Xing-Qiu Chen

List of Publications by Year
in descending order

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140 papers	10,854 citations	57631 44 h-index	31759 101 g-index
145 all docs	145 docs citations	145 times ranked	10116 citing authors

#	Article	IF	Citations
1	Modeling hardness of polycrystalline materials and bulk metallic glasses. Intermetallics, 2011, 19, 1275-1281.	1.8	1,811
2	Dirac semimetal and topological phase transitions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>A</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Bi (<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML") Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 692 Td (display="inline"><mm	1.1	1,529
3	Chemical vapor deposition of layered two-dimensional MoSi ₂ N ₄ materials. Science, 2020, 369, 670-674.	6.0	556
4	Band Gap Narrowing of Titanium Oxide Semiconductors by Noncompensated Anion-Cation Codoping for Enhanced Visible-Light Photoactivity. Physical Review Letters, 2009, 103, 226401.	2.9	347
5	Flexible layer-structured Bi2Te3 thermoelectric on a carbon nanotube scaffold. Nature Materials, 2019, 18, 62-68.	13.3	316
6	Half-Heusler Compounds as a New Class of Three-Dimensional Topological Insulators. Physical Review Letters, 2010, 105, 096404.	2.9	306
7	Thermoelectric performance of a metastable thin-film Heusler alloy. Nature, 2019, 576, 85-90.	13.7	232
8	An Unusual Strong Visibleâ€Light Absorption Band in Red Anatase TiO₂ Photocatalyst Induced by Atomic Hydrogenâ€Occupied Oxygen Vacancies. Advanced Materials, 2018, 30, 1704479.	11.1	231
9	Intercalated architecture of MA2Z4 family layered van der Waals materials with emerging topological, magnetic and superconducting properties. Nature Communications, 2021, 12, 2361.	5.8	199
10	Ab initio prediction of half-metallic properties for the ferromagnetic Heusler alloys Co[sub 2]MSi (M=Ti,V,Cr). Journal of Applied Physics, 2006, 100, 113901.	1.1	180
11	Dirac Node Lines in Pure Alkali Earth Metals. Physical Review Letters, 2016, 117, 096401.	2.9	174
12	Families of Superhard Crystalline Carbon Allotropes Constructed via Cold Compression of Graphite and Nanotubes. Physical Review Letters, 2012, 108, 135501.	2.9	167
13	Extra-electron induced covalent strengthening and generalization of intrinsic ductile-to-brittle criterion. Scientific Reports, 2012, 2, 718.	1.6	165
14	Vacancy Mechanism of High Oxygen Solubility and Nucleation of Stable Oxygen-Enriched Clusters in Fe. Physical Review Letters, 2007, 99, 225502.	2.9	162
15	Electronic and Structural Origin of Ultraincompressibility of5dTransition-Metal DiboridesMB2(M=W,) Tj ETQq1 1 0.784314 rgBT /Ove	2.9	160
16	Structure, bonding, and possible superhardness of CrB<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 85, .	1.1	154
17	Enhancing Charge Separation in Metallic Photocatalysts: A Case Study of the Conducting Molybdenum Dioxide. Advanced Functional Materials, 2016, 26, 4445-4455.	7.8	154
18	Monoclinic dibismuth tetraoxide: A new visible-light-driven photocatalyst for environmental remediation. Applied Catalysis B: Environmental, 2015, 176-177, 444-453.	10.8	153

