Simon P Neville

List of Publications by Year
in descending order

27 papers	586 citations	623188 14 h-index	610482 24 g-index
27 all docs	27 docs citations	27 times ranked	672 citing authors

#	Article	IF	Citations
1	Resolving competing conical intersection pathways: time-resolved X-ray absorption spectroscopy of trans-1,3-butadiene. Physical Chemistry Chemical Physics, 2022, 24, 1345-1354.	1.3	5
2	Formation of electronic coherences in conical intersection-mediated dynamics. Journal of Physics B: Atomic, Molecular and Optical Physics, 2022, 55, 044004.	0.6	9
3	On the measurement of statistical dynamics using the method of Coulomb explosion imaging. AIP Conference Proceedings, 2021, , .	0.3	0
4	Sub-7-femtosecond conical-intersection dynamics probed at the carbon K-edge. Science, 2021, 371, 489-494.	6.0	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. Journal of Physical Chemistry Letters, 2021, 12, 8541-8547.	2.1	9
7	Removing the Deadwood from DFT/MRCI Wave Functions: The p-DFT/MRCI Method. Journal of Chemical Theory and Computation, 2021, 17, 7657-7665.	2.3	4
8	Capturing roaming molecular fragments in real time. Science, 2020, 370, 1072-1077.	6.0	61
9	Propagative block diagonalization diabatization of DFT/MRCI electronic states. Journal of Chemical Physics, 2020, 152, 114110.	1.2	9
10	Ultrafast molecular frame electronic coherences from lab frame scattering anisotropies. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 114001.	0.6	16
11	Electron transfer in photoexcited pyrrole dimers. Journal of Chemical Physics, 2019, 151, 164304.	1.2	2
12	Efficient calculation of X-ray absorption spectra using Chebyshev-Slepian filter diagonalisation. Journal of Chemical Physics, 2019, 150, 184115.	1.2	1
13	The simulation of X-ray absorption spectra from ground and excited electronic states using core-valence separated DFT/MRCI. Journal of Chemical Physics, 2019, 151, 144104.	1.2	19
14	Efficient Solution of the Electronic Eigenvalue Problem Using Wavepacket Propagation. Journal of Chemical Theory and Computation, 2018, 14, 1433-1441.	2.3	3
15	A general approach for the calculation and characterization of x-ray absorption spectra. Journal of Chemical Physics, 2018, 149, 154111.	1.2	13
16	Vacuum ultraviolet excited state dynamics of the smallest ring, cyclopropane. II. Time-resolved photoelectron spectroscopy and ab initio dynamics. Journal of Chemical Physics, 2018, 149, 144311.	1.2	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. Journal of Chemical Physics, 2018, 149, 144310.	1.2	9
18	Ultrafast X-Ray Spectroscopy of Conical Intersections. Physical Review Letters, 2018, 120, 243001.	2.9	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.	1.2	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.	1.2	17
21	Excited state X-ray absorption spectroscopy: Probing both electronic and structural dynamics. Journal of Chemical Physics, 2016, 145, 144307.	1.2	39
22	Electronic and non-adiabatic dynamics: general discussion. Faraday Discussions, 2016, 194, 209-257.	1.6	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.	1.2	21
24	Beyond structure: ultrafast X-ray absorption spectroscopy as a probe of non-adiabatic wavepacket dynamics. Faraday Discussions, 2016, 194, 117-145.	1.6	52
25	Identification of a new electron-transfer relaxation pathway in photoexcited pyrrole dimers. Nature Communications, 2016, 7, 11357.	5.8	15
26	Substituent effects on dynamics at conical intersections: Allene and methyl allenes. Journal of Chemical Physics, 2016, 144, 014305.	1.2	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.	1.2	59