Qing-Miao Hu

List of Publications by Year
in descending order

134 papers	3,855 citations	126907 33 h-index	161849 54 g-index
138 all docs	138 docs citations	138 times ranked	3393 citing authors

#	Article	IF	Citations
1	Phase decomposition and strengthening in HfNbTaTiZr high entropy alloy from first-principles calculations. Acta Materialia, 2022, 225, 117582.	7.9	23
2	Alloying Effect on the Stability of Ti₅Si₃ from Firstâ€Principles Study. Physica Status Solidi (B): Basic Research, 2022, 259, .	1.5	2
3	Theoretical design of BAs/WX2 (XÂ=ÂS, Se) heterostructures for high-performance photovoltaic applications from DFT calculations. Applied Surface Science, 2022, 599, 153865.	6.1	5
4	Generalized stacking fault energies and critical resolved shear stresses of random Î±-Ti-Al alloys from first-principles calculations. Journal of Alloys and Compounds, 2021, 850, 156314.	5.5	29
5	Effects of pressure on the generalized stacking fault energy and twinning propensity of face-centered cubic metals. Journal of Alloys and Compounds, 2021, 866, 158869.	5.5	20
6	New insights into Ï‰-embrittlement in high misfit metastable Î²-titanium alloys: Mechanically-driven Ï‰-mediated amorphization. Materials and Design, 2021, 205, 109724.	7.0	6
7	Twinning pathways in Fe and Feâ€“Cr alloys from first-principles theory. Acta Materialia, 2021, 215, 117094.	7.9	9
8	Interaction between Al and other alloying atoms in Î±-Ti for designing high temperature titanium alloy. Computational Materials Science, 2021, 197, 110620.	3.0	10
9	Structural stability and mechanical properties of B2 ordered refractory AlNbTiVZr high entropy alloys. Journal of Alloys and Compounds, 2021, 886, 161289.	5.5	15
10	Precipitates and alloying elements distribution in near Î± titanium alloy Ti65. Journal of Materials Science and Technology, 2020, 36, 91-96.	10.7	39
11	Ab initio study of the elastic properties of body-centered cubic Ti-Mo-based alloys. Computational Materials Science, 2020, 172, 109320.	3.0	12
12	Understanding crystallographic orientation dependent dissolution rates of 90Cu-10Ni alloy: New insights based on AFM/SKPFM measurements and coordination number/electronic structure calculations. Corrosion Science, 2020, 164, 108320.	6.6	24
13	Phase stability of TiAl-X (X=V, Nb, Ta, Cr, Mo, W, and Mn) alloys. Journal of Alloys and Compounds, 2020, 819, 153291.	5.5	33
14	Large influence of vacancies on the elastic constants of cubic epitaxial tantalum nitride layers grown by reactive magnetron sputtering. Acta Materialia, 2020, 184, 254-266.	7.9	26
15	Influence of lattice distortion on stacking fault energies of CoCrFeNi and Al-CoCrFeNi high entropy alloys. Journal of Alloys and Compounds, 2020, 846, 156321.	5.5	49
16	Unconventional non-uniform local lattice distortion in dilute Ti-Mo solid solution. Acta Materialia, 2020, 197, 91-96.	7.9	16
17	New insights into formation mechanism of interfacial twin boundary Ï‰-phase in metastable Î²-Ti alloys. Materials Characterization, 2020, 164, 110363.	4.4	8
18	The effect of Co and Cr substitutions for Ni on mechanical properties and plastic deformation mechanism of FeMnCoCrNi high entropy alloys. Journal of Materials Science and Technology, 2020, 48, 146-155.	10.7	27

