J Daniel Gezelter

List of Publications by Year
in descending order

46	2,144	331538	233338
papers	citations	21 h-index	45 g-index

49	49	49	2451
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Is the Ewald summation still necessary? Pairwise alternatives to the accepted standard for long-range electrostatics. Journal of Chemical Physics, 2006, 124, 234104.	1.2	508
2	Size-Dependent Spontaneous Alloying of Auâˆ'Ag Nanoparticles. Journal of the American Chemical Society, 2002, 124, 11989-11996.	6.6	416
3	Evidence for stepwise dissociation dynamics in acetone at 248 and 193 nm. Journal of Chemical Physics, 1995, 102, 4447-4460.	1.2	198
4	Calculating the hopping rate for self-diffusion on rough potential energy surfaces: Cage correlations. Journal of Chemical Physics, 1997, 107, 6867-6876.	1.2	118
5	Can imaginary instantaneous normal mode frequencies predict barriers to self-diffusion?. Journal of Chemical Physics, 1997, 107, 4618-4627.	1.2	99
6	Direct Observation of Stretched-Exponential Relaxation in Low-Temperature Lennard-Jones Systems Using the Cage Correlation Function. Physical Review Letters, 1999, 82, 3649-3652.	2.9	73
7	Simulating Interfacial Thermal Conductance at Metal-Solvent Interfaces: The Role of Chemical Capping Agents. Journal of Physical Chemistry C, 2011, 115, 22475-22483.	1.5	49
8	Some problems of correcting the zero-point energy problem in classical trajectories. Chemical Physics Letters, 1992, 193, 512-517.	1.2	47
9	Resonant features in the energy dependence of the rate of ketene isomerization. Journal of Chemical Physics, 1995, 103, 7868-7876.	1.2	41
10	OOPSE: An object-oriented parallel simulation engine for molecular dynamics. Journal of Computational Chemistry, 2005, 26, 252-271.	1.5	37
11	Langevin dynamics for rigid bodies of arbitrary shape. Journal of Chemical Physics, 2008, 128, 234107.	1.2	36
12	A gentler approach to RNEMD: Nonisotropic velocity scaling for computing thermal conductivity and shear viscosity. Journal of Chemical Physics, 2010, 133, 164101.	1.2	36
13	Simulations of Heat Conduction at Thiolate-Capped Gold Surfaces: The Role of Chain Length and Solvent Penetration. Journal of Physical Chemistry C, 2013, 117, 7605-7612.	1.5	35
14	Computational Free Energy Studies of a New Ice Polymorph Which Exhibits Greater Stability than Ice Ih. Journal of Chemical Theory and Computation, 2005, 1, 662-667.	2.3	34
15	Interfacial thermal conductance of thiolate-protected gold nanospheres. Journal of Applied Physics, 2016, 119, .	1.1	29
16	Dynamics of the photodissociation of triplet ketene. Journal of Chemical Physics, 1996, 104, 3546-3554.	1.2	27
17	Calculating the hopping rate for diffusion in molecular liquids: CS2. Journal of Chemical Physics, 1999, 110, 3444-3452.	1.2	26
18	Open Source and Open Data Should Be Standard Practices. Journal of Physical Chemistry Letters, 2015, 6, 1168-1169.	2.1	23

