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	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
2	Deciphering Distinct Overpotential-Dependent Pathways for Electrochemical CO₂ Reduction Catalyzed by an Ironâ€“Terpyridine Complex. Inorganic Chemistry, 2022, 61, 6919-6933.	4.0	10
3	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
4	Exchange Coupling Determines Metal-Dependent Efficiency for Iron- and Cobalt-Catalyzed Photochemical CO₂ Reduction. ACS Catalysis, 2022, 12, 8484-8493.	11.2	12
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	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
13	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
14	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
15	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
16	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
17	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
18	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

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19	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
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