu2	mp-1245	Sr2N	mp-1206854	TiMnP
mp-1071698	EuAu2	mp-10564	SrN2	mp-542995	Nb6Fe16Si7
mp-1078589	EuAu	mp-29973	SrN	mp-1196167	NbFeSi2
mp-1189094	Eu3Au	mp-2049	ZrMo2	mp-1192618	Nb4Fe4Si7
mp-1106137	Eu7Au3	mp-16488	Al9Co2	mp-1209887	NbFeSi
mp-1104457	Eu3Au2	mp-196	Al5Co2	mp-2014	DyP
mp-8683	K5As2Au	mp-284	AlCo	mp-23954	Na2H2Pd
mp-2796	TmAg	mp-1029863	K15Re7N19	mp-9987	Nb2PC
mp-30359	TmAg2	mp-974437	Re2C	mp-1222310	Lu2C
mp-1229012	AgPd	mp-24286	ZrH2	mp-1203767	Lu3C4
mp-985296	Ag3Pd	mp-24658	SmH2	mp-3924	LiNbO2
mp-1436	EuAg2	mp-753721	GdOF	mp-28030	Li8Nb2O9
mp-665747	EuAg	mp-1224869	Gd2C	mp-759900	K2LiNbO4
mp-621667	Eu3Ag2	mp-642655	K2GdF5	mp-556902	KLi4NbO5
mp-542568	EuAg5	mp-8301	Gd2CF2	mp-4156	Li2ZrO3
mp-1202213	Cs8Ga11Cl	mp-1189998	Gd2C3	mp-5418	Li6Zr2O7
mp-2605	CaO	mp-1800	Nd2C3	mp-17208	K2Li14Zr3O14
mp-1078920	LaCu	mp-24096	NdH2	mp-7100	LaOF
mp-2051	LaCu2	mp-1190994	NdHO	mp-1223447	KLaF4
mp-2613	LaCu5	mp-11719	K4ZnP2	mp-866662	K5La4Si4O16F
mp-1194443	LaCu13	mp-1219429	Sc2CO	mp-5152	La2SiO5

Table S6 Phases with stability in the entire range of K potentials

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-2675	MgNi2	mp-999291	PrPd	mp-866755	LiMg149
mp-23	Ni	mp-16705	Pr2O3	mp-29720	Li21Si5
mp-2137	Mg2Ni	mp-1104184	Pr3Pd4	mp-1094889	LiMg
mp-1185599	Mg149Ni	mp-1571	PrPd3	mp-672287	Li13Si4
mp-1094122	Mg	mp-11239	ZrAg	mp-973374	LiMg2
mp-1179656	Rb	mp-2221	Zr2Ag	mp-1185634	Mg149Si
mp-10172	Na	mp-28395	B6P	mp-1094591	Li3Mg

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1184151	Cs	mp-1189967	Pr3Os	mp-11189	Li2MgSiO4
mp-286	YbSe	mp-567339	PrOs2	mp-1220327	NbMo
mp-972364	Yb	mp-510401	GdP	mp-22141	BaIn2
mp-90	Cr	mp-931	ThP	mp-1105101	Ba9In4
mp-867200	Pm	mp-778	Fe2P	mp-31509	BaIn
mp-1018122	Tm	mp-20587	EuS	mp-605809	Ba11In6O3
mp-697068	SiPd2	mp-24650	YH2	mp-28685	Ba8Ni6N7
mp-20622	SiPd3	mp-2114	YN	mp-21653	BaNiN
mp-505071	Si2Pd9	mp-1849	Mn2P	mp-823	TiCo
mp-2	Pd	mp-17751	Y5Ge3	mp-1102138	TiCoP
mp-35	Mn	mp-17381	Y3Ge4	mp-867373	Ti2Co12P7
mp-1203760	Si7Tc4	mp-13360	Y5Ge4	mp-1191331	Ti2Co
mp-1079910	SiTc	mp-2637	YSe	mp-608	TiCo3
mp-113	Tc	mp-29210	Li2Ga	mp-5380	Ca4P2O
mp-1072399	Be5Pt	mp-9568	Li3Ga2	mp-1345	CaP
mp-126	Pt	mp-1205930	Li5Ga4	mp-1225044	Er2C
mp-87	Be	mp-9546	Yb2C3	mp-24192	ErH2
mp-13	Fe	mp-1103975	YbC6	mp-1203719	Er3C4
mp-2197	BaHg	mp-1185628	Mg149Sb	mp-13236	Ho5Si3
mp-8094	Ba2Hg	mp-600561	LiRh	mp-12899	HoSi
mp-122	Ba	mp-1001787	LiRh3	mp-5835	Ho(CoSi)2
mp-38	Pr	mp-510430	Li13In3	mp-977345	Ho2Co3Si5
mp-1185570	Mg149Pb	mp-31324	Li2In	mp-1203317	Ho5(Co2Si7)2
mp-1185637	Mg149Sn	mp-21293	Li3In2	mp-7577	CoSi
mp-2364	PaO2	mp-867226	Li3In	mp-2435	HoCo5
mp-10740	Pa	mp-1184658	HgPd3	mp-2396	HoCo2
mp-1187073	Sr	mp-1077442	CeAu2	mp-622565	Ho3Co
mp-10658	Dy	mp-1025468	CeAu	mp-19905	Co2Si
mp-11698	Tb	mp-1095658	Tb2Au	mp-2379	CoSi2
mp-865934	YbF2	mp-999141	TbAu	mp-569851	Ho10Si17
mp-1958	SrTe	mp-570179	TbAu2	mp-510688	HoCoSi
mp-134	Al	mp-1071422	CeAg2	mp-30969	Ho12Co7
mp-155	Gd	mp-1080709	NdAu	mp-1185589	Mg149Nb
mp-44	U	mp-12788	Nd3Au4	mp-4883	Ba(FeP)2
mp-571261	Pu	mp-567586	Nd17Au36	mp-631	TiC
mp-72	Ti	mp-1102098	Nd2Au	mp-27919	Ti8C5
mp-19876	InNi	mp-1217874	Tb14Ag51	mp-10721	Ti2C
mp-54	Co	mp-30358	TbAg2	mp-1102496	EuH2
mp-12174	HfNi3	mp-2268	TbAg	mp-1640	Ho2C
mp-1018056	HfNi	mp-13392	NdCu	mp-744	HoP
mp-103	Hf	mp-11852	NdCu2	mp-15238	Ho4C5
mp-30849	TaPt2	mp-1140	NdCu5	mp-1154	Ho4C7
mp-50	Ta	mp-30841	UPd3	mp-1202754	Ho3C4
mp-567638	TaPt3	mp-1326	Nb3Sn	mp-1246246	Ca5(CuN2)2
mp-131	Zr	mp-1542	YB2	mp-844	Ca3N2
mp-75	Nb	mp-637	YB4	mp-1882	CaCu5
mp-253	ScCo2	mp-419	YbB6	mp-585949	CaCu
mp-2212	ScCo	mp-864603	YbH2	mp-2686	Ca2N
mp-27162	Sc3Co	mp-1189298	YbB4	mp-12614	Ca2Cu
mp-67	Sc	mp-1186271	NaMg149	mp-1208630	SrC6
mp-8	Re	mp-1185635	Mg149Tl	mp-20181	Ce2C3
mp-569535	Ca2Bi	mp-20831	Gd4Sb3	mp-1199934	Ti3As
mp-132	Ca	mp-510403	GdSb	mp-1201836	Ti5As3
mp-27145	Ca5Bi3	mp-570606	Pr4Ge3	mp-9172	Li4TiO4

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Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-2512	AsPd5	mp-1674	PrSe	mp-38280	LiTiO2
mp-123	Nd	mp-511	PrGe	mp-2931	Li2TiO3
mp-1184115	Er	mp-867190	Pr4Ge7	mp-692	Tb2C
mp-101	Ir	mp-504731	EuF2	mp-645	TbP
mp-2732	PRh2	mp-201	Yb5Sb3	mp-15237	Tb4C5
mp-74	Rh	mp-1857	YbCd	mp-1585	V3Co
mp-145	Lu	mp-1187653	YbCd3	mp-542614	VCo3
mp-1299	SiPt2	mp-770806	Sm2TiO5	mp-555617	Ce10Si8O3
mp-864675	Yb3N2	mp-753192	Yb4Sb2O	mp-2088	CeAl2
mp-864757	YbN2	mp-601	PrP	mp-567305	CeAl3
mp-91	W	mp-13971	Nd2SeO2	mp-1206597	CeAlSi
mp-1057315	Eu	mp-1453	NdSe	mp-1213865	Ce3Al11
mp-33	Ru	mp-7233	La2SeO2	mp-866134	VFe3
mp-49	Os	mp-22266	GdB6	mp-1079399	V3Fe
mp-705522	Sr28In11	mp-1105563	GdB4	mp-20937	Cr3C2
mp-20074	SrIn2	mp-28366	Gd2B5	mp-1196316	Cr7C3
mp-608072	SrIn	mp-2748	CeAs	mp-723	Cr23C6
mp-2286	Li2Se	mp-18051	La2TiO5	mp-866691	La2PC
mp-1018134	Li	mp-1766	TmS	mp-730	P2Pt
mp-1187198	SrMg2	mp-3556	Tm2SO2	mp-13871	P2Pt5
mp-30782	Sr6Mg23	mp-1767	Tm2O3	mp-769173	PrOF
mp-86	Sm	mp-467	Th3N4	mp-11649	Ca3SiO
mp-1519	CaTe	mp-834	ThN	mp-2517	Ca2Si
mp-37	Th	mp-1464	Nd5Ge3	mp-956	U3Si
mp-1079438	Ta2N	mp-172	Nd5Ge4	mp-2800	USi3
mp-1279	TaN	mp-663	NdGe	mp-1563	CaSi
mp-975834	MoRu3	mp-2015	Nd3Ge5	mp-793	Ca5Si3
mp-129	Mo	mp-865834	Yb3GeO	mp-4481	Ca2SiO4
mp-1183252	BIr	mp-1694	Yb2Ge	mp-2090	FeCo
mp-1185513	HfMg149	mp-21300	Yb5Ge4	mp-601848	Fe11Co5
mp-1265	MgO	mp-13973	Gd2SeO2	mp-601820	Fe3Co
mp-352	HfO2	mp-1216020	Zn35Cu17	mp-601842	Fe9Co7
mp-615	YMg	mp-987	ZnCu	mp-12108	VPt2
mp-2652	Y2O3	mp-1368	Zn8Cu5	mp-2678	VPt
mp-1187739	Y	mp-1065	LaSb	mp-2211	V3Pt
mp-865376	YMg3	mp-759	La2Sb	mp-1079997	VPt8
mp-1188082	YMg149	mp-1223	La4Sb3	mp-2705	VPt3
mp-1185557	Mg149Bi	mp-32606	Ba3P2	mp-316	MnV
mp-11534	Np	mp-17566	Ba5P4	mp-28731	V6C5
mp-682	NaF	mp-28823	Ba4P3	mp-20648	V2C
mp-1184119	CuPd3	mp-9968	PrSi	mp-864984	MnV3
mp-1018029	CuPd	mp-1079937	Pr3Si2	mp-3637	YOF
mp-580357	Cu3Pd	mp-27760	PrSi2	mp-4511	La2SO2
mp-30	Cu	mp-1185586	Mg149Be	mp-28255	LaHO
mp-1138	LiF	mp-855	MgBe13	mp-24153	LaH2
mp-11471	ScHg	mp-30842	ZrPd3	mp-1104116	La2H5
mp-861910	Sc3Hg	mp-266	Zr2Pd	mp-1103808	La4H9
mp-19713	Sc3In	mp-13495	ZrPd	mp-568656	SiC
mp-31348	Sc2In	mp-1623	ErS	mp-23715	BaH2
mp-1207100	ScIn	mp-12671	Er2SO2	mp-2091	V3B2
mp-571222	CsBr	mp-679	Er2O3	mp-9973	VB
mp-614603	CsI	mp-1213824	Ce4Ge3	mp-1206441	V5B6
mp-1200207	Cs8Ga11	mp-2563	CeSe	mp-569270	V3B4
mp-1837	TbCu	mp-1200696	Ce5Ge4	mp-9208	V2B3

