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	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
2	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
3	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
4	Melting of Cu under hydrostatic and shock wave loading to high pressures. Journal of Physics Condensed Matter, 2008, 20, 095220.	1.8	77
5	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
6	Homogeneous nucleation and growth of melt in copper. Journal of Chemical Physics, 2007, 127, 164503.	3.0	66
7	Molecular dynamics simulations of melting and the glass transition of nitromethane. Journal of Chemical Physics, 2006, 124, 154504.	3.0	57
8	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
9	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
10	Molecular Dynamics Simulations of the Melting of 1,3,3-Trinitroazetidine. Journal of Physical Chemistry B, 2006, 110, 5721-5726.	2.6	36
11	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
12	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
13	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
14	Payoffs, Not Tradeoffs, in the Adaptation of a Virus to Ostensibly Conflicting Selective Pressures. PLoS Genetics, 2014, 10, e1004611.	3.5	27
15	UV-laser-induced densification of fused silica: a molecular dynamics study. Journal of Non-Crystalline Solids, 2004, 347, 144-152.	3.1	25
16	Melting dynamics of superheated argon: Nucleation and growth. Journal of Chemical Physics, 2007, 126, 034505.	3.0	21
17	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
18	Solidâ€“liquid transitions of sodium chloride at high pressures. Journal of Chemical Physics, 2006, 125, 154510.	3.0	19

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19	Local and bulk melting of Cu at grain boundaries. Physica B: Condensed Matter, 2010, 405, 748-753.	2.7	18
20	Solid-state disordering and melting of silica stishovite: the role of defects. Journal of Physics Condensed Matter, 2006, 18, 659-668.	1.8	17
21	Melting of defective Cu with stacking faults. Journal of Chemical Physics, 2009, 130, 024508.	3.0	16
22	Allosteric Activation via Kinetic Control: Potassium Accelerates a Conformational Change in IMP Dehydrogenase. Biochemistry, 2011, 50, 8508-8518.	2.5	14
23	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
24	Vacancy-induced densification of silica glass. Journal of Non-Crystalline Solids, 2006, 352, 3320-3325.	3.1	13
25	Release melting of shock-loaded single crystal Cu. Journal of Applied Physics, 2009, 105, 066103.	2.5	13
26	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
27	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
28	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
29	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
30	Densification of silica glass at ambient pressure. Journal of Chemical Physics, 2006, 125, 154511.	3.0	9
31	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
32	Spontaneous disordering of nm-grain-sized polycrystals and clusters of silica stishovite. Solid State Communications, 2005, 136, 71-75.	1.9	8
33	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
34	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
35	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
36	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

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37	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
38	Damages to optical silica glass: processes and mechanisms. , 2006, , .		1
39	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
40	Free energy landscape of a minimalist salt bridge model. Protein Science, 2016, 25, 270-276.	7.6	0