Nir Goldman

List of Publications by Year in Descending Order

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	First-Principles Surface Characterization and Water Adsorption of Fe3P Schreibersite. *ACS Earth and Space Chemistry*, **2022**, 6, 512-520	3.2	0
68	Chemistry-mediated Ostwald ripening in carbon-rich C/O systems at extreme conditions.. *Nature Communications*, **2022**, 13, 1424	17.4	0
67	High-Accuracy Semiempirical Quantum Models Based on a Minimal Training Set.. *Journal of Physical Chemistry Letters*, **2022**, 2934-2942	6.4	5
66	Investigating 3,4-bis(3-nitrofurazan-4-yl)furoxan detonation with a rapidly tuned density functional tight binding model. *Journal of Chemical Physics*, **2021**, 154, 164115	3.9	7
65	Semi-Automated Creation of Density Functional Tight Binding Models through Leveraging Chebyshev Polynomial-Based Force Fields. *Journal of Chemical Theory and Computation*, **2021**, 17, 4435-4448	6.4	5
64	Using DFTB to Model Photocatalytic Anatase-Rutile TiO Nanocrystalline Interfaces and Their Band Alignment. *Journal of Chemical Theory and Computation*, **2021**, 17, 5239-5247	6.4	0
63	A Quantum-Based Approach to Predict Primary Radiation Damage in Polymeric Networks. *Journal of Chemical Theory and Computation*, **2021**, 17, 463-473	6.4	3
62	Constitutive Model of Radiation Aging Effects in Filled Silicone Elastomers under Strain. *Journal of Physical Chemistry B*, **2021**, 125, 10047-10057	3.4	3
61	Davis Computational Spectroscopy Workflow-From Structure to Spectra. *Journal of Chemical Information and Modeling*, **2021**, 61, 4486-4496	6.1	1
60	Time resolved x-ray diffraction in shock compressed systems. *Journal of Applied Physics*, **2021**, 129, 040901	2.5	6
59	A first-principles study of hydrogen surface coverage on δ-Pu (100), (111), and (110) surfaces.. *Journal of Chemical Physics*, **2021**, 155, 234702	3.9	0
58	Calculation of the detonation state of HN with quantum accuracy. *Journal of Chemical Physics*, **2020**, 153, 224102	3.9	8
57	Predictive Model of Charge Mobilities in Organic Semiconductor Small Molecules with Force-Matched Potentials. *Journal of Chemical Theory and Computation*, **2020**, 16, 3494-3503	6.4	10
56	Ultrafast shock synthesis of nanocarbon from a liquid precursor. *Nature Communications*, **2020**, 11, 353	17.4	20
55	Active learning for robust, high-complexity reactive atomistic simulations. *Journal of Chemical Physics*, **2020**, 153, 134117	3.9	14
54	Mechanochemical synthesis of glycine oligomers in a virtual rotational diamond anvil cell. *Chemical Science*, **2020**, 11, 7760-7771	9.4	11
53	Many-body reactive force field development for carbon condensation in C/O systems under extreme conditions. *Journal of Chemical Physics*, **2020**, 153, 054103	3.9	13

