J Daniel Gezelter

List of Publications by Year in Descending Order

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	Separation of Enantiomers through Local Vorticity: A Screw Model Mechanism. *Journal of Physical Chemistry B*, **2021**, 125, 11709-11716	3.4	1
45	Thermal Conductivity of GoldPhenylethanethiol (Au144PET60) Nanoarrays: A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2020**, 124, 3389-3395	3.8	2
44	The role of polarizability in the interfacial thermal conductance at the gold-water interface. *Journal of Chemical Physics*, **2020**, 153, 204703	3.9	2
43	Polarizable potentials for metals: The density readjusting embedded atom method (DR-EAM). *Physical Review B*, **2019**, 99,	3.3	7
42	Thermal Transport is Influenced by Nanoparticle Morphology: A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2018**, 122, 1430-1436	3.8	12
41	Why is Ice Slippery? Simulations of Shear Viscosity of the Quasi-Liquid Layer on Ice. *Journal of Physical Chemistry Letters*, **2018**, 9, 3686-3691	6.4	12
40	Friction at Ice-Ih/Water Interfaces Is Governed by Solid/Liquid Hydrogen-Bonding. *Journal of Physical Chemistry C*, **2017**, 121, 26764-26776	3.8	6
39	Real space electrostatics for multipoles. III. Dielectric properties. *Journal of Chemical Physics*, **2016**, 145, 074108	3.9	2
38	Interfacial thermal conductance of thiolate-protected gold nanospheres. *Journal of Applied Physics*, **2016**, 119, 025106	2.5	25
37	CO-Induced Restructuring on Stepped Pt Surfaces: A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2016**, 120, 18180-18190	3.8	5
36	Open Source and Open Data Should Be Standard Practices. *Journal of Physical Chemistry Letters*, **2015**, 6, 1168-9	6.4	15
35	Island Formation on Pt/Pd(557) Surface Alloys in the Presence of Adsorbed CO: A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2015**, 150611154824003	3.8	10
34	Reverse Non-Equilibrium Molecular Dynamics Demonstrate That Surface Passivation Controls Thermal Transport at Semiconductor-Solvent Interfaces. *ACS Nano*, **2015**, 9, 6278-87	16.7	18
33	A Method for Creating Thermal and Angular Momentum Fluxes in Nonperiodic Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 1878-86	6.4	5
32	Nitrile vibrations as reporters of field-induced phase transitions in 4-cyano-4'-pentylbiphenyl (5CB). *Journal of Physical Chemistry B*, **2014**, 118, 8441-8	3.4	
31	Real space electrostatics for multipoles. I. Development of methods. *Journal of Chemical Physics*, **2014**, 141, 134109	3.9	16
30	Real space electrostatics for multipoles. II. Comparisons with the Ewald sum. *Journal of Chemical Physics*, **2014**, 141, 134110	3.9	14

29	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	3.8	29
28	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	3.8	5
27	Simulations of solid-liquid friction at ice-I(h)/water interfaces. *Journal of Chemical Physics*, **2013**, 139, 194710	3.9	5
26	Velocity shearing and scaling RNEMD: a minimally perturbing method for simulating temperature and momentum gradients. *Molecular Physics*, **2012**, 110, 691-701	1.7	16
25	Simulating Interfacial Thermal Conductance at Metal-Solvent Interfaces: The Role of Chemical Capping Agents. *Journal of Physical Chemistry C*, **2011**, 115, 22475-22483	3.8	41
24	The Langevin Hull: Constant pressure and temperature dynamics for non-periodic systems. *Journal of Chemical Theory and Computation*, **2011**, 7, 834-842	6.4	8
23	A gentler approach to RNEMD: nonisotropic velocity scaling for computing thermal conductivity and shear viscosity. *Journal of Chemical Physics*, **2010**, 133, 164101	3.9	29
22	Simulations of Laser-Induced Glass Formation in Ag□u Nanoparticles. *Journal of Physical Chemistry C*, **2008**, 112, 3283-3293	3.8	7
21	Dipolar ordering in the ripple phases of molecular-scale models of lipid membranes. *Journal of Physical Chemistry B*, **2008**, 112, 1968-75	3.4	20
20	Langevin dynamics for rigid bodies of arbitrary shape. *Journal of Chemical Physics*, **2008**, 128, 234107	3.9	27
19	Spontaneous corrugation of dipolar membranes. *Physical Review E*, **2007**, 75, 031602	2.4	2
18	Is the Ewald summation still necessary? Pairwise alternatives to the accepted standard for long-range electrostatics. *Journal of Chemical Physics*, **2006**, 124, 234104	3.9	452
17	Breathing mode dynamics and elastic properties of gold nanoparticles. *Journal of Physical Chemistry B*, **2005**, 109, 16695-9	3.4	8
16	Computational Free Energy Studies of a New Ice Polymorph Which Exhibits Greater Stability than Ice Ih. *Journal of Chemical Theory and Computation*, **2005**, 1, 662-7	6.4	31
15	OOPSE: an object-oriented parallel simulation engine for molecular dynamics. *Journal of Computational Chemistry*, **2005**, 26, 252-71	3.5	35
14	On the structural and transport properties of the soft sticky dipole and related single-point water models. *Journal of Chemical Physics*, **2004**, 120, 9175-84	3.9	21
13	Size-dependent spontaneous alloying of Au-Ag nanoparticles. *Journal of the American Chemical Society*, **2002**, 124, 11989-96	16.4	384
12	Comparing Models for Diffusion in Supercooled Liquids: The Eutectic Composition of the Ag□u Alloy□*Journal of Physical Chemistry A*, **2001**, 105, 2568-2574	2.8	12

11	Random Sequential Adsorption Model for the Differential Coverage of Gold (111) Surfaces by Two Related Silicon Phthalocyanines *Journal of Physical Chemistry B*, **2001**, 105, 6515-6519	3.4	6
10	Rabani, gezelter, and berne reply:. *Physical Review Letters*, **2000**, 85, 467	7.4	7
9	Calculating the hopping rate for diffusion in molecular liquids: CS2. *Journal of Chemical Physics*, **1999**, 110, 3444-3452	3.9	23
8	Direct Observation of Stretched-Exponential Relaxation in Low-Temperature Lennard-Jones Systems Using the Cage Correlation Function. *Physical Review Letters*, **1999**, 82, 3649-3652	7.4	69
7	Response to Comment on a critique of the instantaneous normal mode (INM) approach to diffusion [J. Chem. Phys. 109, 4693 (1998)]. *Journal of Chemical Physics*, **1998**, 109, 4695-4696	3.9	17
6	Can imaginary instantaneous normal mode frequencies predict barriers to self-diffusion?. *Journal of Chemical Physics*, **1997**, 107, 4618-4627	3.9	91
5	Calculating the hopping rate for self-diffusion on rough potential energy surfaces: Cage correlations. *Journal of Chemical Physics*, **1997**, 107, 6867-6876	3.9	110
4	Dynamics of the photodissociation of triplet ketene. *Journal of Chemical Physics*, **1996**, 104, 3546-3554	3.9	23
3	Resonant features in the energy dependence of the rate of ketene isomerization. *Journal of Chemical Physics*, **1995**, 103, 7868-7876	3.9	34
2	Evidence for stepwise dissociation dynamics in acetone at 248 and 193 nm. *Journal of Chemical Physics*, **1995**, 102, 4447-4460	3.9	187
1	Some problems of correcting the zero-point energy problem in classical trajectories. *Chemical Physics Letters*, **1992**, 193, 512-517	2.5	42