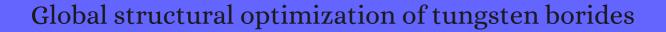
CITATION REPORT List of articles citing



DOI: 10.1103/physrevlett.110.136403 Physical Review Letters, 2013, 110, 136403.

Source: https://exaly.com/paper-pdf/55812407/citation-report.pdf

Version: 2024-04-23

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
247	Orthorhombic C32: a novel superhard sp3 carbon allotrope. 2013 , 15, 14120-5		52
246	Dimension-dependent phase transition and magnetic properties of VS2. 2013 , 1, 10821		154
245	First-principles structural design of superhard material of ZrB4. 2013 , 15, 20894-9		42
244	Unexpectedly hard and highly stable WB3 with a noncompact structure. 2013 , 580, 48-52		39
243	Interstitial-boron solution strengthened WB3+x. 2013 , 103, 171903		62
242	The structural and elastic properties of TMB4(TM =V,Cr,Mn) under pressure: A first-principles study. 2014 , 28, 1450202		1
241	Unexpected structural softening of interstitial boron solid solution WB3+x. 2014 , 105, 211901		7
240	Be2C Monolayer with Quasi-Planar Hexacoordinate Carbons: A Global Minimum Structure. 2014 , 126, 7376-7380		26
239	Lattice stress states of superhard tungsten tetraboride from radial x-ray diffraction under nonhydrostatic compression. <i>Physical Review B</i> , 2014 , 90,	3.3	29
238	Thermodynamic ground state of MgB6 predicted from first principles structure search methods. Journal of Chemical Physics, 2014 , 140, 044710	3.9	11
237	Hardness of FeB4: density functional theory investigation. <i>Journal of Chemical Physics</i> , 2014 , 140, 1745	05 .9	67
236	Phase stability limit of c-BN under hydrostatic and non-hydrostatic pressure conditions. <i>Journal of Chemical Physics</i> , 2014 , 140, 164704	3.9	7
235	Exploring High-Pressure Structures of N2CO. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 27252-27257	3.8	13
234	Novel high-pressure crystal structures of boron trifluoride. 2014 , 75, 1094-1098		2
233	Be(2)C monolayer with quasi-planar hexacoordinate carbons: a global minimum structure. 2014 , 53, 72	48-52	184
232	Structural and relative stabilities, electronic properties, and hardness of iron tetraborides from first prinicples. <i>Inorganic Chemistry</i> , 2014 , 53, 3471-9	5.1	12
231	The stabilities and electronic structures of single-layer bismuth oxyhalides for photocatalytic water splitting. 2014 , 16, 25854-61		90

230	A semiconductive superhard FeBIphase from first-principles calculations. 2014 , 16, 22008-13		13
229	Phase stability and elastic properties of (W0.5Al0.5)C phase with a novel NiAs-type structure. <i>RSC Advances</i> , 2014 , 4, 42585-42590	3.7	
228	Novel heterostructures by stacking layered molybdenum disulfides and nitrides for solar energy conversion. 2014 , 2, 15389-15395		71
227	Hidden Thermodynamic Ground State of Calcium Diazenide. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 650-656	3.8	8
226	Computational search for direct band gap silicon crystals. <i>Physical Review B</i> , 2014 , 90,	3.3	52
225	Crystal structure and physical properties of Mo2B: First-principle calculations. <i>Journal of Applied Physics</i> , 2014 , 115, 113504	2.5	19
224	The metallization and superconductivity of dense hydrogen sulfide. <i>Journal of Chemical Physics</i> , 2014 , 140, 174712	3.9	481
223	All monolayer: the planar tetracoordinate carbon global minimum. 2014 , 6, 10784-91		63
222	High-pressure phase transition of cesium chloride and cesium bromide. 2014 , 16, 17924-9		11
221	Computational materials discovery: the case of the W-B system. 2014 , 70, 85-103		70
220	Structural and mechanical properties of platinum carbide. <i>Inorganic Chemistry</i> , 2014 , 53, 5797-802	5.1	16
219	Crystal Structure of W1⊠ B3 and Phase Equilibria in the Boron-Rich Part of the Systems Mo-Rh-B and W-{Ru,Os,Rh,Ir,Ni,Pd,Pt}-B. 2014 , 35, 384-395		21
218	Exploring Hardness and the Distorted sp2 Hybridization of BB Bonds in WB3. 2014 , 26, 5297-5302		59
217	Formation and stability of tungsten boride nanocomposites in WO3B2O3Mg ternary system: Mechanochemical effects. 2014 , 46, 117-124		14
216	First-principle calculations on the structural and electronic properties of hard C11N4. 2014 , 449, 90-94		5
215	Effect of excess boron oxide on the formation of tungsten boride nanocomposites by mechanically induced self-sustaining reaction. <i>Ceramics International</i> , 2014 , 40, 14235-14246	5.1	11
214	Pressure-induced cation-cation bonding in V2O3. <i>Physical Review B</i> , 2015 , 92,	3.3	12
213	Anomalous Stress Response of Ultrahard WB_{n} Compounds. <i>Physical Review Letters</i> , 2015 , 115, 18550	12 7.4	85

