

Simon P Neville

List of Publications by Year in descending order

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papers

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623734

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672
citing authors

#	ARTICLE	IF	CITATIONS
1	Resolving competing conical intersection pathways: time-resolved X-ray absorption spectroscopy of <i>trans</i> -1,3-butadiene. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1345-1354.	2.8	5
2	Formation of electronic coherences in conical intersection-mediated dynamics. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2022, 55, 044004.	1.5	9
3	On the measurement of statistical dynamics using the method of Coulomb explosion imaging. <i>AIP Conference Proceedings</i> , 2021, , .	0.4	0
4	Sub-7-femtosecond conical-intersection dynamics probed at the carbon K-edge. <i>Science</i> , 2021, 371, 489-494.	12.6	82
5	Sub-7-femtosecond conical-intersection dynamics probed at the carbon K-edge. , 2021, , .		1
6	Vacuum Ultraviolet Excited State Dynamics of the Smallest Ketone: Acetone. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8541-8547.	4.6	9
7	Removing the Deadwood from DFT/MRCI Wave Functions: The p-DFT/MRCI Method. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7657-7665.	5.3	4
8	Capturing roaming molecular fragments in real time. <i>Science</i> , 2020, 370, 1072-1077.	12.6	61
9	Propagative block diagonalization diabaticization of DFT/MRCI electronic states. <i>Journal of Chemical Physics</i> , 2020, 152, 114110.	3.0	9
10	Ultrafast molecular frame electronic coherences from lab frame scattering anisotropies. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2020, 53, 114001.	1.5	16
11	Electron transfer in photoexcited pyrrole dimers. <i>Journal of Chemical Physics</i> , 2019, 151, 164304.	3.0	2
12	Efficient calculation of X-ray absorption spectra using Chebyshev-Slepian filter diagonalisation. <i>Journal of Chemical Physics</i> , 2019, 150, 184115.	3.0	1
13	The simulation of X-ray absorption spectra from ground and excited electronic states using core-valence separated DFT/MRCI. <i>Journal of Chemical Physics</i> , 2019, 151, 144104.	3.0	19
14	Efficient Solution of the Electronic Eigenvalue Problem Using Wavepacket Propagation. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1433-1441.	5.3	3
15	A general approach for the calculation and characterization of x-ray absorption spectra. <i>Journal of Chemical Physics</i> , 2018, 149, 154111.	3.0	13
16	Vacuum ultraviolet excited state dynamics of the smallest ring, cyclopropane. II. Time-resolved photoelectron spectroscopy and <i>ab initio</i> dynamics. <i>Journal of Chemical Physics</i> , 2018, 149, 144311.	3.0	14
17	Vacuum ultraviolet excited state dynamics of the smallest ring, cyclopropane. I. A reinterpretation of the electronic spectrum and the effect of intensity borrowing. <i>Journal of Chemical Physics</i> , 2018, 149, 144310.	3.0	9
18	Ultrafast X-Ray Spectroscopy of Conical Intersections. <i>Physical Review Letters</i> , 2018, 120, 243001.	7.8	77

#	ARTICLE	IF	CITATIONS
19	Non-radiative relaxation dynamics of pyrrole following excitation in the range 249.5â€“200 nm. Chemical Physics Letters, 2017, 683, 179-185.	2.6	19
20	Dynamics in higher lying excited states: Valence to Rydberg transitions in the relaxation paths of pyrrole and methylated derivatives. Journal of Chemical Physics, 2017, 146, 144307.	3.0	17
21	Excited state X-ray absorption spectroscopy: Probing both electronic and structural dynamics. Journal of Chemical Physics, 2016, 145, 144307.	3.0	39
22	Electronic and non-adiabatic dynamics: general discussion. Faraday Discussions, 2016, 194, 209-257.	3.2	3
23	Excited state non-adiabatic dynamics of N-methylpyrrole: A time-resolved photoelectron spectroscopy and quantum dynamics study. Journal of Chemical Physics, 2016, 144, 014309.	3.0	21
24	Beyond structure: ultrafast X-ray absorption spectroscopy as a probe of non-adiabatic wavepacket dynamics. Faraday Discussions, 2016, 194, 117-145.	3.2	52
25	Identification of a new electron-transfer relaxation pathway in photoexcited pyrrole dimers. Nature Communications, 2016, 7, 11357.	12.8	15
26	Substituent effects on dynamics at conical intersections: Allene and methyl allenes. Journal of Chemical Physics, 2016, 144, 014305.	3.0	27
27	Excited state non-adiabatic dynamics of pyrrole: A time-resolved photoelectron spectroscopy and quantum dynamics study. Journal of Chemical Physics, 2015, 142, 074302.	3.0	59