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1610	TbS	mp-1213848	Ce4Ge7	mp-1491	VB2
mp-1527	TbCu2	mp-2154	CeP	mp-8780	Cr2N
mp-11363	TbCu5	mp-1144	ErP	mp-1183691	CrN
mp-1971	HoCu	mp-13415	Ta3B2	mp-24092	GdH2
mp-1240	HoS	mp-1097	TaB	mp-1191288	Eu2Ta2O7
mp-10659	Ho	mp-1108	TaB2	mp-1101654	NaEuO2
mp-30584	HoCu2	mp-10142	Ta3B4	mp-2489	UC
mp-30585	HoCu5	mp-1269	SmS	mp-2486	UC2
mp-674332	U17O31	mp-710	SmP	mp-2625	U2C3
mp-2104	UAs	mp-31380	SmPd	mp-10970	LiErO2
mp-1597	UO2	mp-1104311	Sm3Pd4	mp-12645	LiHoO2
mp-30794	Na15Sn4	mp-662804	Sm10Pd21	mp-1672	CaS
mp-1014265	Zr2N	mp-357	SmPd3	mp-7656	Na5GaO4
mp-1352	ZrN	mp-19830	ErN	mp-27618	Na8Ga2O7
mp-277	Zr3N4	mp-551675	Li3UO4	mp-568151	Ti5Ge3
mp-1183425	Be3Co	mp-8609	Li6UO6	mp-1198692	Ti5Ge4
mp-2773	BeCo	mp-1072248	EuSi2	mp-1699	AlCr2
mp-1071690	Be5Co	mp-21279	EuSi	mp-867780	Al3Cr
mp-554098	Ti6O	mp-1190061	Eu5Si3	mp-31019	Al45Cr7
mp-2591	Ti3O	mp-1751	ThSb	mp-754237	LiTmO2
mp-1215	Ti2O	mp-736	Li3P	mp-21332	LiGdO2
mp-1071163	TiO	mp-11270	MnBe2	mp-540809	Zr2Fe12P7
mp-685008	Ba20As13	mp-1104792	MnBe12	mp-20892	ZrFeP
mp-504425	Nb3As	mp-1153	Li2S	mp-31415	La3TaO7
mp-492	TiN	mp-1934	LiZn	mp-30337	Al5W
mp-8282	Ti2N	mp-975799	LiZn3	mp-1620	Si2W
mp-926	PuP	mp-1077209	TmCu2	mp-1227997	AlSi3W2
mp-999336	NdPd	mp-985	TmCu	mp-11227	Al12W
mp-1045	Nd2O3	mp-2822	TmSe	mp-1018178	Ba2Zn
mp-1104199	Nd3Pd4	mp-30600	TmCu5	mp-303	BaZn5
mp-2333	NdPd3	mp-677	SrCd2	mp-30435	BaZn2
mp-7806	Cr3P	mp-2585	Sr5Sb3	mp-210	BaLi4
mp-21048	CrP	mp-30496	SrCd	mp-672225	BaZn13
mp-570421	Sm2B5	mp-542484	Sr5Cd3	mp-1192350	NbFe2
mp-218	Sm2O3	mp-20995	Eu4As3	mp-1221111	NbFe
mp-8546	SmB4	mp-1106024	Eu5As3	mp-768342	SrNb2O4
mp-6996	SmB6	mp-1169	ScCu	mp-28940	Sr4Nb2O9
mp-1346	B6O	mp-1018149	ScCu2	mp-729	Cr3Si
mp-1960	Li2O	mp-1025122	LuCu2	mp-8937	CrSi2
mp-7083	LaSi	mp-580136	LuCu5	mp-784631	CrNi2
mp-1161	LaSe	mp-1017985	TiAg	mp-19096	Ba2VO4
mp-10961	La5Si3	mp-979115	Ti2Ag	mp-1185655	Mg149Zr
mp-26	La	mp-980769	SmCu	mp-11317	CeFe5
mp-2062	LaSi2	mp-1077154	SmCu2	mp-259	AlMo3
mp-862690	Ac	mp-227	SmCu5	mp-568153	Al22Mo5
mp-655	Na3As	mp-1185593	Mg149P	mp-2733	Al8Mo3
mp-146	V	mp-1185632	Mg149Se	mp-1219908	PdPt
mp-20300	EuP	mp-1077788	BPt2	mp-754225	YbTiO3
mp-21394	EuO	mp-2807	ScP	mp-23714	SrH2
mp-1105092	Eu3P4	mp-22600	Sc3P2	mp-541294	SrNi9P5
mp-2292	La2O3	mp-1188800	Sc3P	mp-18632	SrNi5P3
mp-7283	LaB4	mp-1186074	Na3Pd	mp-1418	FeNi3
mp-2680	LaB6	mp-862658	LiCu3	mp-2213	FeNi
mp-262	Na3B20	mp-742	Ti2Cu	mp-29634	V4P2C

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Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-984	BN	mp-1188441	TiCu4	mp-1195743	V18P9C2
mp-2315	NaB15	mp-2078	TiCu	mp-1029457	Ba(CoN)2
mp-28630	Na3BN2	mp-2643	Ti3Cu4	mp-505765	BaCoN
mp-1187343	RbMg149	mp-12546	TiCu3	mp-28645	CaNiN
mp-1104	LaMg	mp-1079111	EuTiO3	mp-2295	CaNi2
mp-1094174	LaMg3	mp-1025200	Eu2TiO4	mp-774	CaNi5
mp-1104815	LaMg12	mp-12670	Ho2SO2	mvc-9921	MgCr2O4
mp-2616	NpO2	mp-1029	BaF2	mp-1185585	Mg149Cr
mp-1183995	GaCu3	mp-2080	SrBe13	mp-1216160	Y4Zr3O12
mp-1197621	Ga4Cu9	mp-981	SrF2	mp-27731	HfH2
mp-1185639	Mg149Ti	mp-4764	Pr2SeO2	mp-763	MgB2
mp-2334	DyCu	mp-12802	AlCu3	mp-365	MgB4
mp-2470	DyS	mp-985806	Al2Cu	mp-978275	MgB7
mp-1071835	DyCu2	mp-2500	AlCu	mp-24095	PrH2
mp-1225307	DyCu5	mp-593	Al4Cu9	mp-343	PrN
mp-11247	Li3Au	mp-20712	EuGe	mp-532160	Ca14MnP11
mp-1206794	LiAu	mp-1095642	Eu2Ge	mp-30980	NaYO2
mp-567395	Li15Au4	mp-1188934	Eu5Ge3	mp-17891	NaYSiO4
mp-21294	Y2In	mp-530539	Sr4U2O9	mp-30811	Ni4W
mp-22704	YIn	mp-3956	Sr3UO6	mp-5327	Na4UO5
mp-1105835	Y3In5	mp-1898	CeSi2	mp-34842	Na3UO4
mp-20131	YIn3	mp-570175	Ce5Si3	mp-1229032	AgPt4
mp-571095	Na7Ga13	mp-21115	CeSi	mp-1229015	AgPt
mp-2074	Li3Sb	mp-1196829	Ce5Si4	mp-8470	NaPrO2
mp-22903	RbI	mp-11506	Ni3Mo	mp-1477	BaSi2
mp-7956	Na3Sb	mp-11507	Ni4Mo	mp-1619	Ba3Si4
mp-757	Li3As	mp-890	NdIr2	mp-1067235	BaSi
mp-1220249	Pr14Ag51	mp-30522	Nd5Ir3	mp-9905	Ba2Si
mp-1072619	PrAg2	mp-1104605	Nd5Ir2	mp-17612	Ba2SiO4
mp-2525	PrAg	mp-1189686	Nd3Ir	mp-755363	Ba3SiO
mp-985805	AlAg2	mp-1777	Li15Ge4	mp-10923	Ca2Co12P7
mp-1228988	AlAg3	mp-27932	Li9Ge4	mp-3210	Ca(CoP)2
mp-1018131	LuAg2	mp-1188469	La5Ge3	mp-567290	LaN
mp-568953	LuAg4	mp-1084830	LaGe	mp-1019893	La3Si6N11
mp-2647	Al2Au	mp-1211472	La4Ge7	mp-1019967	LaSi3N5
mp-979911	Y2Au	mp-1738	SmAs	mp-569576	La5(SiN3)3
mp-1066254	YAu	mp-19891	Pu2C3	mp-7400	NaAlGe
mp-1018113	YAu2	mp-980757	Sm5Sb3	mp-2970	Na4GeO4
mp-1079811	SmAu	mp-2281	SmSb	mp-31008	Na14Al4O13
mp-2474	YAg	mp-2634	NbN	mp-556168	Na7Al3O8
mp-1216365	Y14Ag51	mp-1079585	Nb2N	mp-9212	NaAlO2
mp-999544	YAg2	mp-2760	Nb6C5	mp-13998	Na5AlO4
mp-2399	YHg	mp-569989	Nb2C	mp-14266	Cu15Si4
mp-1103395	La2Au	mp-12659	Mn2Nb	mp-571056	CsSn
mp-1002136	LaAu	mp-542583	EuTe	mp-2363	HfMo2
mp-1072087	LaAu2	mp-11345	ZrP	mp-22907	DyBi
mp-11237	ScAg	mp-22447	Zr3P	mp-31464	Dy5Bi3
mp-30354	ScAg4	mp-647729	Zr14P9	mp-568646	Ta3Si
mp-1018128	ScAg2	mp-583740	Zr7P4	mp-1989	Ta5Si3
mp-1236	NdAg	mp-2296	Ni3P	mp-1192906	Ba4Ta2O9
mp-18511	NdF3	mp-2790	Ni12P5	mp-11192	TaSi2
mp-1220721	Nd14Ag51	mp-17833	Ba3GeO	mp-504554	Ba5Ta4O15
mp-1072737	NdAg2	mp-13922	Ba2Ge	mp-2631	Ba4Al5
mp-2621	ErAg	mp-9858	Ba3Ge4	mp-4202	BaAl2O4