212	High-Energy Density and Superhard Nitrogen-Rich B-N Compounds. <i>Physical Review Letters</i> , 2015 , 115, 105502	7.4	106
211	Hypervalent Iodine with Linear Chain at High Pressure. Scientific Reports, 2015, 5, 14393	4.9	8
210	Influences of carbon concentration on crystal structures and ideal strengths of B2CxO compounds in the B-C-O system. <i>Scientific Reports</i> , 2015 , 5, 15481	4.9	18
209	The ground-state structure and physical properties of ReB3 and IrB3 predicted from first principles. <i>RSC Advances</i> , 2015 , 5, 25919-25928	3.7	14
208	Influence of boron vacancies on phase stability, bonding and structure of MBI(M = Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W) with AlBItype structure. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 435702	1.8	22
207	Theoretical investigations of physical stability, electronic properties and hardness of transition-metal tungsten borides WBx($x = 2.5, 3$). 2015 , 635, 205-209		18
206	N2H: a novel polymeric hydronitrogen as a high energy density material. 2015 , 3, 4188-4194		42
205	Superhard BC(3) in cubic diamond structure. <i>Physical Review Letters</i> , 2015 , 114, 015502	7.4	147
204	Polytypism in superhard transition-metal triborides. <i>Scientific Reports</i> , 2014 , 4, 5063	4.9	13
203	A new high-pressure polymeric nitrogen phase in potassium azide. <i>RSC Advances</i> , 2015 , 5, 11825-11830	3.7	16
202	An ab initio study of TiS3: a promising electrode material for rechargeable Li and Na ion batteries. <i>RSC Advances</i> , 2015 , 5, 21455-21463	3.7	49
201	Two-dimensional boron-nitrogen-carbon monolayers with tunable direct band gaps. 2015 , 7, 12023-9		63
200	Exploring the metallic phase of N2O under high pressure. <i>RSC Advances</i> , 2015 , 5, 65745-65749	3.7	4
199	Phase diagram, mechanical properties, and electronic structure of Nb-N compounds under pressure. 2015 , 17, 22837-45		20
198	Novel Two-Dimensional Silica Monolayers with Tetrahedral and Octahedral Configurations. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 15654-15660	3.8	18
197	Stable ScS2 nanostructures with tunable electronic and magnetic properties. 2015 , 220, 12-16		10
196	Pressure-induced structural phase transition in iron phosphide. 2015 , 107, 204-209		5
195	Structural stability of W2B5 under high pressure. 2015 , 95, 295-301		

194	Materials discovery via CALYPSO methodology. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 203203 1	.8	63
193	Novel ultra-incompressible phases of Ru2C. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 175505	.8	1
192	Metallic icosahedron phase of sodium at terapascal pressures. <i>Physical Review Letters</i> , 2015 , 114, 12550 †	'·4	56
191	Superhard-driven search of the covalent network in the B3NO system. <i>RSC Advances</i> , 2015 , 5, 35882-358	37	17
190	Porous BN for hydrogen generation and storage. 2015 , 3, 9632-9637		65
189	Influence of B Concentration on the Structural Stability and Mechanical Properties of NbB Compounds. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 23175-23183	8	41
188	Crystal Structures and Electronic Properties of Cesium Xenides at High Pressures. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 24996-25002	8	12
187	Novel . 2015 , 379, 2479-2483		1
186	Structural stability and elastic properties of WB4 under high pressure. 2015 , 29, 1550103		4
185	Structures and stability of novel transition-metal (M=Co,Rh,CoandIr) borides. <i>Physical Review B</i> , 2015 , 92,	.3	7
184	Strength of tungsten triboride under pressure up to 86 GPa from radial X-ray diffraction. <i>Journal of Alloys and Compounds</i> , 2015 , 621, 116-120	i.7	5
183	Cubic CN: A New Superhard Phase of Carbon-Rich Nitride. 2016 , 9,		16
182	Pressure-Induced Phase Transition and Mechanical Properties of MgBr Intermetallics. 2016, 9,		1
181	Structural transitions and electronic properties of sodium superoxide at high pressures. <i>RSC Advances</i> , 2016 , 6, 67910-67915	·7	2
180	Discovering New Materials via A Priori Crystal Structure Prediction. 2016 , 274-326		10
179	Crystal Field Splitting is Limiting the Stability and Strength of Ultra-incompressible Orthorhombic Transition Metal Tetraborides. <i>Scientific Reports</i> , 2016 , 6, 23088	9	17
178	Nonmetallization and band inversion in beryllium dicarbide at high pressure. <i>Scientific Reports</i> , 2016 , 6, 26398	9	1
177	A Crossover from High Stiffness to High Hardness: The Case of Osmium and Its Borides. 2016 , 71, 831-836	5	