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19	Design of defected TaN supercells dataset for structural and elastic properties from ab initio simulations and comparison to experimental data. Data in Brief, 2020, 30, 105411.	1.0	1
20	Prediction on temperature dependent elastic constants of â€œsoftâ€•metal Al by AIMD and QHA. Journal of Materials Science and Technology, 2020, 45, 92-97.	10.7	7
21	Effect of alloying elements on lattice misfit and elasticities of Ni-based single crystal superalloys by first-principle calculations. Solid State Communications, 2020, 310, 113852.	1.9	8
22	Atomic scale modeling of interstitial loop-induced strengthening in nickel. Nuclear Instruments & Methods in Physics Research B, 2019, 452, 36-39.	1.4	0
23	Atomic bonding and electronic stability of the binary sigma phase. Journal of Alloys and Compounds, 2019, 811, 152053.	5.5	7
24	First-principles study of dopant stability and related optical properties in CdSiP2 crystal. Journal of Alloys and Compounds, 2019, 802, 310-317.	5.5	2
25	Site Occupation of Nb in Î³-TiAl: Beyond the Point Defect Gas Approximation. Acta Metallurgica Sinica (English Letters), 2019, 32, 1511-1520.	2.9	5
26	Dynamic recrystallization initiated by direct grain reorientation at high-angle grain boundary in Î±-titanium. Journal of Materials Research, 2019, 34, 1608-1621.	2.6	4
27	Origin of the ductile-to-brittle transition of metastable Î²-titanium alloys: Self-hardening of Ï‰-precipitates. Acta Materialia, 2019, 170, 187-204.	7.9	76
28	Integrated modeling of molar volume of the sigma phase aided by first-principles calculations. Journal of Alloys and Compounds, 2019, 791, 994-1004.	5.5	6
29	Properties of Î²/Ï‰ phase interfaces in Ti and their implications on mechanical properties and Ï‰ morphology. Computational Materials Science, 2019, 158, 49-57.	3.0	6
30	Experimental and DFT characterization of interphase boundaries in titanium and the implications for Ï‰-assisted Î± phase precipitation. Acta Materialia, 2018, 151, 406-415.	7.9	30
31	On the abnormal fast diffusion of solute atoms in Î±-Ti: A first-principles investigation. Journal of Alloys and Compounds, 2018, 740, 156-166.	5.5	28
32	Influence of atomic mixing and atomic order on molar volume of the binary sigma phase. Intermetallics, 2018, 98, 95-105.	3.9	4
33	The surface energy and stress of metals. Surface Science, 2018, 674, 51-68.	1.9	68
34	Strain rate-induced plasticity in bcc Î²-Ti alloy single crystal micropillars containing brittle Ï‰-precipitates. Materials and Design, 2018, 137, 404-413.	7.0	18
35	Influence of atomic order on the enthalpy of formation and bulk modulus of the sigma phase. Fluid Phase Equilibria, 2018, 459, 238-243.	2.5	6
36	Thermal vacancy formation enthalpy of random solid solutions: The FePt case. Computational Materials Science, 2018, 143, 206-211.	3.0	5

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37	Mapping deformation mechanisms in lamellar titanium aluminide. Acta Materialia, 2018, 144, 835-843.	7.9	27
38	First-principles investigations of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.gif" overflow="scroll"><mml:mrow><mml:mi>Ï‰</mml:mi></mml:mrow></mml:math>variant selection during athermal<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.gif" overflow="scroll"><mml:mrow><mml:mi>Î²</mml:mi><mml:mo>â†'</mml:mo><mml:mi>Ï‰</mml:mi></mml:mrow></mml:math>trans of binary Ti-xMo alloy. Computational Materials Science, 2018, 155, 524-533.	3.0	10
39	Effect of Î² (110) texture intensity on Î±-variant selection and microstructure morphology during Î²â†'Î± phase transformation in near Î± titanium alloy. Acta Materialia, 2017, 126, 372-382.	7.9	102
40	Composition-dependent elastic properties in TiNi-Nb from first principle calculations. Journal of Alloys and Compounds, 2017, 706, 260-266.	5.5	11
41	Direct observation of solute interstitials and their clusters in Mg alloys. Materials Characterization, 2017, 128, 226-231.	4.4	10
42	Atomic self-diffusion anisotropy of HCP metals from first-principles calculations. Computational Materials Science, 2017, 128, 236-242.	3.0	12
43	CPA descriptions of random Cu-Au alloys in comparison with SQS approach. Computational Materials Science, 2017, 128, 302-309.	3.0	21
44	Chemical Origin of Termination-Functionalized MXenes: Ti₃C₂T₂ as a Case Study. Journal of Physical Chemistry C, 2017, 121, 19254-19261.	3.1	194
45	Origin of the abnormal diffusion of transition metal atoms in rutile. Physical Review B, 2017, 95, .	3.2	5
46	Longitudinal sound velocities, elastic anisotropy, and phase transition of high-pressure cubic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math> ice to 82 GPa. Physical Review B, 2017, 96, .	3.2	22
47	Stacking fault energy of C-alloyed steels: The effect of magnetism. Acta Materialia, 2017, 122, 72-81.	7.9	30
48	Alloying element's substitution in titanium alloy with improved oxidation resistance and enhanced magnetic properties. Journal of Magnetism and Magnetic Materials, 2017, 422, 20-24.	2.3	4
49	Local lattice distortion in high-entropy alloys. Physical Review Materials, 2017, 1, .	2.4	144
50	First-principles investigation of effects of alloying elements on Ti/TiO2 interface. Metallic Materials, 2017, 55, 291-294.	0.3	0
51	Adsorption of oxygen on low-index surfaces of the TiAl3 alloy. Journal of Experimental and Theoretical Physics, 2016, 123, 991-1007.	0.9	13
52	First-principles study of phase stability and elastic properties of binary Ti-xTM (TM = V,Cr,Nb,Mo) and ternary Ti-15TM-yAl alloys. Materials and Design, 2016, 110, 80-89.	7.0	39
53	Cooperative effect of silicon and other alloying elements on creep resistance of titanium alloys: insight from first-principles calculations. Scientific Reports, 2016, 6, 30611.	3.3	21
54	Strong deformation anisotropies of Ï‰-precipitates and strengthening mechanisms in Ti-10V-2Fe-3Al alloy micropillars: Precipitates shearing vs precipitates disordering. Acta Materialia, 2016, 117, 68-80.	7.9	78