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-30339	ErAg2	mp-1188954	Ba3Ge5	mp-13149	BaAlSi
mp-1225453	Er14Ag51	mp-2627	DyAs	mp-1903	BaAl4
mp-2667	CsAu	mp-510557	CsN3	mp-567701	Ba21Al40
mp-567332	Ce	mp-1079938	TlPd3	mp-9578	Ba3(AlSi)2
mp-20857	CoB	mp-1063174	GdAu2	mp-570400	Ba7Al10
mp-1019608	Cs3BO3	mp-635426	GdAu	mp-5506	Ba(AlSi)2
mp-1056	Tb2O3	mp-2475	SmAg	mp-560978	Ba4Al2O7
mp-1253	BaSe	mp-1219378	Sm14Ag51	mp-11651	Yb3SnO
mp-865782	Yb3SiO	mp-2167	DyAg	mp-570050	Yb2Sn
mp-1216	YbO	mp-1225847	Dy14Ag51	mp-2806	YbSn
mp-10651	YbSi	mp-2618	DyAg2	mp-542915	TiAl3
mp-1207599	Yb2Si	mp-464	HoSe	mp-567705	TiAl2
mp-1077404	YbSi2	mp-8300	Ba4As2O	mp-1823	Ti3Al
mp-567735	Nd5Si3	mp-1221	V3Ge	mp-1953	TiAl
mp-884	NdSi2	mp-752658	Y2SeO2	mp-12894	Y2SO2
mp-9967	NdSi	mp-1753	ThAs	mp-30352	NaAg2
mp-355	Nd5Si4	mp-1405	TbGe	mp-2493	CeN
mp-19879	PPd3	mp-2610	Tb5Ge3	mp-1409	TiNi3
mp-1618	PPd6	mp-1673	Tb5Ge4	mp-1048	TiNi
mp-1820	YbS	mp-1193534	YBe13	mp-1808	Ti2Ni
mp-12673	Lu2SO2	mp-965	TbB2	mp-1018104	Zr2Cd
mp-1427	Lu2O3	mp-568225	TbB4	mp-8299	Sr4As2O
mp-11266	BaCd2	mp-13972	Sm2SeO2	mp-24338	Sr5As3H
mp-9909	Ba5Sb3	mp-21075	HfC	mp-21188	CeNi
mp-527	BaCd	mp-12960	Er5Sb3	mp-580354	CeNi3
mp-8093	Ba2Cd	mp-2191	ErSb	mp-1654	CeNi2
mp-2801	CeCu2	mp-2593	AlNi3	mp-1204381	Ce2Ni7
mp-1096	CeS	mp-622209	Al3Ni	mp-1910	CeNi5
mp-581942	CeCu6	mp-1057	Al3Ni2	mp-1229288	Ce15Ni32
mp-570001	Al6Fe	mp-16515	Al4Ni3	mp-24119	Ca2HN
mp-2658	AlFe	mp-1487	AlNi	mp-644307	Ca(H2N)2
mp-1183162	AlFe3	mp-16514	Al3Ni5	mp-34932	CaHN
mp-13155	Hf2Ag	mp-29621	Ba5Bi3	mp-867264	Re3Os
mp-13156	HfAg	mp-1189863	Tm5Si3	mp-1219509	ReOs
mp-21289	TiZn3	mp-1066975	TmSi	mp-867141	ReOs3
mp-1014229	Ti2Zn	mp-1203324	Zr3Ge	mp-13975	Er2SeO2
mp-1014230	TiZn	mp-17706	Zr5Ge3	mp-1334	Y2C
mp-543051	Lu5Sb3	mp-1025513	ZrGe	mp-9459	Y4C5
mp-516	LuSb	mp-1200749	Zr5Ge4	mp-1200613	Y3C4
mp-2681	Ho5Sb3	mp-865166	HfPd5	mp-1200885	Y4C7
mp-812	Ho2O3	mp-11453	HfPd3	mp-1894	WC
mp-2050	HoSb	mp-11454	Hf2Pd	mp-31167	Er5Si3
mp-2147	SrGe	mp-1007692	HfPd	mp-378	ErSi
mp-2472	SrO	mp-4657	Li5GaO4	mp-749	SmN
mp-30950	Sr3GeO	mp-8253	Na5ReO6	mp-24724	TbH2
mp-2576	Sr2Ge	mp-1199558	Sm5Ir3	mp-1591	Al4C3
mp-1218382	Sr4Bi2O	mp-7342	Sm3Ir	mp-1216546	Tm2C
mp-29620	Sr5Bi3	mp-1104500	Sm5Ir2	mp-7171	TmP
mp-979289	TaW3	mp-1104610	Eu5Pd2	mp-1205180	Tm3C4
mp-1187206	Ta3W	mp-1854	EuPd2	mp-1219177	Sm2C
mp-1217811	TaW	mp-1018147	EuPd	mp-569335	Sm2C3
mp-683	Pr2C3	mp-1105286	Eu3Pd2	mp-3151	Li3TaO4
mp-2384	LaP	mp-1002115	LaPd	mp-755013	Li5TaO5
mp-1038	MgCu2	mp-1104435	La3Pd4	mp-31417	Nd3TaO7

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Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-2481	Mg2Cu	mp-674	LaPd3	mp-755586	NaLaO2
mp-1342	BaO	mp-1105925	La7Pd3	mp-14964	Pr3TaO7
mp-3020	BaNbO3	mp-30753	LaPd5	mp-1222413	LiB3
mp-542201	Ba3Nb2O8	mp-567412	Y5Sn3	mp-27275	Li3BO3
mp-4651	SrTiO3	mp-1199133	Y11Sn10	mp-1001835	LiB
mp-5532	Sr2TiO4	mp-994	YP	mp-1078191	Ba2TeO
mp-3349	Sr3Ti2O7	mp-1219144	Sm2AsSe	mp-2117	TbN
mp-2011	UP	mp-661	AlN	mp-1189033	Tb3Ru
mp-787	U3P4	mp-1472	ZrB2	mp-1101970	TbRu2
mp-1377	ThCu2	mp-27191	Zr9S2	mp-23850	NaH2N
mp-503	ThS	mp-1197374	Zr2S	mp-30883	V4Zn5
mp-1217740	Th14Cu51	mp-708	LaAs	mp-972422	U3Ge
mp-12834	ThCu6	mp-30975	Na3BO3	mp-571370	Fe2NiP
mp-279	LiIr	mp-7664	Na6ZnO4	mp-6499	BaLiBO3
mp-30738	LiIr3	mp-19334	Na4WO5	mp-8204	LiAlB14
mp-30579	ErCu5	mp-1220316	NbW	mp-530274	Al23B50
mp-1024991	ErCu2	mp-3744	NaNbO2	mp-15960	Li5AlO4
mp-1955	ErCu	mp-27247	Na3NbO4	mp-3427	LiAlO2
mp-2491	ErSe	mp-5477	Na5NbO5	mp-567415	Nd2B5
mp-1203025	Np2N3	mp-972071	V3Mo	mp-1632	NdB4
mp-2596	NpN	mp-19391	NaVO2	mp-1929	NdB6
mp-10688	CeO	mp-754829	Na4VO4	mp-1380	Zn3Ru
mp-542313	Ce2O3	mp-8957	Na5TaO5	mp-1205290	Zn6Ru
mp-2629	Ce7O12	mp-1187695	V3Cr	mp-27335	NaAlSi
mp-760323	Ce5O9	mp-1216394	VCr	mp-477	SmGa2
mp-23222	Li3Bi	mp-1187696	VCr3	mp-1195872	Sm3Ga2
mp-23870	NaH	mp-578604	NaCrO2	mp-1776	UN2
mp-504886	Gd2O3	mp-2542	BeO	mp-32590	U4N7
mp-1215377	Zr4O	mp-27757	Be4B	mp-32742	U16N25
mp-1200894	Zr3As	mp-1188434	Y5Ti3	mp-1865	UN
mp-561418	Zr3O	mp-11575	YTi	mp-1216828	U2CN
mp-1682	ZrAs	mp-1101816	Lu2Au	mp-12668	Tb2SO2
mp-972228	Zr3As2	mp-11249	LuAu	mp-485	ZrNi3
mp-1191610	Zr7As4	mp-1018152	LuAu2	mp-556	ZrNi
mp-1203256	Zr14As9	mp-11219	LuB2	mp-328	Zr2Ni
mp-1198302	Nb3Ge	mp-10192	LuP	mp-2717	Zr2Ni7
mp-16842	Nb5Ge3	mp-571495	LuB4	mp-2271	NaPt2
mp-1598	Na3P	mp-1104289	LuB12	mp-1018129	Pt2W
mp-31430	Na2In	mp-1185565	Mg149Mo	mp-5598	Sm2SO2
mp-2352	Na2O	mp-1185556	Mg149H	mp-1139	Co3Mo
mp-769284	Dy2SeO2	mp-21256	Mn7C3	mp-3161	LiAlSi
mp-814	DySe	mp-542830	Mn23C6	mp-976726	LiDyO2
mp-2345	Dy2O3	mp-1188076	ThMg149	mp-754605	LiLuO2
mp-18350	V3P	mp-642644	V2H	mp-1185578	Mg149S
mp-684675	V12P7	mp-554546	Eu2SiO4	mp-24726	TiH2
mp-1192783	V4P3	mp-206	Tb5Si3	mp-4805	Gd2SO2
mp-20541	V2P	mp-1924	TbSi	mp-24727	TmH2
mp-20689	Nb3B2	mp-6964	NaTbO2	mp-1975	TmN
mp-2580	NbB	mp-7500	Na4SiO4	mp-10572	NaPN2
mp-450	NbB2	mp-4533	Na2SiO3	mp-7639	Na2CuP
mp-10255	Nb3B4	mp-754027	NaSmO2	mp-1019519	Ba2NaO
mp-1080021	Nb2B3	mp-8128	NaNdO2	mp-866141	TiFe2Si
mp-3211	Nd2SO2	mp-1569	Be2C	mp-2199	Fe3Si
mp-1748	NdS	mp-2390	YbP	mp-1247744	BaNa

