Shaama Mallikarjun Sharada

List of Publications by Year
in descending order

35 papers	3,969 citations	516215 16 h-index	344852 36 g-index
40 all docs	40 docs citations	40 times ranked	4987 citing authors

#	Article	IF	Citations
1	CO Oxidation with Atomically Dispersed Catalysts: Insights from the Energetic Span Model. ACS Catalysis, 2022, 12, 2064-2076.	5.5	11
2	A computational study of the mechanism of chloroalkane dechlorination with Rh(i) complexes. Physical Chemistry Chemical Physics, 2022, 24, 3518-3522.	1.3	2
3	Kinetics and mechanistic details of bulk ZnO dissolution using a thiolâ€“imidazole system. Chemical Science, 2022, 13, 3208-3215.	3.7	5
4	Modeling and Characterization of Exciplexes in Photoredox CO₂Reduction: Insights from Quantum Chemistry and Fluorescence Spectroscopy. Journal of Physical Chemistry A, 2022, 126, 2319-2329.	1.1	5
5	A matrix completion algorithm for efficient calculation of quantum and variational effects in chemical reactions. Journal of Chemical Physics, 2022, 156, 184119.	1.2	5
6	Organic photoredox catalysts for CO2 reduction: Driving discovery with genetic algorithms. Journal of Chemical Physics, 2022, 156, 184109.	1.2	4
7	Toward Efficient Direct Dynamics Studies of Chemical Reactions: A Novel Matrix Completion Algorithm. Journal of Chemical Theory and Computation, 2022, 18, 4327-4341.	2.3	2
8	Consistent inclusion of continuum solvation in energy decomposition analysis: theory and application to molecular CO₂ reduction catalysts. Chemical Science, 2021, 12, 1398-1414.	3.7	41
9	A framework for constructing linear free energy relationships to design molecular transition metal catalysts. Physical Chemistry Chemical Physics, 2021, 23, 15543-15556.	1.3	5
10	Adsorbate-assisted migration of the metal atom in atomically dispersed catalysts: An ab initio molecular dynamics study. Journal of Chemical Physics, 2021, 154, 234709.	1.2	5
11	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
12	Probing the Ligand Exchange of N-Heterocyclic Carbene-Capped Ag2S Nanocrystals with Amines and Carboxylic Acids. Inorganic Chemistry, 2021, 60, 13699-13706.	1.9	2
13	Photoredox Chemistry with Organic Catalysts: Role of Computational Methods. ACS Omega, 2021, 6, 33253-33264.	1.6	6
14	Perspective and challenges in electrochemical approaches for reactive CO2 separations. IScience, 2021, 24, 103422.	1.9	28
15	Heterobimetallic complexes of IrM (M = Fe^{II}, Co^{II}, and Ni^{II}) core and bridging 2-(diphenylphosphino)pyridine: electronic structure and electrochemical behavior. Dalton Transactions, 2020, 49, 10509-10515.	1.6	5
16	Ab Initio Molecular Dynamics Reveals New Metal-Binding Sites in Atomically Dispersed Pt₁/TiO₂ Catalysts. Journal of Physical Chemistry C, 2020, 124, 24187-24195.	1.5	17
17	A matrix completion algorithm to recover modes orthogonal to the minimum energy path in chemical reactions. Journal of Chemical Physics, 2020, 153, 054122.	1.2	5
18	Computational Analysis of Electron Transfer Kinetics for CO₂ Reduction with Organic Photoredox Catalysts. Journal of Physical Chemistry A, 2020, 124, 5359-5368.	1.1	14

#	Article	IF	Citations
19	Synthesis and Electrocatalytic HER Studies of Carbene-Ligated Cu_{3â€“x}P Nanocrystals. ACS Applied Materials & Interfaces, 2020, 12, 16394-16401.	4.0	19
20	Linear free energy relationships for transition metal chemistry: case study of CH activation with copperâ€“oxygen complexes. Physical Chemistry Chemical Physics, 2020, 22, 7155-7159.	1.3	7
21	A new mechanism of metal-ligand cooperative catalysis in transfer hydrogenation of ketones. Polyhedron, 2020, 182, 114508.	1.0	12
22	Adsorption on transition metal surfaces: Transferability and accuracy of DFT using the ADS41 dataset. Physical Review B, 2019, 100, .	1.1	51
23	A theoretical study of the effect of a non-aqueous proton donor on electrochemical ammonia synthesis. Physical Chemistry Chemical Physics, 2018, 20, 4982-4989.	1.3	86
24	Computational strategies to probe CH activation in dioxo-dicopper complexes. Physical Chemistry Chemical Physics, 2018, 20, 25602-25614.	1.3	9
25	Theoretical Analysis of the Influence of Pore Geometry on Monomolecular Cracking and Dehydrogenation ofn-Butane in BrÃ¸nsted Acidic Zeolites. ACS Catalysis, 2017, 7, 2685-2697.	5.5	42
26	SBH10: A Benchmark Database of Barrier Heights on Transition Metal Surfaces. Journal of Physical Chemistry C, 2017, 121, 19807-19815.	1.5	89
27	Adsorption Thermodynamics and Intrinsic Activation Parameters for Monomolecular Cracking of n-Alkanes on BrÃ¸nsted Acid Sites in Zeolites. Journal of Physical Chemistry C, 2015, 119, 10427-10438.	1.5	48
28	Improved Force-Field Parameters for QM/MM Simulations of the Energies of Adsorption for Molecules in Zeolites and a Free Rotor Correction to the Rigid Rotor Harmonic Oscillator Model for Adsorption Enthalpies. Journal of Physical Chemistry C, 2015, 119, 1840-1850.	1.5	110
29	Wavefunction stability analysis without analytical electronic Hessians: application to orbital-optimised second-order MÃ¸llerâ€“Plesset theory and VV10-containing density functionals. Molecular Physics, 2015, 113, 1802-1808.	0.8	30
30	Ethane and propane dehydrogenation over PtIr/Mg(Al)O. Applied Catalysis A: General, 2015, 506, 25-32.	2.2	64
31	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
32	A finite difference Davidson procedure to sidestep full ab initio hessian calculation: Application to characterization of stationary points and transition state searches. Journal of Chemical Physics, 2014, 140, 164115.	1.2	25
33	Insights into the Kinetics of Cracking and Dehydrogenation Reactions of Light Alkanes in H-MFI. Journal of Physical Chemistry C, 2013, 117, 12600-12611.	1.5	59
34	Automated Transition State Searches without Evaluating the Hessian. Journal of Chemical Theory and Computation, 2012, 8, 5166-5174.	2.3	68
35	A comprehensive singleâ€particle model for solidâ€state polymerization of poly(<scp>L</scp>â€lactic acid). Journal of Applied Polymer Science, 2011, 122, 2966-2980.	1.3	6