

Badri Narayanan

List of Publications by Year in descending order

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papers

4,193
citations

172457

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114465

63
g-index

76
all docs

76
docs citations

76
times ranked

6547
citing authors

#	ARTICLE	IF	CITATIONS
1	Computational Modeling of Battery Materials. , 2022, , 278-290.		0
2	Highly efficient interface stabilization for ambient-temperature quasi-solid-state sodium metal batteries. Chemical Engineering Journal, 2022, 434, 134679.	12.7	15
3	In situ ion irradiation of amorphous TiO ₂ nanotubes. Journal of Materials Research, 2022, 37, 1144-1155.	2.6	8
4	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
5	Investigations of Bis(alkylthiocarbamate)copper Linkage Isomers. Inorganic Chemistry, 2022, 61, 7715-7719.	4.0	2
6	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
7	Defect dynamics in two-dimensional black phosphorus under argon ion irradiation. Nanoscale, 2021, 13, 8575-8590.	5.6	10
8	BLAST: bridging length/timescales via atomistic simulation toolkit. MRS Advances, 2021, 6, 21-31.	0.9	7
9	High temperature stability, metallic character and bonding of the Si ₂ BN planar structure. Journal of Physics Condensed Matter, 2021, 33, 165001.	1.8	2
10	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
11	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
12	Investigation of Delamination-Induced Performance Decay at the Cathode/LLZO Interface. Chemistry of Materials, 2021, 33, 5527-5541.	6.7	24
13	Exemption of lattice collapse in Ni ²⁺ MnO ₂ birnessite regulated by the structural water mobility. Journal of Materials Chemistry A, 2021, 9, 23459-23466.	10.3	12
14	Impact of Stabilizing Cations on Lithium Intercalation in Tunneled Manganese Oxide Cathodes. ACS Applied Energy Materials, 2021, 4, 12099-12111.	5.1	6
15	Visualization of Solid-State Synthesis for Chalcogenide Na Superionic Conductors by in situ Neutron Diffraction. ChemSusChem, 2021, 14, 5161-5166.	6.8	1
16	Active Learning A Neural Network Model For Gold Clusters & Bulk From Sparse First Principles Training Data. ChemCatChem, 2020, 12, 4796-4806.	3.7	17
17	Interface stability of LiCl-rich argyrodite Li ₆ PS ₅ Cl with propylene carbonate boosts high-performance lithium batteries. Electrochimica Acta, 2020, 363, 137128.	5.2	26
18	Perovskite neural trees. Nature Communications, 2020, 11, 2245.	12.8	38

