Lianqing Zheng

List of Publications by Year
in descending order

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40 papers	1,252 citations	430874 18 h-index	361022 35 g-index
40 all docs	40 docs citations	40 times ranked	1194 citing authors

#	Article	IF	Citations
1	Examining the Influence of Bilayer Structure on Energy Transfer and Molecular Photon Upconversion in Metal Ion Linked Multilayers. Journal of Physical Chemistry C, 2020, 124, 23597-23610.	3.1	7
2	Free energy landscape of a minimalist salt bridge model. Protein Science, 2016, 25, 270-276.	7.6	0
3	Comparative exploration of hydrogen sulfide and water transmembrane free energy surfaces via orthogonal space tempering free energy sampling. Journal of Computational Chemistry, 2016, 37, 567-574.	3.3	11
4	Predictive Sampling of Rare Conformational Events in Aqueous Solution: Designing a Generalized Orthogonal Space Tempering Method. Journal of Chemical Theory and Computation, 2016, 12, 41-52.	5.3	11
5	Payoffs, Not Tradeoffs, in the Adaptation of a Virus to Ostensibly Conflicting Selective Pressures. PLoS Genetics, 2014, 10, e1004611.	3.5	27
6	Generalized essential energy space random walks to more effectively accelerate solute sampling in aqueous environment. Journal of Chemical Physics, 2012, 136, 044103.	3.0	14
7	Practically Efficient and Robust Free Energy Calculations: Double-Integration Orthogonal Space Tempering. Journal of Chemical Theory and Computation, 2012, 8, 810-823.	5.3	84
8	The Structure, Thermodynamics, and Solubility of Organic Crystals from Simulation with a Polarizable Force Field. Journal of Chemical Theory and Computation, 2012, 8, 1721-1736.	5.3	77
9	Enhancing QM/MM Molecular Dynamics Sampling in Explicit Environments via an Orthogonal-Space-Random-Walk-Based Strategy. Journal of Physical Chemistry B, 2011, 115, 3924-3935.	2.6	20
10	Allosteric Activation via Kinetic Control: Potassium Accelerates a Conformational Change in IMP Dehydrogenase. Biochemistry, 2011, 50, 8508-8518.	2.5	14
11	Thermal Elimination of Precursors to Poly(phenylenevinylene) with a Macrocounterion versus a Small Counterion: A Coordinated Experimental and Simulation Study. Macromolecules, 2011, 44, 6663-6668.	4.8	2
12	Local and bulk melting of Cu at grain boundaries. Physica B: Condensed Matter, 2010, 405, 748-753.	2.7	18
13	Practically Efficient QM/MM Alchemical Free Energy Simulations: The Orthogonal Space Random Walk Strategy. Journal of Chemical Theory and Computation, 2010, 6, 2253-2266.	5.3	32
14	Release melting of shock-loaded single crystal Cu. Journal of Applied Physics, 2009, 105, 066103.	2.5	13
15	Melting of defective Cu with stacking faults. Journal of Chemical Physics, 2009, 130, 024508.	3.0	16
16	Simultaneous escaping of explicit and hidden free energy barriers: Application of the orthogonal space random walk strategy in generalized ensemble based conformational sampling. Journal of Chemical Physics, 2009, 130, 234105.	3.0	78
17	The relation between shock-state particle velocity and free surface velocity: A molecular dynamics study on single crystal Cu and silica glass. Journal of Applied Physics, 2008, 103, .	2.5	45
18	Melting of Cu under hydrostatic and shock wave loading to high pressures. Journal of Physics Condensed Matter, 2008, 20, 095220.	1.8	77

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19	Random walk in orthogonal space to achieve efficient free-energy simulation of complex systems. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 20227-20232.	7.1	283
20	A hybrid recursion method to robustly ensure convergence efficiencies in the simulated scaling based free energy simulations. Journal of Chemical Physics, 2008, 129, 034105.	3.0	12
21	On the simulated scaling based free energy simulations: Adaptive optimization of the scaling parameter intervals. Journal of Chemical Physics, 2008, 129, 124107.	3.0	8
22	Essential energy space random walks to accelerate molecular dynamics simulations: Convergence improvements via an adaptive-length self-healing strategy. Journal of Chemical Physics, 2008, 129, 014105.	3.0	28
23	Reply to â€œComment on â€˜Melting dynamics of superheated argon: Nucleation and growthâ€™â€•[J. Chem. Phys. 126, 034505 (2007)]. Journal of Chemical Physics, 2007, 126, 187102.	3.0	0
24	Homogeneous nucleation and growth of melt in copper. Journal of Chemical Physics, 2007, 127, 164503.	3.0	66
25	Melting dynamics of superheated argon: Nucleation and growth. Journal of Chemical Physics, 2007, 126, 034505.	3.0	21
26	Molecular Dynamics Simulations of the Melting Mechanisms of Perfect and Imperfect Crystals of Dimethylnitramine. Journal of Physical Chemistry B, 2007, 111, 2891-2895.	2.6	9
27	Densification of silica glass at ambient pressure. Journal of Chemical Physics, 2006, 125, 154511.	3.0	9
28	Solid-state disordering and melting of silica stishovite: the role of defects. Journal of Physics Condensed Matter, 2006, 18, 659-668.	1.8	17
29	Molecular Dynamics Simulations of Hexahydro-1,3,5-trinitro-1,3,5-s-triazine (RDX) Using a Combined Sorescuâ€'Riceâ€'Thompson AMBER Force Field. Journal of Physical Chemistry B, 2006, 110, 26185-26188.	2.6	36
30	On the Accuracy of Force Fields for Predicting the Physical Properties of Dimethylnitramine. Journal of Physical Chemistry B, 2006, 110, 16082-16088.	2.6	6
31	Molecular Dynamics Simulations of the Melting of 1,3,3-Trinitroazetidine. Journal of Physical Chemistry B, 2006, 110, 5721-5726.	2.6	36
32	Vacancy-induced densification of silica glass. Journal of Non-Crystalline Solids, 2006, 352, 3320-3325.	3.1	13
33	Damages to optical silica glass: processes and mechanisms. , 2006, , .		1
34	Molecular dynamics simulations of melting of perfect crystalline hexahydro-1,3,5-trinitro-1,3,5-s-triazine. Journal of Chemical Physics, 2006, 125, 084505.	3.0	35
35	Solidâ€“liquid transitions of sodium chloride at high pressures. Journal of Chemical Physics, 2006, 125, 154510.	3.0	19
36	Molecular dynamics simulations of melting and the glass transition of nitromethane. Journal of Chemical Physics, 2006, 124, 154504.	3.0	57

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37	TENSILE FAILURE OF SINGLE-CRYSTAL AND NANOCRYSTALLINE LENNARD-JONES SOLIDS UNDER UNIAXIAL STRAIN. International Journal of Modern Physics C, 2006, 17, 1551-1561.	1.7	10
38	Spontaneous disordering of nm-grain-sized polycrystals and clusters of silica stishovite. Solid State Communications, 2005, 136, 71-75.	1.9	8
39	Molecular dynamics study of UV-laser-induced densification of fused silica. II. Effects of laser pulse duration, pressure, and temperature, and comparison with pressure-induced densification. Journal of Non-Crystalline Solids, 2005, 351, 3271-3278.	3.1	7
40	UV-laser-induced densification of fused silica: a molecular dynamics study. Journal of Non-Crystalline Solids, 2004, 347, 144-152.	3.1	25