Ryan P Steele

List of Publications by Year
in descending order

32 papers	6,567 citations	471061 17 h-index	433756 31 g-index
34 all docs	34 docs citations	34 times ranked	7217 citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
3	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
4	An improved algorithm for analytical gradient evaluation in resolution-of-the-identity second-order MÃ¸ller-Plesset perturbation theory: Application to alanine tetrapeptide conformational analysis. Journal of Computational Chemistry, 2007, 28, 839-856.	1.5	134
5	The initial and final states of electron and energy transfer processes: Diabatization as motivated by system-solvent interactions. Journal of Chemical Physics, 2009, 130, 234102.	1.2	124
6	Efficient anharmonic vibrational spectroscopy for large molecules using local-mode coordinates. Journal of Chemical Physics, 2014, 141, 104105.	1.2	102
7	How the Shape of an H-Bonded Network Controls Proton-Coupled Water Activation in HONO Formation. Science, 2010, 327, 308-312.	6.0	99
8	Monitoring Water Clusters â€œMeltâ€•Through Vibrational Spectroscopy. Journal of the American Chemical Society, 2017, 139, 7082-7088.	6.6	69
9	Tuning vibrational mode localization with frequency windowing. Journal of Chemical Physics, 2016, 145, 124112.	1.2	47
10	Structural Progression in Clusters of Ionized Water, (H₂O)_{n=1â€“5}⁺. Journal of Physical Chemistry A, 2015, 119, 752-766.	1.1	42
11	Role of Ligand-Bound CO₂ in the Hydrogenation of CO₂ to Formate with a (PNP)Mn Catalyst. ACS Catalysis, 2021, 11, 8358-8369.	5.5	34
12	Vibrational Signatures of Conformer-Specific Intramolecular Interactions in Protonated Tryptophan. Journal of Physical Chemistry A, 2016, 120, 5598-5608.	1.1	32
13	Consecutive Charging of a Molecule-on-Insulator Ensemble Using Single Electron Tunnelling Methods. Nano Letters, 2016, 16, 911-916.	4.5	23
14	Communication: Multiple-timestep ab initio molecular dynamics with electron correlation. Journal of Chemical Physics, 2013, 139, 011102.	1.2	22
15	Vibrational Signatures of Electronic Properties in Oxidized Water: Unraveling the Anomalous Spectrum of the Water Dimer Cation. Journal of the American Chemical Society, 2016, 138, 11936-11945.	6.6	22
16	Ionâ€“Radical Pair Separation in Larger Oxidized Water Clusters, (H₂O)_{n=6â€“21}⁺. Journal of Physical Chemistry A, 2016, 120, 7225-7239.	1.1	21
17	Multiple-Timestep ab Initio Molecular Dynamics Using an Atomic Basis Set Partitioning. Journal of Physical Chemistry A, 2015, 119, 12119-12130.	1.1	17
18	Multiple-Time Step Ab Initio Molecular Dynamics Based on Two-Electron Integral Screening. Journal of Chemical Theory and Computation, 2015, 11, 884-898.	2.3	15

#	Article	IF	Citations
19	Infrared signatures of isomer selectivity and symmetry breaking in the Cs+(H2O)3 complex using many-body potential energy functions. Journal of Chemical Physics, 2020, 153, 044306.	1.2	15
20	Accelerating Ab Initio Path Integral Simulations via Imaginary Multiple-Timestepping. Journal of Chemical Theory and Computation, 2016, 12, 1627-1638.	2.3	12
21	Spectroscopic Signatures of Mode-Dependent Tunnel Splitting in the Iodideâ€“Water Binary Complex. Journal of Physical Chemistry A, 2020, 124, 2991-3001.	1.1	11
22	Probing the Partial Activation of Water by Open-Shell Interactions, Cl(H₂O)_{1â€“4}. Journal of Physical Chemistry A, 2019, 123, 8657-8673.	1.1	9
23	Accelerated ab initio molecular dynamics with response equation extrapolation. Chemical Physics Letters, 2010, 500, 167-171.	1.2	7
24	Signatures of Size-Dependent Structural Patterns in Hydrated Copper(I) Clusters, Cu⁺(H₂O)_{n=1â€“10}. Journal of Physical Chemistry A, 2016, 120, 10252-10263.	1.1	7
25	Accelerating ab initio molecular dynamics simulations by linear prediction methods. Chemical Physics Letters, 2016, 661, 42-47.	1.2	7
26	Stepwise Activation of Water by Open-Shell Interactions, Cl(H₂O)_{n=4â€“8,17}. Journal of Physical Chemistry A, 2020, 124, 3417-3437.	1.1	6
27	Quantum molecular motion in the mixed ion-radical complex, [(H₂O)(H₂S)]⁺. Physical Chemistry Chemical Physics, 2016, 18, 27450-27459.	1.3	5
28	Electronic Structure and Vibrational Signatures of the Delocalized Radical in Hydrated Clusters of Copper(â€œIIâ€) Hydroxide CuOH⁺(H₂O)_{0â€“2}. Journal of Physical Chemistry A, 2021, 125, 3631-3645.	1.1	3
29	Adiabatic Molecular Orbital Tracking in Ab Initio Molecular Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 4675-4685.	2.3	3
30	Nuclear Motion in the Ï*f*-Bound Regime of Metalâ€“H₂ Complexes: [Mg(H₂)_{n=1â€“6}]²⁺. Journal of Physical Chemistry A, 2014, 118, 10057-10066.	1.1	2
31	A tiered approach to Monte Carlo sampling with self-consistent field potentials. Journal of Chemical Physics, 2011, 135, 184107.	1.2	1
32	Nuclear Motion in the Intramolecular Dihydrogen-Bound Regime of an Aminoborane Complex. Journal of Physical Chemistry A, 2019, 123, 6547-6563.	1.1	0