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1193889	HoBe13	mp-1187909	Yb3P	mp-11820	BaNa2
mp-576	B13C2	mp-19340	LiVO2	mp-8648	TiFeSi
mp-574275	Li17Pb4	mp-551835	Ba2I2O	mp-2108	Ti5Si3
mp-30761	Li7Pb2	mp-1196393	Y3Sb	mp-505527	Ti5Si4
mp-30760	Li3Pb	mp-568320	Y4Sb3	mp-305	TiFe
mp-2350	LaS	mp-215	YSb	mp-16253	BaCaSi
mp-614724	Cs3CrF7	mp-7020	LiYO2	mp-21662	TiFeSi2
mp-739	TiP	mp-7137	LiTbO2	mp-1714	FeSi2
mp-1191079	Ti7P4	mp-10004	Mo3P	mp-7092	TiSi
mp-30218	Ti2P	mp-219	MoP	mp-871	FeSi
mp-31214	Ti3P	mp-1552	Mo2C	mp-1077503	TiSi2
mp-616559	Ti2S	mp-7822	Sc5Si3	mp-560889	Ba6Na2Si4O15
mp-1224756	Hf14Cu51	mp-216	Sc2O3	mp-10247	U2CrN3
mp-30581	Hf2Cu	mp-1727	SrSi2	mp-865652	TiMn2Si
mp-1200988	Hf7Cu10	mp-9969	ScSi	mp-27569	Na14Mn2O9
mp-7353	Hf3Cu8	mp-2661	SrSi	mp-1216621	TiW
mp-1102043	LaOs2	mp-18510	Sr2SiO4	mp-1202079	Ti21Mn25
mp-16839	Na3WN3	mp-770771	SrSc2O4	mp-865656	TiMn2W
mp-978	Sr2Sn	mp-30949	Sr3SiO	mp-1949	TiMn2
mp-15698	Sr5As3	mp-746	Sr5Si3	mp-21606	TiMnSi2
mp-17720	Sr5Sn3	mp-1106	Sr2Si	mp-1217077	Ti2Si6W
mp-1698	SrSn	mp-505002	Sc5As3	mp-2726	SrCu5
mp-29424	Sr4As3	mp-17695	Sc5Sn3	mp-21609	SrCuN
mp-570240	La14C14Cl9	mp-1188926	Sc3As2	mp-29136	Sr6Cu3N5
mp-2367	LaC2	mp-2052	ScAs	mp-1025402	SrCu
mp-567694	La2C2Cl	mp-865168	Be3Ni	mp-6406	Na2MgSiO4
mp-1184	La2C3	mp-1033	BeNi	mp-5473	CaMgSi
mp-2795	ZrC	mp-1892	Ba2N	mp-9702	Sr3BPO3
mp-684623	Zr10C9	mp-29199	BaCuN	mp-1079146	Th3Si2
mp-21009	EuSe	mp-1001	BaN2	mp-21238	ThSi
mp-2599	NdN	mp-30428	BaCu	mp-7497	ThSi2
mp-11908	Lu5Si3	mp-10736	Ba3N	mp-3536	MgAl2O4
mp-1001612	LuSi	mp-568643	RbC8	mp-1185596	Mg149Al
mp-504502	Ta3P	mp-14726	Na4TiO4	mp-1094116	MgAl2
mp-22477	Ta2P	mp-242	SrB6	mp-2151	Mg17Al12
mp-1067587	TaP	mp-556695	NaSrBO3	mp-1185597	Mg149Ga
mp-769271	Sr4Ta2O9	mp-16432	Sr3(BO3)2	mp-1770	Mg5Ga2
mp-1077933	GdCu2	mp-1241	BaAg2	mp-30650	Mg2Ga
mp-510404	GdSe	mp-1000	BaTe	mp-23063	Ba4Cl6O
mp-614455	GdCu	mp-11840	BaAg	mp-17143	BaGd2O4
mp-636253	GdCu5	mp-1814	BaAg5	mp-173	MnAl6
mp-9972	YSi	mp-12612	Ba3Ag2	mp-408	Mg2Ge
mp-677445	Y4Si3	mp-504812	Hf3P	mp-2856	Mn4Al11
mp-1534	YS	mp-20672	Hf3P2	mp-771	MnAl
mp-2538	Y5Si3	mp-9953	HfP	mp-865027	Mn3Ge
mp-1216441	Zr14Cu51	mp-504659	Hf2P	mp-1185627	Mg149Mn
mp-193	Zr2Cu	mp-7226	V3Ni	mp-570150	CaAlSi
mp-1188077	Zr7Cu10	mp-171	VNi3	mp-7704	Ca(AlSi)2
mp-1039345	CeMg2	mp-11531	VNi2	mp-721592	Ca6Al7O16
mp-1038976	CeMg5	mp-1216708	V3Ni2	mp-640340	Ca4MgAl3
mp-19918	GdGe	mp-9712	Ba3BPO3	mp-867878	AlFe2Si
mp-1198083	Gd5Ge4	mp-954	BaB6	mp-29110	Al2(FeSi)3
mp-510402	GdS	mp-755417	Ba3(BO3)2	mp-1190708	Al3Fe2Si

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Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-1186974	Sc3Ti	mp-28164	Ba4P2O	mp-1229054	Al53Fe17Si12
mp-7396	Li3Ti	mp-30429	Ba8Ga7	mp-1229249	Al79(Fe13Si9)2
mp-12283	Li5Ti2	mp-1219	BaGa2	mp-351	SiNi
mp-1786	Ti3Au	mp-335	BaGa4	mp-1118	SiNi2
mp-1087547	EuCu	mp-1105598	Y3Co	mp-828	SiNi3
mp-2066	EuCu5	mp-865373	YCo	mp-27276	Si12Ni31
mp-1071732	EuCu2	mp-1294	YCo2	mp-1214980	Al11(CoSi)6
mp-1018148	ScAu2	mp-3952	BaY2O4	mp-1214851	Al3Co3Si4
mp-11256	ScAu	mp-19870	GaFe3	mp-10010	Al(CoSi)2
mp-2462	PrCu5	mp-636368	Ga3Fe	mp-1185642	Mg149Zn
mp-1071904	PrCu2	mp-804	GaN	mp-680671	Mg4Zn7
mp-1079091	PrCu	mp-1804	Fe3N	mp-978269	MgZn2
mp-1095690	Tm2Au	mp-6988	FeN	mp-5529	MnFe2Si
mp-1017507	TmAu	mp-1185592	Mg149Fe	mp-861983	Ti2MnFe
mp-560	TmAu2	mp-22204	Co2P	mp-559904	NaLi3SiO4
mp-1102972	Er2Au	mp-1185590	Mg149I	mp-1221619	MnFeSi2
mp-11243	ErAu	mp-1039148	CaMg	mp-1079460	Ti3Sn
mp-2466	ErAu2	mp-2432	CaMg2	mp-30875	Ti2Sn
mp-1103411	Dy2Au	mp-1184449	CaMg149	mp-676653	Lu4Hf3O12
mp-1007918	DyAu	mp-1185641	Mg149V	mp-1559	Mg3N2
mp-11241	DyAu2	mp-21895	Na15Pb4	mp-1106020	Zr5SiSn3
mp-1080443	YCu	mp-568636	TiCr2	mp-20318	Mn2B
mp-2698	YCu2	mp-11580	TiCrP	mp-10118	Mn3B4
mp-2797	YCu5	mp-1217052	Ti6P2O	mp-1106184	MnB4
mp-2714	Pr2Au	mp-1102537	NbVP	mp-1185549	Mg149Br
mp-1079915	PrAu	mp-3397	Ba2TiO4	mp-1185584	Mg149Cl
mp-30415	PrAu2	mp-292	V3As	mp-18793	LiCrO2
mp-1071698	EuAu2	mp-1199486	Gd5Si4	mp-1199908	Cs7NaSi8
mp-1078589	EuAu	mp-601371	GdSi	mp-2252	ScB2
mp-1189094	Eu3Au	mp-21192	GdSi2	mp-1226479	CrH15N6Cl2O
mp-1106137	Eu7Au3	mp-952	MoPt2	mp-24152	HoH2
mp-1104457	Eu3Au2	mp-999502	MoPt	mp-1206820	HoRu3C
mp-2796	TmAg	mp-1278	Zr2Si	mp-883	HoN
mp-30359	TmAg2	mp-893	ZrSi	mp-977585	Zr3Ti
mp-1229012	AgPd	mp-1207024	Zr3Si2	mp-505569	CeH2
mp-985296	Ag3Pd	mp-8789	Ca4As2O	mp-1104579	Ce2H5
mp-1436	EuAg2	mp-23713	CaH2	mp-1080525	FeB
mp-665747	EuAg	mp-10047	Ca5As3	mp-1915	Fe2B
mp-621667	Eu3Ag2	mp-1194887	Ca4As3	mp-1194531	Fe2B7
mp-542568	EuAg5	mp-680339	Mn4Si7	mp-1121	GaCo
mp-1202213	Cs8Ga11Cl	mp-1431	MnSi	mp-20559	Ga3Co
mp-2605	CaO	mp-20211	Mn3Si	mp-24151	DyH2
mp-1078920	LaCu	mp-5088	NaGdO2	mp-12669	Dy2SO2
mp-2051	LaCu2	mp-13686	Nb5Si3	mp-12574	Dy2C
mp-2613	LaCu5	mp-12104	NbSi2	mp-1212812	Dy4C5
mp-1194443	LaCu13	mp-2836	Dy5Si3	mp-1213387	Dy3C4
mp-972521	SmGe	mp-2620	DySi	mp-570466	Li2Ca
mp-1506	Sm5Ge4	mp-569825	Dy10Si17	mp-865965	Li2CaSi
mp-1447	SmSe	mp-21524	SrNiN	mp-13916	LiCaSi2
mp-9339	NbP	mp-1245	Sr2N	mp-20150	LiCa2Si3
mp-505528	Nb3P	mp-10564	SrN2	mp-30766	Li5Sn2
mp-505064	Nb2P	mp-29973	SrN	mp-573471	Li17Sn4
mp-648999	Nb5P3	mp-2049	ZrMo2	mp-30767	Li7Sn2

