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	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
2	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
3	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
4	vConTACT: an iVirus tool to classify double-stranded DNA viruses that infectArchaeaandBacteria. PeerJ, 2017, 5, e3243.	0.9	219
5	Characterization of the Short-Range Couplings in Excitation Energy Transfer. Journal of Physical Chemistry C, 2008, 112, 1204-1212.	1.5	177
6	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
7	Theory and calculation for the electronic coupling in excitation energy transfer. International Journal of Quantum Chemistry, 2014, 114, 102-115.	1.0	116
8	Triplet-triplet energy-transfer coupling: Theory and calculation. Journal of Chemical Physics, 2006, 124, 044506.	1.2	110
9	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
10	The fragment spin difference scheme for triplet-triplet energy transfer coupling. Journal of Chemical Physics, 2010, 133, 074105.	1.2	58
11	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
12	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
13	The mediated excitation energy transfer: Effects of bridge polarizability. Journal of Chemical Physics, 2008, 129, 084708.	1.2	46
14	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
15	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
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	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
18	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

#	Article	IF	Citations
19	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
20	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
21	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
22	Intrinsically smooth discretisation of Connolly's solvent-excluded molecular surface. Molecular Physics, 2020, 118, .	0.8	13
23	The Excitation Spectra of Naphthalene Dimers: Frenkel and Chargeâ€transfer Excitons. Journal of the Chinese Chemical Society, 2016, 63, 20-32.	0.8	6