176	Anisotropic elastic properties of MB (M = Cr, Mo, W) monoborides: a first-principles investigation. 2016 , 96, 972-990		22
175	High-pressure crystal structures of TaAs from first-principles calculations. 2016 , 240, 37-40		6
174	Low-dimensional ScO2 with tunable electronic and magnetic properties: first-principles studies. Journal of Physics Condensed Matter, 2016 , 28, 015004	1.8	1
173	Catenation of carbon in LaC2 predicted under high pressure. 2016 , 18, 14286-91		5
172	New Insight into the Effect of Alloying Elements on Elastic Behavior, Hardness, and Thermodynamic Properties of Ru2B3. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 21762-21769	3.8	23
171	Structural and electronic phase transitions of ThS2 from first-principles calculations. <i>Physical Review B</i> , 2016 , 94,	3.3	7
170	Ab initio study on structural, electronic properties, and hardness of re-doped W2B5. 2016 , 245, 60-64		5
169	Two-dimensional metallic MoS2: A DFT study. 2016 , 124, 49-53		15
168	Theoretical study of electronic and mechanical properties of Fe2B. RSC Advances, 2016, 6, 73576-73580	3.7	11
167	Theoretical design of diamondlike superhard structures at high pressure. <i>Chinese Physics B</i> , 2016 , 25, 076103	1.2	5
166	Tuning lattice stability and mechanical strength of ultraincompressible tungsten carbides by varying the stacking sequence. <i>Physical Review B</i> , 2016 , 93,	3.3	12
165	High-temperature- and high-pressure-induced formation of the Laves-phase compound XeS2. <i>Physical Review B</i> , 2016 , 93,	3.3	10
164	Strong covalent boron bonding induced extreme hardness of VB3. <i>Journal of Alloys and Compounds</i> , 2016 , 688, 1101-1107	5.7	9
163	Coexistence of Superconductivity and Superhardness in Beryllium Hexaboride Driven by Inherent Multicenter Bonding. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 4898-4904	6.4	8
162	Ground state structures of tantalum tetraboride and triboride: an ab initio study. 2016 , 18, 18074-80		8
161	Prediction of new stable structure, promising electronic and thermodynamic properties of MoS3: Ab initio calculations. 2016 , 325, 246-251		57
160	Fabrication and characterization of superhard tungsten boride layers deposited by radio frequency magnetron sputtering. <i>Ceramics International</i> , 2016 , 42, 12221-12230	5.1	28
159	Structural optimization and physical properties of TcB3 and MoB3 at high-pressure: First-principles. 2016 , 30, 1650131		4

