William J Glover

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3788308/publications.pdf

Version: 2024-02-01

39	1,383	394421	330143
papers	citations	19 h-index	37 g-index

54	54	54	1235
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ultrafast Photoisomerization of Ethylene Studied Using Time-Resolved Extreme Ultraviolet Photoelectron Spectroscopy. Journal of Physical Chemistry A, 2022, 126, 3873-3879.	2.5	6
2	Diabatic Many-Body Expansion: Development and Application to Charge-Transfer Reactions. Journal of Chemical Theory and Computation, 2021, 17, 1497-1511.	5.3	5
3	Accurate Prediction of Absorption Spectral Shifts of Proteorhodopsin Using a Fragment-Based Quantum Mechanical Method. Molecules, 2021, 26, 4486.	3.8	8
4	Active orbital preservation for multiconfigurational self-consistent field. Journal of Chemical Physics, 2021, 155, 071103.	3.0	2
5	Flexible boundary layer using exchange for embedding theories. I. Theory and implementation. Journal of Chemical Physics, 2021, 155, 224112.	3.0	2
6	Flexible boundary layer using exchange for embedding theories. II. QM/MM dynamics of the hydrated electron. Journal of Chemical Physics, 2021, 155, 224113.	3.0	11
7	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.	5.3	14
8	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.	5.3	26
9	SSAIMSâ€"Stochastic-Selection Ab Initio Multiple Spawning for Efficient Nonadiabatic Molecular Dynamics. Journal of Physical Chemistry A, 2020, 124, 6133-6143.	2.5	13
10	Prediction of Excited-State Properties of Oligoacene Crystals Using Fragment-Based Quantum Mechanical Method. Journal of Physical Chemistry A, 2019, 123, 5407-5417.	2.5	18
11	Two-Dimensional Electronic Spectroscopy Reveals the Spectral Dynamics of FÃ¶rster Resonance Energy Transfer. CheM, 2019, 5, 2111-2125.	11.7	15
12	Analytical gradients and derivative couplings for dynamically weighted complete active space self-consistent field. Journal of Chemical Physics, 2019, 151, 201101.	3.0	8
13	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.	3.0	35
14	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.	3.0	51
15	Polarizable Embedding for Excited-State Reactions: Dynamically Weighted Polarizable QM/MM. Journal of Chemical Theory and Computation, 2018, 14, 2137-2144.	5.3	15
16	Temperature dependence of the hydrated electronâ€™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.	3.0	22
17	Short-Range Electron Correlation Stabilizes Noncavity Solvation of the Hydrated Electron. Journal of Chemical Theory and Computation, 2016, 12, 5117-5131.	5.3	35
18	Free Energies of Cavity and Noncavity Hydrated Electrons Near the Instantaneous Air/Water Interface. Journal of Physical Chemistry Letters, 2016, 7, 3192-3198.	4.6	35

#	Article	IF	Citations
19	Ab initio multiple cloning algorithm for quantum nonadiabatic molecular dynamics. Journal of Chemical Physics, 2014, 141, 054110.	3.0	168
20	Communication: Smoothing out excited-state dynamics: Analytical gradients for dynamically weighted complete active space self-consistent field. Journal of Chemical Physics, 2014, 141, 171102.	3.0	19
21	Free Energies of Quantum Particles: The Coupled-Perturbed Quantum Umbrella Sampling Method. Journal of Chemical Theory and Computation, 2014, 10, 4661-4671.	5.3	15
22	Ultrafast internal conversion in ethylene. II. Mechanisms and pathways for quenching and hydrogen elimination. Journal of Chemical Physics, 2012, 136, 124317.	3.0	72
23	Between ethylene and polyenes - the non-adiabatic dynamics of cis-dienes. Faraday Discussions, 2012, 157, 193.	3.2	54
24	Role of Rydberg States in the Photochemical Dynamics of Ethylene. Journal of Physical Chemistry A, 2012, 116, 2808-2818.	2.5	127
25	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, 5887-5894.	2.5	11
26	Response to Comments on â€œDoes the Hydrated Electron Occupy a Cavity?â€• Science, 2011, 331, 1387-1387.	12.6	58
27	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.	3.0	12
28	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.	3.0	19
29	Watching the Solvation of Atoms in Liquids One Solvent Molecule at a Time. Physical Review Letters, 2010, 104, 233005.	7.8	15
30	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.	4.6	21
31	Does the Hydrated Electron Occupy a Cavity?. Science, 2010, 329, 65-69.	12.6	212
32	Nature of Sodium Atoms/(Na⁺, e^{â^'}) Contact Pairs in Liquid Tetrahydrofuran. Journal of Physical Chemistry B, 2010, 114, 11535-11543.	2.6	20
33	Comment on â€œAn electron-water pseudopotential for condensed phase simulationâ€•[J. Chem. Phys. 86, 3462 (1987)]. Journal of Chemical Physics, 2009, 131, 037101; author reply 037102.	3.0	14
34	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.	3.0	27
35	The Structure of the Hydrated Electron. Part 2. A Mixed Quantum/Classical Molecular Dynamics Embedded Cluster Density Functional Theory:â€‰Singleâ^'Excitation Configuration Interaction Study. Journal of Physical Chemistry A, 2007, 111, 5232-5243.	2.5	51
36	A computationally efficient exact pseudopotential method. I. Analytic reformulation of the Phillips-Kleinman theory. Journal of Chemical Physics, 2006, 125, 074102.	3.0	41

#	Article	IF	Citations
37	Comparison of S, Pt, and Hf adsorption on NiAl(110). Surface Science, 2006, 600, 2079-2090.	1.9	26
38	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.	3.0	13
39	Raman spectra of ionic liquids: A simulation study of LaCl3 and its mixtures with alkali chlorides. Journal of Chemical Physics, 2004, 121, 7293-7303.	3.0	64