Miho Isegawa

List of Publications by Year
in descending order

25 papers	695 citations	623734 14 h-index	552781 26 g-index
26 all docs	26 docs citations	26 times ranked	1056 citing authors

#	Article	IF	Citations
1	Ionization Energies and Redox Potentials of Hydrated Transition Metal Ions: Evaluation of Domain-Based Local Pair Natural Orbital Coupled Cluster Approaches. Journal of Chemical Theory and Computation, 2022, 18, 1619-1632.	5.3	9
2	H2 activation by hydrogenase-inspired NiFe catalyst using frustrated Lewis pair: effect of buffer and halide ion in the heterolytic Hâ€“H bond cleavage. RSC Advances, 2021, 11, 28420-28432.	3.6	3
3	Proton-Coupled Electron Transfer in Electrochemical Alanine Formation from Pyruvic Acid: Mechanism of Catalytic Reaction at the Interface between TiO₂ (101) and Water. Journal of Physical Chemistry C, 2021, 125, 12603-12613.	3.1	7
4	Photochemical conversion of CO₂ to CO by a Re complex: theoretical insights into the formation of CO and HCO₃^{â^'} from an experimentally detected monoalkyl carbonate complex. RSC Advances, 2021, 11, 37713-37725.	3.6	6
5	Hydrogen evolution, electron-transfer, and hydride-transfer reactions in a nickelâ€“iron hydrogenase model complex: a theoretical study of the distinctive reactivities for the conformational isomers of nickelâ€“iron hydride. Dalton Transactions, 2021, 51, 312-323.	3.3	3
6	Selective Oxidation of H₂ and CO by NiIr Catalyst in Aqueous Solution: A DFT Mechanistic Study. Inorganic Chemistry, 2020, 59, 1014-1028.	4.0	8
7	[NiFe], [FeFe], and [Fe] hydrogenase models from isomers. Science Advances, 2020, 6, eaaz8181.	10.3	29
8	CO₂ reduction by a Mn electrocatalyst in the presence of a Lewis acid: a DFT study on the reaction mechanism. Sustainable Energy and Fuels, 2019, 3, 1730-1738.	4.9	11
9	Electron and Hydride Transfer in a Redox-Active NiFe Hydride Complex: A DFT Study. ACS Catalysis, 2018, 8, 10419-10429.	11.2	13
10	DFT Study on Fe(IV)-Peroxo Formation and H Atom Transfer Triggered O₂ Activation by NiFe Complex. Organometallics, 2018, 37, 1534-1545.	2.3	11
11	Copper-Catalyzed Enantioselective Boron Conjugate Addition: DFT and AFIR Study on Different Selectivities of Cu(I) and Cu(II) Catalysts. ACS Catalysis, 2017, 7, 5370-5380.	11.2	28
12	Ionization Energies and Aqueous Redox Potentials of Organic Molecules: Comparison of DFT, Correlated ab Initio Theory and Pair Natural Orbital Approaches. Journal of Chemical Theory and Computation, 2016, 12, 2272-2284.	5.3	94
13	Photochemical Ring Opening and Closing of Three Isomers of Diarylethene: Spinâ€“Flip Time-Dependent Density Functional Study. Journal of Physical Chemistry A, 2015, 119, 4191-4199.	2.5	17
14	Ab initio reaction pathways for photodissociation and isomerization of nitromethane on four singlet potential energy surfaces with three roaming paths. Journal of Chemical Physics, 2014, 140, 244310.	3.0	26
15	Complete active space second order perturbation theory (CASPT2) study of N(2D) + H2O reaction paths on D1 and D0 potential energy surfaces: Direct and roaming pathways. Journal of Chemical Physics, 2014, 141, 154303.	3.0	4
16	Predicting pathways for terpene formation from first principles â€“ routes to known and new sesquiterpenes. Chemical Science, 2014, 5, 1555.	7.4	26
17	Quantum Mechanical Fragment Methods Based on Partitioning Atoms or Partitioning Coordinates. Accounts of Chemical Research, 2014, 47, 2731-2738.	15.6	27
18	Polarized Molecular Orbital Model Chemistry 3. The PMO Method Extended to Organic Chemistry. Journal of Chemical Theory and Computation, 2013, 9, 33-45.	5.3	18

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19	Assessment and Validation of Density Functional Approximations for Iron Carbide and Iron Carbide Cation. Journal of Physical Chemistry A, 2013, 117, 169-173.	2.5	23
20	Electrostatically Embedded Molecular Tailoring Approach and Validation for Peptides. Journal of Chemical Theory and Computation, 2013, 9, 1381-1393.	5.3	54
21	Valence excitation energies of alkenes, carbonyl compounds, and azabenzenes by time-dependent density functional theory: Linear response of the ground state compared to collinear and noncollinear spin-flip TDDFT with the Tamm-Dancoff approximation. Journal of Chemical Physics, 2013, 138, 134111.	3.0	62
22	Performance of recent and high-performance approximate density functionals for time-dependent density functional theory calculations of valence and Rydberg electronic transition energies. Journal of Chemical Physics, 2012, 137, 244104.	3.0	165
23	Incorporation of charge transfer into the explicit polarization fragment method by grand canonical density functional theory. Journal of Chemical Physics, 2011, 135, 084107.	3.0	16
24	Polarizable Force Field for Protein with Charge Response Kernel. Journal of Chemical Theory and Computation, 2009, 5, 2809-2821.	5.3	19
25	Electronic polarization effect on low-frequency infrared and Raman spectra of aprotic solvent: Molecular dynamics simulation study with charge response kernel by second order MÃ¸llerâ€“Plesset perturbation method. Journal of Chemical Physics, 2007, 127, 244502.	3.0	14