158	Globally stable structures of LixZn ($x = 1-4$) compounds at high pressures. 2016 , 18, 4437-43		6
157	Discovery of elusive structures of multifunctional transition-metal borides. 2016 , 8, 1055-65		17
156	Structural prediction of ultrahard semi-titanium boride (Ti2B) using the frozen-phonon method. 2016 , 18, 7927-31		11
155	Ultraincompressible, Superhard Materials. 2016 , 46, 465-485		73
154	Novel structures and superconductivities of calcium[]thium alloys at high pressures: A first-principles study. <i>Journal of Alloys and Compounds</i> , 2016 , 669, 101-107	5.7	2
153	Stoner-enhanced paramagnetism in tungsten tetraboride. <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 026005	1.8	Ο
152	CALYPSO structure prediction method and its wide application. 2016 , 112, 406-415		102
151	Stability, chemical bonding behavior, elastic properties and lattice thermal conductivity of molybdenum and tungsten borides under hydrostatic pressure. <i>Ceramics International</i> , 2016 , 42, 2117-2	21/31/2	38
150	Materials discovery at high pressures. 2017 , 2,		266
149	Structural evolution of FeH4 under high pressure. RSC Advances, 2017, 7, 12570-12575	3.7	13
149	Structural evolution of FeH4 under high pressure. <i>RSC Advances</i> , 2017 , 7, 12570-12575 Phase stability, Debye temperature and hardness of semiconducting manganese tetraboride MnB4: First-principles investigations. 2017 , 31, 1750131	3.7	13
	Phase stability, Debye temperature and hardness of semiconducting manganese tetraboride MnB4:	3.7	
148	Phase stability, Debye temperature and hardness of semiconducting manganese tetraboride MnB4: First-principles investigations. 2017 , 31, 1750131 Prediction of novel ultra-incompressibility compounds TM2B (TM=Mo, W, Re and Os) by	3-7	1
148	Phase stability, Debye temperature and hardness of semiconducting manganese tetraboride MnB4: First-principles investigations. 2017 , 31, 1750131 Prediction of novel ultra-incompressibility compounds TM2B (TM=Mo, W, Re and Os) by first-principles calculations. 2017 , 97, 1729-1739	3-7	3
148 147 146	Phase stability, Debye temperature and hardness of semiconducting manganese tetraboride MnB4: First-principles investigations. 2017, 31, 1750131 Prediction of novel ultra-incompressibility compounds TM2B (TM=Mo, W, Re and Os) by first-principles calculations. 2017, 97, 1729-1739 Pressure effect on the hardness of diamond and W2B5: First-principle calculations. 2017, 31, 1750137 Phase stability and incompressibility of tungsten boride (WB) researched by in-situ high pressure	3.7	1 3 5
148 147 146	Phase stability, Debye temperature and hardness of semiconducting manganese tetraboride MnB4: First-principles investigations. 2017, 31, 1750131 Prediction of novel ultra-incompressibility compounds TM2B (TM=Mo, W, Re and Os) by first-principles calculations. 2017, 97, 1729-1739 Pressure effect on the hardness of diamond and W2B5: First-principle calculations. 2017, 31, 1750137 Phase stability and incompressibility of tungsten boride (WB) researched by in-situ high pressure x-ray diffraction. 2017, 521, 6-12	3.7	1 3 5
148 147 146 145	Phase stability, Debye temperature and hardness of semiconducting manganese tetraboride MnB4: First-principles investigations. 2017, 31, 1750131 Prediction of novel ultra-incompressibility compounds TM2B (TM=Mo, W, Re and Os) by first-principles calculations. 2017, 97, 1729-1739 Pressure effect on the hardness of diamond and W2B5: First-principle calculations. 2017, 31, 1750137 Phase stability and incompressibility of tungsten boride (WB) researched by in-situ high pressure x-ray diffraction. 2017, 521, 6-12 Oxidation mechanism of W substituted Mo-Si-B alloys. 2017, 87, 38-44 Boron doped bcc-W films: Achieving excellent mechanical properties and tribological performance	3.7	1 3 5 12 26

140	First-Principles Predictions of Phase Transition and Mechanical Properties of Tungsten Diboride under Pressure. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 7397-7403	3.8	13
139	Pressure-induced metallization and superconducting phase in ReS 2. 2017 , 2,		38
138	Investigation of structural, electronic and anisotropic elastic properties of Ru-doped WB2 compound by increased valence electron concentration. 2017 , 189, 90-95		16
137	Insight into sulfur vacancy-induced insulator to metal transition of Li2S. 2017 , 10, 1750067		12
136	Revealing phase relations between Fe2B7 and FeB4 and hypothetical Fe2B7-type Ru2B7 and Os2B7: first-principles calculations. <i>RSC Advances</i> , 2017 , 7, 44860-44866	3.7	0
135	Prediction of high-pressure phases of Weyl semimetal NbAs and NbP. <i>Scientific Reports</i> , 2017 , 7, 13251	4.9	3
134	Curved-line search algorithm for ab initio atomic structure relaxation. <i>Physical Review B</i> , 2017 , 96,	3.3	O
133	Pressure-induced structural transformations and polymerization in ThC. Scientific Reports, 2017, 7, 4587	72 4.9	10
132	Influence of Re Concentration on the Mechanical Properties of Tungsten Borides from First-Principles Calculations. 2017 , 69, 2009-2013		17
131	Investigations on structural determination of semi-transition-metal borides. 2017 , 19, 31592-31598		14
130	Toxicogenomic responses of human alveolar epithelial cells to tungsten boride nanoparticles. 2017 , 273, 257-265		9
129	Tunable electronic and magnetic properties from structure phase transition of layered vanadium diselenide. 2017 , 32, 574-578		6
128	Novel Superhard sp^{3} Carbon Allotrope from Cold-Compressed C_{70} Peapods. <i>Physical Review Letters</i> , 2017 , 118, 245701	7.4	69
127	Two single-layer porous gallium nitride nanosheets: A first-principles study. 2017 , 250, 18-22		23
126	Correlated High-Pressure Phase Sequence of VO under Strong Compression. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 2388-2393	6.4	13
125	Designing superhard metals: The case of low borides. 2018 , 8, 045305		11
124	High-Pressure Evolution of Crystal Bonding Structures and Properties of FeOOH. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 2181-2185	6.4	57
123	Preparation and Characterization of Amorphous WBC Alloy and Solid Solutions of C in Tungsten Borides. 2018 , 31, 380-388		2

