Neeraj Kumar

List of Publications by Year
in descending order

47 papers	1,449 citations	331670 21 h-index	345221 36 g-index
50 all docs	50 docs citations	50 times ranked	1768 citing authors

#	Article	IF	Citations
1	Homogenous Electrocatalytic Oxygen Reduction Rates Correlate with Reaction Overpotential in Acidic Organic Solutions. ACS Central Science, 2016, 2, 850-856.	11.3	150
2	Mechanism of Catalytic O_2 Reduction by Iron Tetraphenylporphyrin. Journal of the American Chemical Society, 2019, 141, 8315-8326.	13.7	99
3	Electronically Excited States of Vitamin B_{12}: 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
4	Circadian Proteomic Analysis Uncovers Mechanisms of Post-Transcriptional Regulation in Metabolic Pathways. Cell Systems, 2018, 7, 613-626.e5.	6.2	93
5	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
6	Tuning Catalytic Bias of Hydrogen Gas Producing Hydrogenases. Journal of the American Chemical Society, 2020, 142, 1227-1235.	13.7	55
7	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
8	Electronic structure of the S_1 state in methylcobalamin: Insight from CASSCF/MC‑XQDPT2, EOM‑CCSD, and TD‑DFT calculations. Journal of Computational Chemistry, 2013, 34, 987-1004.	3.3	53
9	Bacillus subtilis SepF Binds to the C-Terminus of FtsZ. PLoS ONE, 2012, 7, e43293.	2.5	50
10	Controlling Proton Delivery through Catalyst Structural Dynamics. Angewandte Chemie - International Edition, 2016, 55, 13509-13513.	13.8	48
11	Mechanistic insights into hydride transfer for catalytic hydrogenation of CO_2 with cobalt complexes. Dalton Transactions, 2014, 43, 11803-11806.	3.3	44
12	Manganese-Based Molecular Electrocatalysts for Oxidation of Hydrogen. ACS Catalysis, 2015, 5, 6838-6847.	11.2	43
13	Machine Learning Screening of Metal-Ion Battery Electrode Materials. ACS Applied Materials & Interfaces, 2021, 13, 53355-53362.	8.0	42
14	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
15	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
16	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
17	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
18	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

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19	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
20	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
21	Charge Separation Propensity of the Coenzyme B_{12}–Tyrosine Complex in Adenosylcobalamin-Dependent Methylmalonyl–CoA Mutase Enzyme. Journal of Physical Chemistry Letters, 2012, 3, 1035-1038.	4.6	23
22	Electronic Structure of Cofactor–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
23	Mechanistic Insights for Formation of an Organometallic Co–C Bond in the Methyl Transfer Reaction Catalyzed by Methionine Synthase. Journal of Physical Chemistry B, 2013, 117, 16044-16057.	2.6	22
24	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
25	Co^{2+}/Co^{+} Redox Tuning in Methyltransferases Induced by a Conformational Change at the Axial Ligand. Inorganic Chemistry, 2012, 51, 5533-5538.	4.0	15
26	Time Series ANN Approach for Weather Forecasting. International Journal of Control Theory and Computer Modeling, 2013, 3, 19-25.	0.2	15
27	Electronically excited states of cob(ii)alamin: insights from CASSCF/XMCQDPT2 and TD-DFT calculations. Physical Chemistry Chemical Physics, 2016, 18, 4513-4526.	2.8	15
28	Mechanistic Implications of Reductive Co–C Bond Cleavage in B_{12}-Dependent Methylmalonyl CoA Mutase. Journal of Physical Chemistry B, 2019, 123, 2210-2216.	2.6	15
29	Revealing the Formation Energy–Exfoliation Energy–Structure Correlation of MAB Phases Using Machine Learning and DFT. ACS Applied Materials & Interfaces, 2020, 12, 29424-29431.	8.0	15
30	Decoding the protein–ligand interactions using parallel graph neural networks. Scientific Reports, 2022, 12, 7624.	3.3	15
31	Electronic Structure of One-Electron-Oxidized Form of the Methylcobalamin Cofactor: Spin Density Distribution and Pseudo-Jahn–Teller Effect. Inorganic Chemistry, 2013, 52, 1762-1771.	4.0	14
32	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
33	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
34	Quantum Mechanical Methods Predict Accurate Thermodynamics of Biochemical Reactions. ACS Omega, 2021, 6, 9948-9959.	3.5	12
35	MiMiC: a bioinformatic approach for generation of synthetic communities from metagenomes. Microbial Biotechnology, 2021, 14, 1757-1770.	4.2	12
36	Gonadal steroid levels in rock pigeon eggs do not represent adequately maternal allocation. Scientific Reports, 2018, 8, 11213.	3.3	11

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37	Artificial Intelligence for Autonomous Molecular Design: A Perspective. Molecules, 2021, 26, 6761.	3.8	11
38	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
39	Outer Coordination Sphere Proton Relay Base and Proximity Effects on Hydrogen Oxidation with Iron Electrocatalysts. Organometallics, 2019, 38, 1391-1396.	2.3	7
40	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
41	Enhancement of security in visual cryptography system using cover image share embedded security algorithm (CISEA). , 2011, , .		5
42	Deep Learning Coordinate-Free Quantum Chemistry. Journal of Physical Chemistry A, 2021, 125, 8978-8986.	2.5	5
43	Diverse Analysis of Data Mining and Machine Learning Algorithms to Secure Computer Network. Wireless Personal Communications, 2022, 124, 1033-1059.	2.7	5
44	Bayesian Inference for Integrating *Yarrowia lipolytica* Multiomics Datasets with Metabolic Modeling. ACS Synthetic Biology, 2021, 10, 2968-2981.	3.8	4
45	Density Based Outlier Detection (DBOD) in Data Mining: A Novel Approach. , 2016, , .		3
46	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
47	A Novel Algorithm for Magic Squares. , 2016, , .		0