Sijia S Dong

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1524649/publications.pdf

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17	901	932766 10	940134 16
papers	citations	h-index	g-index

21	21	21	1292
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
2	Automatic Selection of an Active Space for Calculating Electronic Excitation Spectra by MS-CASPT2 or MC-PDFT. Journal of Chemical Theory and Computation, 2018, 14, 2017-2025.	2.3	45
3	Highly Efficient and Diastereoselective Gold(I)â€Catalyzed Synthesis of Tertiary Amines from Secondary Amines and Alkynes: Substrate Scope and Mechanistic Insights. Chemistry - A European Journal, 2011, 17, 12932-12945.	1.7	42
4	Electronic Structures of Group 9 Metallocorroles with Axial Ammines. Inorganic Chemistry, 2011, 50, 764-770.	1.9	18
5	Conformational and Thermodynamic Landscape of GPCR Activation from Theory and Computation. Biophysical Journal, 2016, 110, 2618-2629.	0.2	18
6	Assessment of MC-PDFT Excitation Energies for a Set of QM/MM Models of Rhodopsins. Journal of Chemical Theory and Computation, 2019, 15, 1915-1923.	2.3	16
7	Machine learning dielectric screening for the simulation of excited state properties of molecules and materials. Chemical Science, 2021, 12, 4970-4980.	3.7	16
8	Nature of the 1¹B_u and 2¹A_g Excited States of Butadiene and the Goldilocks Principle of Basis Set Diffuseness. Journal of Chemical Theory and Computation, 2019, 15, 4591-4601.	2.3	15
9	Targeting oncogenic KRAS with molecular brush-conjugated antisense oligonucleotides. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	14
10	Excitation spectra of retinal by multiconfiguration pair-density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 7265-7276.	1.3	13
11	State-Interaction Pair-Density Functional Theory Can Accurately Describe a Spiro Mixed Valence Compound. Journal of Physical Chemistry A, 2019, 123, 2100-2106.	1.1	12
12	Computational predictions of corroles as a class of Hsp90 inhibitors. Molecular BioSystems, 2015, 11, 2907-2914.	2.9	11
13	The Predicted Ensemble of Lowâ€Energy Conformations of Human Somatostatin Receptor Subtypeâ€…5 and the Binding of Antagonists. ChemMedChem, 2015, 10, 650-661.	1.6	6
14	Extended Hamiltonian molecular dynamics: semiclassical trajectories with improved maintenance of zero point energy. Physical Chemistry Chemical Physics, 2018, 20, 30209-30218.	1.3	6
15	Identifying multiple active conformations in the G protein-coupled receptor activation landscape using computational methods. Methods in Cell Biology, 2017, 142, 173-186.	0.5	3
16	Mechanism of halide exchange in reactions of CpRu(PPh₃)₂Cl with haloalkanes. New Journal of Chemistry, 2022, 46, 6603-6608.	1.4	1
17	Computational Prediction of the Class a GPCR Active State Conformations. Biophysical Journal, 2014, 106, 308a.	0.2	0