(2018-2018)

122	Mechanical strength and origin of the strengthening effect of tantalum in superhard W 0.5 Ta 0.5 B monoboride. <i>Ceramics International</i> , 2018 , 44, 10463-10469	5.1	14
121	Structural properties, electronic structures and optical properties of WB2 with different structures: A theoretical investigation. <i>Ceramics International</i> , 2018 , 44, 11438-11447	5.1	40
120	A New Anisotropic Dirac Cone Material: A BS Honeycomb Monolayer. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 1815-1820	6.4	49
119	Prediction of novel stable Fe-V-Si ternary phase. <i>Journal of Alloys and Compounds</i> , 2018 , 732, 567-572	5.7	2
118	Tungsten borides layers deposited by a nanosecond laser pulse. 2018 , 335, 181-187		6
117	Evolution of atomic and electronic structures of TaP under high pressure. 2018, 142, 320-324		
116	Effect of pressure on the structural, electronic and mechanical properties of ultraincompressible WB <i>RSC Advances</i> , 2018 , 8, 35664-35671	3.7	5
115	A first-principles calculation of structural, mechanical, thermodynamic and electronic properties of binary Ni-Y compounds <i>RSC Advances</i> , 2018 , 8, 41575-41586	3.7	4
114	High-Pressure Evolution of Unexpected Chemical Bonding and Promising Superconducting Properties of YB6. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 27820-27828	3.8	7
113	Revealing the stability, elastic properties and electronic structures of Pd-V intermetallics via first principle calculations. 2018 , 8, 105132		3
112	Rare Helium-Bearing Compound FeO_{2}He Stabilized at Deep-Earth Conditions. <i>Physical Review Letters</i> , 2018 , 121, 255703	7.4	38
111	Novel 2D Germanene Dioxide Monolayers: Mechanical Properties, Hole-Mobility Values, and Carrier Mobility. 2018 , 530, 1800214		1
110	Unexpected stable phases of tungsten borides. 2018 , 20, 24665-24670		20
109	Influence of uniaxial strains on the mechanical properties of transition metal borides X2B, XB and XB2 ($X = Cr$, Mo, W). 2018 , 550, 100-111		5
108	The Structure and Properties of Magnesium-Phosphorus Compounds Under Pressure. 2018 , 24, 11402-	11406	5
107	Stability, Elastic Properties, and Deformation of LiBN: A Potential High-Energy Material. <i>Inorganic Chemistry</i> , 2018 , 57, 6333-6339	5.1	
106	First-principles study on structural, mechanical and electronic properties of thorium dichalcogenides under high pressure. 2018 , 508, 147-153		
105	Unraveling the structure and bonding evolution of the newly discovered iron oxide FeO2. <i>Physical Review B</i> , 2018 , 98,	3.3	51

