John A Parkhill

List of Publications by Year
in descending order

35 papers	4,576 citations	430754 18 h-index	377752 34 g-index
35 all docs	35 docs citations	35 times ranked	5853 citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
2	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
3	The TensorMol-0.1 model chemistry: a neural network augmented with long-range physics. Chemical Science, 2018, 9, 2261-2269.	3.7	322
4	Origin of the Size-Dependent Stokes Shift in CsPbBr₃ Perovskite Nanocrystals. Journal of the American Chemical Society, 2017, 139, 12201-12208.	6.6	240
5	Kinetic Energy of Hydrocarbons as a Function of Electron Density and Convolutional Neural Networks. Journal of Chemical Theory and Computation, 2016, 12, 1139-1147.	2.3	101
6	Intrinsic Bond Energies from a Bonds-in-Molecules Neural Network. Journal of Physical Chemistry Letters, 2017, 8, 2689-2694.	2.1	100
7	The many-body expansion combined with neural networks. Journal of Chemical Physics, 2017, 146, 014106.	1.2	95
8	Benchmark results for empirical post-GGA functionals: Difficult exchange problems and independent tests. Physical Chemistry Chemical Physics, 2011, 13, 19325.	1.3	83
9	The perfect quadruples model for electron correlation in a valence active space. Journal of Chemical Physics, 2009, 130, 084101.	1.2	63
10	Metadynamics for training neural network model chemistries: A competitive assessment. Journal of Chemical Physics, 2018, 148, 241710.	1.2	51
11	Nearâ€Infrared Spectroscopy of Nitrogenated Polycyclic Aromatic Hydrocarbon Cations from 0.7 to 2.5 Î¼m. Astrophysical Journal, 2008, 680, 1243-1255.	1.6	39
12	A tractable and accurate electronic structure method for static correlations: The perfect hextuples model. Journal of Chemical Physics, 2010, 133, 024103.	1.2	37
13	Nonadiabatic Dynamics for Electrons at Second-Order: Real-Time TDDFT and OSCF2. Journal of Chemical Theory and Computation, 2015, 11, 2918-2924.	2.3	35
14	A truncation hierarchy of coupled cluster models of strongly correlated systems based on perfect-pairing references: The singles+doubles models. Journal of Chemical Physics, 2010, 133, 124102.	1.2	31
15	Black-Box, Real-Time Simulations of Transient Absorption Spectroscopy. Journal of Physical Chemistry Letters, 2016, 7, 1590-1595.	2.1	31
16	Penalty functions for combining coupled-cluster and perturbation amplitudes in local correlation methods with optimized orbitals. Molecular Physics, 2008, 106, 2309-2324.	0.8	29
17	Detection of electron tunneling across plasmonic nanoparticleâ€“film junctions using nitrile vibrations. Physical Chemistry Chemical Physics, 2017, 19, 5786-5796.	1.3	28
18	A sparse framework for the derivation and implementation of fermion algebra. Molecular Physics, 2010, 108, 513-522.	0.8	19

#	Article	IF	Citations
19	How electronic dynamics with Pauli exclusion produces Fermi-Dirac statistics. Journal of Chemical Physics, 2015, 142, 134113.	1.2	19
20	Feynmanâ€™s clock, a new variational principle, and parallel-in-time quantum dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, E3901-9.	3.3	18
21	Cost-effective description of strong correlation: Efficient implementations of the perfect quadruples and perfect hextuples models. Journal of Chemical Physics, 2016, 145, 134110.	1.2	17
22	Accelerating Realtime TDDFT with Block-Orthogonalized Manbyâ€“Miller Embedding Theory. Journal of Chemical Theory and Computation, 2017, 13, 4173-4178.	2.3	17
23	Orbital optimisation in the perfect pairing hierarchy: applications to full-valence calculations on linear polyacenes. Molecular Physics, 2018, 116, 547-560.	0.8	17
24	Modeling Coherent Anti-Stokes Raman Scattering with Time-Dependent Density Functional Theory: Vacuum and Surface Enhancement.. Journal of Physical Chemistry Letters, 2011, 2, 1849-1854.	2.1	16
25	Compressing physics with an autoencoder: Creating an atomic species representation to improve machine learning models in the chemical sciences. Journal of Chemical Physics, 2019, 151, 084103.	1.2	16
26	Exciton coherence lifetimes from electronic structure. Journal of Chemical Physics, 2012, 136, 104510.	1.2	13
27	Nonradiative Relaxation in Real-Time Electronic Dynamics OSCF2: Organolead Triiodide Perovskite. Journal of Physical Chemistry A, 2016, 120, 6880-6887.	1.1	13
28	On the border between localization and delocalization: tris(iminoxolene)titanium(iv). Dalton Transactions, 2019, 48, 1427-1435.	1.6	11
29	The exchange energy of a uniform electron gas experiencing a new, flexible range separation. Chemical Physics Letters, 2009, 478, 283-286.	1.2	9
30	The formulation and performance of a perturbative correction to the perfect quadruples model. Journal of Chemical Physics, 2011, 134, 154112.	1.2	9
31	A correlated-polaron electronic propagator: Open electronic dynamics beyond the Born-Oppenheimer approximation. Journal of Chemical Physics, 2012, 137, 22A547.	1.2	8
32	The numerical condition of electron correlation theories when only active pairs of electrons are spin-unrestricted. Journal of Chemical Physics, 2009, 130, 184113.	1.2	4
33	Force-field functor theory: classical force-fields which reproduce equilibrium quantum distributions. Frontiers in Chemistry, 2013, 1, 26.	1.8	4
34	Accelerating the computation of bath spectral densities with super-resolution. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	2
35	Response to Commentary on â€œForce-field functor theory: classical force-fields which reproduce equilibrium quantum distributionsâ€• Frontiers in Chemistry, 2013, 1, 33.	1.8	0