Daniel Hollas

List of Publications by Year
in descending order

19 papers	838 citations	567281 15 h-index	794594 19 g-index
19 all docs	19 docs citations	19 times ranked	1105 citing authors

#	Article	IF	Citations
1	Performance of Molecular Mechanics Force Fields for RNA Simulations: Stability of UUCG and GNRA Hairpins. Journal of Chemical Theory and Computation, 2010, 6, 3836-3849.	5.3	339
2	Extensive Molecular Dynamics Simulations Showing That Canonical G8 and Protonated A38H⁺ Forms Are Most Consistent with Crystal Structures of Hairpin Ribozyme. Journal of Physical Chemistry B, 2010, 114, 6642-6652.	2.6	81
3	Nonadiabatic Ab Initio Molecular Dynamics with the Floating Occupation Molecular Orbital-Complete Active Space Configuration Interaction Method. Journal of Chemical Theory and Computation, 2018, 14, 339-350.	5.3	53
4	Reaction selectivity in an ionized water dimer: nonadiabatic ab initio dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 11531.	2.8	48
5	On the importance of initial conditions for excited-state dynamics. Faraday Discussions, 2018, 212, 307-330.	3.2	38
6	Competition between proton transfer and intermolecular Coulombic decay in water. Nature Communications, 2018, 9, 4988.	12.8	34
7	Mechanisms of fluorescence quenching in prototypical aggregation-induced emission systems: excited state dynamics with TD-DFTB. Physical Chemistry Chemical Physics, 2019, 21, 9026-9035.	2.8	28
8	Two Tryptophans Are Better Than One in Accelerating Electron Flow through a Protein. ACS Central Science, 2019, 5, 192-200.	11.3	28
9	Modeling Liquid Photoemission Spectra: Path-Integral Molecular Dynamics Combined with Tuned Range-Separated Hybrid Functionals. Journal of Chemical Theory and Computation, 2016, 12, 5009-5017.	5.3	26
10	Clustering and Photochemistry of Freon CF₂Cl₂ on Argon and Ice Nanoparticles. Journal of Physical Chemistry A, 2014, 118, 4740-4749.	2.5	23
11	UV absorption of Criegee intermediates: quantitative cross sections from high-level ab initio theory. Physical Chemistry Chemical Physics, 2018, 20, 6421-6430.	2.8	23
12	Control of X-ray Induced Electron and Nuclear Dynamics in Ammonia and Glycine Aqueous Solution via Hydrogen Bonding. Journal of Physical Chemistry B, 2015, 119, 10750-10759.	2.6	22
13	On the Performance of Optimally Tuned Range-Separated Hybrid Functionals for X-ray Absorption Modeling. Journal of Chemical Theory and Computation, 2015, 11, 3234-3244.	5.3	20
14	Hamiltonian-Reservoir Replica Exchange and Machine Learning Potentials for Computational Organic Chemistry. Journal of Chemical Theory and Computation, 2020, 16, 3084-3094.	5.3	16
15	Fragmentation of HClâ€“water clusters upon ionization: Non-adiabatic ab initio dynamics study. Chemical Physics Letters, 2015, 622, 80-85.	2.6	15
16	Calculating Photoabsorption Cross-Sections for Atmospheric Volatile Organic Compounds. ACS Earth and Space Chemistry, 2022, 6, 207-217.	2.7	14
17	Aqueous Solution Chemistry of Ammonium Cation in the Auger Time Window. Scientific Reports, 2017, 7, 756.	3.3	12
18	Ultrafast Proton and Electron Dynamics in Core-Ionized Hydrated Hydrogen Peroxide: Photoemission Measurements with Isotopically Substituted Hydrogen Peroxide. Journal of Physical Chemistry C, 2014, 118, 29142-29150.	3.1	10

#	Article	IF	Citations
19	Hydrogen dynamics in solid formic acid: insights from simulations with quantum colored-noise thermostats. Journal of Physics: Conference Series, 2018, 1055, 012003.	0.4	8