104	In situ synthesis, mechanical properties, and microstructure of reactively hot pressed WB4 ceramic with Ni as a sintering additive. <i>Ceramics International</i> , 2018 , 44, 19442-19450	5
103	Screening Surface Structure of MXenes by High-Throughput Computation and Vibrational Spectroscopic Confirmation. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 18501-18509	73
102	High-throughput screening for superhard carbon and boron nitride allotropes with superior stiffness and strength. 2018 , 137, 156-164	15
101	A 2D ferromagnetic semiconductor in monolayer Cr-trihalide and its Janus structures. 2018 , 20, 21755-21763	28
100	Rational design of new phases of tin monosulfide by first-principles structure searches. 2018 , 61, 1	11
99	Microstructure and Properties of M3B2-Type Boride-Based Cermet Coatings Prepared by Laser Cladding Synthesis. 2019 , 9, 476	3
98	Surperhard monoclinic BC 6 N allotropes: First-principles investigations. <i>Chinese Physics B</i> , 2019 , 28, 096 2 01	3
97	Designing ultrastrong 5d transition metal diborides with excellent stability for harsh service environments. 2019 , 21, 16095-16107	4
96	Discovery of superhard materials via CALYPSO methodology. <i>Chinese Physics B</i> , 2019 , 28, 106104 1.2	9
95	Effects of pressure and temperature on thermodynamic properties of WB3 by first-principles predictions. 2019 , 6, 115034	2
94	Phase transition and electronic properties of skutterudite-type IrP under high pressure. 2019 , 21, 21262-2126	i63
93	Atomically thin NiB monolayer: a robust Dirac material. 2019 , 21, 617-622	17
92	Pressure-induced structures and properties in PB compounds. 2019 , 293, 6-10	0
91	Computational discovery and characterization of new BO phases. 2019 , 21, 2499-2506	6
90	Predicted superhard phases of Zr-B compounds under pressure. 2019 , 21, 15609-15614	5
89	An Orthorhombic Phase of Superhard o -BC 4 N *. 2019 , 36, 036201	7
88	Synthesis and characterization of WB2-WB3-B4C hard composites. 2019 , 82, 268-272	5
87	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 2761-2766	17

(2020-2019)

86	Computational Dissection of 2D SiC7 Monolayer: A Direct Band Gap Semiconductor and High Power Conversion Efficiency. 2019 , 2, 1900058		8
85	Computational Design of Mixed-Valence Tin Sulfides as Solar Absorbers. 2019 , 11, 24867-24875		7
84	Mechanical properties, microstructure and grain orientation of hot pressed WB2 ceramics with Co as a sintering additive. <i>Ceramics International</i> , 2019 , 45, 14718-14727	.1	5
83	Phase diagram and bonding states of Ir-P binary compounds at high pressures. <i>Journal of Alloys and Compounds</i> , 2019 , 791, 1257-1262	·7	3
82	Exploring high-pressure iron boride compounds: Structural electronics and mechanical properties. 2019 , 162, 69-75		О
81	Novel graphene-like two-dimensional bilayer germanene dioxide: electronic structure and optical properties <i>RSC Advances</i> , 2019 , 9, 9633-9639	·7	O
80	Theoretical Investigation on the Elastic Properties, Bond Stiffness and Hardness of WX2 ($X = B$ and N). 2019 , 41, 434-440		1
79	Unravelling the structure and strength of the highest boride of tungsten WB4.2. <i>Physical Review B</i> , 2019 , 100,	.3	16
78	First-principles study of high-pressure phase stability and superconductivity of Bi4I4. <i>Physical Review B</i> , 2019 , 100,	.3	4
77	Exploration of high-pressure structural transition and electronic properties of BaFeS. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 115401	.8	1
76	Oxidation resistance of a Mo-W-Si-B alloy at 1000🛮 300 ீ C: The effect of a multicomponent Mo-Si-B coating. 2019 , 470, 289-295		12
75	Mechanochemistry approach to produce in-situ tungsten borides and carbides nanopowders: Experimental study and modeling. 2019 , 224, 47-64		5
74	Prediction of novel ground state and high pressure phases for W2N3: First-principles. 2019 , 156, 215-223		1
73	Theoretical investigation on two novel high-pressure orthorhombic phases of superhard C3N2. Journal of Alloys and Compounds, 2020 , 815, 152324	·7	3
72	Mechanochemical synthesis and annealing of tungsten di- and tetra-boride. 2020, 103, 831-838		5
71	The effect of chemical composition on the structure, chemistry and mechanical properties of magnetron sputtered W-B-C coatings: Modeling and experiments. 2020 , 383, 125274		9
70	Boron-Rich Molybdenum Boride with Unusual Short-Range Vacancy Ordering, Anisotropic Hardness, and Superconductivity. 2020 , 32, 459-467		18
69	PAI-graphene: A new topological semimetallic two-dimensional carbon allotrope with highly tunable anisotropic Dirac cones. 2020 , 170, 477-486		19