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55	Alloying effects on properties of Al 2 O 3 and TiO 2 in connection with oxidation resistance of TiAl. Intermetallics, 2016, 68, 57-62.	3.9	55
56	Generalized stacking fault energy of Î³-Fe. Philosophical Magazine, 2016, 96, 524-541.	1.6	36
57	First-principles calculations of transition metal solute interactions with hydrogen in tungsten. Nuclear Fusion, 2016, 56, 026004.	3.5	33
58	Understanding the martensitic phase transition of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Ni</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:m shape-memory alloys from theoretical calculations. Physical Review B, 2015, 91, .	3.2	14
59	Ab initioprediction of the mechanical properties of alloys: The case of Ni/Mn-doped ferromagnetic Fe. Physical Review B, 2015, 91, .	3.2	20
60	Theoretical investigation of the magnetic and structural transitions of Ni-Co-Mn-Sn metamagnetic shape-memory alloys. Physical Review B, 2015, 92, .	3.2	19
61	Point Defects in TiNi-based Alloys from Ab-initio Calculations. Materials Today: Proceedings, 2015, 2, S615-S618.	1.8	5
62	A Comprehensive Theoretical Investigation of the Molecular Properties of Methyl Bromide (CH₃Br). Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2015, 70, 1025-1030.	1.5	3
63	Elastic constants of random solid solutions by SQS and CPA approaches: the case of fcc Ti-Al. Journal of Physics Condensed Matter, 2015, 27, 315702.	1.8	33
64	Theoretical study of oxygen sorption and diffusion in the volume and on the surface of a Î³-TiAl alloy. Journal of Experimental and Theoretical Physics, 2015, 120, 257-267.	0.9	19
65	Adsorption and diffusion of oxygen on Î³-TiAl(0 0 1) and (1 0 0) surfaces. Computational Materials Science, 2015, 97, 55-63.	3.0	32
66	Initial oxidation of TiAl: An ab-initio investigation. , 2014, , .		2
67	Magnetic effect on the interfacial energy of the Ni(1â€‰1â€‰1)/Cr(1â€‰1â€‰0) interface. Journal of Physics Condensed Matter, 2014, 26, 355001.	1.8	11
68	{112}ã€ˆ111ã€‰ Twinning during Ï‰ to body-centered cubic transition. Acta Materialia, 2014, 62, 122-128.	7.9	74
69	Theoretical investigation of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï‰</mml:mi></mml:math>-related phases in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">TiAl</mml:mi><mml:mo>â^'</mml:mo><mml:mi mathvariant="normal">Nb</mml:mi></mml:math>/Mo alloys. Physical Review B, 2014, 90, .	3.2	32
70	The effect of electron localization on the electronic structure and migration barrier of oxygen vacancies in rutile. Journal of Physics Condensed Matter, 2014, 26, 055602.	1.8	11
71	Generalized stacking fault energies of alloys. Journal of Physics Condensed Matter, 2014, 26, 265005.	1.8	66
72	Structure of Bergman-typeW-TiZrNi approximants to quasicrystal, analyzed by lattice inversion method. Journal of Physics Condensed Matter, 2014, 26, 315003.	1.8	2

