Leif D Jacobson

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/11232280/publications.pdf Version: 2024-02-01



#	Article	IF	CITATION
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	A one-electron model for the aqueous electron that includes many-body electron-water polarization: Bulk equilibrium structure, vertical electron binding energy, and optical absorption spectrum. Journal of Chemical Physics, 2010, 133, 154506.	1.2	89
4	An efficient, fragment-based electronic structure method for molecular systems: Self-consistent polarization with perturbative two-body exchange and dispersion. Journal of Chemical Physics, 2011, 134, 094118.	1.2	82
5	Comment on "Does the Hydrated Electron Occupy a Cavity?― Science, 2011, 331, 1387-1387.	6.0	78
6	Structure of the Aqueous Electron: Assessment of One-Electron Pseudopotential Models in Comparison to Experimental Data and Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2011, 115, 14470-14483.	1.1	69
7	Theoretical Characterization of Four Distinct Isomer Types in Hydrated-Electron Clusters, and Proposed Assignments for Photoelectron Spectra of Water Cluster Anions. Journal of the American Chemical Society, 2011, 133, 19889-19899.	6.6	57
8	Rapid computation of intermolecular interactions in molecular and ionic clusters: self-consistent polarization plus symmetry-adapted perturbation theory. Physical Chemistry Chemical Physics, 2012, 14, 7679.	1.3	56
9	Polarization-Bound Quasi-Continuum States Are Responsible for the "Blue Tail―in the Optical Absorption Spectrum of the Aqueous Electron. Journal of the American Chemical Society, 2010, 132, 10000-10002.	6.6	55
10	Nature's most squishy ion: The important role of solvent polarization in the description of the hydrated electron. International Reviews in Physical Chemistry, 2011, 30, 1-48.	0.9	48
11	The static-exchange electron-water pseudopotential, in conjunction with a polarizable water model: A new Hamiltonian for hydrated-electron simulations. Journal of Chemical Physics, 2009, 130, 124115.	1.2	47
12	Efficient Monomer-Based Quantum Chemistry Methods for Molecular and Ionic Clusters. Annual Reports in Computational Chemistry, 2013, 9, 25-58.	0.9	37
13	A Simple Algorithm for Determining Orthogonal, Self-Consistent Excited-State Wave Functions for a State-Specific Hamiltonian: Application to the Optical Spectrum of the Aqueous Electron. Journal of Chemical Theory and Computation, 2011, 7, 2085-2093.	2.3	15