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	Super-elastic titanium alloy with unstable plastic deformation. Applied Physics Letters, 2005, 87, 091906.	3.3	204
2	Chemical Origin of Termination-Functionalized MXenes: Ti₃C₂T₂ as a Case Study. Journal of Physical Chemistry C, 2017, 121, 19254-19261.	3.1	194
3	Local lattice distortion in high-entropy alloys. Physical Review Materials, 2017, 1, .	2.4	144
4	Stacking fault energies of Mn, Co and Nb alloyed austenitic stainless steels. Acta Materialia, 2011, 59, 5728-5734.	7.9	119
5	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
6	Effect of Î² (110) texture intensity on Î±-variant selection and microstructure morphology during Î²âˆ'Î± phase transformation in near Î± titanium alloy. Acta Materialia, 2017, 126, 372-382.	7.9	102
7	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
8	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
9	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
10	{112}ã€ˆ111ã€‰ Twinning during Ï‰ to body-centered cubic transition. Acta Materialia, 2014, 62, 122-128.	7.9	74
11	(Nd_{1.5}Mg_{0.5})Ni₇-Based Compounds: Structural and Hydrogen Storage Properties. Inorganic Chemistry, 2012, 51, 2976-2983.	4.0	73
12	The surface energy and stress of metals. Surface Science, 2018, 674, 51-68.	1.9	68
13	Generalized stacking fault energies of alloys. Journal of Physics Condensed Matter, 2014, 26, 265005.	1.8	66
14	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
15	First-principles study of fcc-Ag/bcc-Fe interfaces. Physical Review B, 2013, 87, .	3.2	64
16	First-principles investigation of the composition dependent properties ofNi2+xMn1âˆ'xGashape-memory alloys. Physical Review B, 2010, 82, .	3.2	60
17	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
18	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

#	Article	IF	Citations
19	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
20	Energetics and electronic structure of grain boundaries and surfaces of B- and H-dopedNi3Al. Physical Review B, 2003, 67, .	3.2	48
21	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
22	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
23	The effect of Al on the 475 Â°C embrittlement of Feâ€“Cr alloys. Computational Materials Science, 2013, 74, 101-106.	3.0	47
24	Surface properties of 3dtransition metals. Philosophical Magazine, 2011, 91, 3627-3640.	1.6	45
25	Effect of Zr on the properties of (TiZr)Ni alloys from first-principles calculations. Physical Review B, 2007, 76, .	3.2	44
26	Basal-plane stacking fault energy of hexagonal close-packed metals based on the Ising model. Acta Materialia, 2013, 61, 1136-1145.	7.9	44
27	Strengthening of Î³-TiAl-Nb by short-range ordering of point defects. Intermetallics, 2011, 19, 793-796.	3.9	39
28	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
29	Precipitates and alloying elements distribution in near Î± titanium alloy Ti65. Journal of Materials Science and Technology, 2020, 36, 91-96.	10.7	39
30	Geometric and electronic structure ofTi2AlX(X=V,Nb,orTa). Physical Review B, 2003, 68, .	3.2	37
31	Generalized stacking fault energy of Î³-Fe. Philosophical Magazine, 2016, 96, 524-541.	1.6	36
32	Static equation of state of bcc iron. Physical Review B, 2010, 82, .	3.2	35
33	Determining the minimum grain size in severe plastic deformation process via first-principles calculations. Acta Materialia, 2012, 60, 4506-4513.	7.9	35
34	Mechanical properties of structural materials from first-principles. Current Opinion in Solid State and Materials Science, 2006, 10, 19-25.	11.5	34
35	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
36	First-principles calculations of transition metal solute interactions with hydrogen in tungsten. Nuclear Fusion, 2016, 56, 026004.	3.5	33

#	Article	IF	Citations
37	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
38	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
39	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
40	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
41	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
42	Predicted Suppression of the Superconducting Transition of New High-Pressure Yttrium Phases with Increasing Pressure from First-Principles Calculations. Physical Review Letters, 2012, 109, 157004.	7.8	31
43	Point defects and their interaction in TiNi from first-principles calculations. Physical Review B, 2007, 75, .	3.2	30
44	Stacking fault energy of C-alloyed steels: The effect of magnetism. Acta Materialia, 2017, 122, 72-81.	7.9	30
45	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
46	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
47	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
48	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
49	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
50	Mapping deformation mechanisms in lamellar titanium aluminide. Acta Materialia, 2018, 144, 835-843.	7.9	27
51	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
52	Composition-dependent elastic properties and electronic structures of off-stoichiometric TiNi from first-principles calculations. Acta Materialia, 2008, 56, 4913-4920.	7.9	26
53	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
54	The electronic structure and spin polarization of Fe3â^'xMnxSi and Fe3â^'yMnSiy alloys. Journal of Applied Physics, 2010, 107, .	2.5	25

#	Article	IF	Citations
55	First-principles investigations of the five-layer modulated martensitic structure in Ni2Mn(Al Ga1âˆ') alloys. Acta Materialia, 2011, 59, 5938-5945.	7.9	24
56	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
57	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
58	First-principles study of the elastic properties of In-Tl random alloys. Physical Review B, 2010, 82, .	3.2	23
59	Phase stability of Ni<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow		

