Martin Kleinschmidt

List of Publications by Year
in descending order

36 papers	1,421 citations	430442 18 h-index	377514 34 g-index
38 all docs	38 docs citations	38 times ranked	1367 citing authors

#	Article	IF	Citations
1	Spin-orbit coupling of DFT/MRCI wavefunctions: Method, test calculations, and application to thiophene. Journal of Computational Chemistry, 2002, 23, 824-833.	1.5	145
2	Parallel multireference configuration interaction calculations on mini-Î²-carotenes and Î²-carotene. Journal of Chemical Physics, 2009, 130, 044708.	1.2	111
3	SPOCK.CI: A multireference spin-orbit configuration interaction method for large molecules. Journal of Chemical Physics, 2006, 124, 124101.	1.2	105
4	Redesign of the DFT/MRCI Hamiltonian. Journal of Chemical Physics, 2016, 144, 034104.	1.2	99
5	The DFT/MRCI method. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1394.	6.2	99
6	Efficient generation of matrix elements for one-electron spinâ€“orbit operators. Chemical Physics, 2005, 311, 71-79.	0.9	87
7	Excited states of thiophene: ring opening as deactivation mechanism. Physical Chemistry Chemical Physics, 2008, 10, 380-392.	1.3	86
8	Electronic excitation and singlet-triplet coupling in uracil tautomers and uracil-water complexes. European Physical Journal D, 2002, 20, 357-367.	0.6	85
9	Intersystem-crossing and phosphorescence rates in fac-IrIII(ppy)3: A theoretical study involving multi-reference configuration interaction wavefunctions. Journal of Chemical Physics, 2015, 142, 094301.	1.2	75
10	Electronic Coherence Provides a Direct Proof for Energy-Level Crossing in Photoexcited Lutein and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î²</mml:mi></mml:math>-Carotene. Physical Review Letters, 2009, 103, 108302.	2.9	64
11	Phosphorescence or Thermally Activated Delayed Fluorescence? Intersystem Crossing and Radiative Rate Constants of a Three-Coordinate Copper(I) Complex Determined by Quantum-Chemical Methods. Inorganic Chemistry, 2016, 55, 7508-7516.	1.9	57
12	Efficient calculation of electron paramagnetic resonance g-tensors by multireference configuration interaction sum-over-state expansions, using the atomic mean-field spinâ€“orbit method. Journal of Chemical Physics, 2003, 118, 9552-9562.	1.2	44
13	On the performance of DFT/MRCI Hamiltonians for electronic excitations in transition metal complexes: The role of the damping function. Journal of Chemical Physics, 2018, 149, 164106.	1.2	42
14	Quantum-Chemical Studies on Excitation Energy Transfer Processes in BODIPY-Based Donorâ€“Acceptor Systems. Journal of Chemical Theory and Computation, 2015, 11, 4316-4327.	2.3	29
15	The photophysics of 7H-adenine: A quantum chemical investigation including spinâ€“orbit effects. Chemical Physics, 2008, 347, 346-359.	0.9	23
16	Large Inverted Singletâ€“Triplet Energy Gaps Are Not Always Favorable for Triplet Harvesting: Vibronic Coupling Drives the (Reverse) Intersystem Crossing in Heptazine Derivatives. Journal of Physical Chemistry A, 2021, 125, 10044-10051.	1.1	22
17	Electronic excitation spectra and singletâ€“triplet coupling in psoralen and its sulfur and selenium analogs. Journal of Photochemistry and Photobiology A: Chemistry, 2004, 167, 201-212.	2.0	21
18	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

#	Article	IF	Citations
19	Visible Light-Induced Homolytic Cleavage of Perfluoroalkyl Iodides Mediated by Phosphines. Molecules, 2020, 25, 1606.	1.7	19
20	Assessment of Interstate Spinâ€“Orbit Couplings from Linear Response Amplitudes. Journal of Chemical Theory and Computation, 2017, 13, 749-766.	2.3	18
21	Charge-transfer contributions to the excitonic coupling matrix element in BODIPY-based energy transfer cassettes. Chemical Physics, 2017, 482, 265-276.	0.9	16
22	Impact of fluorination on the photophysics of the flavin chromophore: a quantum chemical perspective. Physical Chemistry Chemical Physics, 2019, 21, 9912-9923.	1.3	16
23	Failure of the IDA in FRET Systems at Close Inter-Dye Distances Is Moderated by Frequent Low Î²² Values. Journal of Physical Chemistry B, 2016, 120, 8845-8862.	1.2	15
24	Calculating electron paramagnetic resonance g-matrices for triplet state molecules from multireference spin-orbit configuration interaction wave functions. Journal of Chemical Physics, 2009, 130, 154106.	1.2	14
25	Thioxanthone: on the shape of the first absorption band. Physical Chemistry Chemical Physics, 2010, 12, 9320.	1.3	14
26	On the performance of DFT/MRCI-R and MR-MP2 in spinâ€“orbit coupling calculations on diatomics and polyatomic organic molecules. Molecular Physics, 2017, 115, 109-137.	0.8	14
27	Internal conversion of singlet and triplet states employing numerical DFT/MRCI derivative couplings: Implementation, tests, and application to xanthone. Journal of Chemical Physics, 2021, 155, 014102.	1.2	14
28	On the photophysics of four heteroleptic iridium(III) phenylpyridyl complexes investigated by relativistic multi-configuration methods. Molecular Physics, 0, , 1-16.	0.8	13
29	On the Photophysics of 1,6â€Diphenylâ€1,3,5â€Hexatriene Isomers and Rotamers. ChemPhysChem, 2011, 12, 1872-1879.	1.0	10
30	Kramers-Type Splitting in the X2Î and a4Î£â^' States of CH and CD Calculated in a Hund's Case (a) Basis. Journal of Molecular Spectroscopy, 2002, 211, 179-188.	0.4	9
31	Spinâ€“orbit coupling in keto-porphyrins. Chemical Physics Letters, 2008, 458, 190-194.	1.2	7
32	In search of the dark state of 5-methyl-2-hydroxypyrimidine using a numerical DFT/MRCI gradient. Molecular Physics, 2012, 110, 2429-2438.	0.8	6
33	Acridones: Strongly Emissive HIGHrISC Fluorophores. Journal of Physical Chemistry Letters, 2021, 12, 5703-5709.	2.1	6
34	Quantum Chemical Investigation of Spin-Forbidden Transitions in Dithiosuccinimide. Zeitschrift Fur Physikalische Chemie, 2003, 217, 205-230.	1.4	5
35	Computerâ€Aided Design of Fluorinated Flavin Derivatives by Modulation of Intersystem Crossing and Fluorescence. ChemPhotoChem, 2022, 6, .	1.5	5
36	Synthesis, Structural Characterization, Conformational and Topological Classification of Different Salts in the 2,2-Dimethylpropane-1,3-diamine/HCl/H2O-System. Solids, 2022, 3, 385-396.	1.1	0