Subramanian K R S Sankaranarayanan

List of Publications by Year
in descending order

80 papers	3,903 citations	201674 27 h-index	123424 61 g-index
82 all docs	82 docs citations	82 times ranked	5266 citing authors

#	Article	IF	Citations
1	Learning in continuous action space for developing high dimensional potential energy models. Nature Communications, 2022, 13, 368.	12.8	21
2	Accurate determination of solvation free energies of neutral organic compounds from first principles. Nature Communications, 2022, 13, 414.	12.8	14
3	Reconfigurable perovskite nickelate electronics for artificial intelligence. Science, 2022, 375, 533-539.	12.6	93
4	Multi-reward Reinforcement Learning Based Bond-Order Potential to Study Strain-Assisted Phase Transitions in Phosphorene. Journal of Physical Chemistry Letters, 2022, 13, 1886-1893.	4.6	9
5	Advancing Chemical Separations: Unraveling the Structure and Dynamics of Phase Splitting in Liquidâ€“Liquid Extraction. Journal of Physical Chemistry B, 2022, 126, 2420-2429.	2.6	5
6	Unusual High Hardness and Load-Dependent Mechanical Characteristics of Hydrogenated Carbonâ€“Nitrogen Hybrid Films. ACS Applied Materials & Interfaces, 2022, 14, 20220-20229.	8.0	3
7	AutoPhaseNN: unsupervised physics-aware deep learning of 3D nanoscale Bragg coherent diffraction imaging. Npj Computational Materials, 2022, 8, .	8.7	18
8	Machine learning the metastable phase diagram of covalently bonded carbon. Nature Communications, 2022, 13, .	12.8	9
9	BLAST: bridging length/timescales via atomistic simulation toolkit. MRS Advances, 2021, 6, 21-31.	0.9	7
10	Reinforcement learning in discrete action space applied to inverse defect design. Journal of Physics Communications, 2021, 5, 031001.	1.2	9
11	Bragg Coherent Diffraction Imaging for In Situ Studies in Electrocatalysis. ACS Nano, 2021, 15, 6129-6146.	14.6	24
12	Evolutionary inverse design of defects at graphene 2D lateral interfaces. Journal of Applied Physics, 2021, 129, 185302.	2.5	1
13	Artificial Intelligence-Guided De Novo Molecular Design Targeting COVID-19. ACS Omega, 2021, 6, 12557-12566.	3.5	22
14	Rapid 3D nanoscale coherent imaging via physics-aware deep learning. Applied Physics Reviews, 2021, 8, .	11.3	26
15	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
16	Learning with Delayed Rewardsâ€”A Case Study on Inverse Defect Design in 2D Materials. ACS Applied Materials & Interfaces, 2021, 13, 36455-36464.	8.0	12
17	Multi-objective parametrization of interatomic potentials for large deformation pathways and fracture of two-dimensional materials. Npj Computational Materials, 2021, 7, .	8.7	9
18	Impact of Stabilizing Cations on Lithium Intercalation in Tunneled Manganese Oxide Cathodes. ACS Applied Energy Materials, 2021, 4, 12099-12111.	5.1	6