68	Generative Adversarial Networks for Crystal Structure Prediction. 2020, 6, 1412-1420		35
67	SnP Monolayers: a New Type of Two-Dimensional Materials with High Stability, Carrier Mobility, and Magnetic Properties. 2020 , 15, 155		3
66	Stable Compositions, Structures and Electronic Properties in KLa SystemsUnder Pressure. 2020 , 37, 026201		4
65	Investigating potential hard materials: the case of tetragonal TaMoN. 2020 , 66, 758-764		2
64	Modifying structural polymorphs and tuning electronic properties in pressure-stabilized binary Ir-Sb phases <i>RSC Advances</i> , 2020 , 10, 19185-19191	3.7	
63	New Polymorphs of 2D Indium Selenide with Enhanced Electronic Properties. 2020 , 30, 2001920		19
62	Polymorphism of low dimensional boron nanomaterials driven by electrostatic gating: a computational discovery. 2020 , 12, 10543-10549		2
61	Exploring the structural, mechanical, thermodynamic, and electronic properties of (Ni0.66, Zn0.33)3Sn4 ternary intermetallic compounds by the first-principles study. 2020 , 35, 263-271		
60	First principles study of the elastic and thermodynamic properties of Mg-Al alloys. 2020 , 177, 109587		1
59	Effect of tantalum on phase transition and thermal stability of metastable tungsten tetra-boride. <i>Ceramics International</i> , 2020 , 46, 17217-17223	5.1	6
58	The Effect of Laser Power on the Properties of MB-Type Boride-Based Cermet Coatings Prepared by Laser Cladding Synthesis. 2020 , 13,		5
57	High-pressure study of the structural phase transition in Cu1.875Te. 2021 , 186, 110020		1
56	In-situ synthesis of tungsten boride-carbide composite powders from WO3-B2O3MgI quaternary system via a mechanochemical route. <i>Ceramics International</i> , 2021 , 47, 1640-1650	5.1	2
55	Density functional study on Ag8-xCuxI8 (0⊠8). 2021 , 604, 412668		
54	Ab initio study on crystal structure and phase stability of ZrC2 under high pressure. <i>Chinese Physics B</i> , 2021 , 30, 016101	1.2	2
53	Pressure-Induced Evolution of Crystal and Electronic Structure of Ammonia Borane. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 2036-2043	6.4	2
52	Enhanced Hardness in Transition-Metal Monocarbides via Optimal Occupancy of Bonding Orbitals. 2021 , 13, 14365-14376		3
51	Ground-state structure and physical properties of YB3 predicted from first-principles calculations*. <i>Chinese Physics B</i> , 2021 , 30, 046101	1.2	Ο

(2021-2021)

50	Constrained crystals deep convolutional generative adversarial network for the inverse design of crystal structures. 2021 , 7,		11
49	Structural evolution, lattice dynamics, electronic and thermal properties of VH2 under high pressure. 2021 , 330, 114287		4
48	Probing the mechanical properties of ordered and disordered Pt-Ir alloys by first-principles calculations. 2021 , 405, 127424		2
47	Crystal structures and formation mechanisms of boron-rich tungsten borides. <i>Physical Review B</i> , 2021 , 104,	3.3	3
46	Progress in functional studies of transition metal borides. Chinese Physics B,	1.2	0
45	Energetics of boron near tungsten surfaces: A first-principles study. <i>Journal of Applied Physics</i> , 2021 , 130, 015101	2.5	1
44	Remarkable-cycling-performance anode for Li-ion battery: The bilayer bismuthene. <i>Electrochimica Acta</i> , 2021 , 388, 138641	6.7	0
43	Direct H-He chemical association in superionic FeO2H2He at Deep-Earth conditions. <i>National Science Review</i> ,	10.8	O
42	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. 2020 , 2729-2756	5	1
41	CoB6 monolayer: A robust two-dimensional ferromagnet. <i>Physical Review B</i> , 2019 , 99,	3.3	42
40	Indentation-strain stiffening in tungsten nitrides: Mechanisms and implications. <i>Physical Review Materials</i> , 2020 , 4,	3.2	35
39	Theoretical study of B segregation in Mo(110). <i>Journal of Boron</i> ,		1
38	Structures and properties of functional transition metal borides. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2017 , 66, 036103	0.6	3
37	Effect of tungsten disilicide addition on tungsten boride based composites produced by milling-assisted pressureless sintering. <i>Journal of Boron</i> ,		
36	Theoretical calculations of stabilities and properties of transition metal borocarbides TM3B3C and TM4B3C2 compound. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2019 , 68, 096201	0.6	
35	Stable Structures and Superconductivity in a Y-Si System under High Pressure. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 10388-10393	6.4	3
34	Prediction of LinCd compounds with unusual stoichiometry and valence states. <i>Physical Review Materials</i> , 2020 , 4,	3.2	0
33	Structural evolution and phase transition mechanism of [Formula: see text] under high pressure. <i>Scientific Reports</i> , 2021 , 11, 22090	4.9	

