Patrick J Lestrange

List of Publications by Year
in descending order

13	517	933447 10	1199594 12
papers	citations	h-index	g-index

13	13	13	873
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Interplays of electron and nuclear motions along CO dissociation trajectory in myoglobin revealed by ultrafast X-rays and quantum dynamics calculations. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	10
2	What We Talk About When We Talk About Climate Change. ACS Symposium Series, 2019, , 31-39.	0.5	0
3	Efficient Implementation of Variation after Projection Generalized Hartreeâ€“Fock. Journal of Chemical Theory and Computation, 2018, 14, 588-596.	5.3	14
4	Modeling L_{2,3}-Edge X-ray Absorption Spectroscopy with Real-Time Exact Two-Component Relativistic Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 1998-2006.	5.3	44
5	Realâ€time timeâ€dependent electronic structure theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1341.	14.6	122
6	Time-Dependent Configuration Interaction Using the Graphical Unitary Group Approach: Nonlinear Electric Properties. Advances in Quantum Chemistry, 2018, 76, 295-313.	0.8	19
7	Can Excited State Electronic Coherence Be Tuned via Molecular Structural Modification? A First-Principles Quantum Electronic Dynamics Study of Pyrazolate-Bridged Pt(II) Dimers. Journal of Physical Chemistry A, 2017, 121, 1932-1939.	2.5	15
8	Imaging ultrafast excited state pathways in transition metal complexes by X-ray transient absorption and scattering using X-ray free electron laser source. Faraday Discussions, 2016, 194, 639-658.	3.2	10
9	Ultrafast Excited State Relaxation of a Metalloporphyrin Revealed by Femtosecond X-ray Absorption Spectroscopy. Journal of the American Chemical Society, 2016, 138, 8752-8764.	13.7	77
10	The consequences of improperly describing oscillator strengths beyond the electric dipole approximation. Journal of Chemical Physics, 2015, 143, 234103.	3.0	34
11	Calibration of Energy-Specific TDDFT for Modeling K-edge XAS Spectra of Light Elements. Journal of Chemical Theory and Computation, 2015, 11, 2994-2999.	5.3	78
12	Energy-Specific Equation-of-Motion Coupled-Cluster Methods for High-Energy Excited States: Application to K-edge X-ray Absorption Spectroscopy. Journal of Chemical Theory and Computation, 2015, 11, 4146-4153.	5.3	92
13	Density of States Guided MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2014, 10, 1910-1914.	5.3	2