Simon P Neville

List of Publications by Year
in descending order

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27 papers	586 citations	623734 14 h-index	610901 24 g-index
27 all docs	27 docs citations	27 times ranked	672 citing authors

#	Article	IF	Citations
1	Sub-7-femtosecond conical-intersection dynamics probed at the carbon K-edge. Science, 2021, 371, 489-494.	12.6	82
2	Ultrafast X-Ray Spectroscopy of Conical Intersections. Physical Review Letters, 2018, 120, 243001.	7.8	77
3	Capturing roaming molecular fragments in real time. Science, 2020, 370, 1072-1077.	12.6	61
4	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
5	Beyond structure: ultrafast X-ray absorption spectroscopy as a probe of non-adiabatic wavepacket dynamics. Faraday Discussions, 2016, 194, 117-145.	3.2	52
6	Excited state X-ray absorption spectroscopy: Probing both electronic and structural dynamics. Journal of Chemical Physics, 2016, 145, 144307.	3.0	39
7	Substituent effects on dynamics at conical intersections: Allene and methyl allenes. Journal of Chemical Physics, 2016, 144, 014305.	3.0	27
8	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
9	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
10	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.	3.0	19
11	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
12	Ultrafast molecular frame electronic coherences from lab frame scattering anisotropies. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 114001.	1.5	16
13	Identification of a new electron-transfer relaxation pathway in photoexcited pyrrole dimers. Nature Communications, 2016, 7, 11357.	12.8	15
14	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.	3.0	14
15	A general approach for the calculation and characterization of x-ray absorption spectra. Journal of Chemical Physics, 2018, 149, 154111.	3.0	13
16	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.	3.0	9
17	Propagative block diagonalization diabatization of DFT/MRCI electronic states. Journal of Chemical Physics, 2020, 152, 114110.	3.0	9
18	Vacuum Ultraviolet Excited State Dynamics of the Smallest Ketone: Acetone. Journal of Physical Chemistry Letters, 2021, 12, 8541-8547.	4.6	9

#	Article	IF	Citations
19	Formation of electronic coherences in conical intersection-mediated dynamics. Journal of Physics B: Atomic, Molecular and Optical Physics, 2022, 55, 044004.	1.5	9
20	Resolving competing conical intersection pathways: time-resolved X-ray absorption spectroscopy of trans-1,3-butadiene. Physical Chemistry Chemical Physics, 2022, 24, 1345-1354.	2.8	5
21	Removing the Deadwood from DFT/MRCI Wave Functions: The p-DFT/MRCI Method. Journal of Chemical Theory and Computation, 2021, 17, 7657-7665.	5.3	4
22	Electronic and non-adiabatic dynamics: general discussion. Faraday Discussions, 2016, 194, 209-257.	3.2	3
23	Efficient Solution of the Electronic Eigenvalue Problem Using Wavepacket Propagation. Journal of Chemical Theory and Computation, 2018, 14, 1433-1441.	5.3	3
24	Electron transfer in photoexcited pyrrole dimers. Journal of Chemical Physics, 2019, 151, 164304.	3.0	2
25	Efficient calculation of X-ray absorption spectra using Chebyshev-Slepian filter diagonalisation. Journal of Chemical Physics, 2019, 150, 184115.	3.0	1
26	Sub-7-femtosecond conical-intersection dynamics probed at the carbon K-edge. , 2021, , .		1
27	On the measurement of statistical dynamics using the method of Coulomb explosion imaging. AIP Conference Proceedings, 2021, , .	0.4	0