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	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
2	Manufacture-friendly nanostructured metals stabilized by dual-phase honeycomb shell. Nature Communications, 2022, 13, 2034.	5.8	33
3	Site preference, thermodynamic, and magnetic properties of the ternary Laves phase Ti(Fe<sub>1 â€“) Tj ETQq1 1 0.784314 rgBT /Ov MgZn₂-type. International Journal of Materials Research, 2022, 97, 450-460.	0.1	0
4	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
5	Six-membered-ring inorganic materials: definition and prospects. National Science Review, 2021, 8, nwaa248.	4.6	14
6	A piezoelectric quantum spin Hall insulator with Rashba spin splitting in Janus monolayer SrAlGaSe₄. Journal of Materials Chemistry C, 2021, 9, 7465-7473.	2.7	28
7	Computation and data driven discovery of topological phononic materials. Nature Communications, 2021, 12, 1204.	5.8	98
8	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 mathvariant="normal">N</mml:mi></mml:mrow><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub></mml:mrow></mml: (M=Mo and W). Computational Materials Science, 2021, 188, 110223.	1.4	43
9	Localized Nb clusters in U-Nb liquid alloys: An ab initio molecular dynamics study. Nuclear Materials and Energy, 2021, 26, 100915.	0.6	2
10	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
11	The mechanism of Î¸- to Î±-Al2O3 phase transformation. Journal of Alloys and Compounds, 2021, 863, 158666.	2.8	22
12	Inducing mechanism and model of the critical oxygen content in homogenized steel. Materials and Design, 2021, 205, 109723.	3.3	2
13	Topological phononic materials: Computation and data. Innovation(China), 2021, 2, 100134.	5.2	38
14	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
15	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
16	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
17	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
18	Half-Heusler alloys: Enhancement of ZT after severe plastic deformation (ultra-low thermal) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 62 Td (	3.8	44

#	Article	IF	Citations
19	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
20	Chemical vapor deposition of layered two-dimensional MoSi ₂ N ₄ materials. Science, 2020, 369, 670-674.	6.0	556
21	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
22	Topological phonons in graphene. Physical Review B, 2020, 101, .	1.1	70
23	General principles to high-throughput constructing two-dimensional carbon allotropes*. Chinese Physics B, 2020, 29, 037306.	0.7	8
24	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>, <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:</mml:math>, 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
25	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
26	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
27	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
28	Thermoelectric performance of a metastable thin-film Heusler alloy. Nature, 2019, 576, 85-90.	13.7	232
29	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
30	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
31	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
32	Onâ€Demand Preparation of Î±â€Phaseâ€Dominated Tungsten Films for Highly Qualified Thermal Reflectors. Advanced Materials Interfaces, 2019, 6, 1900031.	1.9	6
33	TiO2 nanoparticles-assisted Î±-Al2O3 direct thermal growth on nickel aluminide intermetallics: Template effect of the oxide with the hexagonal oxygen sublattice. Corrosion Science, 2019, 153, 109-117.	3.0	25
34	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
35	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
36	Flexible layer-structured Bi2Te3 thermoelectric on a carbon nanotube scaffold. Nature Materials, 2019, 18, 62-68.	13.3	316