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19	Hardness of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>T</mml:mi></mml:math>-carbon: Density functional theory calculations. Physical Review B, 2011, 84, .	1.1	140
20	First-principles modeling of anisotropic anodic dissolution of metals and alloys in corrosive environments. Acta Materialia, 2017, 130, 137-146.	3.8	129
21	Unconventional superconducting phase in the weakly correlated noncentrosymmetric<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Mo</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:m Physical Review B, 2010, 82, .	1.1	121
22	Rocksalt SnS and SnSe: Native topological crystalline insulators. Physical Review B, 2013, 88, .	1.1	104
23	Computation and data driven discovery of topological phononic materials. Nature Communications, 2021, 12, 1204.	5.8	98
24	Spin transition in a four-coordinate iron oxide. Nature Chemistry, 2009, 1, 371-376.	6.6	97
25	Topological quantum catalyst: Dirac nodal line states and a potential electrocatalyst of hydrogen evolution in the TiSi family. Science China Materials, 2018, 61, 23-29.	3.5	97
26	Superconductivity in Novel Ge-Based Skutterudites:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo stretchy="false">{</mml:mo><mml:mi>Sr</mml:mi><mml:mo>,</mml:mo><mml:mi>Ba</mml:mi><mml:mo stretchy="false">}</mml:mo><mml:msub><mml:mi>Pt</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:msub><mml:mi>Ge</mml: Physical Review Letters, 2007, 99, 217001.	2.9	90
27	Computational materials discovery: the case of the Wâ€“B system. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 85-103.	0.2	87
28	Vacancy formation enthalpies of high-entropy FeCoCrNi alloy via first-principles calculations and possible implications to its superior radiation tolerance. Journal of Materials Science and Technology, 2018, 34, 355-364.	5.6	87
29	New Family of Three-Dimensional Topological Insulators with Antiperovskite Structure. Physical Review Letters, 2010, 105, 216406.	2.9	80
30	Inclusion flotation-driven channel segregation in solidifying steels. Nature Communications, 2014, 5, 5572.	5.8	79
31	Coexistent three-component and two-component Weyl phonons in TiS, ZrSe, and HfTe. Physical Review B, 2018, 97, .	1.1	75
32	Interstitial-boron solution strengthened WB3+x. Applied Physics Letters, 2013, 103, .	1.5	72
33	First-principles studies of structural stabilities and enthalpies of formation of refractory intermetallics: TM and TM3 (TÂ=ÂTi, Zr, Hf; MÂ=ÂRu, Rh, Pd, Os, Ir, Pt). Intermetallics, 2012, 28, 16-24.	1.8	70
34	Anisotropic magnetic couplings and structure-driven canted to collinear transitions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:m magnetically constrained noncollinear DFT. Physical Review B, 2015, 92, .	1.1	70
35	Topological phonons in graphene. Physical Review B, 2020, 101, .	1.1	70
36	Electronic, optical, and mechanical properties of superhard cold-compressed phases of carbon. Applied Physics Letters, 2011, 99, .	1.5	68

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37	Coexistence of intrinsic piezoelectricity and ferromagnetism induced by small biaxial strain in septuple-atomic-layer VSi₂P₄. Physical Chemistry Chemical Physics, 2020, 22, 28359-28364.	1.3	67
38	Ab initiostudy of ground-state properties of the Laves phase compoundsTiCr2,ZrCr2, andHfCr2. Physical Review B, 2005, 71, .	1.1	64
39	Phononic Weyl nodal straight lines in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MgB</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2020, 101, .	1.1	58
40	Computational and experimental study of phase stability, cohesive properties, magnetism and electronic structure of TiMn2. Acta Materialia, 2003, 51, 1239-1247.	3.8	55
41	First-principles modeling of hardness in transition-metal diborides. Physical Review B, 2009, 80, .	1.1	52
42	First-principles modeling of the hydrogen evolution reaction and its application in electrochemical corrosion of Mg. Acta Materialia, 2020, 183, 377-389.	3.8	50
43	Variable-composition structural optimization and experimental verification of MnB₃and MnB₄. Physical Chemistry Chemical Physics, 2014, 16, 15866-15873.	1.3	49
44	Noninvasively Modifying Band Structures of Wideâ€Bandgap Metal Oxides to Boost Photocatalytic Activity. Advanced Materials, 2018, 30, e1706259.	11.1	48
45	Half-Heusler alloys: Enhancement of ZT after severe plastic deformation (ultra-low thermal) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf	3.8	44
46	Miedemaâ€™s model revisited: The parameter for Ti, Zr, and Hf. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2006, 30, 266-269.	0.7	43
47	Prediction of novel stable compounds in the Mg-Si-O system under exoplanet pressures. Scientific Reports, 2016, 5, 18347.	1.6	43
48	Structure effect on intrinsic piezoelectricity in septuple-atomic-layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si98.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">MSi</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mrow><mml:mi mathvariant="normal">N</mml:mi></mml:mrow><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> (M="Mo and W". Computational Materials Science, 2021, 188, 110223.	1.4	43
49	display="inline"><mml:mrow><mml:mi>d</mml:mi></mml:mrow></mml:math>perovskites<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>R</mml:mi></mml:mrow></mml:math>TcO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:m	1.1	42
50	Phononic Weyl points and one-way topologically protected nontrivial phononic surface arc states in noncentrosymmetric WC-type materials. Physical Review B, 2019, 99, .	1.1	41
51	Ab initiostudy of ground-state properties of the Laves-phase compoundZrMn2. Physical Review B, 2005, 72, .	1.1	40
52	The electronic, elastic, and structural properties of Tiâ€“Pd intermetallics and associated hydrides from first principles calculations. Intermetallics, 2010, 18, 998-1006.	1.8	40
53	Relativistic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math> +BSE study of the optical properties of Ruddlesden-Popper iridates. Physical Review Materials, 2018, 2, .	0.0	40
54	Bonding and strength of solid nitrogen in the cubic gauche (cg-N) structure. Physical Review B, 2008, 77, .	1.1	39

