Nir Goldman

List of Publications by Year
in descending order

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74 papers	2,764 citations	201575 27 h-index	182361 51 g-index
75 all docs	75 docs citations	75 times ranked	2278 citing authors

#	Article	IF	Citations
1	Dynamic Ionization of Water under Extreme Conditions. Physical Review Letters, 2005, 94, 125508.	2.9	212
2	Nitrogen-Rich Heterocycles as Reactivity Retardants in Shocked Insensitive Explosives. Journal of the American Chemical Society, 2009, 131, 5483-5487.	6.6	189
3	High-nitrogen energetic materials derived from azotetrazolate. Journal of Energetic Materials, 1998, 16, 119-127.	1.0	155
4	Shock synthesis of amino acids from impacting cometary and icy planet surface analogues. Nature Geoscience, 2013, 6, 1045-1049.	5.4	129
5	Water Dimers in the Atmosphere III: Equilibrium Constant from a Flexible Potentialâ€. Journal of Physical Chemistry A, 2006, 110, 5411-5419.	1.1	120
6	Synthesis of glycine-containing complexes in impacts of comets on early Earth. Nature Chemistry, 2010, 2, 949-954.	6.6	120
7	Spectroscopic determination of the water dimer intermolecular potential-energy surface. Journal of Chemical Physics, 2002, 116, 10148-10163.	1.2	118
8	Bonding in the Superionic Phase of Water. Physical Review Letters, 2005, 94, 217801.	2.9	99
9	Catalytic behaviour of dense hot water. Nature Chemistry, 2009, 1, 57-62.	6.6	95
10	Ab initio simulation of the equation of state and kinetics of shocked water. Journal of Chemical Physics, 2009, 130, 124517.	1.2	91
11	Water Dimers in the Atmosphere:â€‰Equilibrium Constant for Water Dimerization from the VRT(ASP-W) Potential Surface. Journal of Physical Chemistry A, 2001, 105, 515-519.	1.1	85
12	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.	0.7	85
13	Ultrafast transformation of graphite to diamond: An ab initio study of graphite under shock compression. Journal of Chemical Physics, 2008, 128, 184701.	1.2	84
14	Water Dimers in the Atmosphere II:Â Results from the VRT(ASP-W)III Potential Surface. Journal of Physical Chemistry A, 2004, 108, 787-794.	1.1	65
15	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.	0.8	59
16	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, 4777-4789.	1.2	55
17	ChIMES: A Force Matched Potential with Explicit Three-Body Interactions for Molten Carbon. Journal of Chemical Theory and Computation, 2017, 13, 6222-6229.	2.3	54
18	Dissociative melting of ice VII at high pressure. Journal of Chemical Physics, 2009, 130, 124514.	1.2	45

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19	Prebiotic Chemistry within a Simple Impacting Icy Mixture. Journal of Physical Chemistry A, 2013, 117, 5124-5131.	1.1	45
20	A â€˜first principlesâ€™ 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.	1.6	43
21	Quantum mechanical corrections to simulated shock Hugoniot temperatures. Journal of Chemical Physics, 2009, 131, 204103.	1.2	40
22	Ultrafast Shock Initiation of Exothermic Chemistry in Hydrogen Peroxide. Journal of Physical Chemistry A, 2013, 117, 13051-13058.	1.1	33
23	Ultrafast dynamic response of single-crystal Î²-HMX (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine). Journal of Applied Physics, 2018, 123, .	1.1	33
24	Ultrafast shock synthesis of nanocarbon from a liquid precursor. Nature Communications, 2020, 11, 353.	5.8	33
25	Carbyne Fiber Synthesis within Evaporating Metallic Liquid Carbon. Journal of Physical Chemistry C, 2015, 119, 21605-21611.	1.5	32
26	Extending the Density Functional Tight Binding Method to Carbon Under Extreme Conditions. Journal of Physical Chemistry C, 2012, 116, 2198-2204.	1.5	29
27	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.	1.5	28
28	Using Force-Matched Potentials To Improve the Accuracy of Density Functional Tight Binding for Reactive Conditions. Journal of Chemical Theory and Computation, 2015, 11, 4530-4535.	2.3	28
29	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.	2.3	28
30	Development of a Multicenter Density Functional Tight Binding Model for Plutonium Surface Hydriding. Journal of Chemical Theory and Computation, 2018, 14, 2652-2660.	2.3	27
31	Synthesis of functionalized nitrogen-containing polycyclic aromatic hydrocarbons and other prebiotic compounds in impacting glycine solutions. Chemical Science, 2019, 10, 6091-6098.	3.7	27
32	Chemical Degradation Pathways in Siloxane Polymers Following Phenyl Excitations. Journal of Physical Chemistry B, 2018, 122, 12201-12210.	1.2	25
33	Using Force Matching To Determine Reactive Force Fields for Water under Extreme Thermodynamic Conditions. Journal of Chemical Theory and Computation, 2017, 13, 135-146.	2.3	24
34	Application of the ChIMES Force Field to Nonreactive Molecular Systems: Water at Ambient Conditions. Journal of Chemical Theory and Computation, 2019, 15, 436-447.	2.3	23
35	A First-Principles Study of Hydrogen Diffusivity and Dissociation on Î´-Pu (100) and (111) Surfaces. Journal of Physical Chemistry C, 2017, 121, 17950-17957.	1.5	21
36	Active learning for robust, high-complexity reactive atomistic simulations. Journal of Chemical Physics, 2020, 153, 134117.	1.2	21