52	Quantum Accurate Prediction of Plutonium Plutonium Dihydride Phase Equilibrium Using a Lattice Gas Model. *Journal of Physical Chemistry C*, **2020**, 124, 20881-20888	3.8	2
51	Free Energies of Reaction for Aqueous Glycine Condensation Chemistry at Extreme Temperatures. *Geophysical Monograph Series*, **2020**, 271-283	1.1	4
50	Anisotropic Hydrolysis Susceptibility in Deformed Polydimethylsiloxanes. *Journal of Physical Chemistry B*, **2019**, 123, 7926-7935	3.4	4
49	Synthesis of functionalized nitrogen-containing polycyclic aromatic hydrocarbons and other prebiotic compounds in impacting glycine solutions. *Chemical Science*, **2019**, 10, 6091-6098	9.4	21
48	Force Matching Approaches to Extend Density Functional Theory to Large Time and Length Scales. *Challenges and Advances in Computational Chemistry and Physics*, **2019**, 71-93	0.7	5
47	Application of the ChIMES Force Field to Nonreactive Molecular Systems: Water at Ambient Conditions. *Journal of Chemical Theory and Computation*, **2019**, 15, 436-447	6.4	17
46	Development of a Multicenter Density Functional Tight Binding Model for Plutonium Surface Hydriding. *Journal of Chemical Theory and Computation*, **2018**, 14, 2652-2660	6.4	21
45	Generating Converged Accurate Free Energy Surfaces for Chemical Reactions with a Force-Matched Semiempirical Model. *Journal of Chemical Theory and Computation*, **2018**, 14, 2207-2218	6.4	25
44	Effects of pressure on the structure and lattice dynamics of ammonium perchlorate: A combined experimental and theoretical study. *Journal of Chemical Physics*, **2018**, 149, 034501	3.9	4
43	Chemical Degradation Pathways in Siloxane Polymers Following Phenyl Excitations. *Journal of Physical Chemistry B*, **2018**, 122, 12201-12210	3.4	16
42	Ultrafast dynamic response of single-crystal HMX (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine). *Journal of Applied Physics*, **2018**, 123, 205902	2.5	24
41	Mechanochemical formation of heterogeneous diamond structures during rapid uniaxial compression in graphite. *Physical Review B*, **2018**, 97,	3.3	12
40	Using Force Matching To Determine Reactive Force Fields for Water under Extreme Thermodynamic Conditions. *Journal of Chemical Theory and Computation*, **2017**, 13, 135-146	6.4	22
39	A First-Principles Study of Hydrogen Diffusivity and Dissociation on Pu (100) and (111) Surfaces. *Journal of Physical Chemistry C*, **2017**, 121, 17950-17957	3.8	14
38	ChIMES: A Force Matched Potential with Explicit Three-Body Interactions for Molten Carbon. *Journal of Chemical Theory and Computation*, **2017**, 13, 6222-6229	6.4	36
37	Carbyne Fiber Synthesis within Evaporating Metallic Liquid Carbon. *Journal of Physical Chemistry C*, **2015**, 119, 21605-21611	3.8	27
36	PREBIOTIC HYDROCARBON SYNTHESIS IN IMPACTING REDUCED ASTROPHYSICAL ICY MIXTURES. *Astrophysical Journal*, **2015**, 803, 91	4.7	11
35	Using force-matched potentials to improve the accuracy of density functional tight binding for reactive conditions. *Journal of Chemical Theory and Computation*, **2015**, 11, 4530-5	6.4	26

34	Multi-center semi-empirical quantum models for carbon under extreme thermodynamic conditions. *Chemical Physics Letters*, **2015**, 622, 128-136	2.5	13
33	Accelerated reaction simulations: A virtual squeeze on chemistry. *Nature Chemistry*, **2014**, 6, 1033-4	17.6	4
32	Graphene and nano-diamond synthesis in expansions of molten liquid carbon. *Journal of Chemical Physics*, **2014**, 141, 164709	3.9	3
31	A density functional tight binding model with an extended basis set and three-body repulsion for hydrogen under extreme thermodynamic conditions. *Journal of Physical Chemistry A*, **2014**, 118, 5520-8	2.8	17
30	Nitrogen oxides as a chemistry trap in detonating oxygen-rich materials. *Journal of Physical Chemistry A*, **2014**, 118, 2897-903	2.8	16
29	Ultrafast shock initiation of exothermic chemistry in hydrogen peroxide. *Journal of Physical Chemistry A*, **2013**, 117, 13051-8	2.8	29
28	Shock synthesis of amino acids from impacting cometary and icy planet surface analogues. *Nature Geoscience*, **2013**, 6, 1045-1049	18.3	102
27	Prebiotic chemistry within a simple impacting icy mixture. *Journal of Physical Chemistry A*, **2013**, 117, 5124-31	2.8	35
26	Determination of a Density Functional Tight Binding Model with an Extended Basis Set and Three-Body Repulsion for Carbon Under Extreme Pressures and Temperatures. *Journal of Physical Chemistry C*, **2013**, 117, 7885-7894	3.8	24
25	Reply to "comment on Ţprebiotic chemistry within a simple impacting icy mixtureŤ". *Journal of Physical Chemistry A*, **2013**, 117, 14295-7	2.8	
24	Extending the Density Functional Tight Binding Method to Carbon Under Extreme Conditions. *Journal of Physical Chemistry C*, **2012**, 116, 2198-2204	3.8	28
23	Gold Cluster Diffusion Kinetics on Stoichiometric and Reduced Surfaces of Rutile TiO2(110). *Journal of Physical Chemistry C*, **2011**, 115, 11611-11617	3.8	14
22	Synthesis of glycine-containing complexes in impacts of comets on early Earth. *Nature Chemistry*, **2010**, 2, 949-54	17.6	99
21	Quantum mechanical corrections to simulated shock Hugoniot temperatures. *Journal of Chemical Physics*, **2009**, 131, 204103	3.9	36
20	Ab initio simulation of the equation of state and kinetics of shocked water. *Journal of Chemical Physics*, **2009**, 130, 124517	3.9	83
19	Catalytic behaviour of dense hot water. *Nature Chemistry*, **2009**, 1, 57-62	17.6	85
18	Dissociative melting of ice VII at high pressure. *Journal of Chemical Physics*, **2009**, 130, 124514	3.9	43
17	Nitrogen-rich heterocycles as reactivity retardants in shocked insensitive explosives. *Journal of the American Chemical Society*, **2009**, 131, 5483-7	16.4	160

