Mudit Dixit

List of Publications by Year in descending order

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42 papers	2,909 citations	318942 23 h-index	340414 39 g-index
42 all docs	42 docs citations	42 times ranked	4100 citing authors

#	Article	IF	Citations
1	Tantalum based single, double, and triple atom catalysts supported on g-C₂N monolayer for effective nitrogen reduction reaction: a comparative DFT investigation. Catalysis Science and Technology, 2022, 12, 310-319.	2.1	20
2	Copper acetate catalysed Câ€“C bond formation en route to the synthesis of spiro indanedione cyclopropylpyrazolones. Organic and Biomolecular Chemistry, 2022, , .	1.5	0
3	A terpyridine based hydrogel system for reversible transmissive-to-dark electrochromism and bright-to-quenched electrofluorochromism. Chemical Communications, 2022, 58, 8368-8371.	2.2	13
4	Unraveling the Mechanistic Details of Ruâ€“Bis(pyridyl)borate Complex Catalyst for the Dehydrogenation of Ammonia Borane. Inorganic Chemistry, 2022, 61, 10283-10293.	1.9	2
5	Solvent manipulation of the pre-reduction metalâ€“ligand complex and particle-ligand binding for controlled synthesis of Pd nanoparticles. Nanoscale, 2021, 13, 206-217.	2.8	18
6	Review of Computational Studies of NCM Cathode Materials for Liâ€ion Batteries. Israel Journal of Chemistry, 2020, 60, 850-862.	1.0	40
7	Layered Cathode Materials for Lithium-Ion Batteries: Review of Computational Studies on LiNi_{1â€“xâ€“y}Co_xMn_yO₂ and LiNi_{1â€“xâ€“y}Co_xAl_yO₂. Chemistry of Materials, 2020, 32, 915-952.	3.2	196
8	Assessing the viability of K-Mo₂C for reverse waterâ€“gas shift scale-up: molecular to laboratory to pilot scale. Energy and Environmental Science, 2020, 13, 2524-2539.	15.6	51
9	Predicting Metalâ€“Support Interactions in Oxide-Supported Single-Atom Catalysts. Industrial & Engineering Chemistry Research, 2019, 58, 20236-20246.	1.8	25
10	The role of nanoparticle size and ligand coverage in size focusing of colloidal metal nanoparticles. Nanoscale Advances, 2019, 1, 4052-4066.	2.2	61
11	Understanding the Gas Phase Chemistry of Alkanes with First-Principles Calculations. Journal of Chemical & Engineering Data, 2018, 63, 2430-2437.	1.0	1
12	Mechanistic Studies on the Michael Addition of Amines and Hydrazines To Nitrostyrenes: Nitroalkane Elimination via a Retro-aza-Henry-Type Process. Journal of Organic Chemistry, 2018, 83, 1176-1184.	1.7	28
13	Pushing the limit of layered transition metal oxide cathodes for high-energy density rechargeable Li ion batteries. Energy and Environmental Science, 2018, 11, 1271-1279.	15.6	322
14	Comment on â€œSubstrate Folding Modes in Trichodiene Synthase: A Determinant of Chemo- and Stereoselectivityâ€• ACS Catalysis, 2018, 8, 1371-1375.	5.5	17
15	From Surface ZrO₂ Coating to Bulk Zr Doping by High Temperature Annealing of Nickelâ€Rich Lithiated Oxides and Their Enhanced Electrochemical Performance in Lithium Ion Batteries. Advanced Energy Materials, 2018, 8, 1701682.	10.2	443
16	Predicting accurate cathode properties of layered oxide materials using the SCAN meta-GGA density functional. Npj Computational Materials, 2018, 4, .	3.5	99
17	Understanding Alkane Dehydrogenation through Alcohol Dehydration on Î³-Al₂O₃. Industrial & Engineering Chemistry Research, 2018, 57, 16657-16663.	1.8	15
18	Computational Study of Methane Activation on Î³-Al₂O₃. ACS Omega, 2018, 3, 18242-18250.	1.6	30