Material ID	Formula	Material ID	Formula	Material ID	Formula
mp-18254	Nb7P4	mp-16488	Al9Co2	mp-1185265	Li3Sn
mp-983509	Na3Cd	mp-196	Al5Co2	mp-990440	Na2ZrO3
mp-1217395	Th4C3	mp-284	AlCo	mp-28559	Na6Be8O11
mp-1164	ThC	mp-974437	Re2C	mp-28588	Na2BeO2
mp-643	ThO2	mp-24286	ZrH2	mp-1105633	Y3Ni
mp-1217298	Th5C	mp-24658	SmH2	mp-582134	Y3Ni2
mp-1188514	Th2C3	mp-753721	GdOF	mp-1364	YNi
mp-7224	ThC2	mp-1224869	Gd2C	mp-2152	YNi5
mp-20711	Fe3Ge	mp-8301	Gd2CF2	mp-574339	Y2Ni7
mp-601833	Fe13Ge3	mp-1189998	Gd2C3	mp-1200338	Y15Ni32
mp-1363	Na2Au	mp-1800	Nd2C3	mp-569196	YNi3
mp-2744	LiPd	mp-24096	NdH2	mp-35730	BaUO3
mp-728	Li2Pd	mp-1190994	NdHO	mp-583034	Ba2U2O7
mp-1079855	LiPd7	mp-1219429	Sc2CO	mp-557448	Ba2CaUO6
mp-1197547	Li15Pd4	mp-24237	ScH2	mp-1845	CaBe13
mp-861936	LiPd3	mp-29941	Sc2C	mp-11449	HfMn2
mp-1560	LaTe	mp-15661	Sc4C3	mp-1212189	HfMnP
mp-1103990	EuC6	mp-28733	Sc3C4	mp-33090	V2N
mp-17904	Nd2TiO5	mp-1173761	Na2CeO3	mp-1018027	VN
mp-1025059	LaAg2	mp-3972	Ce2SO2	mp-1188283	V8N
mp-1948	LaAg	mp-510522	Zr5Sn3	mp-1215471	Zr2HC
mp-11283	ZrBe5	mp-543001	Zr5Sn4	mp-1185594	Mg149In
mp-30445	ZrBe13	mp-559426	Pr2Zr2O7	mp-30228	Li4HN
mp-2544	Zr2Be17	mp-1842	NbAl3	mp-2251	Li3N
mp-541787	Na8Hg3	mp-18427	Nb2Al	mp-1201065	Li15H9N8
mp-31205	Zr3Fe	mp-1104164	Ba3Au2	mp-23702	LiH2N
mp-1190681	ZrFe2	mp-1214417	BaC6	mp-1200910	Li7H5N4
mp-582924	Zr6Fe23	mp-570775	BaAu	mp-20147	ZrMnP
mp-2823	NdP	mp-30363	BaAu2	mp-1112	CeCo2
mp-2116	ZrMn2	mp-9488	SmOF	mp-864889	ZrZn3
mp-12662	Re24Mo5	mp-1025489	SmSi	mp-1401	ZrZn2
mp-1981	Ba2Sn	mp-1106373	Sm5Si3	mp-570276	ZrZn
mp-872	BaSn	mp-8298	Sr4P2O	mp-3236	Pr2SO2
mp-567276	TaV2	mp-32635	Sr3P2	mp-2495	PrS
mp-637224	Pu2O3	mp-7931	SrP	mp-1213975	CaB4
mp-24720	PuH2	mp-505622	Mn4N	mp-865	CaB6
mp-1959	PuO2	mp-9981	Mn2N	mp-1102980	NbFeP
mp-639805	Ta3Ge	mp-28861	CsC8	mp-1206854	TiMnP
mp-17593	Ta5Ge3	mp-2157	Co3W	mp-542995	Nb6Fe16Si7
mp-1210753	Li2Al	mp-1222825	Lu4Zr3O12	mp-1196167	NbFeSi2
mp-23703	LiH	mp-29792	CaNb2O4	mp-1192618	Nb4Fe4Si7
mp-16506	Li3Al2	mp-1228030	Ba4Bi2O	mp-1209887	NbFeSi
mp-10890	LiAl3	mp-567280	Yb5Bi3	mp-2014	DyP
mp-1067	LiAl	mp-23171	PrBi	mp-23954	Na2H2Pd
mp-18337	Be3N2	mp-1105548	Pr5Bi3	mp-9987	Nb2PC
mp-11427	GdPd	mp-17412	BaPr2O4	mp-1222310	Lu2C
mp-21427	GdPd3	mp-5977	Nd2Zr2O7	mp-1203767	Lu3C4
mp-1190736	Ca8Al3	mp-988	Si3N4	mp-3924	LiNbO2
mp-2741	CaF2	mp-1223129	Li4SiO4	mp-28030	Li8Nb2O9
mp-2404	CaAl2	mp-1201871	Li7Si3	mp-4156	Li2ZrO3
mp-9774	Ba4Sb2O	mp-1105932	Li2MgSi	mp-5418	Li6Zr2O7
mp-1500	BaS	mp-1222798	Li14MgSi4	mp-7100	LaOF
mp-2602	NdAs	mp-1367	Mg2Si	mp-5152	La2SiO5

Table S7 Candidates of Li-ion & electron insulators

Material ID	Formula	Structural type	Band gap (eV)	Density (g/cm ³)
mp-2542	BeO	Experimental	7.463	2.967
mp-981	SrF2	Experimental	6.776	4.134
mp-568662	BaCl2	Experimental	5.612	3.394
mp-23193	KCl	Experimental	5.045	1.904
mp-573697	CsCl	Experimental	5.017	3.175
mp-23295	RbCl	Experimental	5.016	2.672
mp-23251	KBr	Experimental	4.515	2.624
mp-567744	SrBr2	Experimental	4.470	3.756
mp-643	ThO2	Experimental	4.464	9.884
mp-571222	CsBr	Experimental	4.425	3.485
mp-23063	Ba4OCl6	Experimental	4.373	3.778
mp-22867	RbBr	Experimental	4.372	3.164
mp-27791	SrBe3O4	Experimental	4.127	3.568
mp-2652	Y2O3	Experimental	4.106	4.892
mp-22916	NaBr	Experimental	4.090	3.121
mp-661	AlN	Experimental	4.054	3.201
mp-22898	KI	Experimental	4.043	2.972
mp-1427	Lu2O3	Experimental	4.031	9.495
mp-1767	Tm2O3	Experimental	3.991	8.919
mp-29909	Ba4OI6	Experimental	3.988	4.813
mp-679	Er2O3	Experimental	3.982	8.654
mp-812	Ho2O3	Experimental	3.961	8.404
mp-22903	RbI	Experimental	3.954	3.360
mp-2345	Dy2O3	Experimental	3.936	8.144
mp-1056	Tb2O3	Experimental	3.912	7.837
mp-218	Sm2O3	Experimental	3.878	6.962
mp-614603	CsI	Experimental	3.856	3.555
mp-553921	Pm2O3	Experimental	3.775	6.605
mp-18337	Be3N2	Experimental	3.717	2.703
mp-1045	Nd2O3	Experimental	3.711	6.396
mp-2605	CaO	Experimental	3.692	3.287
mp-16705	Pr2O3	Experimental	3.659	6.090
mp-2292	La2O3	Experimental	3.590	5.840
mp-23268	NaI	Experimental	3.569	3.572
mp-11107	Ac2O3	Experimental	3.562	8.975
mp-1216	YbO	Experimental	3.531	11.723
mp-23260	BaI2	Experimental	3.436	4.899
mp-23713	CaH2	Experimental	3.186	1.959
mp-12671	Er2O2S	Experimental	3.182	8.210
mp-12670	Ho2O2S	Experimental	3.138	7.992
mp-12668	Tb2O2S	Experimental	3.134	7.501
mp-12669	Dy2O2S	Experimental	3.115	7.771
mp-4511	La2O2S	Experimental	3.080	5.700
mp-5598	Sm2O2S	Experimental	3.057	6.730
mp-3211	Nd2O2S	Experimental	3.016	6.222
mp-3236	Pr2O2S	Experimental	3.005	5.945
mp-865934	YbF2	Theoretical	6.733	7.541
mp-865716	YbCl2	Theoretical	5.400	4.773

Table S8 Candidates of Na-ion & electron insulators

Material ID	Formula	Structural type	Band gap (eV)	Density (g/cm ³)
mp-1138	LiF	Experimental	8.720	2.530
mp-11347	TbF3	Experimental	7.948	7.164
mp-3700	LiYF4	Experimental	7.837	3.808