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19	Quantum-Chemically Informed Machine Learning: Prediction of Energies of Organic Molecules with 10 to 14 Non-hydrogen Atoms. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5804-5811.	2.5	28
20	Machine learning enabled autonomous microstructural characterization in 3D samples. <i>Npj Computational Materials</i> , 2020, 6, .	8.7	308
21	The Role of Local Inhomogeneities on Dendrite Growth in LLZO-Based Solid Electrolytes. <i>Journal of the Electrochemical Society</i> , 2020, 167, 100537.	2.9	51
22	A Longâ€Cycleâ€Life Lithiumâ€CO ₂ Battery with Carbon Neutrality. <i>Advanced Materials</i> , 2019, 31, e1902518.	21.0	138
23	Teaching an Old Dog New Tricks: Machine Learning an Improved TIP3P Potential Model for Liquidâ€Vapor Phase Phenomena. <i>Journal of Physical Chemistry C</i> , 2019, 123, 22643-22655.	3.1	9
24	Machine learning prediction of accurate atomization energies of organic molecules from low-fidelity quantum chemical calculations. <i>MRS Communications</i> , 2019, 9, 891-899.	1.8	38
25	Machine learning coarse grained models for water. <i>Nature Communications</i> , 2019, 10, 379.	12.8	108
26	Accurate quantum chemical energies for 133â€000 organic molecules. <i>Chemical Science</i> , 2019, 10, 7449-7455.	7.4	53
27	Machine learning a bond order potential model to study thermal transport in WSe ₂ nanostructures. <i>Nanoscale</i> , 2019, 11, 10381-10392.	5.6	22
28	Ligand dynamics control structure, elasticity, and high-pressure behavior of nanoparticle superlattices. <i>Nanoscale</i> , 2019, 11, 10655-10666.	5.6	20
29	Machine Learning Applied to a Variable Charge Atomistic Model for Cu/Hf Binary Alloy Oxide Heterostructures. <i>Chemistry of Materials</i> , 2019, 31, 3089-3102.	6.7	15
30	Perovskite nickelates as bio-electronic interfaces. <i>Nature Communications</i> , 2019, 10, 1651.	12.8	33
31	A coarse-grained deep neural network model for liquid water. <i>Applied Physics Letters</i> , 2019, 115, .	3.3	13
32	Machine Learning Classical Interatomic Potentials for Molecular Dynamics from First-Principles Training Data. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6941-6957.	3.1	72
33	Perovskite nickelates as electric-field sensors in salt water. <i>Nature</i> , 2018, 553, 68-72.	27.8	146
34	Quantitative Observation of Threshold Defect Behavior in Memristive Devices with <i>Operando</i> X-ray Microscopy. <i>ACS Nano</i> , 2018, 12, 4938-4945.	14.6	12
35	A lithiumâ€oxygen battery with a long cycle life in an air-like atmosphere. <i>Nature</i> , 2018, 555, 502-506.	27.8	433
36	Operando tribochemical formation of onion-like-carbon leads to macroscale superlubricity. <i>Nature Communications</i> , 2018, 9, 1164.	12.8	199

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37	Defect Dynamics in 2-D MoS ₂ Probed by Using Machine Learning, Atomistic Simulations, and High-Resolution Microscopy. ACS Nano, 2018, 12, 8006-8016.	14.6	72
38	Crude-Oil-Repellent Membranes by Atomic Layer Deposition: Oxide Interface Engineering. ACS Nano, 2018, 12, 8678-8685.	14.6	150
39	Tuning the electrolyte network structure to invoke quasi-solid state sulfur conversion and suppress lithium dendrite formation in Li-S batteries. Nature Energy, 2018, 3, 783-791.	39.5	421
40	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
41	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
42	Quantitative 3D evolution of colloidal nanoparticle oxidation in solution. Science, 2017, 356, 303-307.	12.6	125
43	Silicene growth through island migration and coalescence. Nanoscale, 2017, 9, 10186-10192.	5.6	15
44	Evolutionary Optimization of a Charge Transfer Ionic Potential Model for Ta/Ta-Oxide Heterointerfaces. Chemistry of Materials, 2017, 29, 3603-3614.	6.7	22
45	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
46	Ultrafast Three-Dimensional X-ray Imaging of Deformation Modes in ZnO Nanocrystals. Nano Letters, 2017, 17, 1102-1108.	9.1	25
47	Effect of the Hydrofluoroether Cosolvent Structure in Acetonitrile-Based Solvate Electrolytes on the Li ⁺ Solvation Structure and Li-S Battery Performance. ACS Applied Materials & Interfaces, 2017, 9, 39357-39370.	8.0	58
48	Machine learnt bond order potential to model metal-organic (Co-C) heterostructures. Nanoscale, 2017, 9, 18229-18239.	5.6	11
49	Habituation based synaptic plasticity and organismic learning in a quantum perovskite. Nature Communications, 2017, 8, 240.	12.8	84
50	Thermomechanical Response of Self-Assembled Nanoparticle Membranes. ACS Nano, 2017, 11, 8026-8033.	14.6	17
51	Computational Studies of Solubilities of LiO ₂ and Li ₂ O ₂ in Aprotic Solvents. Journal of the Electrochemical Society, 2017, 164, E3696-E3701.	2.9	26
52	Machine Learning Force Field Parameters from Ab Initio Data. Journal of Chemical Theory and Computation, 2017, 13, 4492-4503.	5.3	105
53	Alloy-assisted deposition of three-dimensional arrays of atomic gold catalyst for crystal growth studies. Nature Communications, 2017, 8, 2014.	12.8	21
54	Cavitation and radicals drive the sonochemical synthesis of functional polymer spheres. Applied Physics Letters, 2016, 109, .	3.3	5

