

William J Glover

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

38
papers

1,127
citations

16
h-index

33
g-index

54
ext. papers

1,258
ext. citations

5.9
avg, IF

4.66
L-index

#	Paper	IF	Citations
38	Accurate Prediction of Absorption Spectral Shifts of Proteorhodopsin Using a Fragment-Based Quantum Mechanical Method. <i>Molecules</i> , 2021 , 26,	4.8	2
37	Diabatic Many-Body Expansion: Development and Application to Charge-Transfer Reactions. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 1497-1511	6.4	2
36	Active orbital preservation for multiconfigurational self-consistent field. <i>Journal of Chemical Physics</i> , 2021 , 155, 071103	3.9	0
35	Flexible boundary layer using exchange for embedding theories. I. Theory and implementation.. <i>Journal of Chemical Physics</i> , 2021 , 155, 224112	3.9	1
34	Flexible boundary layer using exchange for embedding theories. II. QM/MM dynamics of the hydrated electron.. <i>Journal of Chemical Physics</i> , 2021 , 155, 224113	3.9	4
33	Fragment Quantum Mechanical Method for Excited States of Proteins: Development and Application to the Green Fluorescent Protein. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 5174-5188	6.4	12
32	SSAIMS-Stochastic-Selection Multiple Spawning for Efficient Nonadiabatic Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 6133-6143	2.8	10
31	The Fluxional Nature of the Hydrated Electron: Energy and Entropy Contributions to Aqueous Electron Free Energies. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 1263-1270	6.4	9
30	Prediction of Excited-State Properties of Oligoacene Crystals Using Fragment-Based Quantum Mechanical Method. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 5407-5417	2.8	15
29	Two-Dimensional Electronic Spectroscopy Reveals the Spectral Dynamics of Förster Resonance Energy Transfer. <i>Chem</i> , 2019 , 5, 2111-2125	16.2	9
28	Analytical gradients and derivative couplings for dynamically weighted complete active space self-consistent field. <i>Journal of Chemical Physics</i> , 2019 , 151, 201101	3.9	5
27	Excited state non-adiabatic dynamics of the smallest polyene, trans 1,3-butadiene. I. Time-resolved photoelectron-photoion coincidence spectroscopy. <i>Journal of Chemical Physics</i> , 2018 , 148, 164302	3.9	28
26	Excited state non-adiabatic dynamics of the smallest polyene, trans 1,3-butadiene. II. Ab initio multiple spawning simulations. <i>Journal of Chemical Physics</i> , 2018 , 148, 164303	3.9	37
25	Polarizable Embedding for Excited-State Reactions: Dynamically Weighted Polarizable QM/MM. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 2137-2144	6.4	9
24	Temperature dependence of the hydrated electron's excited-state relaxation. I. Simulation predictions of resonance Raman and pump-probe transient absorption spectra of cavity and non-cavity models. <i>Journal of Chemical Physics</i> , 2017 , 147, 074503	3.9	14
23	Short-Range Electron Correlation Stabilizes Noncavity Solvation of the Hydrated Electron. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 5117-5131	6.4	26
22	Free Energies of Cavity and Noncavity Hydrated Electrons Near the Instantaneous Air/Water Interface. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 3192-8	6.4	27

21	Free Energies of Quantum Particles: The Coupled-Perturbed Quantum Umbrella Sampling Method. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4661-71	6.4	13
20	Ab initio multiple cloning algorithm for quantum nonadiabatic molecular dynamics. <i>Journal of Chemical Physics</i> , 2014 , 141, 054110	3.9	135
19	Communication: Smoothing out excited-state dynamics: analytical gradients for dynamically weighted complete active space self-consistent field. <i>Journal of Chemical Physics</i> , 2014 , 141, 171102	3.9	15
18	Between ethylene and polyenes--the non-adiabatic dynamics of cis-dienes. <i>Faraday Discussions</i> , 2012 , 157, 193-212; discussion 243-84	3.6	49
17	Role of Rydberg states in the photochemical dynamics of ethylene. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 2808-18	2.8	119
16	Ultrafast internal conversion in ethylene. II. Mechanisms and pathways for quenching and hydrogen elimination. <i>Journal of Chemical Physics</i> , 2012 , 136, 124317	3.9	59
15	Simulating the formation of sodium:electron tight-contact pairs: watching the solvation of atoms in liquids one molecule at a time. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 5887-94	2.8	8
14	Response to Comments on "Does the Hydrated Electron Occupy a Cavity?". <i>Science</i> , 2011 , 331, 1387-1387	3.3	52
13	First principles multielectron mixed quantum/classical simulations in the condensed phase. II. The charge-transfer-to-solvent states of sodium anions in liquid tetrahydrofuran. <i>Journal of Chemical Physics</i> , 2010 , 132, 144102	3.9	12
12	First principles multielectron mixed quantum/classical simulations in the condensed phase. I. An efficient Fourier-grid method for solving the many-electron problem. <i>Journal of Chemical Physics</i> , 2010 , 132, 144101	3.9	16
11	Watching the solvation of atoms in liquids one solvent molecule at a time. <i>Physical Review Letters</i> , 2010 , 104, 233005	7.4	13
10	How Does a Solvent Affect Chemical Bonds? Mixed Quantum/Classical Simulations with a Full CI Treatment of the Bonding Electrons. <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 165-169	6.4	16
9	Does the hydrated electron occupy a cavity?. <i>Science</i> , 2010 , 329, 65-9	33.3	181
8	Nature of sodium atoms/(Na(+), e(-)) contact pairs in liquid tetrahydrofuran. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 11535-43	3.4	16
7	Comment on "An electron-water pseudopotential for condensed phase simulation" [J. Chem. Phys. 86, 3462 (1987)]. <i>Journal of Chemical Physics</i> , 2009 , 131, 037101; author reply 037102	3.9	12
6	The roles of electronic exchange and correlation in charge-transfer- to-solvent dynamics: Many-electron nonadiabatic mixed quantum/classical simulations of photoexcited sodium anions in the condensed phase. <i>Journal of Chemical Physics</i> , 2008 , 129, 164505	3.9	21
5	The structure of the hydrated electron. Part 2. A mixed quantum/classical molecular dynamics embedded cluster density functional theory: single-excitation configuration interaction study. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 5232-43	2.8	50
4	A computationally efficient exact pseudopotential method. II. Application to the molecular pseudopotential of an excess electron interacting with tetrahydrofuran (THF). <i>Journal of Chemical Physics</i> , 2006 , 125, 074103	3.9	11

3	A computationally efficient exact pseudopotential method. I. Analytic reformulation of the Phillips-Kleinman theory. <i>Journal of Chemical Physics</i> , 2006 , 125, 074102	3.9	37
2	Comparison of S, Pt, and Hf adsorption on NiAl(110). <i>Surface Science</i> , 2006 , 600, 2079-2090	1.8	22
1	Raman spectra of ionic liquids: a simulation study of LaCl ₃ and its mixtures with alkali chlorides. <i>Journal of Chemical Physics</i> , 2004 , 121, 7293-303	3.9	58