Kuan-Yu Liu

List of Publications by Year
in descending order

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Version: 2024-02-01

8 papers	762 citations	1163117 8 h-index	1588992 8 g-index
8 all docs	8 docs citations	8 times ranked	600 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	Understanding the many-body expansion for large systems. II. Accuracy considerations. Journal of Chemical Physics, 2016, 144, 164105.	3.0	65
3	Accurate and Efficient ab Initio Calculations for Supramolecular Complexes: Symmetry-Adapted Perturbation Theory with Many-Body Dispersion. Journal of Physical Chemistry Letters, 2019, 10, 2706-2714.	4.6	51
4	Energy-Screened Many-Body Expansion: A Practical Yet Accurate Fragmentation Method for Quantum Chemistry. Journal of Chemical Theory and Computation, 2020, 16, 475-487.	5.3	48
5	Understanding the many-body expansion for large systems. III. Critical role of four-body terms, counterpoise corrections, and cutoffs. Journal of Chemical Physics, 2017, 147, 161729.	3.0	30
6	Variational Formulation of the Generalized Many-Body Expansion with Self-Consistent Charge Embedding: Simple and Correct Analytic Energy Gradient for Fragment-Basedab InitioMolecular Dynamics. Journal of Physical Chemistry Letters, 2019, 10, 3877-3886.	4.6	19
7	Self-consistent charge embedding at very low cost, with application to symmetry-adapted perturbation theory. Journal of Chemical Physics, 2019, 151, 031102.	3.0	17
8	Accuracy of finiteâ€difference harmonic frequencies in density functional theory. Journal of Computational Chemistry, 2017, 38, 1678-1684.	3.3	14