Zhigang Zhang

List of Publications by Year
in descending order

31 papers	933 citations	623734 14 h-index	454955 30 g-index
32 all docs	32 docs citations	32 times ranked	1181 citing authors

#	Article	IF	Citations
1	An optimized molecular potential for carbon dioxide. Journal of Chemical Physics, 2005, 122, 214507.	3.0	188
2	Equation of state of the H2O, CO2, and H2Oâ€“CO2 systems up to 10 GPa and 2573.15K: Molecular dynamics simulations with ab initio potential surface. Geochimica Et Cosmochimica Acta, 2006, 70, 2311-2324.	3.9	157
3	Prediction of the PVT properties of water over wide range of temperatures and pressures from molecular dynamics simulation. Physics of the Earth and Planetary Interiors, 2005, 149, 335-354.	1.9	101
4	Relief history and denudation evolution of the northern Tibet margin: Constraints from 40Ar/39Ar and (Uâ€“Th)/He dating and implications for far-field effect of rising plateau. Tectonophysics, 2016, 675, 196-208.	2.2	60
5	Elastic properties of MgSiO3-perovskite under lower mantle conditions and the composition of the deep Earth. Earth and Planetary Science Letters, 2013, 379, 1-12.	4.4	55
6	Lithium chloride ionic association in dilute aqueous solution: a constrained molecular dynamics study. Chemical Physics, 2004, 297, 221-233.	1.9	50
7	Stability and Reactions of CaCO₃ Polymorphs in the Earth's Deep Mantle. Journal of Geophysical Research: Solid Earth, 2018, 123, 6491-6500.	3.4	32
8	New Highâ€Pressure Phase of CaCO₃ at the Topmost Lower Mantle: Implication for the Deepâ€Mantle Carbon Transportation. Geophysical Research Letters, 2018, 45, 1355-1360.	4.0	30
9	The structure, dynamics and solvation mechanisms of ions in water from long time molecular dynamics simulations: a case study of CaCl2(aq) aqueous solutions. Molecular Physics, 2008, 106, 2685-2697.	1.7	26
10	Molecular dynamics simulation of the CH4 and CH4â€“H2O systems up to 10GPa and 2573K. Geochimica Et Cosmochimica Acta, 2007, 71, 2036-2055.	3.9	25
11	Partitioning of sulfur between solid and liquid iron under Earthâ€™s core conditions: Constraints from atomistic simulations with machine learning potentials. Geochimica Et Cosmochimica Acta, 2020, 291, 5-18.	3.9	23
12	An accurate model for calculating C2H6 solubility in pure water and aqueous NaCl solutions. Fluid Phase Equilibria, 2005, 238, 77-86.	2.5	17
13	High pressure equation of state for molten CaCO3 from first principles simulations. Diqiu Huaxue, 2015, 34, 13-20.	0.5	16
14	Some thermodynamic properties of larnite (Î²-Ca₂SiO₄) constrained by highT/Pexperiment and/or theoretical simulation. American Mineralogist, 2016, 101, 277-288.	1.9	16
15	Phase equilibria of the system methaneâ€“ethane from temperature scaling Gibbs Ensemble Monte Carlo simulation. Geochimica Et Cosmochimica Acta, 2002, 66, 3431-3439.	3.9	15
16	Modelling of phase equilibria in CH4â€“C2H6â€“C3H8â€“nC4H10â€“NaClâ€“H2O systems. Applied Geochemistry, 2015, 56, 23-36.	3.0	14
17	Compressional behavior of MgCr2O4 spinel from first-principles simulation. Science China Earth Sciences, 2016, 59, 989-996.	5.2	14
18	Two-phase thermodynamic model for computing entropies of liquids reanalyzed. Journal of Chemical Physics, 2017, 147, 194505.	3.0	14

#	Article	IF	Citations
19	Solvation properties of Li+and Clâ^'in water: molecular dynamics simulation with a non-rigid model. Molecular Physics, 2003, 101, 1501-1510.	1.7	12
20	Magnesium partitioning between silicate melt and liquid iron using first-principles molecular dynamics: Implications for the early thermal history of the Earth's core. Earth and Planetary Science Letters, 2020, 531, 115934.	4.4	10
21	Evaluation of the pressureâ€"volumeâ€"temperature (PVT) data of water from experiments and molecular simulations since 1990. Physics of the Earth and Planetary Interiors, 2015, 245, 88-102.	1.9	9
22	Spinel and post-spinel phase assemblages in Zn2TiO4: an experimental and theoretical study. Physics and Chemistry of Minerals, 2017, 44, 109-123.	0.8	9
23	The effect of Si and S on the stability of bcc iron with respect to tetragonal strain at the Earth's inner core conditions. Geophysical Research Letters, 2013, 40, 2958-2962.	4.0	8
24	A new Ca3MgSi2O8 compound and some of its thermodynamic properties. Journal of Solid State Chemistry, 2017, 255, 145-149.	2.9	7
25	Extension of the IAPWS-95 formulation and an improved calculation approach for saturated properties. Physics of the Earth and Planetary Interiors, 2011, 185, 53-60.	1.9	6
26	Equations of state for aqueous solutions under mantle conditions. Science China Earth Sciences, 2016, 59, 1095-1106.	5.2	5
27	Equations of state of Co2TiO4-Sp, Co2TiO4-CM, and Co2TiO4-CT, and their phase transitions: an experimental and theoretical study. Physics and Chemistry of Minerals, 2019, 46, 571-582.	0.8	4
28	Crystal Structure and Some Thermodynamic Properties of Ca7MgSi4O16-Bredigite. Crystals, 2021, 11, 14.	2.2	4
29	Response to â€œComment on â€˜An optimized potential for carbon dioxideâ€™â€‰â€•[J. Chem. Phys. 129, 087101 (2008)]. Journal of Chemical Physics, 2008, 129, 087102.	3.0	3
30	Free energies of Feâ€"Oâ€"Si ternary liquids at high temperatures and pressures: Implications for the evolution of the Earthâ€™s core composition. Geophysical Research Letters, 0, , .	4.0	2
31	Thermoelastic properties of MgSiO3-majorite at high temperatures and pressures: A first principles study. Physics of the Earth and Planetary Interiors, 2020, 303, 106491.	1.9	1