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73	Basal-plane stacking fault energy of hexagonal close-packed metals based on the Ising model. Acta Materialia, 2013, 61, 1136-1145.	7.9	44
74	The effect of long-range order on the elastic properties of Cu₃Au. Journal of Physics Condensed Matter, 2013, 25, 085401.	1.8	20
75	Magnetic ordering and physical stability ofX2Mn1+xSn1â^'x(X=Ru, Os, Co, Rh, Ni, Pd, Cu, and Ag) Heusler alloys from a first-principles study. Physical Review B, 2013, 88, .	3.2	11
76	Lattice parameters and relative stability of Î±â€³ phase in binary titanium alloys from first-principles calculations. Solid State Communications, 2013, 159, 70-75.	1.9	47
77	Trapping of interstitial defects: filling the gap between the experimental measurements and DFT calculations. Journal of Physics Condensed Matter, 2013, 25, 435402.	1.8	3
78	Ab initioinvestigation of the elastic properties of Ni<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>Fe. Physical Review B, 2013, 88, .	3.2	14
79	The effect of Al on the 475 Â°C embrittlement of Feâ€“Cr alloys. Computational Materials Science, 2013, 74, 101-106.	3.0	47
80	Magnetic properties and temperature-dependent half-metallicity of Co₂Mn(Ga_{1â^'x}Z_x) (Z=Si, Ge, Sn) from first-principles calculation. Journal of Physics Condensed Matter, 2013, 25, 156003.	1.8	6
81	First-principles investigations of oxygen adsorption at TiNi surface and the TiO2/TiOâ€“TiNi interface. Physica B: Condensed Matter, 2013, 426, 118-126.	2.7	17
82	First-principles study of fcc-Ag/bcc-Fe interfaces. Physical Review B, 2013, 87, .	3.2	64
83	INVESTIGATION ON EFFECTS OF ALLOYING ON OXIDATION RESISTANCE OF Î³-TiAl BY USING FIRST PRINCIPLE. Jinshu Xuebao/Acta Metallurgica Sinica, 2013, 49, 385.	0.3	6
84	Phase stability of Ni<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow		

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91	Role of magnetic and atomic ordering in the martensitic transformation of Ni-Mn-In from a first-principles study. Physical Review B, 2012, 86, .	3.2	48
92	Composition dependent elastic modulus and phase stability of Ni2MnGa based ferromagnetic shape memory alloys. Science China Technological Sciences, 2012, 55, 295-305.	4.0	16
93	Electronic and magnetic properties of Fe3â^'x Cr x Si ordered alloys from first principles. Journal of Materials Science, 2012, 47, 797-803.	3.7	14
94	Energetic effects of dopants on the eutectoid decomposition of Nbâ€“Siin situcomposites. Philosophical Magazine Letters, 2011, 91, 640-647.	1.2	5
95	Strengthening of Î³-TiAl-Nb by short-range ordering of point defects. Intermetallics, 2011, 19, 793-796.	3.9	39
96	Surface properties of 3dtransition metals. Philosophical Magazine, 2011, 91, 3627-3640.	1.6	45
97	Stacking fault energies of Mn, Co and Nb alloyed austenitic stainless steels. Acta Materialia, 2011, 59, 5728-5734.	7.9	119
98	First-principles investigations of the five-layer modulated martensitic structure in Ni2Mn(Al Ga1â^') alloys. Acta Materialia, 2011, 59, 5938-5945.	7.9	24
99	Composition and orientation dependence of the interfacial energy in Feâ€“Cr stainless steel alloys. Physica Status Solidi (B): Basic Research, 2011, 248, 2087-2090.	1.5	3
100	The effect of defects on the electronic and magnetic properties of Fe₂MnSi Heusler alloy. Physica Status Solidi (B): Basic Research, 2011, 248, 2893-2898.	1.5	24
101	Theoretical investigation of the effects of composition and atomic disordering on the properties of Ni2Mn(Al1â^'xGax) alloy. Acta Materialia, 2011, 59, 971-980.	7.9	28
102	Site preference and elastic properties of Fe-, Co-, and Cu-doped Ni<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>MnGa shape memory alloys from first principles. Physical Review B, 2011, 84, .	3.2	56
103	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>P</mml:mi><mml:msub><mml:mn>6</mml:mn><mml:mn>2</mml:mn></mml:msub><mml:mn> of yttrium above 206 GPa from first principles. Physical Review B, 2011, 84, .	3.2	11
104	Interplay between temperature and composition effects on the martensitic transformation in Ni2+xMn1â^'xGa alloys. Applied Physics Letters, 2011, 98, 261903.	3.3	12
105	Temperature dependence of elastic properties of Ni<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn><mml:mo>+</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Mn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Ga and Ni<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display=. Physical Review B, 2011,	3.2	27
106	The electronic structure and spin polarization of Fe3â^'xMnxSi and Fe3â^'yMnSiy alloys. Journal of Applied Physics, 2010, 107, .	2.5	25
107	First-principles determination of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</mml:mi><mml:mtext>â^'</mml:mtext><mml:msup><mml:mi>Î±</mml:mi><mml:mo>â€² energy in Fe-Cr alloys. Physical Review B, 2010, 82, .	3.2	32
108	Magnetoelastic effects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>Ni</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mtext> from first-principles calculations. Physical Review B, 2010, 81, .	3.2	18

