Qi-Jun Hong

List of Publications by Year
in descending order

35 papers	1,924 citations	394421 19 h-index	377865 34 g-index
36 all docs	36 docs citations	36 times ranked	2328 citing authors

#	Article	IF	Citations
1	Multicomponent multisublattice alloys, nonconfigurational entropy and other additions to the Alloy Theoretic Automated Toolkit. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2009, 33, 266-278.	1.6	638
2	CO2 fixation into methanol at Cu/ZrO2 interface from first principles kinetic Monte Carlo. Journal of Catalysis, 2009, 263, 114-122.	6.2	188
3	Theoretical prediction of high melting temperature for a Moâ€“Ruâ€“Taâ€“W HCP multiprincipal element alloy. Npj Computational Materials, 2021, 7, .	8.7	186
4	Prediction of the material with highest known melting point fromab initiomolecular dynamics calculations. Physical Review B, 2015, 92, .	3.2	126
5	Methods for First-Principles Alloy Thermodynamics. Jom, 2013, 65, 1523-1532.	1.9	64
6	Mechanism of CO2 hydrogenation over Cu/ZrO2(2Ì...12) interface from first-principles kinetics Monte Carlo simulations. Surface Science, 2010, 604, 1869-1876.	1.9	62
7	Software tools for high-throughput CALPHAD from first-principles data. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2017, 58, 70-81.	1.6	57
8	Carbides and Nitrides of Zirconium and Hafnium. Materials, 2019, 12, 2728.	2.9	56
9	The free energy of mechanically unstable phases. Nature Communications, 2015, 6, 7559.	12.8	54
10	Solid-liquid coexistence in small systems: A statistical method to calculate melting temperatures. Journal of Chemical Physics, 2013, 139, 094114.	3.0	48
11	First-principles study of phase equilibrium in Tiâ€“V, Tiâ€“Nb, and Tiâ€“Ta alloys. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2016, 54, 125-133.	1.6	42
12	Free energy calculation of mechanically unstable but dynamically stabilized bcc titanium. Physical Review B, 2017, 95, .	3.2	40
13	Combined computational and experimental investigation of the refractory properties of La2Zr2O7. Acta Materialia, 2015, 84, 275-282.	7.9	36
14	Combined computational and experimental investigation of high temperature thermodynamics and structure of cubic ZrO2 and HfO2. Scientific Reports, 2018, 8, 14962.	3.3	35
15	First-principles calculations of thermal properties of the mechanically unstable phases of the PtTi and NiTi shape memory alloys. Acta Materialia, 2018, 147, 296-303.	7.9	26
16	The Thermodynamic Database Database. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 61, 173-178.	1.6	25
17	High-throughput calculations in the context of alloy design. MRS Bulletin, 2019, 44, 252-256.	3.5	24
18	A user guide for SLUSCHI: Solid and Liquid in Ultra Small Coexistence with Hovering Interfaces. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2016, 52, 88-97.	1.6	23

#	Article	IF	Citations
19	Equation of state of solid, liquid and gaseous tantalum from first principles. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2015, 51, 133-143.	1.6	21
20	Invited paper: Reconciling SGTE and ab initio enthalpies of the elements. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 60, 1-6.	1.6	18
21	Reentrant melting of sodium, magnesium, and aluminum: General trend. Physical Review B, 2019, 100, .	3.2	17
22	Direct first-principles chemical potential calculations of liquids. Journal of Chemical Physics, 2012, 137, 094114.	3.0	14
23	A combined experimental and theoretical study of enthalpy of phase transition and fusion of yttria above 2000ÂÂ°C using â€œdrop-n-catchâ€•calorimetry and first-principles calculation. Acta Materialia, 2017, 124, 204-209.	7.9	14
24	Ab initiocalculation of anisotropic interfacial excess free energies. Physical Review B, 2014, 89, .	3.2	12
25	Energetics of melting of Yb2O3 and Lu2O3 from drop and catch calorimetry and first principles computations. Journal of Chemical Thermodynamics, 2019, 132, 405-410.	2.0	12
26	Epicycle method for elasticity limit calculations. Physical Review B, 2017, 95, .	3.2	11
27	Software tools for thermodynamic calculation of mechanically unstable phases from first-principles data. Computer Physics Communications, 2020, 246, 106712.	7.5	9
28	Identifying rhenium substitute candidate multiprincipal-element alloys from electronic structure and thermodynamic criteria. Journal of Materials Research, 2019, 34, 3296-3304.	2.6	8
29	Simulations provide a rare look at real melting. Science, 2014, 346, 704-705.	12.6	7
30	Assessing Phase Diagram Accuracy. Journal of Phase Equilibria and Diffusion, 2019, 40, 170-175.	1.4	6
31	Computational Assessment of Novel Predicted Compounds in Ni-Re Alloy System. Journal of Phase Equilibria and Diffusion, 2021, 42, 315-320.	1.4	3
32	Tetrahedron-tiling method for crystal structure prediction. Physical Review Materials, 2017, 1, .	2.4	3
33	First-principles thermal compatibility between Ru-based Re-substitute alloys and Ir coatings. Computational Materials Science, 2019, 170, 109199.	3.0	2
34	Rapid screening of high-throughput ground state predictions. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2021, 74, 102306.	1.6	2
35	Interactive Exploration of High-Dimensional Phase Diagrams. Jom, 0, , 1.	1.9	0