32	Effects of substrate bias voltage on the phase structure, mechanical and wear resistance properties of tungsten boride films. <i>Ceramics International</i> , 2022 ,	5.1	O
31	Boosting the photocatalytic H evolution activity of type-II g-GaN/ScCO van der Waals heterostructure using applied biaxial strain and external electric field RSC Advances, 2022, 12, 7391-74	40 ²⁷	1
30	Orthorhombic ScB3 and hexagonal ScB6 with high hardness. <i>Physical Review B</i> , 2022 , 105,	3.3	0
29	Hardening Effects in Superhard Transition-Metal Borides. <i>Accounts of Materials Research</i> , 2022 , 3, 100-	1 0,9 5	1
28	Stability and mechanical properties of W1\(\mathbb{M}\)moxB4.2 (x. Physical Review Materials, 2021 , 5,	3.2	O
27	A DFT study to determine the structure and composition of EW2B5-x. <i>Journal of Alloys and Compounds</i> , 2022 , 164962	5.7	O
26	Efficient Synthesis of WB-WB Powders with Selectivity for WB Content Inorganic Chemistry, 2022,	5.1	1
25	Energetics of intrinsic point defects and hydrogen in tungsten borides: A first-principles study. <i>Nuclear Fusion</i> ,	3.3	O
24	Theoretical Methods for Structural Phase Transitions in Elemental Solids at Extreme Conditions: Statics and Dynamics. <i>Journal of Physics Condensed Matter</i> ,	1.8	
23	New Insights into the Traditional Charge Compensation Theory: Amphoteric Behavior of TiO2 under the Guidance of SupplyDemand Relationship. <i>ACS Omega</i> , 2022 , 7, 21225-21232	3.9	
22	First-principles study on the thermodynamic, electronic and mechanical properties of MgAlBi ternary compounds. <i>Journal of Materials Research and Technology</i> , 2022 , 19, 2848-2862	5.5	O
21	Structural and electro-catalytic properties of copper clusters: a study via deep learning and first principles . <i>Journal of Chemical Physics</i> ,	3.9	
20	Prediction of Core Electron Reactivity and High Oxidation States in Radium under High Pressure. Journal of Physical Chemistry C,	3.8	
19	Force-based gradient descent method for ab initio atomic structure relaxation. 2022, 106,		O
18	Pressure-induced novel structure with graphene-like boron-layer in titanium monoboride.		0
17	Size-controlled preparations of tungsten and molybdenum borides in calcium or aluminum melt. 2022 ,		O
16	Polymeric Hydronitrogen N4H: A Promising High-Energy-Density Material and High-Temperature Superconductor.		О
15	Two-dimensional semiconductors of $Cr X3H3$ (X = O, S, Se, and Te) structures with large magnetic anisotropy and high Curie temperature.		O

CITATION REPORT

14	First-principles study on the elastic anisotropy and thermal properties of MgI compounds. 2022 , 171, 111034	О
13	Roles of hydrogen in structural stability and electronic property of bulk hydrogenated amorphous silicon. 2023 , 216, 111846	1
12	First-principles predictions of stable structure of AuAl2 under high pressure. 2023 , 359, 115009	О
11	Stabilized Nitrogen Framework Anions in the Gaß System.	О
10	Impact of vacancies on structure, stability and properties of hexagonal transition metal diborides, MB2 (M = Sc, Y, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Mn, and Fe). 2022 , 101629	0
9	Strain and thickness effects on the electronic structures of low-energy two-dimensional CdxTey phases. 2022 , 24, 29772-29780	o
8	First-principle prediction of one-dimensional silicon allotropes: Promising new candidate for chemical and electrochemical hydrogen storage. 2022 ,	О
7	Structure, Stability, and Electronic Properties of Hydrogenated Monolayer 2D Silicon Allotropes by First-Principles Calculation. 2200426	o
6	A noise-robust data assimilation method for crystal structure determination using powder diffraction intensity. 2022 , 157, 224112	О
5	Pressure-induced enhancement of thermoelectric performance of CoP3 by the structural phase transition. 2023 , 248, 118773	O
4	First-principles calculations to investigate mechanical, electronic, optical, and thermodynamic properties of Zr-based ternary compounds. 2023 , 23, 1417-1434	0
3	Direct transformation of tungsten trioxide monohydrate into ammonium paratungstate tetrahydrate in ammonium salt solutions. 2023 , 30, 121-131	0
2	Current Status and Future Scope of Phase Diagram Studies. 2023 , 63, 407-418	0
1	Surface stability and H adsorption and diffusion near surfaces of W borides: a first-principles study. 2023 , 63, 066002	O