Material ID	Formula	Structural type	Band gap (eV)	Density (g/cm ³)
mp-18511	NdF ₃	Experimental	7.806	6.338
mp-561430	LiLuF ₄	Experimental	7.764	6.111
mp-2542	BeO	Experimental	7.463	2.967
mp-555932	RbEr ₃ F ₁₀	Experimental	7.282	6.591
mp-2741	CaF ₂	Experimental	7.248	3.090
mp-7104	CsCaF ₃	Experimental	7.234	3.970
mp-18040	KPrF ₄	Experimental	7.143	4.446
mp-3448	KMgF ₃	Experimental	6.954	3.002
mp-28726	KYF ₄	Experimental	6.910	3.355
mp-981	SrF ₂	Experimental	6.776	4.134
mp-13230	K ₃ YF ₆	Experimental	6.699	2.722
mp-5926	KCaF ₃	Experimental	6.650	2.609
mp-1029	BaF ₂	Experimental	6.624	4.695
mp-31212	K ₂ MgF ₄	Experimental	6.454	2.727
mp-37722	KBH ₄	Experimental	6.268	1.201
mp-24123	Rb(BH) ₆	Experimental	5.642	1.600
mp-24239	K(BH) ₆	Experimental	5.639	1.166
mp-560114	Er ₃ O ₂ F ₅	Experimental	5.614	8.077
mp-568662	BaCl ₂	Experimental	5.612	3.394
mp-17673	Lu ₃ O ₂ F ₅	Experimental	5.605	8.719
mp-24136	Cs(BH) ₆	Experimental	5.480	1.818
mp-23432	BaClF	Experimental	5.443	4.355
mp-1070599	CsYbCl ₃	Experimental	5.385	4.286
mp-1072193	ErOF	Experimental	5.173	8.532
mp-27275	Li ₃ BO ₃	Experimental	5.157	2.092
mp-1078265	Cs ₂ YbCl ₄	Experimental	5.132	3.791
mp-3575	Ca ₃ (BO ₃) ₂	Experimental	5.107	3.007
mp-1072114	HoOF	Experimental	5.087	8.377
mp-23193	KCl	Experimental	5.045	1.904
mp-573697	CsCl	Experimental	5.017	3.175
mp-23295	RbCl	Experimental	5.016	2.672
mp-1072208	DyOF	Experimental	5.014	8.141
mp-1960	Li ₂ O	Experimental	4.992	1.963
mp-14093	TbOF	Experimental	4.935	7.861
mp-3637	YOF	Experimental	4.930	5.056
mp-16432	Sr ₃ (BO ₃) ₂	Experimental	4.700	4.096
mp-15960	Li ₅ AlO ₄	Experimental	4.692	2.184
mp-9488	SmOF	Experimental	4.663	7.048
mp-1265	MgO	Experimental	4.638	3.471
mp-17612	Ba ₂ SiO ₄	Experimental	4.632	5.230
mp-3427	LiAlO ₂	Experimental	4.593	2.530
mp-9172	Li ₄ TiO ₄	Experimental	4.549	2.498
mp-6499	BaLiBO ₃	Experimental	4.519	4.266
mp-23251	KBr	Experimental	4.515	2.624
mp-5634	NdOF	Experimental	4.498	6.514
mp-984	BN	Experimental	4.494	1.956
mp-18510	Sr ₂ SiO ₄	Experimental	4.480	4.373
mp-1201301	K ₂ Hf ₂ O ₅	Experimental	4.468	6.157
mp-7020	LiYO ₂	Experimental	4.465	3.971
mp-643	ThO ₂	Experimental	4.464	9.884
mp-571222	CsBr	Experimental	4.425	3.485
mp-23063	Ba ₄ Cl ₆ O	Experimental	4.373	3.778
mp-27456	BaBr ₂	Experimental	4.373	4.586
mp-22867	RbBr	Experimental	4.372	3.164

(Continued)

Material ID	Formula	Structural type	Band gap (eV)	Density (g/cm ³)
mp-510557	CsN ₃	Experimental	4.261	3.178
mp-6632	Ca ₅ B ₃ O ₉ F	Experimental	4.237	2.814
mp-3393	Sr ₃ Al ₂ O ₆	Experimental	4.205	4.017
mp-827	KN ₃	Experimental	4.202	1.908
mp-4481	Ca ₂ SiO ₄	Experimental	4.201	2.891
mp-743	RbN ₃	Experimental	4.198	2.634
mp-555218	Ba ₄ Br ₆ O	Experimental	4.181	4.506
mp-554346	KSr ₄ (BO ₃) ₃	Experimental	4.172	3.994
mp-3094	SrAl ₂ O ₄	Experimental	4.153	3.442
mp-695998	K ₂ ZnH ₄	Experimental	4.149	2.083
mp-3397	Ba ₂ TiO ₄	Experimental	4.144	4.965
mp-27791	SrBe ₃ O ₄	Experimental	4.127	3.568
mp-2652	Y ₂ O ₃	Experimental	4.106	4.892
mp-4202	BaAl ₂ O ₄	Experimental	4.097	3.939
mp-352	HfO ₂	Experimental	4.068	9.968
mp-661	AlN	Experimental	4.054	3.201
mp-22898	KI	Experimental	4.043	2.972
mp-707218	Ba ₃ AlHO ₄	Experimental	4.041	5.188
mp-1427	Lu ₂ O ₃	Experimental	4.031	9.495
mp-557753	K ₃ PO ₄	Experimental	3.999	2.510
mp-1767	Tm ₂ O ₃	Experimental	3.991	8.919
mp-29909	Ba ₄ I ₆ O	Experimental	3.988	4.813
mp-679	Er ₂ O ₃	Experimental	3.982	8.654
mp-812	Ho ₂ O ₃	Experimental	3.961	8.404
mp-22903	RbI	Experimental	3.954	3.360
mp-5418	Li ₆ Zr ₂ O ₇	Experimental	3.944	3.433
mp-2345	Dy ₂ O ₃	Experimental	3.936	8.144
mp-1056	Tb ₂ O ₃	Experimental	3.912	7.837
mp-2983	Ba(PN ₂) ₂	Experimental	3.912	4.600
mp-31116	LaScO ₃	Experimental	3.897	5.670
mp-218	Sm ₂ O ₃	Experimental	3.878	6.962
mp-3564	BaSc ₂ O ₄	Experimental	3.872	4.796
mp-614603	CsI	Experimental	3.856	3.555
mp-777297	K ₅ H(CN ₂) ₂	Experimental	3.850	1.984
mp-4156	Li ₂ ZrO ₃	Experimental	3.841	4.032
mp-23859	CaHCl	Experimental	3.840	2.490
mp-4974	La ₂ Zr ₂ O ₇	Experimental	3.833	5.883
mp-4571	CaZrO ₃	Experimental	3.826	4.467
mp-216	Sc ₂ O ₃	Experimental	3.814	3.751
mp-568284	SrI ₂	Experimental	3.802	4.243
mp-1199246	Ba ₅ B ₃ BrO ₉	Experimental	3.780	4.786
mp-1201345	Ba ₅ B ₃ ClO ₉	Experimental	3.749	4.652
mp-18337	Be ₃ N ₂	Experimental	3.717	2.703
mp-1045	Nd ₂ O ₃	Experimental	3.711	6.396
mp-984055	Ca ₇ (H ₆ Cl) ₂	Experimental	3.696	2.176
mp-2605	CaO	Experimental	3.692	3.287
mp-16594	K ₃ TbSi ₂ O ₇	Experimental	3.688	3.528
mp-16705	Pr ₂ O ₃	Experimental	3.659	6.090
mp-4387	SrZrO ₃	Experimental	3.626	5.252
mp-3952	BaY ₂ O ₄	Experimental	3.593	5.602
mp-2292	La ₂ O ₃	Experimental	3.590	5.840
mp-29910	Sr ₄ I ₆ O	Experimental	3.586	4.673
mp-560978	Ba ₄ Al ₂ O ₇	Experimental	3.574	5.080
mp-23956	K ₂ MgH ₄	Experimental	3.554	1.585

Material ID	Formula	Structural type	Band gap (eV)	Density (g/cm ³)
mp-1153	Li ₂ S	Experimental	3.538	1.630
mp-3933	Mg ₂ PN ₃	Experimental	3.537	3.045
mp-8430	KLiS	Experimental	3.537	1.965
mp-1216	YbO	Experimental	3.531	11.723
mp-551203	Sr ₂ I ₂ O	Experimental	3.480	4.483
mp-31417	Nd ₃ TaO ₇	Experimental	3.472	7.403
mp-4056	CaSc ₂ O ₄	Experimental	3.456	3.819
mp-2472	SrO	Experimental	3.449	4.878
mp-5977	Nd ₂ Zr ₂ O ₇	Experimental	3.443	6.152
mp-23260	BaI ₂	Experimental	3.436	4.899
mp-14964	Pr ₃ TaO ₇	Experimental	3.418	7.233
mp-3834	BaZrO ₃	Experimental	3.410	5.958
mp-5001	Li ₃ BN ₂	Experimental	3.402	1.732
mp-1079891	Ba ₂ Br ₂ O	Experimental	3.401	4.492
mp-2892	BaNd ₂ O ₄	Experimental	3.394	6.612
mp-753721	GdOF	Experimental	3.375	7.541
mp-17904	Nd ₂ TiO ₅	Experimental	3.348	5.729
mp-1195324	Pr ₂ TiO ₅	Experimental	3.346	5.528
mp-770806	Sm ₂ TiO ₅	Experimental	3.336	6.106
mp-974713	K ₂ H ₄ Pt	Experimental	3.316	3.533
mp-18051	La ₂ TiO ₅	Experimental	3.292	5.361
mp-974482	K ₄ Hf ₅ O ₁₂	Experimental	3.274	6.730
mp-28030	Li ₈ Nb ₂ O ₉	Experimental	3.242	3.396
mp-23714	SrH ₂	Experimental	3.236	3.318
mp-643047	Ba ₃ (H ₆ Ir) ₂	Experimental	3.208	5.662
mp-23713	CaH ₂	Experimental	3.186	1.959
mp-12671	Er ₂ SO ₂	Experimental	3.182	8.210
mp-23703	LiH	Experimental	3.175	0.825
mp-551835	Ba ₂ I ₂ O	Experimental	3.152	4.792
mp-10408	K ₂ CN ₂	Experimental	3.143	2.097
mp-3556	Tm ₂ SO ₂	Experimental	3.140	8.430
mp-23702	LiH ₂ N	Experimental	3.124	1.120
mp-12669	Dy ₂ SO ₂	Experimental	3.115	7.771
mp-17143	BaGd ₂ O ₄	Experimental	3.109	7.389
mp-2286	Li ₂ Se	Experimental	3.107	2.827
mp-4511	La ₂ SO ₂	Experimental	3.080	5.700
mp-2931	Li ₂ TiO ₃	Experimental	3.069	3.336
mp-504554	Ba ₅ Ta ₄ O ₁₅	Experimental	3.059	7.685
mp-5598	Sm ₂ SO ₂	Experimental	3.057	6.730
mp-8335	Ba ₂ ZrO ₄	Experimental	3.028	5.804
mp-3211	Nd ₂ SO ₂	Experimental	3.016	6.222
mp-3236	Pr ₂ SO ₂	Experimental	3.005	5.945
mp-1212889	DyF ₃	Theoretical	7.871	7.692
mp-1211343	KNdF ₄	Theoretical	7.166	4.592
mp-1209185	RbPrF ₄	Theoretical	6.859	4.923
mp-17077	K ₂ YF ₅	Theoretical	6.810	3.211
mp-865934	YbF ₂	Theoretical	6.733	7.541
mp-1219553	RbBH ₄	Theoretical	6.212	1.887
mp-1185319	LiCl	Theoretical	5.927	1.660
mp-1225884	CsBH ₄	Theoretical	5.816	2.372
mp-865716	YbCl ₂	Theoretical	5.400	4.773
mp-1097916	CsCaCl ₃	Theoretical	5.383	2.836
mp-1213703	Cs ₃ Ca ₂ Cl ₇	Theoretical	5.186	2.860
mp-1025185	Cs ₂ CaCl ₄	Theoretical	5.113	2.875