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19	Structureâ€“Activity Relationships in Alkane Dehydrogenation on Î³-Al₂O₃: Site-Dependent Reactions. ACS Catalysis, 2018, 8, 11570-11578.	5.5	75
20	A promising drug candidate for the treatment of glaucoma based on a P2Y6-receptor agonist. Purinergic Signalling, 2018, 14, 271-284.	1.1	14
21	Unraveling the Effects of Al Doping on the Electrochemical Properties of LiNi_{0.5}Co_{0.2}Mn_{0.3}O₂Using First Principles. Journal of the Electrochemical Society, 2017, 164, A6359-A6365.	1.3	118
22	Chemical Control in the Battle against Fidelity in Promiscuous Natural Product Biosynthesis: The Case of Trichodiene Synthase. ACS Catalysis, 2017, 7, 812-818.	5.5	48
23	Elucidating the role of oxygen coverage in CO₂ reduction on Mo₂C. Catalysis Science and Technology, 2017, 7, 5521-5529.	2.1	23
24	Origin of Structural Degradation During Cycling and Low Thermal Stability of Ni-Rich Layered Transition Metal-Based Electrode Materials. Journal of Physical Chemistry C, 2017, 121, 22628-22636.	1.5	199
25	Study of Cathode Materials for Lithium-Ion Batteries: Recent Progress and New Challenges. Inorganics, 2017, 5, 32.	1.2	68
26	Is it True That the Normal Valenceâ€Length Correlation Is Irrelevant for Metalâ€“Metal Bonds?. Chemistry - A European Journal, 2016, 22, 5269-5276.	1.7	11
27	Nucleoside-2â€²,3â€²/3â€²,5â€²-bis(thio)phosphate antioxidants are also capable of disassembly of amyloid beta₄₂-Zn(<scp>ii</scp>)/Cu(<scp>ii</scp>) aggregates via Zn(<scp>ii</scp>)/Cu(<scp>ii</scp>)-chelation. Organic and Biomolecular Chemistry, 2016, 14, 4640-4653.	1.5	9
28	Stabilizing nickel-rich layered cathode materials by a high-charge cation doping strategy: zirconium-doped LiNi_{0.6}Co_{0.2}Mn_{0.2}O₂. Journal of Materials Chemistry A, 2016, 4, 16073-16084.	5.2	295
29	Practical Aspects of Multiscale Classical and Quantum Simulations of Enzyme Reactions. Methods in Enzymology, 2016, 577, 251-286.	0.4	8
30	First principles model calculations of the biosynthetic pathway in selinadiene synthase. Bioorganic and Medicinal Chemistry, 2016, 24, 4867-4870.	1.4	11
31	Improving Energy Density and Structural Stability of Manganese Oxide Cathodes for Na-Ion Batteries by Structural Lithium Substitution. Chemistry of Materials, 2016, 28, 9064-9076.	3.2	191
32	Hydrogen adsorption in ZIF-7: A DFT and ab-initio molecular dynamics study. Chemical Physics Letters, 2016, 651, 178-182.	1.2	12
33	Thermodynamic and kinetic studies of LiNi_{0.5}Co_{0.2}Mn_{0.3}O₂ as a positive electrode material for Li-ion batteries using first principles. Physical Chemistry Chemical Physics, 2016, 18, 6799-6812.	1.3	126
34	Studies of Aluminum-Doped LiNi_{0.5}Co_{0.2}Mn_{0.3}O₂: Electrochemical Behavior, Aging, Structural Transformations, and Thermal Characteristics. Journal of the Electrochemical Society, 2015, 162, A1014-A1027.	1.3	121
35	Classical and Quantum Modeling of Li and Na Diffusion in FePO₄. Journal of Physical Chemistry C, 2015, 119, 15801-15809.	1.5	29
36	Magnetism in olivine-type LiCo_{1â€“x}Fe_xPO₄cathode materials: bridging theory and experiment. Physical Chemistry Chemical Physics, 2015, 17, 31202-31215.	1.3	16

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37	Identification of Highly Promising Antioxidants/Neuroprotectants Based on Nucleoside 5â€²-Phosphorothioate Scaffold. Synthesis, Activity, and Mechanisms of Action. Journal of Medicinal Chemistry, 2015, 58, 8427-8443.	2.9	13
38	Photoelectrochemical splitting of water with nanocrystalline Zn1â^'xMnxO thin films: First-principle DFT computations supporting the systematic experimental endeavor. International Journal of Hydrogen Energy, 2014, 39, 3637-3648.	3.8	22
39	Atomistic details of effect of disulfide bond reduction on active site of Phytase B from Aspergillus niger: A MD Study. Bioinformation, 2013, 9, 963-967.	0.2	7
40	Scandium-Decorated MOF-5 as Potential Candidates for Room-Temperature Hydrogen Storage: A Solution for the Clustering Problem in MOFs. Journal of Physical Chemistry C, 2012, 116, 17336-17342.	1.5	50
41	Thiocyanato Bridged Heterodinuclear Complex [Cu(bpy)2(Âµ-NCS)Ru(bpy)2(NO3)](PF6)2 and Its Binding with Cd(II), Hg(II), Pb(II) and Ag(I) Ions. , 2012, , 231-247.		1
42	Ab initio and periodic DFT investigation of hydrogen storage on light metal-decorated MOF-5. International Journal of Hydrogen Energy, 2011, 36, 10816-10827.	3.8	61