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37	Computational design of flexible electrides with nontrivial band topology. Physical Review Materials, 2019, 3, .	0.9	18
38	First-principles study on the effects of twin boundaries on anodic dissolution of Mg. Physical Review Materials, 2019, 3, .	0.9	14
39	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:m from first principles, x-ray diffraction, and calorimetric experiments. Physical Review B, 2018, 97, .	1.1	6
40	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
41	Noninvasively Modifying Band Structures of Wideâ€Bandgap Metal Oxides to Boost Photocatalytic Activity. Advanced Materials, 2018, 30, e1706259.	11.1	48
42	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
43	Tunable metal-insulator transition, Rashba effect and Weyl Fermions in a relativistic charge-ordered ferroelectric oxide. Nature Communications, 2018, 9, 492.	5.8	31
44	Coexistent three-component and two-component Weyl phonons in TiS, ZrSe, and HfTe. Physical Review B, 2018, 97, .	1.1	75
45	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
46	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
47	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
48	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:m +BSE study of the optical properties of Ruddlesden-Popper iridates. Physical Review Materials, 2018, 2, .	3.1	40
49	Topologically Entangled Rashba-Split Shockley States on the Surface of Grey Arsenic. Physical Review Letters, 2017, 118, 046802.	2.9	27
50	First-principles modeling of anisotropic anodic dissolution of metals and alloys in corrosive environments. Acta Materialia, 2017, 130, 137-146.	3.8	129
51	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
52	A simple and efficient criterion for ready screening of potential topological insulators. Science Bulletin, 2017, 62, 1649-1653.	4.3	10
53	Enhancing Charge Separation in Metallic Photocatalysts: A Case Study of the Conducting Molybdenum Dioxide. Advanced Functional Materials, 2016, 26, 4445-4455.	7.8	154
54	Electron and hole doping in the relativistic Mott insulator <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">Sr</mml:mi><mml:mn mathvariant="bold">2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">IrO</mml:mi><mml:mn mathvariant="bold">4</mml:mn></mml:msub></mml:mrow></mml:math> : A first-principles study using	1.1	27

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55	Ductile-to-brittle transition and materialsâ€™ resistance to amorphization by irradiation damage. RSC Advances, 2016, 6, 44561-44568.	1.7	14
56	Dirac Node Lines in Pure Alkali Earth Metals. Physical Review Letters, 2016, 117, 096401.	2.9	174
57	Prediction of novel stable compounds in the Mg-Si-O system under exoplanet pressures. Scientific Reports, 2016, 5, 18347.	1.6	43
58	Thermally stable coherent domain boundaries in complex-structured Cr₂Nb intermetallics. Philosophical Magazine, 2016, 96, 58-70.	0.7	10
59	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
60	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:math> magnetically constrained noncollinear DFT. Physical Review B, 2015, 92, .	1.1	70
61	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:msub></mml:mrow></mml:math> Physical Review B, 2015, 92, .	1.1	9
62	First-principles study of the large-gap three-dimensional topological insulatorsM3Bi2(M=Ca, Sr, Ba). Physical Review B, 2015, 92, .	1.1	8
63	Topological Metal of NaBi with Ultralow Lattice Thermal Conductivity and Electron-phonon Superconductivity. Scientific Reports, 2015, 5, 8446.	1.6	7
64	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
65	Stable compositions and structures in the Naâ€“Bi system. Physical Chemistry Chemical Physics, 2015, 17, 6933-6947.	1.3	18
66	Monoclinic dibismuth tetraoxide: A new visible-light-driven photocatalyst for environmental remediation. Applied Catalysis B: Environmental, 2015, 176-177, 444-453.	10.8	153
67	Crystal structures and constitution of the binary system iridium-boron. Science China Materials, 2015, 58, 649-668.	3.5	22
68	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
69	Inclusion flotation-driven channel segregation in solidifying steels. Nature Communications, 2014, 5, 5572.	5.8	79
70	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
71	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
72	Variable-composition structural optimization and experimental verification of MnB₃and MnB₄. Physical Chemistry Chemical Physics, 2014, 16, 15866-15873.	1.3	49

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73	First-principles study of ground-state properties of U₂Mo. Physical Chemistry Chemical Physics, 2014, 16, 26974-26982.	1.3	26
74	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
75	Computational materials discovery: the case of the Wâ€“B system. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 85-103.	0.2	87
76	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:m Physical Review B, 2014, 89, .	1.1	36
77	Unified mechanism for hydrogen trapping at metal vacancies. International Journal of Hydrogen Energy, 2014, 39, 11321-11327.	3.8	30
78	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
79	The system Taâ€“Vâ€“Si: Thermodynamic modeling. Journal of Solid State Chemistry, 2013, 199, 171-180.	1.4	5
80	Rocksalt SnS and SnSe: Native topological crystalline insulators. Physical Review B, 2013, 88, .	1.1	104
81	Tuning the vertical location of helical surface states in topological insulator heterostructures via dual-proximity effects. Scientific Reports, 2013, 3, 1233.	1.6	38
82	Interstitial-boron solution strengthened WB3+x. Applied Physics Letters, 2013, 103, .	1.5	72
83	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
84	Extra-electron induced covalent strengthening and generalization of intrinsic ductile-to-brittle criterion. Scientific Reports, 2012, 2, 718.	1.6	165
85	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
86	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
87	Families of Superhard Crystalline Carbon Allotropes Constructed via Cold Compression of Graphite and Nanotubes. Physical Review Letters, 2012, 108, 135501.	2.9	167
88	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 50 132 Td (display="inline"><mm	1.1	1,529
89	The system Taâ€“Vâ€“Si: Crystal structure and phase equilibria. Journal of Solid State Chemistry, 2012, 187, 114-123.	1.4	9
90	Electronic, optical, and mechanical properties of superhard cold-compressed phases of carbon. Applied Physics Letters, 2011, 99, .	1.5	68