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19	Angstrom-Scale Transparent Overcoats: Interfacial Nitrogen-Driven Atomic Intermingling Promotes Lubricity and Surface Protection of Ultrathin Carbon. Nano Letters, 2021, 21, 8960-8969.	9.1	5
20	Solution Processable High Performance Multiwall Carbon Nanotubeâ€“Si Heterojunctions. Advanced Electronic Materials, 2020, 6, 2000617.	5.1	3
21	Active Learning A Neural Network Model For Gold Clusters & Bulk From Sparse First Principles Training Data. ChemCatChem, 2020, 12, 4796-4806.	3.7	17
22	Accelerating copolymer inverse design using monte carlo tree search. Nanoscale, 2020, 12, 23653-23662.	5.6	22
23	Screening of Therapeutic Agents for COVID-19 Using Machine Learning and Ensemble Docking Studies. Journal of Physical Chemistry Letters, 2020, 11, 7058-7065.	4.6	82
24	Inverse design of metasurfaces with non-local interactions. Npj Computational Materials, 2020, 6, .	8.7	39
25	Active learning a coarse-grained neural network model for bulk water from sparse training data. Molecular Systems Design and Engineering, 2020, 5, 902-910.	3.4	8
26	Creation of Single-Photon Emitters in WSe₂ Monolayers Using Nanometer-Sized Gold Tips. Nano Letters, 2020, 20, 5866-5872.	9.1	33
27	Active Learning the Potential Energy Landscape for Water Clusters from Sparse Training Data. Journal of Physical Chemistry C, 2020, 124, 4907-4916.	3.1	25
28	Organismic materials for beyond von Neumann machines. Applied Physics Reviews, 2020, 7, .	11.3	30
29	Machine learning enabled autonomous microstructural characterization in 3D samples. Npj Computational Materials, 2020, 6, .	8.7	308
30	Machine learning for multi-fidelity scale bridging and dynamical simulations of materials. JPhys Materials, 2020, 3, 031002.	4.2	11
31	Combinatorial Black-Box Optimization with Expert Advice. , 2020, , .		3
32	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
33	Ironâ€Nanoparticle Driven Tribochemistry Leading to Superlubric Sliding Interfaces. Advanced Materials Interfaces, 2019, 6, 1901416.	3.7	41
34	Machine learning coarse grained models for water. Nature Communications, 2019, 10, 379.	12.8	108
35	Machine learning a bond order potential model to study thermal transport in WSe₂ nanostructures. Nanoscale, 2019, 11, 10381-10392.	5.6	22
36	Ligand dynamics control structure, elasticity, and high-pressure behavior of nanoparticle superlattices. Nanoscale, 2019, 11, 10655-10666.	5.6	20

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37	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
38	â€œTeamwork Makes the Dream Workâ€: Tribal Competition Evolutionary Search as a Surrogate for Free-Energy-Based Structural Predictions. Journal of Physical Chemistry A, 2019, 123, 3903-3910.	2.5	1
39	A coarse-grained deep neural network model for liquid water. Applied Physics Letters, 2019, 115, .	3.3	13
40	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
41	Boosting contact sliding and wear protection via atomic intermixing and tailoring of nanoscale interfaces. Science Advances, 2019, 5, eaau7886.	10.3	22
42	Three-Dimensional Integrated X-ray Diffraction Imaging of a Native Strain in Multi-Layered WSe₂. Nano Letters, 2018, 18, 1993-2000.	9.1	9
43	Perovskite nickelates as electric-field sensors in salt water. Nature, 2018, 553, 68-72.	27.8	146
44	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
45	Crude-Oil-Repellent Membranes by Atomic Layer Deposition: Oxide Interface Engineering. ACS Nano, 2018, 12, 8678-8685.	14.6	150
46	Active site localization of methane oxidation on Pt nanocrystals. Nature Communications, 2018, 9, 3422.	12.8	58
47	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
48	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
49	Quantitative 3D evolution of colloidal nanoparticle oxidation in solution. Science, 2017, 356, 303-307.	12.6	125
50	Silicene growth through island migration and coalescence. Nanoscale, 2017, 9, 10186-10192.	5.6	15
51	Evolutionary Optimization of a Charge Transfer Ionic Potential Model for Ta/Ta-Oxide Heterointerfaces. Chemistry of Materials, 2017, 29, 3603-3614.	6.7	22
52	Ultrafast Three-Dimensional X-ray Imaging of Deformation Modes in ZnO Nanocrystals. Nano Letters, 2017, 17, 1102-1108.	9.1	25
53	Ultrafast Three-Dimensional Integrated Imaging of Strain in Core/Shell Semiconductor/Metal Nanostructures. Nano Letters, 2017, 17, 7696-7701.	9.1	14
54	Machine learnt bond order potential to model metalâ€“organic (Coâ€“C) heterostructures. Nanoscale, 2017, 9, 18229-18239.	5.6	11

