Ralph A Wheeler

List of Publications by Year
in descending order

29 papers	1,173 citations	471509 17 h-index	552781 26 g-index
31 all docs	31 docs citations	31 times ranked	1295 citing authors

#	Article	IF	Citations
1	Structure factor lineshape model gives approximate nanoscale size of polar aggregates in the ionic liquid N-methyl-N-propylpyrrolidinium bis(trifluoromethylsulfonyl)imide. Physical Chemistry Chemical Physics, 2021, 23, 9061-9064.	2.8	1
2	viewSq, a Visual Molecular Dynamics (VMD) module for calculating, analyzing, and visualizing X-ray and neutron structure factors from atomistic simulations. Computer Physics Communications, 2021, 264, 107881.	7.5	22
3	Temperature Dependence of Static Structure Factor Peak Intensities for a Pyrrolidinium-Based Ionic Liquid. Journal of Physical Chemistry B, 2019, 123, 1672-1678.	2.6	9
4	Distinguishing the Protonation State of the Histidine Ligand to the Oxidized Ironâ€“Sulfur Cluster from the MitoNEET Family of Proteins. ChemPhysChem, 2017, 18, 39-41.	2.1	3
5	Distinguishing Protonation States of Histidine Ligands to the Oxidized Rieske Ironâ€“Sulfur Cluster through ¹⁵N Vibrational Frequency Shifts. ChemPhysChem, 2016, 17, 216-220.	2.1	2
6	Pressure Annealing as a Complement to Temperature Annealing To Find Low-Energy Structures of Oligomeric Molecules. Journal of Chemical Theory and Computation, 2009, 5, 1883-1894.	5.3	0
7	Flexible proteinâ€“flexible ligand docking with disrupted velocity simulated annealing. Proteins: Structure, Function and Bioinformatics, 2008, 71, 440-454.	2.6	30
8	Wavelet Transforms for Determining Time-Dependent Vibrational Frequencies. Journal of Chemical Theory and Computation, 2005, 1, 769-771.	5.3	10
9	Simulating Thermochemistry of p-Benzo-quinone Reduction and Binding of Ubiquinone in the Photosynthetic Reaction Center. ACS Symposium Series, 2004, , 51-69.	0.5	0
10	New perspectives on multiple-copy, mean-field molecular dynamics methods. Journal of Molecular Graphics and Modelling, 2004, 22, 349-357.	2.4	2
11	Practical multiple-copy methods for sampling classical statistical mechanical ensembles. Chemical Physics Letters, 2004, 386, 330-335.	2.6	3
12	Harmonic Vibrational Frequencies:â€‰ Scaling Factors for HF, B3LYP, and MP2 Methods in Combination with Correlation Consistent Basis Sets. Journal of Physical Chemistry A, 2004, 108, 9213-9217.	2.5	405
13	Introduction to the Molecular Bioenergetics of Electron, Proton, and Energy Transfer. ACS Symposium Series, 2004, , 1-6.	0.5	9
14	A Quantum Chemical View of the Initial Photochemical Event in Photosynthesis. ACS Symposium Series, 2004, , 7-35.	0.5	0
15	Optimal Spectrum Estimation in Statistical Mechanics. ChemPhysChem, 2003, 4, 1227-1230.	2.1	20
16	Quasiharmonic Vibrations of Water, Water Dimer, and Liquid Water from Principal Component Analysis of Quantum or QM/MM Trajectories. ChemPhysChem, 2003, 4, 382-384.	2.1	37
17	Vibrational Assignments for High Molecular Weight Linear Polyethylenimine (LPEI) Based on Monomeric and Tetrameric Model Compounds. Macromolecules, 2003, 36, 7348-7351.	4.8	40
18	Rigorous classical-mechanical derivation of a multiple-copy algorithm for sampling statistical mechanical ensembles. Physical Review E, 2001, 64, 026701.	2.1	6

#	Article	IF	Citations
19	Amino Acid Protonation States Determine Binding Sites of the Secondary Ubiquinone and Its Anion in theRhodobacter sphaeroidesPhotosynthetic Reaction Center1. Journal of Physical Chemistry B, 1999, 103, 5380-5387.	2.6	60
20	Compatibility of correlation-consistent basis sets with a hybrid Hartree-Fock/density functional method. Journal of Computational Chemistry, 1999, 20, 207-216.	3.3	37
21	Oxidative Aromatic Substitutions:â€‰ Hartreeâ^'Fock/Density Functional and ab Initio Molecular Orbital Studies of Benzene and Toluene Nitrosation. Journal of Physical Chemistry A, 1999, 103, 4261-4269.	2.5	42
22	ViPA: A computer program for vector projection analysis of normal vibrational modes of molecules. Computer Physics Communications, 1998, 113, 78-84.	7.5	27
23	Vibrational projection analysis: New tool for quantitatively comparing vibrational normal modes of similar molecules. Journal of Computational Chemistry, 1998, 19, 1663-1674.	3.3	41
24	Trimethyl-p-benzoquinone Provides Excellent Structural, Spectroscopic, and Thermochemical Models for Plastoquinone-1 and Its Radical Anion. Journal of Physical Chemistry A, 1997, 101, 1160-1165.	2.5	34
25	A Comparison of the Properties of Various Fused-Ring Quinones and Their Radical Anions Using Hartreeâ^'Fock and Hybrid Hartreeâ^'Fock/Density Functional Methods. Journal of Physical Chemistry A, 1997, 101, 7154-7166.	2.5	54
26	Ï€-Donor Substituent Effects on Calculated Structures, Spin Properties, and Vibrations of Radical Anions ofp-Chloranil,p-Fluoranil, andp-Benzoquinone. Journal of Physical Chemistry A, 1997, 101, 8351-8359.	2.5	55
27	Structures and Properties of Ubiquinone-1 and Its Radical Anion from Hybrid Hartreeâ^'Fock/Density Functional Studies. Journal of Physical Chemistry A, 1997, 101, 5799-5804.	2.5	36
28	.pi.-Donor Substituent Effects on Calculated Structures and Vibrational Frequencies of p-Benzoquinone, p-Fluoranil, and p-Chloranil. The Journal of Physical Chemistry, 1995, 99, 8125-8134.	2.9	69
29	Densityâ€functional methods give accurate vibrational frequencies and spin densities for phenoxyl radical. Journal of Chemical Physics, 1995, 102, 1689-1698.	3.0	119