

# John A Parkhill

## List of Publications by Year in descending order

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35  
papers

4,576  
citations

430442

18  
h-index

377514

34  
g-index

35  
all docs

35  
docs citations

35  
times ranked

5853  
citing authors

#	ARTICLE	IF	CITATIONS
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
2	Compressing physics with an autoencoder: Creating an atomic species representation to improve machine learning models in the chemical sciences. <i>Journal of Chemical Physics</i> , 2019, 151, 084103.	1.2	16
3	On the border between localization and delocalization: tris(iminoxolene)titanium(iv). <i>Dalton Transactions</i> , 2019, 48, 1427-1435.	1.6	11
4	The TensorMol-0.1 model chemistry: a neural network augmented with long-range physics. <i>Chemical Science</i> , 2018, 9, 2261-2269.	3.7	322
5	Metadynamics for training neural network model chemistries: A competitive assessment. <i>Journal of Chemical Physics</i> , 2018, 148, 241710.	1.2	51
6	Orbital optimisation in the perfect pairing hierarchy: applications to full-valence calculations on linear polyacenes. <i>Molecular Physics</i> , 2018, 116, 547-560.	0.8	17
7	The many-body expansion combined with neural networks. <i>Journal of Chemical Physics</i> , 2017, 146, 014106.	1.2	95
8	Detection of electron tunneling across plasmonic nanoparticleâ€“film junctions using nitrile vibrations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5786-5796.	1.3	28
9	Intrinsic Bond Energies from a Bonds-in-Molecules Neural Network. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2689-2694.	2.1	100
10	Accelerating Realtime TDDFT with Block-Orthogonalized Manbyâ€“Miller Embedding Theory. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4173-4178.	2.3	17
11	Origin of the Size-Dependent Stokes Shift in CsPbBr <sub>3</sub> Perovskite Nanocrystals. <i>Journal of the American Chemical Society</i> , 2017, 139, 12201-12208.	6.6	240
12	Cost-effective description of strong correlation: Efficient implementations of the perfect quadruples and perfect hexuples models. <i>Journal of Chemical Physics</i> , 2016, 145, 134110.	1.2	17
13	Black-Box, Real-Time Simulations of Transient Absorption Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1590-1595.	2.1	31
14	Nonradiative Relaxation in Real-Time Electronic Dynamics OSCF2: Organolead Triiodide Perovskite. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6880-6887.	1.1	13
15	Accelerating the computation of bath spectral densities with super-resolution. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	2
16	Kinetic Energy of Hydrocarbons as a Function of Electron Density and Convolutional Neural Networks. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1139-1147.	2.3	101
17	How electronic dynamics with Pauli exclusion produces Fermi-Dirac statistics. <i>Journal of Chemical Physics</i> , 2015, 142, 134113.	1.2	19
18	Nonadiabatic Dynamics for Electrons at Second-Order: Real-Time TDDFT and OSCF2. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2918-2924.	2.3	35

#	ARTICLE	IF	CITATIONS
19	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
20	Feynman's clock, a new variational principle, and parallel-in-time quantum dynamics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, E3901-9.	3.3	18
21	Force-field functor theory: classical force-fields which reproduce equilibrium quantum distributions. <i>Frontiers in Chemistry</i> , 2013, 1, 26.	1.8	4
22	Response to Commentary on "Force-field functor theory: classical force-fields which reproduce equilibrium quantum distributions". <i>Frontiers in Chemistry</i> , 2013, 1, 33.	1.8	0
23	Exciton coherence lifetimes from electronic structure. <i>Journal of Chemical Physics</i> , 2012, 136, 104510.	1.2	13
24	A correlated-polaron electronic propagator: Open electronic dynamics beyond the Born-Oppenheimer approximation. <i>Journal of Chemical Physics</i> , 2012, 137, 22A547.	1.2	8
25	Modeling Coherent Anti-Stokes Raman Scattering with Time-Dependent Density Functional Theory: Vacuum and Surface Enhancement.. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1849-1854.	2.1	16
26	Benchmark results for empirical post-GGA functionals: Difficult exchange problems and independent tests. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 19325.	1.3	83
27	The formulation and performance of a perturbative correction to the perfect quadruples model. <i>Journal of Chemical Physics</i> , 2011, 134, 154112.	1.2	9
28	A tractable and accurate electronic structure method for static correlations: The perfect hexuples model. <i>Journal of Chemical Physics</i> , 2010, 133, 024103.	1.2	37
29	A truncation hierarchy of coupled cluster models of strongly correlated systems based on perfect-pairing references: The singles+doubles models. <i>Journal of Chemical Physics</i> , 2010, 133, 124102.	1.2	31
30	A sparse framework for the derivation and implementation of fermion algebra. <i>Molecular Physics</i> , 2010, 108, 513-522.	0.8	19
31	The numerical condition of electron correlation theories when only active pairs of electrons are spin-unrestricted. <i>Journal of Chemical Physics</i> , 2009, 130, 184113.	1.2	4
32	The exchange energy of a uniform electron gas experiencing a new, flexible range separation. <i>Chemical Physics Letters</i> , 2009, 478, 283-286.	1.2	9
33	The perfect quadruples model for electron correlation in a valence active space. <i>Journal of Chemical Physics</i> , 2009, 130, 084101.	1.2	63
34	Penalty functions for combining coupled-cluster and perturbation amplitudes in local correlation methods with optimized orbitals. <i>Molecular Physics</i> , 2008, 106, 2309-2324.	0.8	29
35	Near-Infrared Spectroscopy of Nitrogenated Polycyclic Aromatic Hydrocarbon Cations from 0.7 to 2.5 $\mu\text{m}$ . <i>Astrophysical Journal</i> , 2008, 680, 1243-1255.	1.6	39