(Continued)

Material ID	Formula	Structural type	Band gap (eV)	Density (g/cm ³)
mp-1223129	Li ₄ SiO ₄	Theoretical	5.093	2.317
mp-1210775	LuOF	Theoretical	5.025	8.727
mp-1207669	TmOF	Theoretical	4.860	8.197
mp-1228149	Ba ₃ Sr ₉ Al ₄ (O ₄ F) ₄	Theoretical	4.604	4.992
mp-769173	PrOF	Theoretical	4.437	6.241
mp-1218249	SrLa ₄ Si ₃ O ₁₃	Theoretical	4.428	5.169
mp-755417	Ba ₃ (BO ₃) ₂	Theoretical	4.170	4.752
mp-1189614	BaThO ₃	Theoretical	4.044	7.431
mp-1216160	Y ₄ Zr ₃ O ₁₂	Theoretical	4.032	5.250
mp-1227337	Ca ₆ Al ₇ O ₁₆ F	Theoretical	3.871	2.658
mp-1227232	Ca ₆ Al ₇ ClO ₁₆	Theoretical	3.797	2.695
mp-755558	BaLa ₂ O ₄	Theoretical	3.711	5.426
mp-755895	Ba ₃ Zr ₂ O ₇	Theoretical	3.030	5.860

Table S9 Candidates of K-ion & electron insulators

Material ID	Formula	Structural type	Band gap (eV)	Density (g/cm ³)
mp-1138	LiF	Experimental	8.720	2.530
mp-18511	NdF ₃	Experimental	7.806	6.338
mp-2542	BeO	Experimental	7.463	2.967
mp-2741	CaF ₂	Experimental	7.248	3.090
mp-981	SrF ₂	Experimental	6.776	4.134
mp-1029	BaF ₂	Experimental	6.624	4.695
mp-682	NaF	Experimental	6.095	2.693
mp-27275	Li ₃ BO ₃	Experimental	5.157	2.092
mp-3536	MgAl ₂ O ₄	Experimental	5.122	3.465
mp-1960	Li ₂ O	Experimental	4.992	1.963
mp-3637	YOF	Experimental	4.930	5.056
mp-10572	NaPN ₂	Experimental	4.868	3.085
mp-16432	Sr ₃ (BO ₃) ₂	Experimental	4.700	4.096
mp-15960	Li ₅ AlO ₄	Experimental	4.692	2.184
mp-11189	Li ₂ MgSiO ₄	Experimental	4.677	2.484
mp-9488	SmOF	Experimental	4.663	7.048
mp-1265	MgO	Experimental	4.638	3.471
mp-17612	Ba ₂ SiO ₄	Experimental	4.632	5.230
mp-3427	LiAlO ₂	Experimental	4.593	2.530
mp-976726	LiDyO ₂	Experimental	4.574	6.581
mp-7100	LaOF	Experimental	4.567	5.889
mp-7137	LiTbO ₂	Experimental	4.553	6.371
mp-9172	Li ₄ TiO ₄	Experimental	4.549	2.498
mp-3151	Li ₃ TaO ₄	Experimental	4.540	5.701
mp-6499	BaLiBO ₃	Experimental	4.519	4.266
mp-10970	LiErO ₂	Experimental	4.508	6.677
mp-559904	NaLi ₃ SiO ₄	Experimental	4.500	2.397
mp-5152	La ₂ SiO ₅	Experimental	4.496	5.347
mp-984	BN	Experimental	4.494	1.956
mp-18510	Sr ₂ SiO ₄	Experimental	4.480	4.373
mp-7020	LiYO ₂	Experimental	4.465	3.971
mp-643	ThO ₂	Experimental	4.464	9.884
mp-571222	CsBr	Experimental	4.425	3.485
mp-12645	LiHoO ₂	Experimental	4.418	6.480
mp-23063	Ba ₄ Cl ₆ O	Experimental	4.373	3.778
mp-510557	CsN ₃	Experimental	4.261	3.178
mp-988	Si ₃ N ₄	Experimental	4.258	3.134
mp-4481	Ca ₂ SiO ₄	Experimental	4.201	2.891

Material ID	Formula	Structural type	Band gap (eV)	Density (g/cm ³)
mp-560889	Ba ₆ Na ₂ Si ₄ O ₁₅	Experimental	4.172	4.738
mp-3397	Ba ₂ TiO ₄	Experimental	4.144	4.965
mp-30980	NaYO ₂	Experimental	4.132	4.251
mp-2652	Y ₂ O ₃	Experimental	4.106	4.892
mp-4202	BaAl ₂ O ₄	Experimental	4.097	3.939
mp-23870	NaH	Experimental	4.070	1.417
mp-352	HfO ₂	Experimental	4.068	9.968
mp-661	AlN	Experimental	4.054	3.201
mp-1427	Lu ₂ O ₃	Experimental	4.031	9.495
mp-6964	NaTbO ₂	Experimental	4.006	6.269
mp-1767	Tm ₂ O ₃	Experimental	3.991	8.919
mp-679	Er ₂ O ₃	Experimental	3.982	8.654
mp-812	Ho ₂ O ₃	Experimental	3.961	8.404
mp-22903	RbI	Experimental	3.954	3.360
mp-5418	Li ₆ Zr ₂ O ₇	Experimental	3.944	3.433
mp-2345	Dy ₂ O ₃	Experimental	3.936	8.144
mp-1056	Tb ₂ O ₃	Experimental	3.912	7.837
mp-1192906	Ba ₄ Ta ₂ O ₉	Experimental	3.896	6.359
mp-218	Sm ₂ O ₃	Experimental	3.878	6.962
mp-4533	Na ₂ SiO ₃	Experimental	3.863	2.540
mp-556695	NaSrBO ₃	Experimental	3.860	3.706
mp-614603	CsI	Experimental	3.856	3.555
mp-4156	Li ₂ ZrO ₃	Experimental	3.841	4.032
mp-9212	NaAlO ₂	Experimental	3.815	2.669
mp-216	Sc ₂ O ₃	Experimental	3.814	3.751
mp-19334	Na ₄ WO ₅	Experimental	3.809	4.695
mp-4657	Li ₅ GaO ₄	Experimental	3.792	2.824
mp-27247	Na ₃ NbO ₄	Experimental	3.782	3.680
mp-6406	Na ₂ MgSiO ₄	Experimental	3.774	2.575
mp-28940	Sr ₄ Nb ₂ O ₉	Experimental	3.728	4.623
mp-18337	Be ₃ N ₂	Experimental	3.717	2.703
mp-1045	Nd ₂ O ₃	Experimental	3.711	6.396
mp-2605	CaO	Experimental	3.692	3.287
mp-16705	Pr ₂ O ₃	Experimental	3.659	6.090
mp-28559	Na ₆ Be ₈ O ₁₁	Experimental	3.621	2.402
mp-3952	BaY ₂ O ₄	Experimental	3.593	5.602
mp-2292	La ₂ O ₃	Experimental	3.590	5.840
mp-560978	Ba ₄ Al ₂ O ₇	Experimental	3.574	5.080
mp-559426	Pr ₂ Zr ₂ O ₇	Experimental	3.573	6.009
mp-1153	Li ₂ S	Experimental	3.538	1.630
mp-1216	YbO	Experimental	3.531	11.723
mp-31417	Nd ₃ TaO ₇	Experimental	3.472	7.403
mp-31415	La ₃ TaO ₇	Experimental	3.459	7.036
mp-2472	SrO	Experimental	3.449	4.878
mp-5977	Nd ₂ Zr ₂ O ₇	Experimental	3.443	6.152
mp-14964	Pr ₃ TaO ₇	Experimental	3.418	7.233
mp-753721	GdOF	Experimental	3.375	7.541
mp-17904	Nd ₂ TiO ₅	Experimental	3.348	5.729
mp-8128	NaNdO ₂	Experimental	3.339	5.242
mp-770806	Sm ₂ TiO ₅	Experimental	3.336	6.106
mp-14726	Na ₄ TiO ₄	Experimental	3.319	2.589
mp-18051	La ₂ TiO ₅	Experimental	3.292	5.361
mp-21332	LiGdO ₂	Experimental	3.284	6.169
mp-28030	Li ₈ Nb ₂ O ₉	Experimental	3.242	3.396

(Continued)

