

Nir Goldman

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

69
papers

2,323
citations

25
h-index

47
g-index

75
ext. papers

2,552
ext. citations

5.4
avg. IF

5.15
L-index

#	Paper	IF	Citations
69	Dynamic ionization of water under extreme conditions. <i>Physical Review Letters</i> , 2005 , 94, 125508	7.4	190
68	Nitrogen-rich heterocycles as reactivity retardants in shocked insensitive explosives. <i>Journal of the American Chemical Society</i> , 2009 , 131, 5483-7	16.4	160
67	High-nitrogen energetic materials derived from azotetrazolate. <i>Journal of Energetic Materials</i> , 1998 , 16, 119-127	1.6	136
66	Spectroscopic determination of the water dimer intermolecular potential-energy surface. <i>Journal of Chemical Physics</i> , 2002 , 116, 10148-10163	3.9	116
65	Water dimers in the atmosphere III: equilibrium constant from a flexible potential. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 5411-9	2.8	108
64	Shock synthesis of amino acids from impacting cometary and icy planet surface analogues. <i>Nature Geoscience</i> , 2013 , 6, 1045-1049	18.3	102
63	Synthesis of glycine-containing complexes in impacts of comets on early Earth. <i>Nature Chemistry</i> , 2010 , 2, 949-54	17.6	99
62	Bonding in the superionic phase of water. <i>Physical Review Letters</i> , 2005 , 94, 217801	7.4	95
61	Catalytic behaviour of dense hot water. <i>Nature Chemistry</i> , 2009 , 1, 57-62	17.6	85
60	Ab initio simulation of the equation of state and kinetics of shocked water. <i>Journal of Chemical Physics</i> , 2009 , 130, 124517	3.9	83
59	Water Dimers in the Atmosphere: Equilibrium Constant for Water Dimerization from the VRT(ASP-W) Potential Surface. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 515-519	2.8	81
58	Characterization of hydrogen bond acceptor molecules at the water surface using near-edge x-ray absorption fine-structure spectroscopy and density functional theory. <i>Journal of Physics Condensed Matter</i> , 2002 , 14, L221-L226	1.8	79
57	Ultrafast transformation of graphite to diamond: an ab initio study of graphite under shock compression. <i>Journal of Chemical Physics</i> , 2008 , 128, 184701	3.9	74
56	Water Dimers in the Atmosphere II: Results from the VRT(ASP-W)III Potential Surface. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 787-794	2.8	63
55	Complete characterization of the water dimer vibrational ground state and testing the VRT(ASP-W)III, SAPT-5st, and VRT(MCY-5f) surfaces. <i>Molecular Physics</i> , 2003 , 101, 3477-3492	1.7	58
54	Elucidating the role of many-body forces in liquid water. I. Simulations of water clusters on the VRT(ASP-W) potential surfaces. <i>Journal of Chemical Physics</i> , 2004 , 120, 4777-89	3.9	52
53	Dissociative melting of ice VII at high pressure. <i>Journal of Chemical Physics</i> , 2009 , 130, 124514	3.9	43

52	A First principles potential energy surface for liquid water from VRT spectroscopy of water clusters. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2005 , 363, 493-508	3	42
51	ChIMES: A Force Matched Potential with Explicit Three-Body Interactions for Molten Carbon. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 6222-6229	6.4	36
50	Quantum mechanical corrections to simulated shock Hugoniot temperatures. <i>Journal of Chemical Physics</i> , 2009 , 131, 204103	3.9	36
49	Prebiotic chemistry within a simple impacting icy mixture. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 5124-31	2.8	35
48	Ultrafast shock initiation of exothermic chemistry in hydrogen peroxide. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 13051-8	2.8	29
47	Extending the Density Functional Tight Binding Method to Carbon Under Extreme Conditions. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 2198-2204	3.8	28
46	Carbyne Fiber Synthesis within Evaporating Metallic Liquid Carbon. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 21605-21611	3.8	27
45	Using force-matched potentials to improve the accuracy of density functional tight binding for reactive conditions. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 4530-5	6.4	26
44	Generating Converged Accurate Free Energy Surfaces for Chemical Reactions with a Force-Matched Semiempirical Model. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 2207-2218	6.4	25
43	Determination of a Density Functional Tight Binding Model with an Extended Basis Set and Three-Body Repulsion for Carbon Under Extreme Pressures and Temperatures. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 7885-7894	3.8	24
42	Ultrafast dynamic response of single-crystal HMX (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine). <i>Journal of Applied Physics</i> , 2018 , 123, 205902	2.5	24
41	Using Force Matching To Determine Reactive Force Fields for Water under Extreme Thermodynamic Conditions. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 135-146	6.4	22
40	Synthesis of functionalized nitrogen-containing polycyclic aromatic hydrocarbons and other prebiotic compounds in impacting glycine solutions. <i>Chemical Science</i> , 2019 , 10, 6091-6098	9.4	21
39	Development of a Multicenter Density Functional Tight Binding Model for Plutonium Surface Hydriding. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 2652-2660	6.4	21
38	Ultrafast shock synthesis of nanocarbon from a liquid precursor. <i>Nature Communications</i> , 2020 , 11, 353	17.4	20
37	A density functional tight binding model with an extended basis set and three-body repulsion for hydrogen under extreme thermodynamic conditions. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 5520-8	2.8	17
36	Application of the ChIMES Force Field to Nonreactive Molecular Systems: Water at Ambient Conditions. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 436-447	6.4	17
35	Nitrogen oxides as a chemistry trap in detonating oxygen-rich materials. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 2897-903	2.8	16

