Zhi-Qiang You

List of Publications by Year
in descending order

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23 papers	4,647 citations	430442 18 h-index	642321 23 g-index
23 all docs	23 docs citations	23 times ranked	5619 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.	1.2	518
2	Intrinsically smooth discretisation of Connolly's solvent-excluded molecular surface. Molecular Physics, 2020, 118, .	0.8	13
3	What Is the Optoelectronic Effect of the Capsule on the Guest Molecule in Aqueous Host/Guest Complexes? A Combined Computational and Spectroscopic Perspective. Journal of Physical Chemistry C, 2017, 121, 15481-15488.	1.5	17
4	vConTACT: an iVirus tool to classify double-stranded DNA viruses that infectArchaeaandBacteria. PeerJ, 2017, 5, e3243.	0.9	219
5	The Hydrated Electron at the Surface of Neat Liquid Water Appears To Be Indistinguishable from the Bulk Species. Journal of the American Chemical Society, 2016, 138, 10879-10886.	6.6	56
6	The Excitation Spectra of Naphthalene Dimers: Frenkel and Chargeâ€transfer Excitons. Journal of the Chinese Chemical Society, 2016, 63, 20-32.	0.8	6
7	Reparameterization of an Accurate, Few-Parameter Implicit Solvation Model for Quantum Chemistry: Composite Method for Implicit Representation of Solvent, CMIRS v. 1.1. Journal of Chemical Theory and Computation, 2016, 12, 4338-4346.	2.3	18
8	Comparison of the Marcus and Pekar partitions in the context of non-equilibrium, polarizable-continuum solvation models. Journal of Chemical Physics, 2015, 143, 204104.	1.2	52
9	Calculating Electron-Transfer Coupling with Density Functional Theory: The Long-Range-Corrected Density Functionals. Journal of Physical Chemistry B, 2015, 119, 7480-7490.	1.2	31
10	Experimental Benchmark Data and Systematic Evaluation of Two a Posteriori, Polarizable-Continuum Corrections for Vertical Excitation Energies in Solution. Journal of Physical Chemistry A, 2015, 119, 5446-5464.	1.1	120
11	A Structural Model for a Self-Assembled Nanotube Provides Insight into Its Exciton Dynamics. Journal of Physical Chemistry C, 2015, 119, 13948-13956.	1.5	21
12	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
13	Theory and calculation for the electronic coupling in excitation energy transfer. International Journal of Quantum Chemistry, 2014, 114, 102-115.	1.0	116
14	Ab Initio Implementation of the Frenkelâ€“Davydov Exciton Model: A Naturally Parallelizable Approach to Computing Collective Excitations in Crystals and Aggregates. Journal of Chemical Theory and Computation, 2014, 10, 5366-5376.	2.3	74
15	The role of CHâ€“Ï€ interaction in the charge transfer properties in tris(8-hydroxyquinolinato)aluminium(iii). Physical Chemistry Chemical Physics, 2011, 13, 20704.	1.3	15
16	Ab Inito Study on Triplet Excitation Energy Transfer in Photosynthetic Light-Harvesting Complexes. Journal of Physical Chemistry A, 2011, 115, 4092-4100.	1.1	30
17	Theoretical characterization of photoinduced electron transfer in rigidly linked donorâ€“acceptor molecules: the fragment charge difference and the generalized Mullikenâ€“Hush schemes. Molecular Physics, 2010, 108, 2775-2789.	0.8	19
18	The fragment spin difference scheme for triplet-triplet energy transfer coupling. Journal of Chemical Physics, 2010, 133, 074105.	1.2	58

#	Article	IF	Citations
19	Characterization of the Short-Range Couplings in Excitation Energy Transfer. Journal of Physical Chemistry C, 2008, 112, 1204-1212.	1.5	177
20	The mediated excitation energy transfer: Effects of bridge polarizability. Journal of Chemical Physics, 2008, 129, 084708.	1.2	46
21	Triplet-triplet energy-transfer coupling: Theory and calculation. Journal of Chemical Physics, 2006, 124, 044506.	1.2	110
22	Charge Transport Properties of Tris(8-hydroxyquinolinato)aluminum(III):Â Why It Is an Electron Transporter. Journal of the American Chemical Society, 2005, 127, 66-67.	6.6	330
23	Calculating electron transfer couplings by the Spin-Flip approach: energy splitting and dynamical correlation effects. Chemical Physics Letters, 2004, 390, 116-123.	1.2	40