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55	Superconductivity and spin fluctuations in{Th,U}Pt4Ge12skutterudites. Physical Review B, 2008, 78, .	1.1	38
56	Tuning the vertical location of helical surface states in topological insulator heterostructures via dual-proximity effects. Scientific Reports, 2013, 3, 1233.	1.6	38
57	Effects of dilute substitutional solutes on interstitial carbon in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math>-Fe: Interactions and associated carbon diffusion from first-principles calculations. Physical Review B, 2014, 90, .	1.1	38
58	Topological phononic materials: Computation and data. Innovation(China), 2021, 2, 100134.	5.2	38
59	The standard enthalpies of formation of binary intermetallic compounds of some late 4d and 5d transition metals by high temperature direct synthesis calorimetry. Journal of Alloys and Compounds, 2010, 492, 105-115.	2.8	36
60	Structural transitions and transport-half-metallic ferromagnetism in LaMnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>at elevated pressure. Physical Review B, 2012, 85, .	1.1	36
61	Ground-state phase in the three-dimensional topological Dirac semimetal<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Na</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi>Bi</mml:mi><mml:mn>1−</mml:mn></mml:msub></mml:math>Physical Review B, 2014, 89, .	1.1	36
62	Manufacture-friendly nanostructured metals stabilized by dual-phase honeycomb shell. Nature Communications, 2022, 13, 2034.	5.8	33
63	Strain-driven onset of nontrivial topological insulating states in Zintl Sr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub><mml:mi>X</mml:mi></mml:mrow></mml:math>compounds		

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73	Site preference, thermodynamic, and magnetic properties of the ternary Laves phase Ti(Fe_{1â€“x}Al_x)₂ with the crystal structure of the MgZn₂-type. International Journal of Materials Research, 2006, 97, 450-460.	0.8	24
74	From trans-polyacetylene to zigzag-edged graphene nanoribbons. Chemical Physics Letters, 2009, 483, 120-123.	1.2	24
75	Two-dimensional layered MSi₂N₄ (M = Mo, W) as promising thermal management materials: a comparative study. Physical Chemistry Chemical Physics, 2022, 24, 3086-3093.	1.3	24
76	Comment on â€œEnthalpies of formation of binary Laves phasesâ€•[Intermetallics, 10 (2002) 579â€“595]. Intermetallics, 2004, 12, 59-62.	1.8	23
77	The standard enthalpies of formation of some intermetallic compounds of early 4d and 5d transition metals by high temperature direct synthesis calorimetry. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2009, 33, 55-62.	0.7	23
78	Underlying Topological Dirac Nodal Line Mechanism of the Anomalously Large Electron-Phonon Coupling Strength on a Be (0001) Surface. Physical Review Letters, 2019, 123, 136802.	2.9	23
79	Crystal structures and constitution of the binary system iridium-boron. Science China Materials, 2015, 58, 649-668.	3.5	22
80	The mechanism of Î¸- to Î±-Al2O3 phase transformation. Journal of Alloys and Compounds, 2021, 863, 158666.	2.8	22
81	High-throughput modeling of atomic diffusion migration energy barrier of fcc metals. Progress in Natural Science: Materials International, 2019, 29, 341-348.	1.8	20
82	Crystal structure, phase stability and elastic properties of the Laves phase ZrTiCu2. Intermetallics, 2008, 16, 651-657.	1.8	19
83	Polymeric forms of carbon in dense lithium carbide. Journal of Physics Condensed Matter, 2010, 22, 292201.	0.7	19
84	Density functional study of structural and phase stabilities for RMn2 Laves phases (R = Sc, Y, Lu, Ti, Zr,) Tj ETQq0 0 0 rgBT /Overlock 10 T	2.8	18
85	On the ternary Laves phases {Sc,Ti}2M3Si (M=Cr, Mn, Fe, Co, Ni) with MgZn2-type. Journal of Alloys and Compounds, 2007, 429, 10-18.	2.8	18
86	Laves phases in the ternary systems Tiâ€“{Pd, Pt}â€“Al. Intermetallics, 2009, 17, 336-342.	1.8	18
87	Stable compositions and structures in the Naâ€“Bi system. Physical Chemistry Chemical Physics, 2015, 17, 6933-6947.	1.3	18
88	Fast and Huge Anisotropic Diffusion of Cu (Ag) and Its Resistance on the Sn Self-diffusivity in Solid Î²â€“Sn. Journal of Materials Science and Technology, 2016, 32, 121-128.	5.6	18
89	Computational design of flexible electrides with nontrivial band topology. Physical Review Materials, 2019, 3, .	0.9	18
90	A new polymorphic material? Structural degeneracy of ZrMn 2. Europhysics Letters, 2004, 67, 807-813.	0.7	17

