Matthias Loipersberger

List of Publications by Year
in descending order

20 papers	1,059 citations	687363 13 h-index	794594 19 g-index
21 all docs	21 docs citations	21 times ranked	791 citing authors

#	Article	IF	Citations
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
2	Metalâ€“Ligand Cooperativity via Exchange Coupling Promotes Iron- Catalyzed Electrochemical CO₂ Reduction at Low Overpotentials. Journal of the American Chemical Society, 2020, 142, 20489-20501.	13.7	77
3	From Intermolecular Interaction Energies and Observable Shifts to Component Contributions and Back Again: A Tale of Variational Energy Decomposition Analysis. Annual Review of Physical Chemistry, 2021, 72, 641-666.	10.8	55
4	Mechanistic Insights into Co and Fe Quaterpyridine-Based CO₂ Reduction Catalysts: Metalâ€“Ligand Orbital Interaction as the Key Driving Force for Distinct Pathways. Journal of the American Chemical Society, 2021, 143, 744-763.	13.7	52
5	Development of an Advanced Force Field for Water Using Variational Energy Decomposition Analysis. Journal of Chemical Theory and Computation, 2019, 15, 5001-5013.	5.3	49
6	Templating Bicarbonate in the Second Coordination Sphere Enhances Electrochemical CO₂ Reduction Catalyzed by Iron Porphyrins. Journal of the American Chemical Society, 2022, 144, 11656-11663.	13.7	45
7	Consistent inclusion of continuum solvation in energy decomposition analysis: theory and application to molecular CO₂ reduction catalysts. Chemical Science, 2021, 12, 1398-1414.	7.4	41
8	Revealing the nature of electron correlation in transition metal complexes with symmetry breaking and chemical intuition. Journal of Chemical Physics, 2021, 154, 194109.	3.0	36
9	Regularized Second-Order MÃ¸llerâ€“Plesset Theory: A More Accurate Alternative to Conventional MP2 for Noncovalent Interactions and Transition Metal Thermochemistry for the Same Computational Cost. Journal of Physical Chemistry Letters, 2021, 12, 12084-12097.	4.6	32
10	Controlled Single-Electron Transfer via Metalâ€“Ligand Cooperativity Drives Divergent Nickel-Electrocatalyzed Radical Pathways. Journal of the American Chemical Society, 2021, 143, 6990-7001.	13.7	24
11	Computational Study of an Iron(II) Polypyridine Electrocatalyst for CO₂ Reduction: Key Roles for Intramolecular Interactions in CO₂ Binding and Proton Transfer. Inorganic Chemistry, 2020, 59, 8146-8160.	4.0	23
12	Variational Forwardâ€“Backward Charge Transfer Analysis Based on Absolutely Localized Molecular Orbitals: Energetics and Molecular Properties. Journal of Chemical Theory and Computation, 2020, 16, 1073-1089.	5.3	21
13	Probing radicalâ€“molecule interactions with a second generation energy decomposition analysis of DFT calculations using absolutely localized molecular orbitals. Physical Chemistry Chemical Physics, 2020, 22, 12867-12885.	2.8	17
14	Two New Methods To Generate Internal Coordinates for Molecular Wave Packet Dynamics in Reduced Dimensions. Journal of Chemical Theory and Computation, 2016, 12, 5698-5708.	5.3	14
15	Energy Decomposition Analysis for Interactions of Radicals: Theory and Implementation at the MP2 Level with Application to Hydration of Halogenated Benzene Cations and Complexes between CO₂^{â€“}Â· and Pyridine and Imidazole. Journal of Physical Chemistry A, 2019, 123, 9621-9633.	2.5	12
16	Exchange Coupling Determines Metal-Dependent Efficiency for Iron- and Cobalt-Catalyzed Photochemical CO₂ Reduction. ACS Catalysis, 2022, 12, 8484-8493.	11.2	12
17	Exploring the Limits of Second- and Third-Order MÃ¸llerâ€“Plesset Perturbation Theories for Noncovalent Interactions: Revisiting MP2.5 and Assessing the Importance of Regularization and Reference Orbitals. Journal of Chemical Theory and Computation, 2021, 17, 5582-5599.	5.3	11
18	Deciphering Distinct Overpotential-Dependent Pathways for Electrochemical CO₂ Reduction Catalyzed by an Ironâ€“Terpyridine Complex. Inorganic Chemistry, 2022, 61, 6919-6933.	4.0	10

#	Article	IF	Citations
19	Revisiting the Bonding Model for Gold(I) Species: The Importance of Pauli Repulsion Revealed in a Gold(I)â€Cyclobutadiene Complex. Angewandte Chemie - International Edition, 2022, 61, .	13.8	8
20	Revisiting the Bonding Model for Gold(I) Species: The Importance of Pauli Repulsion Revealed in a Gold(I)â€Cyclobutadiene Complex. Angewandte Chemie, 0, , .	2.0	0