Jie J Bao

List of Publications by Year
in descending order

11 papers	870 citations	1039406 9 h-index	1281420 11 g-index
14 all docs	14 docs citations	14 times ranked	1113 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	Multi-state pair-density functional theory. Faraday Discussions, 2020, 224, 348-372.	1.6	28
4	Multiconfiguration Pair-Density Functional Theory. Annual Review of Physical Chemistry, 2021, 72, 541-564.	4.8	28
5	Automatic Active Space Selection for Calculating Electronic Excitation Energies Based on High-Spin Unrestricted Hartreeâ€“Fock Orbitals. Journal of Chemical Theory and Computation, 2019, 15, 5308-5318.	2.3	27
6	Compressed-State Multistate Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 7444-7452.	2.3	23
7	Electronic structure of strongly correlated systems: recent developments in multiconfiguration pair-density functional theory and multiconfiguration nonclassical-energy functional theory. Chemical Science, 2022, 13, 7685-7706.	3.7	18
8	Weak Interactions in Alkaline Earth Metal Dimers by Pair-Density Functional Theory. Journal of Physical Chemistry Letters, 2019, 10, 799-805.	2.1	12
9	Multiconfiguration pair-density functional theory for doublet excitation energies and excited state geometries: the excited states of CN. Physical Chemistry Chemical Physics, 2017, 19, 30089-30096.	1.3	10
10	Multireference Methods for Calculating the Dissociation Enthalpy of Tetrahedral P4 to Two P2. Journal of Physical Chemistry A, 2018, 122, 5742-5749.	1.1	8
11	Zero-Field Splitting Calculations by Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 2199-2207.	2.3	6