

Sijia S Dong

List of Publications by Year in descending order

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17
papers

901
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932766

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1292
citing authors

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