

# Ralph A Wheeler

## List of Publications by Year in descending order

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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	Harmonic Vibrational Frequencies: Scaling Factors for HF, B3LYP, and MP2 Methods in Combination with Correlation Consistent Basis Sets. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9213-9217.	2.5	405
2	Density-functional methods give accurate vibrational frequencies and spin densities for phenoxyl radical. <i>Journal of Chemical Physics</i> , 1995, 102, 1689-1698.	3.0	119
3	$\pi$ -Donor Substituent Effects on Calculated Structures and Vibrational Frequencies of p-Benzoquinone, p-Fluoranil, and p-Chloranil. <i>The Journal of Physical Chemistry</i> , 1995, 99, 8125-8134.	2.9	69
4	Amino Acid Protonation States Determine Binding Sites of the Secondary Ubiquinone and Its Anion in the Rhodospirillum rubrum Photosynthetic Reaction Center. <i>Journal of Physical Chemistry B</i> , 1999, 103, 5380-5387.	2.6	60
5	$\pi$ -Donor Substituent Effects on Calculated Structures, Spin Properties, and Vibrations of Radical Anions of p-Chloranil, p-Fluoranil, and p-Benzoquinone. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8351-8359.	2.5	55
6	A Comparison of the Properties of Various Fused-Ring Quinones and Their Radical Anions Using Hartree-Fock and Hybrid Hartree-Fock/Density Functional Methods. <i>Journal of Physical Chemistry A</i> , 1997, 101, 7154-7166.	2.5	54
7	Oxidative Aromatic Substitutions: Hartree-Fock/Density Functional and ab Initio Molecular Orbital Studies of Benzene and Toluene Nitrosation. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4261-4269.	2.5	42
8	Vibrational projection analysis: New tool for quantitatively comparing vibrational normal modes of similar molecules. <i>Journal of Computational Chemistry</i> , 1998, 19, 1663-1674.	3.3	41
9	Vibrational Assignments for High Molecular Weight Linear Polyethylenimine (LPEI) Based on Monomeric and Tetrameric Model Compounds. <i>Macromolecules</i> , 2003, 36, 7348-7351.	4.8	40
10	Compatibility of correlation-consistent basis sets with a hybrid Hartree-Fock/density functional method. <i>Journal of Computational Chemistry</i> , 1999, 20, 207-216.	3.3	37
11	Quasiharmonic Vibrations of Water, Water Dimer, and Liquid Water from Principal Component Analysis of Quantum or QM/MM Trajectories. <i>ChemPhysChem</i> , 2003, 4, 382-384.	2.1	37
12	Structures and Properties of Ubiquinone-1 and Its Radical Anion from Hybrid Hartree-Fock/Density Functional Studies. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5799-5804.	2.5	36
13	Trimethyl-p-benzoquinone Provides Excellent Structural, Spectroscopic, and Thermochemical Models for Plastoquinone-1 and Its Radical Anion. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1160-1165.	2.5	34
14	Flexible protein flexible ligand docking with disrupted velocity simulated annealing. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 71, 440-454.	2.6	30
15	ViPA: A computer program for vector projection analysis of normal vibrational modes of molecules. <i>Computer Physics Communications</i> , 1998, 113, 78-84.	7.5	27
16	viewSq, a Visual Molecular Dynamics (VMD) module for calculating, analyzing, and visualizing X-ray and neutron structure factors from atomistic simulations. <i>Computer Physics Communications</i> , 2021, 264, 107881.	7.5	22
17	Optimal Spectrum Estimation in Statistical Mechanics. <i>ChemPhysChem</i> , 2003, 4, 1227-1230.	2.1	20
18	Wavelet Transforms for Determining Time-Dependent Vibrational Frequencies. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 769-771.	5.3	10

#	ARTICLE	IF	CITATIONS
19	Introduction to the Molecular Bioenergetics of Electron, Proton, and Energy Transfer. ACS Symposium Series, 2004, , 1-6.	0.5	9
20	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
21	Rigorous classical-mechanical derivation of a multiple-copy algorithm for sampling statistical mechanical ensembles. Physical Review E, 2001, 64, 026701.	2.1	6
22	Practical multiple-copy methods for sampling classical statistical mechanical ensembles. Chemical Physics Letters, 2004, 386, 330-335.	2.6	3
23	Distinguishing the Protonation State of the Histidine Ligand to the Oxidized Iron-Sulfur Cluster from the MitoNEET Family of Proteins. ChemPhysChem, 2017, 18, 39-41.	2.1	3
24	New perspectives on multiple-copy, mean-field molecular dynamics methods. Journal of Molecular Graphics and Modelling, 2004, 22, 349-357.	2.4	2
25	Distinguishing Protonation States of Histidine Ligands to the Oxidized Rieske Iron-Sulfur Cluster through <sup>15</sup> N Vibrational Frequency Shifts. ChemPhysChem, 2016, 17, 216-220.	2.1	2
26	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
27	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
28	A Quantum Chemical View of the Initial Photochemical Event in Photosynthesis. ACS Symposium Series, 2004, , 7-35.	0.5	0
29	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