#	Article	IF	Citations
19	Dipolar Ordering in the Ripple Phases of Molecular-Scale Models of Lipid Membranes. Journal of Physical Chemistry B, 2008, 112, 1968-1975.	1.2	22
20	Velocity shearing and scaling RNEMD: a minimally perturbing method for simulating temperature and momentum gradients. Molecular Physics, 2012, 110, 691-701.	0.8	22
21	On the structural and transport properties of the soft sticky dipole and related single-point water models. Journal of Chemical Physics, 2004, 120, 9175-9184.	1.2	21
22	Reverse Non-Equilibrium Molecular Dynamics Demonstrate That Surface Passivation Controls Thermal Transport at Semiconductorâ€“Solvent Interfaces. ACS Nano, 2015, 9, 6278-6287.	7.3	21
23	Response to â€œComment on a critique of the instantaneous normal mode (INM) approach to diffusionâ€• [J. Chem. Phys. 109, 4693 (1998)]. Journal of Chemical Physics, 1998, 109, 4695-4696.	1.2	20
24	Thermal Transport is Influenced by Nanoparticle Morphology: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2018, 122, 1430-1436.	1.5	20
25	Real space electrostatics for multipoles. I. Development of methods. Journal of Chemical Physics, 2014, 141, 134109.	1.2	19
26	Why is Ice Slippery? Simulations of Shear Viscosity of the Quasi-Liquid Layer on Ice. Journal of Physical Chemistry Letters, 2018, 9, 3686-3691.	2.1	17
27	Real space electrostatics for multipoles. II. Comparisons with the Ewald sum. Journal of Chemical Physics, 2014, 141, 134110.	1.2	14
28	Comparing Models for Diffusion in Supercooled Liquids:Â The Eutectic Composition of the Agâ^'Cu Alloyâ€. Journal of Physical Chemistry A, 2001, 105, 2568-2574.	1.1	12
29	Friction at Ice-I_h/Water Interfaces Is Governed by Solid/Liquid Hydrogen-Bonding. Journal of Physical Chemistry C, 2017, 121, 26764-26776.	1.5	12
30	Polarizable potentials for metals: The density readjusting embedded atom method (DR-EAM). Physical Review B, 2019, 99, .	1.1	12
31	The Langevin Hull: Constant Pressure and Temperature Dynamics for Nonperiodic Systems. Journal of Chemical Theory and Computation, 2011, 7, 834-842.	2.3	11
32	Simulations of Laser-Induced Glass Formation in Agâ^'Cu Nanoparticles. Journal of Physical Chemistry C, 2008, 112, 3283-3293.	1.5	10
33	Island Formation on Pt/Pd(557) Surface Alloys in the Presence of Adsorbed CO: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2015, 119, 14239-14247.	1.5	10
34	CO-Induced Restructuring on Stepped Pt Surfaces: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2016, 120, 18180-18190.	1.5	9
35	Breathing Mode Dynamics and Elastic Properties of Gold Nanoparticles. Journal of Physical Chemistry B, 2005, 109, 16695-16699.	1.2	8
36	Simulations of solid-liquid friction at ice-Ih/water interfaces. Journal of Chemical Physics, 2013, 139, 194710.	1.2	8

#	Article	IF	Citations
37	Rabani, Gezelter, and Berne Reply:. Physical Review Letters, 2000, 85, 467-467.	2.9	7
38	A Method for Creating Thermal and Angular Momentum Fluxes in Nonperiodic Simulations. Journal of Chemical Theory and Computation, 2014, 10, 1878-1886.	2.3	7
39	Random Sequential Adsorption Model for the Differential Coverage of Gold (111) Surfaces by Two Related Silicon Phthalocyaninesâ€. Journal of Physical Chemistry B, 2001, 105, 6515-6519.	1.2	6
40	The role of polarizability in the interfacial thermal conductance at the goldâ€“water interface. Journal of Chemical Physics, 2020, 153, 204703.	1.2	6
41	Molecular Dynamics Simulations of the Surface Reconstructions of Pt(557) and Au(557) under Exposure to CO. Journal of Physical Chemistry C, 2013, 117, 14579-14587.	1.5	5
42	Thermal Conductivity of Goldâ€“Phenylethanethiol (Au144PET60) Nanoarrays: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2020, 124, 3389-3395.	1.5	4
43	Separation of Enantiomers through Local Vorticity: A Screw Model Mechanism. Journal of Physical Chemistry B, 2021, 125, 11709-11716.	1.2	4
44	Real space electrostatics for multipoles. III. Dielectric properties. Journal of Chemical Physics, 2016, 145, 074108.	1.2	3
45	Spontaneous corrugation of dipolar membranes. Physical Review E, 2007, 75, 031602.	0.8	2
46	Nitrile Vibrations as Reporters of Field-Induced Phase Transitions in 4-Cyano-4â€²-pentylbiphenyl (5CB). Journal of Physical Chemistry B, 2014, 118, 8441-8448.	1.2	0