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91	Superconductivity and Magnetism in MPt₄Ge₁₂, M = Ca, Ba, Sr, Eu. Journal of the Physical Society of Japan, 2008, 77, 121-127.	0.7	17
92	Anisotropy in electronic, optical, and mechanical properties of superhard body-centered tetragonal C4 phase of carbon. Applied Physics Letters, 2010, 97, 061910.	1.5	17
93	Atom order and thermodynamic properties of the ternary Laves phase Ti(TiyNixAl1â€“xâ€“y)2. Zeitschrift Fur Kristallographie - Crystalline Materials, 2006, 221, .	0.4	16
94	Two-dimensional topological semimetal states in monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>2</mml:mn></mml:r , and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>2</mml:mn></mml:mm.	1.1	16
95	Thermodynamic modeling of Laves phases in the Taâ€“V system: Reassessment using first-principles results. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2011, 35, 103-108.	0.7	15
96	Vacancy formation enthalpy of filled<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>d</mml:mi></mml:math>-band noble metals by hybrid functionals. Physical Review B, 2014, 90, .	1.1	15
97	Ductile-to-brittle transition and materialsâ€™ resistance to amorphization by irradiation damage. RSC Advances, 2016, 6, 44561-44568.	1.7	14
98	Evolution of local atomic structure during solidification of U116Nb12 liquid: An ab initio molecular dynamics study. Journal of Alloys and Compounds, 2019, 787, 267-275.	2.8	14
99	Six-membered-ring inorganic materials: definition and prospects. National Science Review, 2021, 8, nwaa248.	4.6	14
100	First-principles study on the effects of twin boundaries on anodic dissolution of Mg. Physical Review Materials, 2019, 3, .	0.9	14
101	Structural, thermodynamic, and transport properties of Laves-phaseZrMn2from x-ray and neutron diffraction and first principles. Physical Review B, 2006, 74, .	1.1	13
102	Ab initiostudy of structural stability, elastic, vibrational, and electronic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">Pd</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2007, 76, .	1.1	13
103	Pressure-induced behavior of the hydrogen-dominant compoundSiH4(H2)2from first-principles calculations. Physical Review B, 2010, 82, .	1.1	13
104	Crystal chemistry of the G-phases in the {Ti, Zr, Hf}â€“Niâ€“Si systems. Journal of Solid State Chemistry, 2007, 180, 733-741.	1.4	12
105	Ab initiostudy of structural, magnetic, vibrational, and thermodynamic properties of the Laves-phase compoundHfMn2. Physical Review B, 2007, 76, .	1.1	11
106	Topological massive Dirac fermions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi></mml:math>-tungsten. Physical Review B, 2019, 99, .	1.1	11
107	Topological nodal line and superconductivity of highly thermally stable two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">TiB</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review B, 2021, 104, .	1.1	11
108	Thermally stable coherent domain boundaries in complex-structured Cr₂Nb intermetallics. Philosophical Magazine, 2016, 96, 58-70.	0.7	10

