

J Daniel Gezelter

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46
papers

1,893
citations

19
h-index

43
g-index

49
ext. papers

2,026
ext. citations

4.5
avg, IF

4.83
L-index

#	Paper	IF	Citations
46	Is the Ewald summation still necessary? Pairwise alternatives to the accepted standard for long-range electrostatics. <i>Journal of Chemical Physics</i> , 2006 , 124, 234104	3.9	452
45	Size-dependent spontaneous alloying of Au-Ag nanoparticles. <i>Journal of the American Chemical Society</i> , 2002 , 124, 11989-96	16.4	384
44	Evidence for stepwise dissociation dynamics in acetone at 248 and 193 nm. <i>Journal of Chemical Physics</i> , 1995 , 102, 4447-4460	3.9	187
43	Calculating the hopping rate for self-diffusion on rough potential energy surfaces: Cage correlations. <i>Journal of Chemical Physics</i> , 1997 , 107, 6867-6876	3.9	110
42	Can imaginary instantaneous normal mode frequencies predict barriers to self-diffusion?. <i>Journal of Chemical Physics</i> , 1997 , 107, 4618-4627	3.9	91
41	Direct Observation of Stretched-Exponential Relaxation in Low-Temperature Lennard-Jones Systems Using the Cage Correlation Function. <i>Physical Review Letters</i> , 1999 , 82, 3649-3652	7.4	69
40	Some problems of correcting the zero-point energy problem in classical trajectories. <i>Chemical Physics Letters</i> , 1992 , 193, 512-517	2.5	42
39	Simulating Interfacial Thermal Conductance at Metal-Solvent Interfaces: The Role of Chemical Capping Agents. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 22475-22483	3.8	41
38	OOPSE: an object-oriented parallel simulation engine for molecular dynamics. <i>Journal of Computational Chemistry</i> , 2005 , 26, 252-71	3.5	35
37	Resonant features in the energy dependence of the rate of ketene isomerization. <i>Journal of Chemical Physics</i> , 1995 , 103, 7868-7876	3.9	34
36	Computational Free Energy Studies of a New Ice Polymorph Which Exhibits Greater Stability than Ice Ih. <i>Journal of Chemical Theory and Computation</i> , 2005 , 1, 662-7	6.4	31
35	Simulations of Heat Conduction at Thiolate-Capped Gold Surfaces: The Role of Chain Length and Solvent Penetration. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 7605-7612	3.8	29
34	A gentler approach to RNEMD: nonisotropic velocity scaling for computing thermal conductivity and shear viscosity. <i>Journal of Chemical Physics</i> , 2010 , 133, 164101	3.9	29
33	Langevin dynamics for rigid bodies of arbitrary shape. <i>Journal of Chemical Physics</i> , 2008 , 128, 234107	3.9	27
32	Interfacial thermal conductance of thiolate-protected gold nanospheres. <i>Journal of Applied Physics</i> , 2016 , 119, 025106	2.5	25
31	Calculating the hopping rate for diffusion in molecular liquids: CS ₂ . <i>Journal of Chemical Physics</i> , 1999 , 110, 3444-3452	3.9	23
30	Dynamics of the photodissociation of triplet ketene. <i>Journal of Chemical Physics</i> , 1996 , 104, 3546-3554	3.9	23

29	On the structural and transport properties of the soft sticky dipole and related single-point water models. <i>Journal of Chemical Physics</i> , 2004 , 120, 9175-84	3.9	21
28	Dipolar ordering in the ripple phases of molecular-scale models of lipid membranes. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 1968-75	3.4	20
27	Reverse Non-Equilibrium Molecular Dynamics Demonstrate That Surface Passivation Controls Thermal Transport at Semiconductor-Solvent Interfaces. <i>ACS Nano</i> , 2015 , 9, 6278-87	16.7	18
26	Response to Comment on a critique of the instantaneous normal mode (INM) approach to diffusion [J. Chem. Phys. 109, 4693 (1998)]. <i>Journal of Chemical Physics</i> , 1998 , 109, 4695-4696	3.9	17
25	Real space electrostatics for multipoles. I. Development of methods. <i>Journal of Chemical Physics</i> , 2014 , 141, 134109	3.9	16
24	Velocity shearing and scaling RNEMD: a minimally perturbing method for simulating temperature and momentum gradients. <i>Molecular Physics</i> , 2012 , 110, 691-701	1.7	16
23	Open Source and Open Data Should Be Standard Practices. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 1168-9	6.4	15
22	Real space electrostatics for multipoles. II. Comparisons with the Ewald sum. <i>Journal of Chemical Physics</i> , 2014 , 141, 134110	3.9	14
21	Thermal Transport is Influenced by Nanoparticle Morphology: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 1430-1436	3.8	12
20	Why is Ice Slippery? Simulations of Shear Viscosity of the Quasi-Liquid Layer on Ice. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 3686-3691	6.4	12
19	Comparing Models for Diffusion in Supercooled Liquids: The Eutectic Composition of the AgCu Alloy. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 2568-2574	2.8	12
18	Island Formation on Pt/Pd(557) Surface Alloys in the Presence of Adsorbed CO: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2015 , 150611154824003	3.8	10
17	The Langevin Hull: Constant pressure and temperature dynamics for non-periodic systems. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 834-842	6.4	8
16	Breathing mode dynamics and elastic properties of gold nanoparticles. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 16695-9	3.4	8
15	Polarizable potentials for metals: The density readjusting embedded atom method (DR-EAM). <i>Physical Review B</i> , 2019 , 99,	3.3	7
14	Simulations of Laser-Induced Glass Formation in AgCu Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 3283-3293	3.8	7
13	Rabani, gezelter, and berne reply:. <i>Physical Review Letters</i> , 2000 , 85, 467	7.4	7
12	Friction at Ice-Ih/Water Interfaces Is Governed by Solid/Liquid Hydrogen-Bonding. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 26764-26776	3.8	6

11	Random Sequential Adsorption Model for the Differential Coverage of Gold (111) Surfaces by Two Related Silicon Phthalocyanines <i>Journal of Physical Chemistry B</i> , 2001 , 105, 6515-6519	3.4	6
10	A Method for Creating Thermal and Angular Momentum Fluxes in Nonperiodic Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 1878-86	6.4	5
9	Molecular Dynamics Simulations of the Surface Reconstructions of Pt(557) and Au(557) under Exposure to CO. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 14579-14587	3.8	5
8	Simulations of solid-liquid friction at ice-I(h)/water interfaces. <i>Journal of Chemical Physics</i> , 2013 , 139, 194710	3.9	5
7	CO-Induced Restructuring on Stepped Pt Surfaces: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 18180-18190	3.8	5
6	Thermal Conductivity of Gold/Phenylethanethiol (Au144PET60) Nanoarrays: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 3389-3395	3.8	2
5	Spontaneous corrugation of dipolar membranes. <i>Physical Review E</i> , 2007 , 75, 031602	2.4	2
4	The role of polarizability in the interfacial thermal conductance at the gold-water interface. <i>Journal of Chemical Physics</i> , 2020 , 153, 204703	3.9	2
3	Real space electrostatics for multipoles. III. Dielectric properties. <i>Journal of Chemical Physics</i> , 2016 , 145, 074108	3.9	2
2	Separation of Enantiomers through Local Vorticity: A Screw Model Mechanism. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 11709-11716	3.4	1
1	Nitrile vibrations as reporters of field-induced phase transitions in 4-cyano-4'-pentylbiphenyl (5CB). <i>Journal of Physical Chemistry B</i> , 2014 , 118, 8441-8	3.4	