## Guang-Jun Guo

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Why can water cages adsorb aqueous methane? A potential of mean force calculation on hydrate nucleation mechanisms. Physical Chemistry Chemical Physics, 2009, 11, 10427.	1.3	121
2	Using the face-saturated incomplete cage analysis to quantify the cage compositions and cage linking structures of amorphous phase hydrates. Physical Chemistry Chemical Physics, 2011, 13, 12048.	1.3	105
3	Microcanonical molecular simulations of methane hydrate nucleation and growth: evidence that direct nucleation to sI hydrate is among the multiple nucleation pathways. Physical Chemistry Chemical Physics, 2015, 17, 8870-8876.	1.3	94
4	Solubility of Aqueous Methane under Metastable Conditions: Implications for Gas Hydrate Nucleation. Journal of Physical Chemistry B, 2013, 117, 6498-6504.	1.2	89
5	Equilibrium molecular dynamics calculation of the bulk viscosity of liquid water. Molecular Physics, 2001, 99, 283-289.	0.8	70
6	Effect of Methane Adsorption on the Lifetime of a Dodecahedral Water Cluster Immersed in Liquid Water:  A Molecular Dynamics Study on the Hydrate Nucleation Mechanisms. Journal of Physical Chemistry C, 2007, 111, 2595-2606.	1.5	70
7	Metallogenic geodynamic background of Mesozoic gold deposits in granite-greenstone terrains of North China Craton. Science in China Series D: Earth Sciences, 1998, 41, 113-120.	0.9	64
8	Can the dodecahedral water cluster naturally form in methane aqueous solutions? A molecular dynamics study on the hydrate nucleation mechanisms. Journal of Chemical Physics, 2008, 128, 194504.	1.2	63
9	Lifetimes of cagelike water clusters immersed in bulk liquid water: A molecular dynamics study on gas hydrate nucleation mechanisms. Journal of Chemical Physics, 2004, 121, 1542-1547.	1.2	60
10	Effects of ensembles on methane hydrate nucleation kinetics. Physical Chemistry Chemical Physics, 2016, 18, 15602-15608.	1.3	53
11	Viscosity and stress autocorrelation function in supercooled water: a molecular dynamics study. Molecular Physics, 2002, 100, 2617-2627.	0.8	34
12	The effects of ice on methane hydrate nucleation: a microcanonical molecular dynamics study. Physical Chemistry Chemical Physics, 2017, 19, 19496-19505.	1.3	33
13	Bridging solution properties to gas hydrate nucleation through guest dynamics. Physical Chemistry Chemical Physics, 2018, 20, 24535-24538.	1.3	33
14	Mechanolysis mechanisms of the fused aromatic rings of anthracite coal under shear stress. Fuel, 2019, 253, 1247-1255.	3.4	33
15	Molecular Insight into the Growth of Hydrogen and Methane Binary Hydrates. Journal of Physical Chemistry C, 2018, 122, 7771-7778.	1.5	30
16	A molecular dynamics study of bulk and shear viscosity of liquid iron using embedded-atom potential. Physics and Chemistry of Minerals, 2000, 27, 164-169.	0.3	25
17	Finite-size effect at both high and low temperatures in molecular dynamics calculations of the self-diffusion coefficient and viscosity of liquid silica. Journal of Physics Condensed Matter, 2004, 16, 9127-9135.	0.7	25
18	Insight on the stability of polycrystalline natural gas hydrates by molecular dynamics simulations. Fuel, 2021, 289, 119946.	3.4	23

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19	Molecular dynamics calculation of the bulk viscosity of liquid iron–nickel alloy and the mechanisms for the bulk attenuation of seismic waves in the Earth's outer core. Physics of the Earth and Planetary Interiors, 2000, 122, 289-298.	0.7	21
20	Mechanisms of methane generation from anthracite at low temperatures: Insights from quantum chemistry calculations. International Journal of Hydrogen Energy, 2017, 42, 18922-18929.	3.8	20
21	Molecular Insights into Guest and Composition Dependence of Mixed Hydrate Nucleation. Journal of Physical Chemistry C, 2020, 124, 25078-25086.	1.5	20
22	Gas generation mechanisms of bituminous coal under shear stress based on ReaxFF molecular dynamics simulation. Fuel, 2021, 298, 120240.	3.4	20
23	Does Local Structure Bias How a Crystal Nucleus Evolves?. Journal of Physical Chemistry Letters, 2018, 9, 6991-6998.	2.1	19
24	Might a 2,2-Dimethylbutane Molecule Serve as a Site to Promote Gas Hydrate Nucleation?. Journal of Physical Chemistry C, 2019, 123, 20579-20586.	1.5	19
25	Nanopore Surfaces Control the Shale Gas Adsorption via Roughness and Layer-Accumulated Adsorption Potential: A Molecular Dynamics Study. Energy & Fuels, 2021, 35, 4893-4900.	2.5	16
26	Open questions on methane hydrate nucleation. Communications Chemistry, 2021, 4, .	2.0	15
27	Effects of cage type and adsorption face on the cage–methane adsorption interaction: Implications for hydrate nucleation studies. Chemical Physics Letters, 2013, 575, 54-58.	1.2	14
28	Effect of H-bond topology on the lifetimes of cagelike water clusters immersed in liquid water and the probability distribution of these lifetimes: Implications for hydrate nucleation mechanisms. Chemical Physics Letters, 2005, 413, 415-419.	1.2	13
29	Effect of guests on the adsorption interaction between a hydrate cage and guests. RSC Advances, 2016, 6, 106443-106452.	1.7	13
30	Equations of state of CaSiO3 Perovskite: a molecular dynamics study. Physics and Chemistry of Minerals, 2006, 33, 126-137.	0.3	10
31	Partitioning of Si and O between liquid iron and silicate melt: A twoâ€phase abâ€initio molecular dynamics study. Geophysical Research Letters, 2009, 36, .	1.5	9
32	Stress Sensitivity for the Occurrence of Coalbed Gas Outbursts: A Reactive Force Field Molecular Dynamics Study. Energy & Fuels, 2021, 35, 5801-5807.	2.5	9
33	Effects of gas reservoir configuration and pore radius on shale gas nanoflow: A molecular dynamics study. Journal of Chemical Physics, 2018, 148, 204703.	1.2	8
34	Comment on "Computation of the viscosity of a liquid from time averages of stress fluctuationsâ€. Physical Review E, 2003, 67, 043101.	0.8	7
35	Effects of italicized angle and turning angle on shale gas nanoflows in non-straight nanopores: A nonequilibrium molecular dynamics study. Fuel, 2020, 278, 118275.	3.4	6
36	Strong temperature dependence of the first pressure derivative of isothermal bulk modulus at zero pressure. Journal of Geophysical Research, 2007, 112, .	3.3	5

#	Article	IF	CITATIONS
37	Comment on "lterative Cup Overlapping: An Efficient Identification Algorithm for Cage Structures of Amorphous Phase Hydrates― Journal of Physical Chemistry B, 2021, 125, 5451-5453.	1.2	5