Material ID	Formula	Structural type	Band gap (eV)	Density (g/cm ³)
mp-23714	SrH2	Experimental	3.236	3.318
mp-7500	Na4SiO4	Experimental	3.227	2.569
mp-8470	NaPrO2	Experimental	3.200	5.018
mp-18793	LiCrO2	Experimental	3.188	4.101
mp-23713	CaH2	Experimental	3.186	1.959
mp-12671	Er2SO2	Experimental	3.182	8.210
mp-23703	LiH	Experimental	3.175	0.825
mp-551835	Ba2I2O	Experimental	3.152	4.792
mp-5088	NaGdO2	Experimental	3.150	6.044
mp-3556	Tm2SO2	Experimental	3.140	8.430
mp-12670	Ho2SO2	Experimental	3.138	7.992
mp-12668	Tb2SO2	Experimental	3.134	7.501
mp-23702	LiH2N	Experimental	3.124	1.120
mp-1019967	LaSi3N5	Experimental	3.123	4.485
mp-12669	Dy2SO2	Experimental	3.115	7.771
mp-17143	BaGd2O4	Experimental	3.109	7.389
mp-2286	Li2Se	Experimental	3.107	2.827
mp-12673	Lu2SO2	Experimental	3.093	8.920
mp-4511	La2SO2	Experimental	3.080	5.700
mp-17412	BaPr2O4	Experimental	3.076	6.395
mp-2931	Li2TiO3	Experimental	3.069	3.336
mp-504554	Ba5Ta4O15	Experimental	3.059	7.685
mp-5598	Sm2SO2	Experimental	3.057	6.730
mp-578604	NaCrO2	Experimental	3.036	4.140
mp-644307	Ca(H2N)2	Experimental	3.035	1.727
mp-3211	Nd2SO2	Experimental	3.016	6.222
mp-1019893	La3Si6N11	Experimental	3.015	4.789
mp-3236	Pr2SO2	Experimental	3.005	5.945
mp-865934	YbF2	Theoretical	6.733	7.541
mp-1223129	Li4SiO4	Theoretical	5.093	2.317
mp-676653	Lu4Hf3O12	Theoretical	4.596	9.845
mp-542201	Ba3Nb2O8	Theoretical	4.580	5.081
mp-754605	LiLuO2	Theoretical	4.501	7.422
mp-769173	PrOF	Theoretical	4.437	6.241
mp-990440	Na2ZrO3	Theoretical	4.416	3.957
mp-754237	LiTmO2	Theoretical	4.315	6.974
mp-17891	NaYSiO4	Theoretical	4.284	3.567
mp-769271	Sr4Ta2O9	Theoretical	4.197	5.850
mp-755417	Ba3(BO3)2	Theoretical	4.170	4.752
mp-1222825	Lu4Zr3O12	Theoretical	4.118	7.895
mp-1216160	Y4Zr3O12	Theoretical	4.032	5.250
mp-755013	Li5TaO5	Theoretical	3.720	4.430
mp-754027	NaSmO2	Theoretical	3.656	5.675
mp-770771	SrSc2O4	Theoretical	3.436	4.512
mp-755586	NaLaO2	Theoretical	3.242	4.856

Table S10 Candidates of multi-ions (Li-ions & Na-ions) and electron insulators

Material ID	Formula	Structural type	Band gap (eV)	Density (g/cm ³)
mp-2542	BeO	Experimental	7.463	2.967
mp-981	SrF2	Experimental	6.776	4.134
mp-568662	BaCl2	Experimental	5.612	3.394
mp-23193	KCl	Experimental	5.045	1.904
mp-573697	CsCl	Experimental	5.017	3.175
mp-23295	RbCl	Experimental	5.016	2.672

Material ID	Formula	Structural type	Band gap (eV)	Density (g/cm ³)
mp-23251	KBr	Experimental	4.515	2.624
mp-643	ThO ₂	Experimental	4.464	9.884
mp-571222	CsBr	Experimental	4.425	3.485
mp-23063	Ba ₄ Cl ₆ O	Experimental	4.373	3.778
mp-22867	RbBr	Experimental	4.372	3.164
mp-27791	SrBe ₃ O ₄	Experimental	4.127	3.568
mp-2652	Y ₂ O ₃	Experimental	4.106	4.892
mp-661	AlN	Experimental	4.054	3.201
mp-22898	KI	Experimental	4.043	2.972
mp-1427	Lu ₂ O ₃	Experimental	4.031	9.495
mp-1767	Tm ₂ O ₃	Experimental	3.991	8.919
mp-29909	Ba ₄ I ₆ O	Experimental	3.988	4.813
mp-679	Er ₂ O ₃	Experimental	3.982	8.654
mp-812	Ho ₂ O ₃	Experimental	3.961	8.404
mp-22903	RbI	Experimental	3.954	3.360
mp-2345	Dy ₂ O ₃	Experimental	3.936	8.144
mp-1056	Tb ₂ O ₃	Experimental	3.912	7.837
mp-218	Sm ₂ O ₃	Experimental	3.878	6.962
mp-614603	CsI	Experimental	3.856	3.555
mp-18337	Be ₃ N ₂	Experimental	3.717	2.703
mp-1045	Nd ₂ O ₃	Experimental	3.711	6.396
mp-2605	CaO	Experimental	3.692	3.287
mp-16705	Pr ₂ O ₃	Experimental	3.659	6.090
mp-2292	La ₂ O ₃	Experimental	3.590	5.840
mp-1216	YbO	Experimental	3.531	11.723
mp-23260	BaI ₂	Experimental	3.436	4.899
mp-23713	CaH ₂	Experimental	3.186	1.959
mp-12671	Er ₂ SO ₂	Experimental	3.182	8.210
mp-12669	Dy ₂ SO ₂	Experimental	3.115	7.771
mp-4511	La ₂ SO ₂	Experimental	3.080	5.700
mp-5598	Sm ₂ SO ₂	Experimental	3.057	6.730
mp-3211	Nd ₂ SO ₂	Experimental	3.016	6.222
mp-3236	Pr ₂ SO ₂	Experimental	3.005	5.945
mp-865934	YbF ₂	Theoretical	6.733	7.541
mp-865716	YbCl ₂	Theoretical	5.400	4.773

Table S11 Candidates of multi-ions (Li-ions & K-ions) and electron insulators

Material ID	Formula	Structural type	Band gap (eV)	Density (g/cm ³)
mp-2542	BeO	Experimental	7.463	2.967
mp-981	SrF ₂	Experimental	6.776	4.134
mp-643	ThO ₂	Experimental	4.464	9.884
mp-571222	CsBr	Experimental	4.425	3.485
mp-23063	Ba ₄ Cl ₆ O	Experimental	4.373	3.778
mp-2652	Y ₂ O ₃	Experimental	4.106	4.892
mp-661	AlN	Experimental	4.054	3.201
mp-1427	Lu ₂ O ₃	Experimental	4.031	9.495
mp-1767	Tm ₂ O ₃	Experimental	3.991	8.919
mp-679	Er ₂ O ₃	Experimental	3.982	8.654
mp-812	Ho ₂ O ₃	Experimental	3.961	8.404
mp-22903	RbI	Experimental	3.954	3.360
mp-2345	Dy ₂ O ₃	Experimental	3.936	8.144
mp-1056	Tb ₂ O ₃	Experimental	3.912	7.837
mp-218	Sm ₂ O ₃	Experimental	3.878	6.962
mp-614603	CsI	Experimental	3.856	3.555

(Continued)

Material ID	Formula	Structural type	Band gap (eV)	Density (g/cm ³)
mp-18337	Be ₃ N ₂	Experimental	3.717	2.703
mp-1045	Nd ₂ O ₃	Experimental	3.711	6.396
mp-2605	CaO	Experimental	3.692	3.287
mp-16705	Pr ₂ O ₃	Experimental	3.659	6.090
mp-2292	La ₂ O ₃	Experimental	3.590	5.840
mp-1216	YbO	Experimental	3.531	11.723
mp-23713	CaH ₂	Experimental	3.186	1.959
mp-12671	Er ₂ SO ₂	Experimental	3.182	8.210
mp-12670	Ho ₂ SO ₂	Experimental	3.138	7.992
mp-12668	Tb ₂ SO ₂	Experimental	3.134	7.501
mp-12669	Dy ₂ SO ₂	Experimental	3.115	7.771
mp-4511	La ₂ SO ₂	Experimental	3.080	5.700
mp-5598	Sm ₂ SO ₂	Experimental	3.057	6.730
mp-3211	Nd ₂ SO ₂	Experimental	3.016	6.222
mp-3236	Pr ₂ SO ₂	Experimental	3.005	5.945
mp-865934	YbF ₂	Theoretical	6.733	7.541

Table S12 Candidates of multi-ions (Li-ions & Na-ions & K-ions) and electron insulators

Material ID	Formula	Structural type	Band gap (eV)	Density (g/cm ³)
mp-2542	BeO	Experimental	7.463	2.967
mp-981	SrF ₂	Experimental	6.776	4.134
mp-643	ThO ₂	Experimental	4.464	9.884
mp-571222	CsBr	Experimental	4.425	3.485
mp-23063	Ba ₄ Cl ₆ O	Experimental	4.373	3.778
mp-2652	Y ₂ O ₃	Experimental	4.106	4.892
mp-661	AlN	Experimental	4.054	3.201
mp-1427	Lu ₂ O ₃	Experimental	4.031	9.495
mp-1767	Tm ₂ O ₃	Experimental	3.991	8.919
mp-679	Er ₂ O ₃	Experimental	3.982	8.654
mp-812	Ho ₂ O ₃	Experimental	3.961	8.404
mp-22903	RbI	Experimental	3.954	3.360
mp-2345	Dy ₂ O ₃	Experimental	3.936	8.144
mp-1056	Tb ₂ O ₃	Experimental	3.912	7.837
mp-218	Sm ₂ O ₃	Experimental	3.878	6.962
mp-614603	CsI	Experimental	3.856	3.555
mp-18337	Be ₃ N ₂	Experimental	3.717	2.703
mp-1045	Nd ₂ O ₃	Experimental	3.711	6.396
mp-2605	CaO	Experimental	3.692	3.287
mp-16705	Pr ₂ O ₃	Experimental	3.659	6.090
mp-2292	La ₂ O ₃	Experimental	3.590	5.840
mp-1216	YbO	Experimental	3.531	11.723
mp-23713	CaH ₂	Experimental	3.186	1.959
mp-12671	Er ₂ SO ₂	Experimental	3.182	8.210
mp-12669	Dy ₂ SO ₂	Experimental	3.115	7.771
mp-4511	La ₂ SO ₂	Experimental	3.080	5.700
mp-5598	Sm ₂ SO ₂	Experimental	3.057	6.730
mp-3211	Nd ₂ SO ₂	Experimental	3.016	6.222
mp-3236	Pr ₂ SO ₂	Experimental	3.005	5.945
mp-865934	YbF ₂	Theoretical	6.733	7.541