

William J Glover

List of Publications by Year in descending order

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39
papers

1,383
citations

394286

19
h-index

330025

37
g-index

54
all docs

54
docs citations

54
times ranked

1235
citing authors

#	ARTICLE	IF	CITATIONS
1	Does the Hydrated Electron Occupy a Cavity?. <i>Science</i> , 2010, 329, 65-69.	6.0	212
2	<i>Ab initio</i> multiple cloning algorithm for quantum nonadiabatic molecular dynamics. <i>Journal of Chemical Physics</i> , 2014, 141, 054110.	1.2	168
3	Role of Rydberg States in the Photochemical Dynamics of Ethylene. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2808-2818.	1.1	127
4	Ultrafast internal conversion in ethylene. II. Mechanisms and pathways for quenching and hydrogen elimination. <i>Journal of Chemical Physics</i> , 2012, 136, 124317.	1.2	72
5	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, 7293-7303.	1.2	64
6	Response to Comments on "Does the Hydrated Electron Occupy a Cavity?". <i>Science</i> , 2011, 331, 1387-1387.	6.0	58
7	Between ethylene and polyenes - the non-adiabatic dynamics of cis-dienes. <i>Faraday Discussions</i> , 2012, 157, 193.	1.6	54
8	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, 5232-5243.	1.1	51
9	Excited state non-adiabatic dynamics of the smallest polyene, <i>trans</i> 1,3-butadiene. II. <i>Ab initio</i> multiple spawning simulations. <i>Journal of Chemical Physics</i> , 2018, 148, 164303.	1.2	51
10	A computationally efficient exact pseudopotential method. I. Analytic reformulation of the Phillips-Kleinman theory. <i>Journal of Chemical Physics</i> , 2006, 125, 074102.	1.2	41
11	Short-Range Electron Correlation Stabilizes Noncavity Solvation of the Hydrated Electron. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5117-5131.	2.3	35
12	Free Energies of Cavity and Noncavity Hydrated Electrons Near the Instantaneous Air/Water Interface. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3192-3198.	2.1	35
13	Excited state non-adiabatic dynamics of the smallest polyene, <i>trans</i> 1,3-butadiene. I. Time-resolved photoelectron-photoion coincidence spectroscopy. <i>Journal of Chemical Physics</i> , 2018, 148, 164302.	1.2	35
14	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.	1.2	27
15	Comparison of S, Pt, and Hf adsorption on NiAl(110). <i>Surface Science</i> , 2006, 600, 2079-2090.	0.8	26
16	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.	2.3	26
17	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.	1.2	22
18	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.	2.1	21

#	ARTICLE	IF	CITATIONS
19	Nature of Sodium Atoms/(Na ⁺ , e ⁻) Contact Pairs in Liquid Tetrahydrofuran. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11535-11543.	1.2	20
20	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.	1.2	19
21	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.	1.2	19
22	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.	1.1	18
23	Watching the Solvation of Atoms in Liquids One Solvent Molecule at a Time. <i>Physical Review Letters</i> , 2010, 104, 233005.	2.9	15
24	Free Energies of Quantum Particles: The Coupled-Perturbed Quantum Umbrella Sampling Method. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4661-4671.	2.3	15
25	Polarizable Embedding for Excited-State Reactions: Dynamically Weighted Polarizable QM/MM. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2137-2144.	2.3	15
26	Two-Dimensional Electronic Spectroscopy Reveals the Spectral Dynamics of Förster Resonance Energy Transfer. <i>CheM</i> , 2019, 5, 2111-2125.	5.8	15
27	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.	1.2	14
28	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.	2.3	14
29	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.	1.2	13
30	SSAIMS "Stochastic-Selection" Multiple Spawning for Efficient Nonadiabatic Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6133-6143.	1.1	13
31	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.	1.2	12
32	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, 5887-5894.	1.1	11
33	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.	1.2	11
34	Analytical gradients and derivative couplings for dynamically weighted complete active space self-consistent field. <i>Journal of Chemical Physics</i> , 2019, 151, 201101.	1.2	8
35	Accurate Prediction of Absorption Spectral Shifts of Proteorhodopsin Using a Fragment-Based Quantum Mechanical Method. <i>Molecules</i> , 2021, 26, 4486.	1.7	8
36	Ultrafast Photoisomerization of Ethylene Studied Using Time-Resolved Extreme Ultraviolet Photoelectron Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3873-3879.	1.1	6

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37	Diabatic Many-Body Expansion: Development and Application to Charge-Transfer Reactions. Journal of Chemical Theory and Computation, 2021, 17, 1497-1511.	2.3	5
38	Active orbital preservation for multiconfigurational self-consistent field. Journal of Chemical Physics, 2021, 155, 071103.	1.2	2
39	Flexible boundary layer using exchange for embedding theories. I. Theory and implementation. Journal of Chemical Physics, 2021, 155, 224112.	1.2	2