Badri Narayanan

List of Publications by Year
in descending order

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75 papers	4,193 citations	172457 29 h-index	114465 63 g-index
76 all docs	76 docs citations	76 times ranked	6547 citing authors

#	Article	IF	Citations
1	A lithiumâ€“oxygen battery with a long cycle life in an air-like atmosphere. Nature, 2018, 555, 502-506.	27.8	433
2	Tuning the electrolyte network structure to invoke quasi-solid state sulfur conversion and suppress lithium dendrite formation in Liâ€“S batteries. Nature Energy, 2018, 3, 783-791.	39.5	421
3	Carbon-based tribofilms from lubricating oils. Nature, 2016, 536, 67-71.	27.8	370
4	Machine learning enabled autonomous microstructural characterization in 3D samples. Npj Computational Materials, 2020, 6, .	8.7	308
5	Operando tribochemical formation of onion-like-carbon leads to macroscale superlubricity. Nature Communications, 2018, 9, 1164.	12.8	199
6	Crude-Oil-Repellent Membranes by Atomic Layer Deposition: Oxide Interface Engineering. ACS Nano, 2018, 12, 8678-8685.	14.6	150
7	Perovskite nickelates as electric-field sensors in salt water. Nature, 2018, 553, 68-72.	27.8	146
8	Tunable MoS2 bandgap in MoS2-graphene heterostructures. Applied Physics Letters, 2014, 105, .	3.3	142
9	A Longâ€Cycleâ€Life Lithiumâ€“CO₂ Battery with Carbon Neutrality. Advanced Materials, 2019, 31, e1902518.	21.0	138
10	Quantitative 3D evolution of colloidal nanoparticle oxidation in solution. Science, 2017, 356, 303-307.	12.6	125
11	Machine learning coarse grained models for water. Nature Communications, 2019, 10, 379.	12.8	108
12	Machine Learning Force Field Parameters from Ab Initio Data. Journal of Chemical Theory and Computation, 2017, 13, 4492-4503.	5.3	105
13	Habituation based synaptic plasticity and organismic learning in a quantum perovskite. Nature Communications, 2017, 8, 240.	12.8	84
14	Ab Initio-Based Bond Order Potential to Investigate Low Thermal Conductivity of Stanene Nanostructures. Journal of Physical Chemistry Letters, 2016, 7, 3752-3759.	4.6	80
15	Defect Dynamics in 2-D MoS₂ Probed by Using Machine Learning, Atomistic Simulations, and High-Resolution Microscopy. ACS Nano, 2018, 12, 8006-8016.	14.6	72
16	Machine Learning Classical Interatomic Potentials for Molecular Dynamics from First-Principles Training Data. Journal of Physical Chemistry C, 2019, 123, 6941-6957.	3.1	72
17	Metal-induced rapid transformation of diamond into single and multilayer graphene on wafer scale. Nature Communications, 2016, 7, 12099.	12.8	70
18	Towards accurate prediction of catalytic activity in IrO₂ nanoclusters via first principles-based variable charge force field. Journal of Materials Chemistry A, 2015, 3, 18970-18982.	10.3	62

