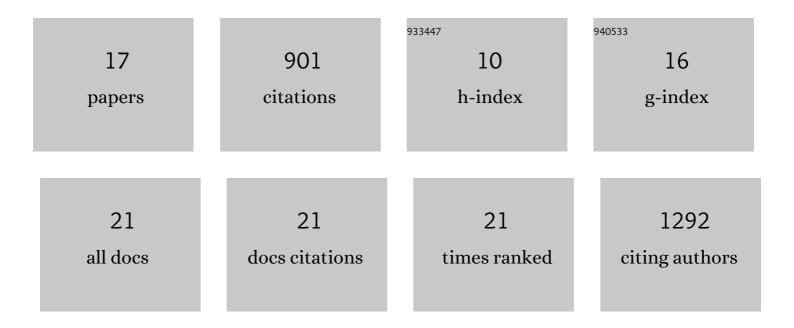
Sijia S Dong

List of Publications by Year in descending order

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SULLA S DONC

| # | Article | IF | CITATIONS |
|----|---|-----|-----------|
| 1 | OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964. | 5.3 | 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. | 5.3 | 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. | 3.3 | 42 |
| 4 | Electronic Structures of Group 9 Metallocorroles with Axial Ammines. Inorganic Chemistry, 2011, 50, 764-770. | 4.0 | 18 |
| 5 | Conformational and Thermodynamic Landscape of GPCR Activation from Theory and Computation. Biophysical Journal, 2016, 110, 2618-2629. | 0.5 | 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. | 5.3 | 16 |
| 7 | Machine learning dielectric screening for the simulation of excited state properties of molecules and materials. Chemical Science, 2021, 12, 4970-4980. | 7.4 | 16 |
| 8 | Nature of the 1 ¹ B _u and 2 ¹ A _g Excited States of Butadiene and the Goldilocks Principle of Basis Set Diffuseness. Journal of Chemical Theory and Computation, 2019, 15, 4591-4601. | 5.3 | 15 |
| 9 | Targeting oncogenic KRAS with molecular brush-conjugated antisense oligonucleotides. Proceedings of the United States of America, 2022, 119, . | 7.1 | 14 |
| 10 | Excitation spectra of retinal by multiconfiguration pair-density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 7265-7276. | 2.8 | 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. | 2.5 | 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. | 3.2 | 6 |
| 14 | Extended Hamiltonian molecular dynamics: semiclassical trajectories with improved maintenance of zero point energy. Physical Chemistry Chemical Physics, 2018, 20, 30209-30218. | 2.8 | 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. | 1.1 | 3 |
| 16 | Mechanism of halide exchange in reactions of CpRu(PPh ₃) ₂ Cl with haloalkanes. New Journal of Chemistry, 2022, 46, 6603-6608. | 2.8 | 1 |
| 17 | Computational Prediction of the Class a GPCR Active State Conformations. Biophysical Journal, 2014, 106, 308a. | 0.5 | 0 |