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	Theoretical prediction of high melting temperature for a Moâ€“Ruâ€“Taâ€“W HCP multiprincipal element alloy. Npj Computational Materials, 2021, 7, .	8.7	186
2	Computational Assessment of Novel Predicted Compounds in Ni-Re Alloy System. Journal of Phase Equilibria and Diffusion, 2021, 42, 315-320.	1.4	3
3	Rapid screening of high-throughput ground state predictions. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2021, 74, 102306.	1.6	2
4	Software tools for thermodynamic calculation of mechanically unstable phases from first-principles data. Computer Physics Communications, 2020, 246, 106712.	7.5	9
5	Reentrant melting of sodium, magnesium, and aluminum: General trend. Physical Review B, 2019, 100, .	3.2	17
6	Carbides and Nitrides of Zirconium and Hafnium. Materials, 2019, 12, 2728.	2.9	56
7	First-principles thermal compatibility between Ru-based Re-substitute alloys and Ir coatings. Computational Materials Science, 2019, 170, 109199.	3.0	2
8	Assessing Phase Diagram Accuracy. Journal of Phase Equilibria and Diffusion, 2019, 40, 170-175.	1.4	6
9	Identifying rhenium substitute candidate multiprincipal-element alloys from electronic structure and thermodynamic criteria. Journal of Materials Research, 2019, 34, 3296-3304.	2.6	8
10	High-throughput calculations in the context of alloy design. MRS Bulletin, 2019, 44, 252-256.	3.5	24
11	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
12	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
13	The Thermodynamic Database Database. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 61, 173-178.	1.6	25
14	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
15	Combined computational and experimental investigation of high temperature thermodynamics and structure of cubic ZrO2 and HfO2. Scientific Reports, 2018, 8, 14962.	3.3	35
16	Free energy calculation of mechanically unstable but dynamically stabilized bcc titanium. Physical Review B, 2017, 95, .	3.2	40
17	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
18	Epicycle method for elasticity limit calculations. Physical Review B, 2017, 95, .	3.2	11

#	Article	IF	Citations
19	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
20	Tetrahedron-tiling method for crystal structure prediction. Physical Review Materials, 2017, 1, .	2.4	3
21	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
22	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
23	The free energy of mechanically unstable phases. Nature Communications, 2015, 6, 7559.	12.8	54
24	Prediction of the material with highest known melting point fromab initiomolecular dynamics calculations. Physical Review B, 2015, 92, .	3.2	126
25	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
26	Combined computational and experimental investigation of the refractory properties of La2Zr2O7. Acta Materialia, 2015, 84, 275-282.	7.9	36
27	Simulations provide a rare look at real melting. Science, 2014, 346, 704-705.	12.6	7
28	Ab initiocalculation of anisotropic interfacial excess free energies. Physical Review B, 2014, 89, .	3.2	12
29	Solid-liquid coexistence in small systems: A statistical method to calculate melting temperatures. Journal of Chemical Physics, 2013, 139, 094114.	3.0	48
30	Methods for First-Principles Alloy Thermodynamics. Jom, 2013, 65, 1523-1532.	1.9	64
31	Direct first-principles chemical potential calculations of liquids. Journal of Chemical Physics, 2012, 137, 094114.	3.0	14
32	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
33	CO2 fixation into methanol at Cu/ZrO2 interface from first principles kinetic Monte Carlo. Journal of Catalysis, 2009, 263, 114-122.	6.2	188
34	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
35	Interactive Exploration of High-Dimensional Phase Diagrams. Jom, 0, , 1.	1.9	0