Neeraj Kumar

List of Publications by Year
in descending order

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47	1,449	331670	345221
papers	citations	21 h-index	36 g-index

50	50	50	1768
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Synthesis and analysis of prediction errors and error fusion based prior for prediction algorithms. Multimedia Tools and Applications, 2022, 81, 19835-19847.	3.9	1
2	High-Throughput Virtual Screening and Validation of a SARS-CoV-2 Main Protease Noncovalent Inhibitor. Journal of Chemical Information and Modeling, 2022, 62, 116-128.	5.4	54
3	Diverse Analysis of Data Mining and Machine Learning Algorithms to Secure Computer Network. Wireless Personal Communications, 2022, 124, 1033-1059.	2.7	5
4	Decoding the proteinâ€“ligand interactions using parallel graph neural networks. Scientific Reports, 2022, 12, 7624.	3.3	15
5	Accurate Prediction of Voltage of Battery Electrode Materials Using Attention-Based Graph Neural Networks. ACS Applied Materials & Interfaces, 2022, 14, 26587-26594.	8.0	13
6	Quantum Mechanical Methods Predict Accurate Thermodynamics of Biochemical Reactions. ACS Omega, 2021, 6, 9948-9959.	3.5	12
7	High-throughput screening of the ReFRAME, Pandemic Box, and COVID Box drug repurposing libraries against SARS-CoV-2 nsp15 endoribonuclease to identify small-molecule inhibitors of viral activity. PLoS ONE, 2021, 16, e0250019.	2.5	27
8	Machine Learning Screening of Metal-Ion Battery Electrode Materials. ACS Applied Materials & Interfaces, 2021, 13, 53355-53362.	8.0	42
9	MiMiC: a bioinformatic approach for generation of synthetic communities from metagenomes. Microbial Biotechnology, 2021, 14, 1757-1770.	4.2	12
10	Deep Learning Coordinate-Free Quantum Chemistry. Journal of Physical Chemistry A, 2021, 125, 8978-8986.	2.5	5
11	Bayesian Inference for Integrating Yarrowia lipolytica Multiomics Datasets with Metabolic Modeling. ACS Synthetic Biology, 2021, 10, 2968-2981.	3.8	4
12	3D-Scaffold: A Deep Learning Framework to Generate 3D Coordinates of Drug-like Molecules with Desired Scaffolds. Journal of Physical Chemistry B, 2021, 125, 12166-12176.	2.6	30
13	Artificial Intelligence for Autonomous Molecular Design: A Perspective. Molecules, 2021, 26, 6761.	3.8	11
14	Tuning Catalytic Bias of Hydrogen Gas Producing Hydrogenases. Journal of the American Chemical Society, 2020, 142, 1227-1235.	13.7	55
15	Explaining discrepancies in the study of maternal effects: the role of context and embryo. Current Opinion in Behavioral Sciences, 2020, 36, 185-192.	3.9	12
16	Revealing the Formation Energyâ€“Exfoliation Energyâ€“Structure Correlation of MAB Phases Using Machine Learning and DFT. ACS Applied Materials & Interfaces, 2020, 12, 29424-29431.	8.0	15
17	Steroid receptors and their regulation in avian extraembryonic membranes provide a novel substrate for hormone mediated maternal effects. Scientific Reports, 2019, 9, 11501.	3.3	8
18	Mechanism of Catalytic O₂ Reduction by Iron Tetraphenylporphyrin. Journal of the American Chemical Society, 2019, 141, 8315-8326.	13.7	99