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91	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
92	Exceptionally strong magnetism in the 4<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" 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
93	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
94	Modeling hardness of polycrystalline materials and bulk metallic glasses. Intermetallics, 2011, 19, 1275-1281.	1.8	1,811
95	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
96	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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109	Laves phases in the ternary systems Tiâ€“{Pd, Pt}â€“Al. Intermetallics, 2009, 17, 336-342.	1.8	18
110	Hybrid density-functional calculation of the electronic and magnetic structures of tetragonal CuO. Physical Review B, 2009, 80, .	1.1	27
111	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
112	BaPt₄Ge₁₂: A Skutterudite Based Entirely on a Ge Framework. Advanced Materials, 2008, 20, 1325-1328.	11.1	7
113	On the ternary Laves phases Ti(Mn1â^'xAlx)2 with MgZn2-type. Intermetallics, 2008, 16, 16-26.	1.8	27
114	Crystal structure, phase stability and elastic properties of the Laves phase ZrTiCu2. Intermetallics, 2008, 16, 651-657.	1.8	19
115	Pressure Response of Novel Superconducting {Sr,Ba}Pt4Ge12. Journal of the Physical Society of Japan, 2008, 77, 350-352.	0.7	5
116	Bonding and strength of solid nitrogen in the cubic gauche (cg-N) structure. Physical Review B, 2008, 77, .	1.1	39
117	Superconductivity and spin fluctuations in{Th,U}Pt4Ge12skutterudites. Physical Review B, 2008, 78, .	1.1	38
118	Electronic and Structural Origin of Ultraincompressibility of5dTransition-Metal DiboridesMB2(M=W,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.9	160
119	Superconductivity and Magnetism in MPt₄Ge₁₂, M = Ca, Ba, Sr, Eu. Journal of the Physical Society of Japan, 2008, 77, 121-127.	0.7	17
120	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
121	Ab initiostudy of structural, magnetic, vibrational, and thermodynamic properties of the Laves-phase compoundHfMn2. Physical Review B, 2007, 76, .	1.1	11
122	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
123	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
124	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:mi> Physical Review Letters, 2007, 99, 217001.	2.9	90
125	Vacancy Mechanism of High Oxygen Solubility and Nucleation of Stable Oxygen-Enriched Clusters in Fe. Physical Review Letters, 2007, 99, 225502.	2.9	162
126	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

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127	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
128	Structural, thermodynamic, and transport properties of Laves-phaseZrMn2from x-ray and neutron diffraction and first principles. Physical Review B, 2006, 74, .	1.1	13
129	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
130	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
131	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
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	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
134	Ab initiostudy of ground-state properties of the Laves-phase compoundZrMn2. Physical Review B, 2005, 72, .	1.1	40
135	Ab initiostudy of ground-state properties of the Laves phase compoundsTiCr2,ZrCr2, andHfCr2. Physical Review B, 2005, 71, .	1.1	64
136	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
137	Comment on â€œEnthalpies of formation of binary Laves phasesâ€•[Intermetallics, 10 (2002) 579â€“595]. Intermetallics, 2004, 12, 59-62.	1.8	23
138	A new polymorphic material? Structural degeneracy of ZrMn 2. Europhysics Letters, 2004, 67, 807-813.	0.7	17
139	Computational and experimental study of phase stability, cohesive properties, magnetism and electronic structure of TiMn2. Acta Materialia, 2003, 51, 1239-1247.	3.8	55
140	An ab initio study on the dynamical properties of U-Nb alloy melt. Chinese Physics B, 0, , .	0.7	0