34	Chemical Degradation Pathways in Siloxane Polymers Following Phenyl Excitations. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 12201-12210	3.4	16
33	A First-Principles Study of Hydrogen Diffusivity and Dissociation on EPu (100) and (111) Surfaces. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 17950-17957	3.8	14
32	Gold Cluster Diffusion Kinetics on Stoichiometric and Reduced Surfaces of Rutile TiO ₂ (110). <i>Journal of Physical Chemistry C</i> , 2011 , 115, 11611-11617	3.8	14
31	First principles simulation of a superionic phase of hydrogen fluoride (HF) at high pressures and temperatures. <i>Journal of Chemical Physics</i> , 2006 , 125, 44501	3.9	14
30	Active learning for robust, high-complexity reactive atomistic simulations. <i>Journal of Chemical Physics</i> , 2020 , 153, 134117	3.9	14
29	Multi-center semi-empirical quantum models for carbon under extreme thermodynamic conditions. <i>Chemical Physics Letters</i> , 2015 , 622, 128-136	2.5	13
28	Many-body reactive force field development for carbon condensation in C/O systems under extreme conditions. <i>Journal of Chemical Physics</i> , 2020 , 153, 054103	3.9	13
27	X-ray scattering intensities of water at extreme pressure and temperature. <i>Journal of Chemical Physics</i> , 2007 , 126, 134505	3.9	12
26	Mechanochemical formation of heterogeneous diamond structures during rapid uniaxial compression in graphite. <i>Physical Review B</i> , 2018 , 97,	3.3	12
25	PREBIOTIC HYDROCARBON SYNTHESIS IN IMPACTING REDUCED ASTROPHYSICAL ICY MIXTURES. <i>Astrophysical Journal</i> , 2015 , 803, 91	4.7	11
24	Mechanochemical synthesis of glycine oligomers in a virtual rotational diamond anvil cell. <i>Chemical Science</i> , 2020 , 11, 7760-7771	9.4	11
23	Predictive Model of Charge Mobilities in Organic Semiconductor Small Molecules with Force-Matched Potentials. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 3494-3503	6.4	10
22	Calculation of the detonation state of HN with quantum accuracy. <i>Journal of Chemical Physics</i> , 2020 , 153, 224102	3.9	8
21	New phases of hydrogen-bonded systems at extreme conditions. <i>Phase Transitions</i> , 2007 , 80, 1073-1084	1.3	8
20	Investigating 3,4-bis(3-nitrofurazan-4-yl)furoxan detonation with a rapidly tuned density functional tight binding model. <i>Journal of Chemical Physics</i> , 2021 , 154, 164115	3.9	7
19	Time resolved x-ray diffraction in shock compressed systems. <i>Journal of Applied Physics</i> , 2021 , 129, 040901	1.5	6
18	Force Matching Approaches to Extend Density Functional Theory to Large Time and Length Scales. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019 , 71-93	0.7	5
17	Semi-Automated Creation of Density Functional Tight Binding Models through Leveraging Chebyshev Polynomial-Based Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 4435-4448	6.4	5

16	High-Accuracy Semiempirical Quantum Models Based on a Minimal Training Set.. <i>Journal of Physical Chemistry Letters</i> , 2022 , 2934-2942	6.4	5
15	Anisotropic Hydrolysis Susceptibility in Deformed Polydimethylsiloxanes. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 7926-7935	3.4	4
14	Effects of pressure on the structure and lattice dynamics of ammonium perchlorate: A combined experimental and theoretical study. <i>Journal of Chemical Physics</i> , 2018 , 149, 034501	3.9	4
13	Accelerated reaction simulations: A virtual squeeze on chemistry. <i>Nature Chemistry</i> , 2014 , 6, 1033-4	17.6	4
12	Mesocrystalline Ordering and Phase Transformation of Iron Oxide Biominerals in the Ultrahard Teeth of <i>Cryptochiton stelleri</i> . <i>Small Structures</i> , 2100202	8.7	4
11	Free Energies of Reaction for Aqueous Glycine Condensation Chemistry at Extreme Temperatures. <i>Geophysical Monograph Series</i> , 2020 , 271-283	1.1	4
10	Graphene and nano-diamond synthesis in expansions of molten liquid carbon. <i>Journal of Chemical Physics</i> , 2014 , 141, 164709	3.9	3
9	A Quantum-Based Approach to Predict Primary Radiation Damage in Polymeric Networks. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 463-473	6.4	3
8	Constitutive Model of Radiation Aging Effects in Filled Silicone Elastomers under Strain. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 10047-10057	3.4	3
7	Quantum Accurate Prediction of Plutonium Plutonium Dihydride Phase Equilibrium Using a Lattice Gas Model. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 20881-20888	3.8	2
6	Davis Computational Spectroscopy Workflow-From Structure to Spectra. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 4486-4496	6.1	1
5	Using DFTB to Model Photocatalytic Anatase-Rutile TiO Nanocrystalline Interfaces and Their Band Alignment. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 5239-5247	6.4	0
4	First-Principles Surface Characterization and Water Adsorption of Fe ₃ P Schreibersite. <i>ACS Earth and Space Chemistry</i> , 2022 , 6, 512-520	3.2	0
3	Chemistry-mediated Ostwald ripening in carbon-rich C/O systems at extreme conditions.. <i>Nature Communications</i> , 2022 , 13, 1424	17.4	0
2	A first-principles study of hydrogen surface coverage on Pu (100), (111), and (110) surfaces.. <i>Journal of Chemical Physics</i> , 2021 , 155, 234702	3.9	0
1	Reply to "comment on "Prebiotic chemistry within a simple impacting icy mixture". <i>Journal of Physical Chemistry A</i> , 2013 , 117, 14295-7	2.8	