16	Ultrafast transformation of graphite to diamond: an ab initio study of graphite under shock compression. *Journal of Chemical Physics*, **2008**, 128, 184701	3.9	74
15	New phases of hydrogen-bonded systems at extreme conditions. *Phase Transitions*, **2007**, 80, 1073-1084	1.3	8
14	X-ray scattering intensities of water at extreme pressure and temperature. *Journal of Chemical Physics*, **2007**, 126, 134505	3.9	12
13	First principles simulation of a superionic phase of hydrogen fluoride (HF) at high pressures and temperatures. *Journal of Chemical Physics*, **2006**, 125, 44501	3.9	14
12	Water dimers in the atmosphere III: equilibrium constant from a flexible potential. *Journal of Physical Chemistry A*, **2006**, 110, 5411-9	2.8	108
11	Dynamic ionization of water under extreme conditions. *Physical Review Letters*, **2005**, 94, 125508	7.4	190
10	Bonding in the superionic phase of water. *Physical Review Letters*, **2005**, 94, 217801	7.4	95
9	A first principles potential energy surface for liquid water from VRT spectroscopy of water clusters. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2005**, 363, 493-508	3	42
8	Elucidating the role of many-body forces in liquid water. I. Simulations of water clusters on the VRT(ASP-W) potential surfaces. *Journal of Chemical Physics*, **2004**, 120, 4777-89	3.9	52
7	Water Dimers in the Atmosphere II: Results from the VRT(ASP-W)III Potential Surface. *Journal of Physical Chemistry A*, **2004**, 108, 787-794	2.8	63
6	Complete characterization of the water dimer vibrational ground state and testing the VRT(ASP-W)III, SAPT-5st, and VRT(MCY-5f) surfaces. *Molecular Physics*, **2003**, 101, 3477-3492	1.7	58
5	Spectroscopic determination of the water dimer intermolecular potential-energy surface. *Journal of Chemical Physics*, **2002**, 116, 10148-10163	3.9	116
4	Characterization of hydrogen bond acceptor molecules at the water surface using near-edge x-ray absorption fine-structure spectroscopy and density functional theory. *Journal of Physics Condensed Matter*, **2002**, 14, L221-L226	1.8	79
3	Water Dimers in the Atmosphere: Equilibrium Constant for Water Dimerization from the VRT(ASP-W) Potential Surface. *Journal of Physical Chemistry A*, **2001**, 105, 515-519	2.8	81
2	High-nitrogen energetic materials derived from azotetrazolate. *Journal of Energetic Materials*, **1998**, 16, 119-127	1.6	136
1	Mesocrystalline Ordering and Phase Transformation of Iron Oxide Biominerals in the Ultrahard Teeth of Cryptochiton stelleri. *Small Structures*,2100202	8.7	4