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19	Effect of the Hydrofluoroether Cosolvent Structure in Acetonitrile-Based Solvate Electrolytes on the Li⁺ Solvation Structure and Liâ€“S Battery Performance. ACS Applied Materials & Interfaces, 2017, 9, 39357-39370.	8.0	58
20	Strongly correlated perovskite lithium ion shuttles. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 9672-9677.	7.1	55
21	Accurate quantum chemical energies for 133â€‰000 organic molecules. Chemical Science, 2019, 10, 7449-7455.	7.4	53
22	A reactive force field for lithiumâ€“aluminum silicates with applications to eucryptite phases. Modelling and Simulation in Materials Science and Engineering, 2012, 20, 015002.	2.0	51
23	The Role of Local Inhomogeneities on Dendrite Growth in LLZO-Based Solid Electrolytes. Journal of the Electrochemical Society, 2020, 167, 100537.	2.9	51
24	Self-Assembly of Collagen on Flat Surfaces: The Interplay of Collagenâ€“Collagen and Collagenâ€“Substrate Interactions. Langmuir, 2014, 30, 1343-1350.	3.5	40
25	Machine learning prediction of accurate atomization energies of organic molecules from low-fidelity quantum chemical calculations. MRS Communications, 2019, 9, 891-899.	1.8	38
26	Perovskite neural trees. Nature Communications, 2020, 11, 2245.	12.8	38
27	Perovskite nickelates as bio-electronic interfaces. Nature Communications, 2019, 10, 1651.	12.8	33
28	In Situ 3D Imaging of Catalysis Induced Strain in Gold Nanoparticles. Journal of Physical Chemistry Letters, 2016, 7, 3008-3013.	4.6	32
29	Atomistic origin of superior performance of ionic liquid electrolytes for Al-ion batteries. Physical Chemistry Chemical Physics, 2014, 16, 20387-20391.	2.8	30
30	Quantum-Chemically Informed Machine Learning: Prediction of Energies of Organic Molecules with 10 to 14 Non-hydrogen Atoms. Journal of Physical Chemistry A, 2020, 124, 5804-5811.	2.5	28
31	Describing the Diverse Geometries of Gold from Nanoclusters to Bulkâ€”A First-Principles-Based Hybrid Bond-Order Potential. Journal of Physical Chemistry C, 2016, 120, 13787-13800.	3.1	26
32	Computational Studies of Solubilities of LiO₂and Li₂O₂in Aprotic Solvents. Journal of the Electrochemical Society, 2017, 164, E3696-E3701.	2.9	26
33	Interface stability of LiCl-rich argyrodite Li6PS5Cl with propylene carbonate boosts high-performance lithium batteries. Electrochimica Acta, 2020, 363, 137128.	5.2	26
34	Ultrafast Three-Dimensional X-ray Imaging of Deformation Modes in ZnO Nanocrystals. Nano Letters, 2017, 17, 1102-1108.	9.1	25
35	A Self-Limiting Electro-Ablation Technique for the Top-Down Synthesis of Large-Area Monolayer Flakes of 2D Materials. Scientific Reports, 2016, 6, 28195.	3.3	24
36	Investigation of Delamination-Induced Performance Decay at the Cathode/LLZO Interface. Chemistry of Materials, 2021, 33, 5527-5541.	6.7	24

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37	Development of a Modified Embedded Atom Force Field for Zirconium Nitride Using Multi-Objective Evolutionary Optimization. Journal of Physical Chemistry C, 2016, 120, 17475-17483.	3.1	23
38	Evolutionary Optimization of a Charge Transfer Ionic Potential Model for Ta/Ta-Oxide Heterointerfaces. Chemistry of Materials, 2017, 29, 3603-3614.	6.7	22
39	Machine learning a bond order potential model to study thermal transport in WSe₂ nanostructures. Nanoscale, 2019, 11, 10381-10392.	5.6	22
40	Unraveling the Planar-Globular Transition in Gold Nanoclusters through Evolutionary Search. Scientific Reports, 2016, 6, 34974.	3.3	21
41	Heterogeneous Pyrolysis: A Route for Epitaxial Growth of hBN Atomic Layers on Copper Using Separate Boron and Nitrogen Precursors. Nano Letters, 2017, 17, 2404-2413.	9.1	21
42	Alloy-assisted deposition of three-dimensional arrays of atomic gold catalyst for crystal growth studies. Nature Communications, 2017, 8, 2014.	12.8	21
43	Ligand dynamics control structure, elasticity, and high-pressure behavior of nanoparticle superlattices. Nanoscale, 2019, 11, 10655-10666.	5.6	20
44	Elastic constants of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î²</mml:mi></mml:math>-eucryptite studied by density functional theory. Physical Review B, 2010, 81, .	3.2	19
45	Carbon monoxide-induced reduction and healing of graphene oxide. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2013, 31, .	2.1	17
46	Thermomechanical Response of Self-Assembled Nanoparticle Membranes. ACS Nano, 2017, 11, 8026-8033.	14.6	17
47	Active Learning A Neural Network Model For Gold Clusters & Bulk From Sparse First Principles Training Data. ChemCatChem, 2020, 12, 4796-4806.	3.7	17
48	Silicene growth through island migration and coalescence. Nanoscale, 2017, 9, 10186-10192.	5.6	15
49	Machine Learning Applied to a Variable Charge Atomistic Model for Cu/Hf Binary Alloy Oxide Heterostructures. Chemistry of Materials, 2019, 31, 3089-3102.	6.7	15
50	Highly efficient interface stabilization for ambient-temperature quasi-solid-state sodium metal batteries. Chemical Engineering Journal, 2022, 434, 134679.	12.7	15
51	Migration mechanism for atomic hydrogen in porous carbon materials. Applied Physics Letters, 2012, 100, .	3.3	14
52	Atomic-scale mechanism for pressure-induced amorphization of Î²-eucryptite. Journal of Applied Physics, 2013, 114, 083520.	2.5	13
53	A coarse-grained deep neural network model for liquid water. Applied Physics Letters, 2019, 115, .	3.3	13
54	Quantitative Observation of Threshold Defect Behavior in Memristive Devices with Operando X-ray Microscopy. ACS Nano, 2018, 12, 4938-4945.	14.6	12