#	Article	IF	Citations
73	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:mte from first-principles calculations. Physical Review B, 2010, 81, .	3.2	18
74	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
75	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
76	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
77	Hardness and elastic properties of covalent/ionic solid solutions from first-principles theory. Journal of Applied Physics, 2008, 103, .	2.5	16
78	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
79	Unconventional non-uniform local lattice distortion in dilute Ti-Mo solid solution. Acta Materialia, 2020, 197, 91-96.	7.9	16
80	Atomic-Scale Modeling of the Dynamics of Titanium Oxidation. Journal of Physical Chemistry C, 2012, 116, 24201-24205.	3.1	15
81	Structural stability and mechanical properties of B2 ordered refractory AlNbTiVZr high entropy alloys. Journal of Alloys and Compounds, 2021, 886, 161289.	5.5	15
82	Predicting hardness of covalentâ•ionic solid solution from first-principles theory. Applied Physics Letters, 2007, 91, .	3.3	14
83	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
84	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
85	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:msub><mml:mn shape-memory alloys from theoretical calculations. Physical Review B, 2015, 91, .	3.2	14
86	Adsorption of oxygen on low-index surfaces of the TiAl3 alloy. Journal of Experimental and Theoretical Physics, 2016, 123, 991-1007.	0.9	13
87	Interplay between temperature and composition effects on the martensitic transformation in Ni2+xMn1â^'xGa alloys. Applied Physics Letters, 2011, 98, 261903.	3.3	12
88	Atomic self-diffusion anisotropy of HCP metals from first-principles calculations. Computational Materials Science, 2017, 128, 236-242.	3.0	12
89	Ab initio study of the elastic properties of body-centered cubic Ti-Mo-based alloys. Computational Materials Science, 2020, 172, 109320.	3.0	12
90	Rare earth elements in Î±-Ti: A first-principles investigation. Computational Materials Science, 2009, 46, 1187-1191.	3.0	11

#	Article	IF	Citations
91	<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
92	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
93	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
94	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
95	Composition-dependent elastic properties in TiNi-Nb from first principle calculations. Journal of Alloys and Compounds, 2017, 706, 260-266.	5.5	11
96	First-principles investigations of ordering in binary Î±-Ti solid solutions. Philosophical Magazine, 2003, 83, 217-229.	1.6	10
97	Direct observation of solute interstitials and their clusters in Mg alloys. Materials Characterization, 2017, 128, 226-231.	4.4	10
98	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
99	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
100	Twinning pathways in Fe and Feâ€“Cr alloys from first-principles theory. Acta Materialia, 2021, 215, 117094.	7.9	9
101	Binding of an Oxide Layer to a Metal: The Case of Ti(101Ì…0)/TiO2(100). Journal of Physical Chemistry C, 2012, 116, 4224-4233.	3.1	8
102	New insights into formation mechanism of interfacial twin boundary Ï‰-phase in metastable Î²-Ti alloys. Materials Characterization, 2020, 164, 110363.	4.4	8
103	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
104	Atomic bonding and electronic stability of the binary sigma phase. Journal of Alloys and Compounds, 2019, 811, 152053.	5.5	7
105	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
106	Theoretical investigations of interstitial atoms in bcc metals: Local lattice distortion and diffusion barrier. Computational Materials Science, 2012, 58, 67-70.	3.0	6
107	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
108	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

#	Article	IF	Citations
109	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
110	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
111	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
112	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
113	Energetic effects of dopants on the eutectoid decomposition of Nbâ€“Siin situcomposites. Philosophical Magazine Letters, 2011, 91, 640-647.	1.2	5
114	Point Defects in TiNi-based Alloys from Ab-initio Calculations. Materials Today: Proceedings, 2015, 2, S615-S618.	1.8	5
115	Origin of the abnormal diffusion of transition metal atoms in rutile. Physical Review B, 2017, 95, .	3.2	5
116	Thermal vacancy formation enthalpy of random solid solutions: The FePt case. Computational Materials Science, 2018, 143, 206-211.	3.0	5
117	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
118	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
119	Study of Nickel Segregation at the TiNi-Titanium Oxide Interface. Materials Science Forum, 0, 738-739, 269-273.	0.3	4
120	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
121	Influence of atomic mixing and atomic order on molar volume of the binary sigma phase. Intermetallics, 2018, 98, 95-105.	3.9	4
122	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
123	Features of hydrogen interaction in the Pd-based alloys with 3d transition metals. Journal of Surface Investigation, 2007, 1, 754-758.	0.5	3
124	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
125	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
126	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

#	Article	IF	Citations
127	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
128	Initial oxidation of TiAl: An ab-initio investigation. , 2014, , .		2
129	Structure of Bergman-typeW-TiZrNi approximants to quasicrystal, analyzed by lattice inversion method. Journal of Physics Condensed Matter, 2014, 26, 315003.	1.8	2
130	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
131	Alloying Effect on the Stability of Ti₅Si₃ from Firstâ€Principles Study. Physica Status Solidi (B): Basic Research, 2022, 259, .	1.5	2
132	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
133	Atomic scale modeling of interstitial loop-induced strengthening in nickel. Nuclear Instruments & Methods in Physics Research B, 2019, 452, 36-39.	1.4	0
134	First-principles investigation of effects of alloying elements on Ti/TiO2 interface. Metallic Materials, 2017, 55, 291-294.	0.3	0