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19	Revisiting mechanisms and functions of prenatal hormone-mediated maternal effects using avian species as a model. Philosophical Transactions of the Royal Society B: Biological Sciences, 2019, 374, 20180115.	4.0	90
20	Avian yolk androgens are metabolized instead of taken up by the embryo during the first days of incubation. Journal of Experimental Biology, 2019, 222, .	1.7	16
21	Mechanistic Implications of Reductive Coâ€“C Bond Cleavage in B₁₂-Dependent Methylmalonyl CoA Mutase. Journal of Physical Chemistry B, 2019, 123, 2210-2216.	2.6	15
22	Outer Coordination Sphere Proton Relay Base and Proximity Effects on Hydrogen Oxidation with Iron Electrocatalysts. Organometallics, 2019, 38, 1391-1396.	2.3	7
23	Circadian Proteomic Analysis Uncovers Mechanisms of Post-Transcriptional Regulation in Metabolic Pathways. Cell Systems, 2018, 7, 613-626.e5.	6.2	93
24	Gonadal steroid levels in rock pigeon eggs do not represent adequately maternal allocation. Scientific Reports, 2018, 8, 11213.	3.3	11
25	Prediction of Metabolite Concentrations, Rate Constants and Post-Translational Regulation Using Maximum Entropy-Based Simulations with Application to Central Metabolism of Neurospora crassa. Processes, 2018, 6, 63.	2.8	24
26	Early embryonic modification of maternal hormones differs systematically among embryos of different laying order: A study in birds. General and Comparative Endocrinology, 2018, 269, 53-59.	1.8	24
27	High-Throughput Simulations Reveal Membrane-Mediated Effects of Alcohols on MscL Gating. Journal of the American Chemical Society, 2017, 139, 2664-2671.	13.7	41
28	Controlling Proton Delivery through Catalyst Structural Dynamics. Angewandte Chemie - International Edition, 2016, 55, 13509-13513.	13.8	48
29	Density Based Outlier Detection (DBOD) in Data Mining: A Novel Approach. , 2016, , .		3
30	Homogenous Electrocatalytic Oxygen Reduction Rates Correlate with Reaction Overpotential in Acidic Organic Solutions. ACS Central Science, 2016, 2, 850-856.	11.3	150
31	Electronically excited states of cob(<scp>ii</scp>)alamin: insights from CASSCF/XMCQDPT2 and TD-DFT calculations. Physical Chemistry Chemical Physics, 2016, 18, 4513-4526.	2.8	15
32	A Novel Algorithm for Magic Squares. , 2016, , .		0
33	Increasing the rate of hydrogen oxidation without increasing the overpotential: a bio-inspired iron molecular electrocatalyst with an outer coordination sphere proton relay. Chemical Science, 2015, 6, 2737-2745.	7.4	40
34	Manganese-Based Molecular Electrocatalysts for Oxidation of Hydrogen. ACS Catalysis, 2015, 5, 6838-6847.	11.2	43
35	Mechanistic insights into hydride transfer for catalytic hydrogenation of CO₂ with cobalt complexes. Dalton Transactions, 2014, 43, 11803-11806.	3.3	44
36	Mechanistic Insights for Formation of an Organometallic Coâ€“C Bond in the Methyl Transfer Reaction Catalyzed by Methionine Synthase. Journal of Physical Chemistry B, 2013, 117, 16044-16057.	2.6	22

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37	Molecular Recognition of Aromatic Rings by Flavin: Electrostatics and Dispersion Determine Ring Positioning above Isoalloxazine. Journal of Physical Chemistry A, 2013, 117, 12946-12952.	2.5	6
38	Electronic Structure of One-Electron-Oxidized Form of the Methylcobalamin Cofactor: Spin Density Distribution and Pseudo-Jahnâ€“Teller Effect. Inorganic Chemistry, 2013, 52, 1762-1771.	4.0	14
39	Electronic structure of the S₁ state in methylcobalamin: Insight from CASSCF/MCâ€XQDPT2, EOMâ€CCSD, and TDâ€DFT calculations. Journal of Computational Chemistry, 2013, 34, 987-1004.	3.3	53
40	Time Series ANN Approach for Weather Forecasting. International Journal of Control Theory and Computer Modeling, 2013, 3, 19-25.	0.2	15
41	Co²⁺/Co⁺ Redox Tuning in Methyltransferases Induced by a Conformational Change at the Axial Ligand. Inorganic Chemistry, 2012, 51, 5533-5538.	4.0	15
42	Charge Separation Propensity of the Coenzyme B₁₂â€“Tyrosine Complex in Adenosylcobalamin-Dependent Methylmalonylâ€“CoA Mutase Enzyme. Journal of Physical Chemistry Letters, 2012, 3, 1035-1038.	4.6	23
43	Bacillus subtilis SepF Binds to the C-Terminus of FtsZ. PLoS ONE, 2012, 7, e43293.	2.5	50
44	Role of the Axial Base in the Modulation of the Cob(I)alamin Electronic Properties: Insight from QM/MM, DFT, and CASSCF Calculations. Journal of Chemical Theory and Computation, 2011, 7, 1541-1551.	5.3	31
45	Electronically Excited States of Vitamin B₁₂: Benchmark Calculations Including Time-Dependent Density Functional Theory and Correlated ab Initio Methods. Journal of Physical Chemistry A, 2011, 115, 1280-1292.	2.5	94
46	Electronic Structure of Cofactorâ€'Substrate Reactant Complex Involved in the Methyl Transfer Reaction Catalyzed by Cobalamin-Dependent Methionine Synthase. Journal of Physical Chemistry B, 2011, 115, 6722-6731.	2.6	22
47	Enhancement of security in visual cryptography system using cover image share embedded security algorithm (CISEA). , 2011, , .		5