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37	Mechanochemical synthesis of glycine oligomers in a virtual rotational diamond anvil cell. Chemical Science, 2020, 11, 7760-7771.	3.7	21
38	Mechanochemical formation of heterogeneous diamond structures during rapid uniaxial compression in graphite. Physical Review B, 2018, 97, .	1.1	20
39	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, 5520-5528.	1.1	18
40	Nitrogen Oxides As a Chemistry Trap in Detonating Oxygen-Rich Materials. Journal of Physical Chemistry A, 2014, 118, 2897-2903.	1.1	18
41	Gold Cluster Diffusion Kinetics on Stoichiometric and Reduced Surfaces of Rutile TiO₂(110). Journal of Physical Chemistry C, 2011, 115, 11611-11617.	1.5	17
42	Many-body reactive force field development for carbon condensation in C/O systems under extreme conditions. Journal of Chemical Physics, 2020, 153, 054103.	1.2	17
43	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.	2.3	16
44	First principles simulation of a superionic phase of hydrogen fluoride (HF) at high pressures and temperatures. Journal of Chemical Physics, 2006, 125, 044501.	1.2	15
45	Multi-center semi-empirical quantum models for carbon under extreme thermodynamic conditions. Chemical Physics Letters, 2015, 622, 128-136.	1.2	14
46	Calculation of the detonation state of HN3 with quantum accuracy. Journal of Chemical Physics, 2020, 153, 224102.	1.2	14
47	X-ray scattering intensities of water at extreme pressure and temperature. Journal of Chemical Physics, 2007, 126, 134505.	1.2	12
48	PREBIOTIC HYDROCARBON SYNTHESIS IN IMPACTING REDUCED ASTROPHYSICAL ICY MIXTURES. Astrophysical Journal, 2015, 803, 91.	1.6	12
49	Predictive Model of Charge Mobilities in Organic Semiconductor Small Molecules with Force-Matched Potentials. Journal of Chemical Theory and Computation, 2020, 16, 3494-3503.	2.3	12
50	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.	1.2	12
51	Constitutive Model of Radiation Aging Effects in Filled Silicone Elastomers under Strain. Journal of Physical Chemistry B, 2021, 125, 10047-10057.	1.2	12
52	High-Accuracy Semiempirical Quantum Models Based on a Minimal Training Set. Journal of Physical Chemistry Letters, 2022, 13, 2934-2942.	2.1	12
53	Mesocrystalline Ordering and Phase Transformation of Iron Oxide Biominerals in the Ultrahard Teeth of Cryptochiton stelleri. Small Structures, 2022, 3, .	6.9	11
54	Efficient and universal characterization of atomic structures through a topological graph order parameter. Npj Computational Materials, 2022, 8, .	3.5	11

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55	New phases of hydrogen-bonded systems at extreme conditions. Phase Transitions, 2007, 80, 1073-1084.	0.6	9
56	Time resolved x-ray diffraction in shock compressed systems. Journal of Applied Physics, 2021, 129, 040901.	1.1	9
57	Pressure-driven symmetry transitions in dense <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:math> ice. Physical Review B, 2022, 105, .	1.1	9
58	A Quantum-Based Approach to Predict Primary Radiation Damage in Polymeric Networks. Journal of Chemical Theory and Computation, 2021, 17, 463-473.	2.3	8
59	A virtual squeeze on chemistry. Nature Chemistry, 2014, 6, 1033-1034.	6.6	7
60	Anisotropic Hydrolysis Susceptibility in Deformed Polydimethylsiloxanes. Journal of Physical Chemistry B, 2019, 123, 7926-7935.	1.2	7
61	Graphene and nano-diamond synthesis in expansions of molten liquid carbon. Journal of Chemical Physics, 2014, 141, 164709.	1.2	6
62	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.	1.2	6
63	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.	0.6	5
64	Quantum Accurate Prediction of Plutoniumâ€“Plutonium Dihydride Phase Equilibrium Using a Lattice Gas Model. Journal of Physical Chemistry C, 2020, 124, 20881-20888.	1.5	4
65	Davis Computational Spectroscopy Workflowâ€”From Structure to Spectra. Journal of Chemical Information and Modeling, 2021, 61, 4486-4496.	2.5	4
66	Polymer degradation through chemical change: a quantum-based test of inferred reactions in irradiated polydimethylsiloxane. Physical Chemistry Chemical Physics, 2022, 24, 8142-8157.	1.3	4
67	Chemistry-mediated Ostwald ripening in carbon-rich C/O systems at extreme conditions. Nature Communications, 2022, 13, 1424.	5.8	4
68	Machineâ€Learning a Solution for Reactive Atomistic Simulations of Energetic Materials. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.0	4
69	Using DFTB to Model Photocatalytic Anataseâ€“Rutile TiO2 Nanocrystalline Interfaces and Their Band Alignment. Journal of Chemical Theory and Computation, 2021, 17, 5239-5247.	2.3	3
70	Comparing the Expense and Accuracy of Methods to Simulate Atomic Vibrations in Rubrene. Journal of Chemical Theory and Computation, 2021, , .	2.3	3
71	First-Principles Surface Characterization and Water Adsorption of Fe₃P Schreibersite. ACS Earth and Space Chemistry, 2022, 6, 512-520.	1.2	2
72	A first-principles study of hydrogen surface coverage on Î´-Pu (100), (111), and (110) surfaces. Journal of Chemical Physics, 2021, 155, 234702.	1.2	2

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73	Reply to â€œComment on â€˜Prebiotic Chemistry Within a Simple Impacting Icy Mixtureâ€™â€•. Journal of Physical Chemistry A, 2013, 117, 14295-14297.	1.1	0
74	Quantifying the atomistic free-volume morphology of materials with graph theory. Computational Materials Science, 2022, 213, 111623.	1.4	0