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	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
2	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
3	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
4	SBH10: A Benchmark Database of Barrier Heights on Transition Metal Surfaces. Journal of Physical Chemistry C, 2017, 121, 19807-19815.	1.5	89
5	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
6	Automated Transition State Searches without Evaluating the Hessian. Journal of Chemical Theory and Computation, 2012, 8, 5166-5174.	2.3	68
7	Ethane and propane dehydrogenation over PtIr/Mg(Al)O. Applied Catalysis A: General, 2015, 506, 25-32.	2.2	64
8	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
9	Adsorption on transition metal surfaces: Transferability and accuracy of DFT using the ADS41 dataset. Physical Review B, 2019, 100, .	1.1	51
10	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
11	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
12	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
13	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
14	Perspective and challenges in electrochemical approaches for reactive CO2 separations. IScience, 2021, 24, 103422.	1.9	28
15	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
16	Synthesis and Electrocatalytic HER Studies of Carbene-Ligated Cu_{3â€“x}P Nanocrystals. ACS Applied Materials & Interfaces, 2020, 12, 16394-16401.	4.0	19
17	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
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	A new mechanism of metal-ligand cooperative catalysis in transfer hydrogenation of ketones. Polyhedron, 2020, 182, 114508.	1.0	12
20	CO Oxidation with Atomically Dispersed Catalysts: Insights from the Energetic Span Model. ACS Catalysis, 2022, 12, 2064-2076.	5.5	11
21	Computational strategies to probe CH activation in dioxo-dicopper complexes. Physical Chemistry Chemical Physics, 2018, 20, 25602-25614.	1.3	9
22	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
23	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
24	Photoredox Chemistry with Organic Catalysts: Role of Computational Methods. ACS Omega, 2021, 6, 33253-33264.	1.6	6
25	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
26	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
27	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
28	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
29	Kinetics and mechanistic details of bulk ZnO dissolution using a thiolâ€“imidazole system. Chemical Science, 2022, 13, 3208-3215.	3.7	5
30	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
31	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
32	Organic photoredox catalysts for CO2 reduction: Driving discovery with genetic algorithms. Journal of Chemical Physics, 2022, 156, 184109.	1.2	4
33	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
34	A computational study of the mechanism of chloroalkane dechlorination with Rh(i) complexes. Physical Chemistry Chemical Physics, 2022, 24, 3518-3522.	1.3	2
35	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