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109	First-principles investigation of the composition dependent properties ofNi2+xMn1â^'xGashape-memory alloys. Physical Review B, 2010, 82, .	3.2	60
110	First-principles study of the elastic properties of In-Tl random alloys. Physical Review B, 2010, 82, .	3.2	23
111	Static equation of state of bcc iron. Physical Review B, 2010, 82, .	3.2	35
112	Site occupancy, magnetic moments, and elastic constants of off-stoichiometric<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ni</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub first-principles calculations. Physical Review B, 2009, 79, .	3.2	64
113	Rare earth elements in Î±-Ti: A first-principles investigation. Computational Materials Science, 2009, 46, 1187-1191.	3.0	11
114	Composition-dependent elastic properties and electronic structures of off-stoichiometric TiNi from first-principles calculations. Acta Materialia, 2008, 56, 4913-4920.	7.9	26
115	Hardness and elastic properties of covalent/ionic solid solutions from first-principles theory. Journal of Applied Physics, 2008, 103, .	2.5	16
116	First-principles Investigations of Point Defect Behavior and Elastic Properties of TiNi Based Alloys. Materials Research Society Symposia Proceedings, 2008, 1128, 90301.	0.1	2
117	Phase stability and elastic modulus of Ti alloys containing Nb, Zr, and/or Sn from first-principles calculations. Applied Physics Letters, 2008, 93, .	3.3	80
118	Elastic stability of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î²</mml:mi><mml:mtext>-Ti</mml:mtext></mml:mrow></mml:math>under pressure calculated using a first-principles plane-wave pseudopotential method. Physical Review B, 2008, 78, .	3.2	32
119	Effect of Zr on the properties of (TiZr)Ni alloys from first-principles calculations. Physical Review B, 2007, 76, .	3.2	44
120	Interaction between hydrogen and the alloying atom in palladium. Physical Review B, 2007, 76, .	3.2	21
121	Towards an Exact Treatment of Exchange and Correlation in Materials: Application to the â€œCO Adsorption Puzzleâ€•and Other Systems. Physical Review Letters, 2007, 98, 176103.	7.8	110
122	Predicting hardness of covalentâˆ•ionic solid solution from first-principles theory. Applied Physics Letters, 2007, 91, .	3.3	14
123	Point defects and their interaction in TiNi from first-principles calculations. Physical Review B, 2007, 75, .	3.2	30
124	Features of hydrogen interaction in the Pd-based alloys with 3d transition metals. Journal of Surface Investigation, 2007, 1, 754-758.	0.5	3
125	Mechanical properties of structural materials from first-principles. Current Opinion in Solid State and Materials Science, 2006, 10, 19-25.	11.5	34
126	Super-elastic titanium alloy with unstable plastic deformation. Applied Physics Letters, 2005, 87, 091906.	3.3	204

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127	Concentrated Point Defects in and Order-Disorder Transition Temperature of Intermetallic Compounds. Physical Review Letters, 2004, 92, 185505.	7.8	19
128	Bonding characteristics of micro-alloyed B2 NiAl in relation to site occupancies and phase stability. Acta Materialia, 2003, 51, 5545-5554.	7.9	19
129	First-principles investigations of ordering in binary Î±-Ti solid solutions. Philosophical Magazine, 2003, 83, 217-229.	1.6	10
130	Geometric and electronic structure ofTi2AlX(X=V,Nb,orTa). Physical Review B, 2003, 68, .	3.2	37
131	Energetics and electronic structure of grain boundaries and surfaces of B- and H-dopedNi3Al. Physical Review B, 2003, 67, .	3.2	48
132	First-principles investigation of solute-hydrogen interaction in a Î±-Ti solid solution. Physical Review B, 2002, 66, .	3.2	22
133	First-principles investigations of the soluteâ€“vacancy interaction energy and its effect on the creep properties of Î±-titanium. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2001, 81, 2809-2821.	0.6	17
134	Study of Nickel Segregation at the TiNi-Titanium Oxide Interface. Materials Science Forum, 0, 738-739, 269-273.	0.3	4