William J Glover

List of Publications by Citations

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	Does the hydrated electron occupy a cavity?. *Science*, **2010**, 329, 65-9	33.3	181
37	Ab initio multiple cloning algorithm for quantum nonadiabatic molecular dynamics. *Journal of Chemical Physics*, **2014**, 141, 054110	3.9	135
36	Role of Rydberg states in the photochemical dynamics of ethylene. *Journal of Physical Chemistry A*, **2012**, 116, 2808-18	2.8	119
35	Ultrafast internal conversion in ethylene. II. Mechanisms and pathways for quenching and hydrogen elimination. *Journal of Chemical Physics*, **2012**, 136, 124317	3.9	59
34	Raman spectra of ionic liquids: a simulation study of LaCl3 and its mixtures with alkali chlorides. *Journal of Chemical Physics*, **2004**, 121, 7293-303	3.9	58
33	Response to Comments on "Does the Hydrated Electron Occupy a Cavity?". *Science*, **2011**, 331, 1387-1387	33.3	52
32	The structure of the hydrated electron. Part 2. A mixed quantum/classical molecular dynamics embedded cluster density functional theory: single-excitation configuration interaction study. *Journal of Physical Chemistry A*, **2007**, 111, 5232-43	2.8	50
31	Between ethylene and polyenes--the non-adiabatic dynamics of cis-dienes. *Faraday Discussions*, **2012**, 157, 193-212; discussion 243-84	3.6	49
30	Excited state non-adiabatic dynamics of the smallest polyene, trans 1,3-butadiene. II. Ab initio multiple spawning simulations. *Journal of Chemical Physics*, **2018**, 148, 164303	3.9	37
29	A computationally efficient exact pseudopotential method. I. Analytic reformulation of the Phillips-Kleinman theory. *Journal of Chemical Physics*, **2006**, 125, 074102	3.9	37
28	Excited state non-adiabatic dynamics of the smallest polyene, trans 1,3-butadiene. I. Time-resolved photoelectron-photoion coincidence spectroscopy. *Journal of Chemical Physics*, **2018**, 148, 164302	3.9	28
27	Free Energies of Cavity and Noncavity Hydrated Electrons Near the Instantaneous Air/Water Interface. *Journal of Physical Chemistry Letters*, **2016**, 7, 3192-8	6.4	27
26	Short-Range Electron Correlation Stabilizes Noncavity Solvation of the Hydrated Electron. *Journal of Chemical Theory and Computation*, **2016**, 12, 5117-5131	6.4	26
25	Comparison of S, Pt, and Hf adsorption on NiAl(110). *Surface Science*, **2006**, 600, 2079-2090	1.8	22
24	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. *Journal of Chemical Physics*, **2008**, 129, 164505	3.9	21
23	First principles multielectron mixed quantum/classical simulations in the condensed phase. I. An efficient Fourier-grid method for solving the many-electron problem. *Journal of Chemical Physics*, **2010**, 132, 144101	3.9	16
22	How Does a Solvent Affect Chemical Bonds? Mixed Quantum/Classical Simulations with a Full CI Treatment of the Bonding Electrons. *Journal of Physical Chemistry Letters*, **2010**, 1, 165-169	6.4	16

21	Nature of sodium atoms/(Na(+), e(-)) contact pairs in liquid tetrahydrofuran. *Journal of Physical Chemistry B*, **2010**, 114, 11535-43	3.4	16
20	Prediction of Excited-State Properties of Oligoacene Crystals Using Fragment-Based Quantum Mechanical Method. *Journal of Physical Chemistry A*, **2019**, 123, 5407-5417	2.8	15
19	Communication: Smoothing out excited-state dynamics: analytical gradients for dynamically weighted complete active space self-consistent field. *Journal of Chemical Physics*, **2014**, 141, 171102	3.9	15
18	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. *Journal of Chemical Physics*, **2017**, 147, 074503	3.9	14
17	Free Energies of Quantum Particles: The Coupled-Perturbed Quantum Umbrella Sampling Method. *Journal of Chemical Theory and Computation*, **2014**, 10, 4661-71	6.4	13
16	Watching the solvation of atoms in liquids one solvent molecule at a time. *Physical Review Letters*, **2010**, 104, 233005	7.4	13
15	Fragment Quantum Mechanical Method for Excited States of Proteins: Development and Application to the Green Fluorescent Protein. *Journal of Chemical Theory and Computation*, **2020**, 16, 5174-5188	6.4	12
14	First principles multielectron mixed quantum/classical simulations in the condensed phase. II. The charge-transfer-to-solvent states of sodium anions in liquid tetrahydrofuran. *Journal of Chemical Physics*, **2010**, 132, 144102	3.9	12
13	Comment on "An electron-water pseudopotential for condensed phase simulation" [J. Chem. Phys. 86, 3462 (1987)]. *Journal of Chemical Physics*, **2009**, 131, 037101; author reply 037102	3.9	12
12	A computationally efficient exact pseudopotential method. II. Application to the molecular pseudopotential of an excess electron interacting with tetrahydrofuran (THF). *Journal of Chemical Physics*, **2006**, 125, 074103	3.9	11
11	SSAIMS-Stochastic-Selection Multiple Spawning for Efficient Nonadiabatic Molecular Dynamics. *Journal of Physical Chemistry A*, **2020**, 124, 6133-6143	2.8	10
10	Two-Dimensional Electronic Spectroscopy Reveals the Spectral Dynamics of Förster Resonance Energy Transfer. *CheM*, **2019**, 5, 2111-2125	16.2	9
9	Polarizable Embedding for Excited-State Reactions: Dynamically Weighted Polarizable QM/MM. *Journal of Chemical Theory and Computation*, **2018**, 14, 2137-2144	6.4	9
8	The Fluxional Nature of the Hydrated Electron: Energy and Entropy Contributions to Aqueous Electron Free Energies. *Journal of Chemical Theory and Computation*, **2020**, 16, 1263-1270	6.4	9
7	Simulating the formation of sodium:electron tight-contact pairs: watching the solvation of atoms in liquids one molecule at a time. *Journal of Physical Chemistry A*, **2011**, 115, 5887-94	2.8	8
6	Analytical gradients and derivative couplings for dynamically weighted complete active space self-consistent field. *Journal of Chemical Physics*, **2019**, 151, 201101	3.9	5
5	Flexible boundary layer using exchange for embedding theories. II. QM/MM dynamics of the hydrated electron.. *Journal of Chemical Physics*, **2021**, 155, 224113	3.9	4
4	Accurate Prediction of Absorption Spectral Shifts of Proteorhodopsin Using a Fragment-Based Quantum Mechanical Method. *Molecules*, **2021**, 26,	4.8	2

3	Diabatic Many-Body Expansion: Development and Application to Charge-Transfer Reactions. *Journal of Chemical Theory and Computation*, **2021**, 17, 1497-1511	6.4	2
2	Flexible boundary layer using exchange for embedding theories. I. Theory and implementation.. *Journal of Chemical Physics*, **2021**, 155, 224112	3.9	1
1	Active orbital preservation for multiconfigurational self-consistent field. *Journal of Chemical Physics* , **2021**, 155, 071103	3.9	0