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55	Exemption of lattice collapse in Niâ€“MnO₂ birnessite regulated by the structural water mobility. Journal of Materials Chemistry A, 2021, 9, 23459-23466.	10.3	12
56	Machine learnt bond order potential to model metalâ€“organic (Coâ€“C) heterostructures. Nanoscale, 2017, 9, 18229-18239.	5.6	11
57	Synthesis of Fluorine-Doped Lithium Argyrodite Solid Electrolytes for Solid-State Lithium Metal Batteries. ACS Applied Materials & Interfaces, 2022, 14, 11483-11492.	8.0	11
58	Strong correlations between structural order and passive state at waterâ€“copper oxide interfaces. Electrochimica Acta, 2015, 179, 386-393.	5.2	10
59	Pressure-induced phase transformation in Î²-eucryptite: An X-ray diffraction and density functional theory study. Scripta Materialia, 2016, 122, 64-67.	5.2	10
60	Defect dynamics in two-dimensional black phosphorus under argon ion irradiation. Nanoscale, 2021, 13, 8575-8590.	5.6	10
61	Graph-Based Approaches for Predicting Solvation Energy in Multiple Solvents: Open Datasets and Machine Learning Models. Journal of Physical Chemistry A, 2021, 125, 5990-5998.	2.5	10
62	Teaching an Old Dog New Tricks: Machine Learning an Improved TIP3P Potential Model for Liquidâ€“Vapor Phase Phenomena. Journal of Physical Chemistry C, 2019, 123, 22643-22655.	3.1	9
63	In situ ion irradiation of amorphous TiO2 nanotubes. Journal of Materials Research, 2022, 37, 1144-1155.	2.6	8
64	BLAST: bridging length/timescales via atomistic simulation toolkit. MRS Advances, 2021, 6, 21-31.	0.9	7
65	Impact of Stabilizing Cations on Lithium Intercalation in Tunneled Manganese Oxide Cathodes. ACS Applied Energy Materials, 2021, 4, 12099-12111.	5.1	6
66	Radiation effects and tolerance mechanism in Î²-eucryptite. Journal of Applied Physics, 2013, 113, 033504.	2.5	5
67	Cavitation and radicals drive the sonochemical synthesis of functional polymer spheres. Applied Physics Letters, 2016, 109, .	3.3	5
68	Nanoscale origin and evolution of kinetically induced defects in carbon spheres. Carbon, 2016, 96, 647-660.	10.3	5
69	Configurational-Bias Monte Carlo Back-Mapping Algorithm for Efficient and Rapid Conversion of Coarse-Grained Water Structures into Atomistic Models. Journal of Physical Chemistry B, 2018, 122, 7102-7110.	2.6	3
70	High temperature stability, metallic character and bonding of the Si2BN planar structure. Journal of Physics Condensed Matter, 2021, 33, 165001.	1.8	2
71	One-Dimensional Lateral Force Anisotropy at the Atomic Scale in Sliding Single Molecules on a Surface. Nano Letters, 2021, 21, 6391-6397.	9.1	2
72	Investigations of Bis(alkylthiocarbamato)copper Linkage Isomers. Inorganic Chemistry, 2022, 61, 7715-7719.	4.0	2

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73	Revitalizing Iron Redox by Anion-Insertion-Assisted Ferro- and Ferri-Hydroxides Conversion at Low Alkalinity. Journal of the American Chemical Society, 2022, 144, 11938-11942.	13.7	2
74	Visualization of Solidâ€State Synthesis for Chalcogenide Na Superionic Conductors by inâ€situ Neutron Diffraction. ChemSusChem, 2021, 14, 5161-5166.	6.8	1
75	Computational Modeling of Battery Materials. , 2022, , 278-290.		0