Itai Leven

List of Publications by Year
in descending order

23 papers	1,029 citations	567281 15 h-index	752698 20 g-index
24 all docs	24 docs citations	24 times ranked	1207 citing authors

#	Article	IF	Citations
1	Can electric fields drive chemistry for an aqueous microdroplet?. Nature Communications, 2022, 13, 280.	12.8	102
2	NewtonNet: a Newtonian message passing network for deep learning of interatomic potentials and forces. , 2022, 1, 333-343.		42
3	A benchmark dataset for Hydrogen Combustion. Scientific Data, 2022, 9, 215.	5.3	6
4	Recent Advances for Improving the Accuracy, Transferability, and Efficiency of Reactive Force Fields. Journal of Chemical Theory and Computation, 2021, 17, 3237-3251.	5.3	41
5	Proton Traffic Jam: Effect of Nanoconfinement and Acid Concentration on Proton Hopping Mechanism. Angewandte Chemie - International Edition, 2021, 60, 25419-25427.	13.8	14
6	RÃ¼cktitelbild: Proton Traffic Jam: Effect of Nanoconfinement and Acid Concentration on Proton Hopping Mechanism (Angew. Chem. 48/2021). Angewandte Chemie, 2021, 133, 25788-25788.	2.0	0
7	Protein C-GeM: A Coarse-Grained Electron Model for Fast and Accurate Protein Electrostatics Prediction. Journal of Chemical Information and Modeling, 2021, 61, 4357-4369.	5.4	9
8	Stochastic Constrained Extended System Dynamics for Solving Charge Equilibration Models. Journal of Chemical Theory and Computation, 2020, 16, 5991-5998.	5.3	5
9	A Reactive Force Field with Coarse-Grained Electrons for Liquid Water. Journal of Physical Chemistry Letters, 2020, 11, 9240-9247.	4.6	18
10	Inertial extended-Lagrangian scheme for solving charge equilibration models. Physical Chemistry Chemical Physics, 2019, 21, 18652-18659.	2.8	16
11	Development of an Advanced Force Field for Water Using Variational Energy Decomposition Analysis. Journal of Chemical Theory and Computation, 2019, 15, 5001-5013.	5.3	49
12	Quantifying the two-state facilitated diffusion model of proteinâ€"DNA interactions. Nucleic Acids Research, 2019, 47, 5530-5538.	14.5	25
13	C-GeM: Coarse-Grained Electron Model for Predicting the Electrostatic Potential in Molecules. Journal of Physical Chemistry Letters, 2019, 10, 6820-6826.	4.6	20
14	Interlayer Potential for Homogeneous Graphene and Hexagonal Boron Nitride Systems: Reparametrization for Many-Body Dispersion Effects. Journal of Physical Chemistry C, 2017, 121, 22826-22835.	3.1	61
15	Smallest Archimedean Screw: Facet Dynamics and Friction in Multiwalled Nanotubes. Nano Letters, 2017, 17, 5321-5328.	9.1	16
16	Interlayer Potential for Graphene/<i>h</i>-BN Heterostructures. Journal of Chemical Theory and Computation, 2016, 12, 2896-2905.	5.3	107
17	Multiwalled nanotube faceting unravelled. Nature Nanotechnology, 2016, 11, 1082-1086.	31.5	47
18	Coherent commensurate electronic states at the interface between misoriented graphene layers. Nature Nanotechnology, 2016, 11, 752-757.	31.5	107

#	Article	IF	Citations
19	Nanotube Motion on Layered Materials: A Registry Perspective. Journal of Physical Chemistry C, 2016, 120, 4466-4470.	3.1	14
20	Inter-layer potential for hexagonal boron nitride. Journal of Chemical Physics, 2014, 140, 104106.	3.0	72
21	Robust Superlubricity in Graphene/<i>h</i>-BN Heterojunctions. Journal of Physical Chemistry Letters, 2013, 4, 115-120.	4.6	184
22	Ultrahigh Torsional Stiffness and Strength of Boron Nitride Nanotubes. Nano Letters, 2012, 12, 6347-6352.	9.1	72
23	Proton Traffic Jam: Effect of Nanoconfinement and Acid Concentration on Proton Hopping Mechanism. Angewandte Chemie, 0, , .	2.0	2