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55	Habituation based synaptic plasticity and organismic learning in a quantum perovskite. Nature Communications, 2017, 8, 240.	12.8	84
56	Thermomechanical Response of Self-Assembled Nanoparticle Membranes. ACS Nano, 2017, 11, 8026-8033.	14.6	17
57	Machine Learning Force Field Parameters from Ab Initio Data. Journal of Chemical Theory and Computation, 2017, 13, 4492-4503.	5.3	105
58	Unraveling the Planar-Globular Transition in Gold Nanoclusters through Evolutionary Search. Scientific Reports, 2016, 6, 34974.	3.3	21
59	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
60	Carbon-based tribofilms from lubricating oils. Nature, 2016, 536, 67-71.	27.8	370
61	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
62	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
63	In Situ 3D Imaging of Catalysis Induced Strain in Gold Nanoparticles. Journal of Physical Chemistry Letters, 2016, 7, 3008-3013.	4.6	32
64	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
65	Subnanometre ligand-shell asymmetry leads to Janus-like nanoparticle membranes. Nature Materials, 2015, 14, 912-917.	27.5	71
66	Femtosecond Laser Pulse Driven Melting in Gold Nanorod Aqueous Colloidal Suspension: Identification of a Transition from Stretched to Exponential Kinetics. Scientific Reports, 2015, 5, 8146.	3.3	13
67	Strong correlations between structural order and passive state at waterâ€"copper oxide interfaces. Electrochimica Acta, 2015, 179, 386-393.	5.2	10
68	Macroscale superlubricity enabled by graphene nanoscroll formation. Science, 2015, 348, 1118-1122.	12.6	665
69	Non-equilibrium effects evidenced by vibrational spectra during the coil-to-globule transition in poly(N-isopropylacrylamide) subjected to an ultrafast heatingâ€"cooling cycle. Soft Matter, 2014, 10, 1462-1480.	2.7	22
70	Thermodynamic considerations for solubility and conformational transitions of poly-N-isopropyl-acrylamide. Physical Chemistry Chemical Physics, 2013, 15, 12667.	2.8	27
71	Chloride ions induce order-disorder transition at water-oxide interfaces. Physical Review E, 2013, 88, 062119.	2.1	7
72	Role of Solvation Dynamics and Local Ordering of Water in Inducing Conformational Transitions in Poly(N-isopropylacrylamide) Oligomers through the LCST. Journal of Physical Chemistry B, 2012, 116, 2651-2663.	2.6	171

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73	Reactive Molecular Dynamics Study of Chloride Ion Interaction with Copper Oxide Surfaces in Aqueous Media. ACS Applied Materials & Interfaces, 2012, 4, 1225-1232.	8.0	44
74	Optically Directed Mesoscale Assembly and Patterning of Electrically Conductive Organicâ€“Inorganic Hybrid Structures. Advanced Materials, 2012, 24, OP242-6.	21.0	7
75	Compositional tuning of ultrathin surface oxides on metal and alloy substrates using photons: Dynamic simulations and experiments. Physical Review B, 2010, 81, .	3.2	13
76	Electric Field Control of Surface Oxygen Dynamics and its Effect on the Atomic Scale Structure and Morphology of a Growing Ultrathin Oxide Film. Journal of Physical Chemistry C, 2010, 114, 6631-6639.	3.1	18
77	Atomistic Simulation of Field Enhanced Oxidation of Al (100) Beyond the Mott Potential. Physical Review Letters, 2009, 102, 095504.	7.8	45
78	Electric field tuning of oxygen stoichiometry at oxide surfaces: molecular dynamics simulations studies of zirconia. Energy and Environmental Science, 2009, 2, 1196.	30.8	28
79	On the Low-Temperature Oxidation and Ultrathin Oxide Growth on Zirconium in the Presence of Atomic Oxygen: A Modeling Study. Journal of Physical Chemistry C, 2008, 112, 17877-17882.	3.1	29
80	Molecular dynamics simulation study of nanoscale passive oxide growth on Ni-Al alloy surfaces at low temperatures. Physical Review B, 2008, 78, .	3.2	45