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109	A simple and efficient criterion for ready screening of potential topological insulators. Science Bulletin, 2017, 62, 1649-1653.	4.3	10
110	Structural, elastic, and electronic properties of topological semimetal WC-type MX family by first-principles calculation*. Chinese Physics B, 2019, 28, 077105.	0.7	10
111	The system Taâ€“Vâ€“Si: Crystal structure and phase equilibria. Journal of Solid State Chemistry, 2012, 187, 114-123.	1.4	9
112	Combined fast reversible liquidlike elastic deformation with topological phase transition in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Na</mml:mi><mml:mn>3</mml:mn></mml: Physical Review B, 2015, 92, .	1.1	9
113	First-Principles Investigation of Thermodynamic Decomposition of Interfacial Oxides in Hot Compression Bonding. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2020, 51, 874-886.	1.1	9
114	Thickness dependent structural and electronic properties of CuO grown on SrTiO₃(100): a hybrid density functional theory study. Journal of Physics Condensed Matter, 2011, 23, 045004.	0.7	8
115	First-principles study of the large-gap three-dimensional topological insulatorsM3Bi2(M=Ca, Sr, Ba). Physical Review B, 2015, 92, .	1.1	8
116	The electronic and mechanical properties of tetragonal YB2C as explored by first-principles methods. Journal of Alloys and Compounds, 2017, 726, 173-178.	2.8	8
117	First-principles study of hydrogen trapping behavior in face centered cubic metals (M=Ni, Cu and Al) with monovacancy. International Journal of Hydrogen Energy, 2020, 45, 25555-25566.	3.8	8
118	General principles to high-throughput constructing two-dimensional carbon allotropes*. Chinese Physics B, 2020, 29, 037306.	0.7	8
119	First-principles comprehensive study of electronic and mechanical properties of novel uranium hydrides at different pressures. Progress in Natural Science: Materials International, 2020, 30, 251-259.	1.8	8
120	BaPt₄Ge₁₂: A Skutterudite Based Entirely on a Ge Framework. Advanced Materials, 2008, 20, 1325-1328.	11.1	7
121	First-principles studies of hydrogen behavior interacting with oxygen-enriched nanostructured particles in the ODS steels. International Journal of Hydrogen Energy, 2014, 39, 18506-18519.	3.8	7
122	Topological Metal of NaBi with Ultralow Lattice Thermal Conductivity and Electron-phonon Superconductivity. Scientific Reports, 2015, 5, 8446.	1.6	7
123	One-Step Growth of Bilayer 2Hâ€“1Tâ€² MoTe₂ van der Waals Heterostructures with Interlayer-Coupled Resonant Phonon Vibration. ACS Nano, 2022, 16, 11268-11277.	7.3	7
124	Towards a Mechanism Underlying the Stability of the Tetragonal CuO Phase: Comparison with NiO and CoO by Hybrid Density Functional Calculation. Chinese Physics Letters, 2014, 31, 027402.	1.3	6
125	Structural, thermodynamic, and electronic properties of Laves-phase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NbMn</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:m from first principles, x-ray diffraction, and calorimetric experiments. Physical Review B, 2018, 97, .	1.1	6
126	Comprehensive first-principles study of transition-metal substitution in the Î³ phase of nickel-based superalloys. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 61, 41-49.	0.7	6

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127	Onâ€Demand Preparation of Î±â€Phaseâ€Dominated Tungsten Films for Highly Qualified Thermal Reflectors. Advanced Materials Interfaces, 2019, 6, 1900031.	1.9	6
128	Comment on â€œProposed model for calculating the standard formation enthalpy of binary transition-metal systemsâ€•[Appl. Phys. Lett. 81, 1219 (2002)]. Applied Physics Letters, 2005, 86, 216103.	1.5	5
129	Pressure Response of Novel Superconducting {Sr,Ba}Pt4Ge12. Journal of the Physical Society of Japan, 2008, 77, 350-352.	0.7	5
130	The system Taâ€“Vâ€“Si: Thermodynamic modeling. Journal of Solid State Chemistry, 2013, 199, 171-180.	1.4	5
131	Thermochemistry of some binary lead and transition metal compounds by high temperature direct synthesis calorimetry. Journal of Alloys and Compounds, 2015, 633, 183-187.	2.8	5
132	Publisher's Note:Ab initiostudy of ground-state properties of the Laves phase compoundsTiCr2,ZrCr2, andHfCr2[Phys. Rev. B71, 174101 (2005)]. Physical Review B, 2005, 71, .	1.1	4
133	Boosting the discovery of 3D topological materials: mixing chemistry with physics via a two-step computational screening strategy. National Science Review, 2018, 5, 316-318.	4.6	2
134	Localized Nb clusters in U-Nb liquid alloys: An ab initio molecular dynamics study. Nuclear Materials and Energy, 2021, 26, 100915.	0.6	2
135	Inducing mechanism and model of the critical oxygen content in homogenized steel. Materials and Design, 2021, 205, 109723.	3.3	2
136	Coupling of magnetic ordering and vibrational properties: a density functional theory study of magnetic and structural phase transitions. Phase Transitions, 2007, 80, 445-468.	0.6	1
137	Modeling Activity and Interaction Coefficients of Components of Multicomponent Alloy Melts: An Example of Iron Melt. High Temperature Materials and Processes, 2013, 32, 215-221.	0.6	0
138	An ab initio study on the dynamical properties of U-Nb alloy melt. Chinese Physics B, 0, , .	0.7	0
139	Implications for the Nb aggregation inherited from melt to Î³ phase of U-Nb alloy. Journal of Alloys and Compounds, 2021, 885, 160537.	2.8	0
140	Site preference, thermodynamic, and magnetic properties of the ternary Laves phase Ti(Fe<sub>1 â€“) Tj ETQq0 0 0 rgBT /Overlock 10 T MgZn₂-type. International Journal of Materials Research, 2022, 97, 450-460.	0.1	0