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55	Unraveling the Planar-Globular Transition in Gold Nanoclusters through Evolutionary Search. <i>Scientific Reports</i> , 2016, 6, 34974.	3.3	21
56	A Self-Limiting Electro-Ablation Technique for the Top-Down Synthesis of Large-Area Monolayer Flakes of 2D Materials. <i>Scientific Reports</i> , 2016, 6, 28195.	3.3	24
57	Pressure-induced phase transformation in β -eucryptite: An X-ray diffraction and density functional theory study. <i>Scripta Materialia</i> , 2016, 122, 64-67.	5.2	10
58	Carbon-based tribofilms from lubricating oils. <i>Nature</i> , 2016, 536, 67-71.	27.8	370
59	Development of a Modified Embedded Atom Force Field for Zirconium Nitride Using Multi-Objective Evolutionary Optimization. <i>Journal of Physical Chemistry C</i> , 2016, 120, 17475-17483.	3.1	23
60	Ab Initio-Based Bond Order Potential to Investigate Low Thermal Conductivity of Stanene Nanostructures. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3752-3759.	4.6	80
61	In Situ 3D Imaging of Catalysis Induced Strain in Gold Nanoparticles. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3008-3013.	4.6	32
62	Metal-induced rapid transformation of diamond into single and multilayer graphene on wafer scale. <i>Nature Communications</i> , 2016, 7, 12099.	12.8	70
63	Describing the Diverse Geometries of Gold from Nanoclusters to Bulk—A First-Principles-Based Hybrid Bond-Order Potential. <i>Journal of Physical Chemistry C</i> , 2016, 120, 13787-13800.	3.1	26
64	Nanoscale origin and evolution of kinetically induced defects in carbon spheres. <i>Carbon</i> , 2016, 96, 647-660.	10.3	5
65	Strong correlations between structural order and passive state at water-copper oxide interfaces. <i>Electrochimica Acta</i> , 2015, 179, 386-393.	5.2	10
66	Towards accurate prediction of catalytic activity in IrO_2 nanoclusters via first principles-based variable charge force field. <i>Journal of Materials Chemistry A</i> , 2015, 3, 18970-18982.	10.3	62
67	Self-Assembly of Collagen on Flat Surfaces: The Interplay of Collagen-Substrate Interactions. <i>Langmuir</i> , 2014, 30, 1343-1350.	3.5	40
68	Atomistic origin of superior performance of ionic liquid electrolytes for Al-ion batteries. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20387-20391.	2.8	30
69	Tunable MoS_2 bandgap in MoS_2 -graphene heterostructures. <i>Applied Physics Letters</i> , 2014, 105, .	3.3	142
70	Atomic-scale mechanism for pressure-induced amorphization of β -eucryptite. <i>Journal of Applied Physics</i> , 2013, 114, 083520.	2.5	13
71	Carbon monoxide-induced reduction and healing of graphene oxide. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2013, 31, .	2.1	17
72	Radiation effects and tolerance mechanism in β -eucryptite. <i>Journal of Applied Physics</i> , 2013, 113, 033504.	2.5	5

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73	A reactive force field for lithium–aluminum silicates with applications to eucryptite phases. Modelling and Simulation in Materials Science and Engineering, 2012, 20, 015002.	2.0	51
74	Migration mechanism for atomic hydrogen in porous carbon materials. Applied Physics Letters, 2012, 100, .	3.3	14
75	Elastic constants of $\hat{\epsilon}^2$ -eucryptite studied by density functional theory. Physical Review B, 2010, 81, .	3.2	19