Tim Kowalczyk

List of Publications by Year
in descending order

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29 papers	5,547 citations	361413 20 h-index	454955 30 g-index
33 all docs	33 docs citations	33 times ranked	7034 citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
2	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	3.0	589
3	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
4	Constrained Density Functional Theory. Chemical Reviews, 2012, 112, 321-370.	47.7	454
5	The Diabatic Picture of Electron Transfer, Reaction Barriers, and Molecular Dynamics. Annual Review of Physical Chemistry, 2010, 61, 149-170.	10.8	280
6	Assessment of the Î”SCF density functional theory approach for electronic excitations in organic dyes. Journal of Chemical Physics, 2011, 134, 054128.	3.0	152
7	Twoâ€Đimensional Tetrathiafulvalene Covalent Organic Frameworks: Towards Latticed Conductive Organic Salts. Chemistry - A European Journal, 2014, 20, 14608-14613.	3.3	147
8	What Can Density Functional Theory Tell Us about Artificial Catalytic Water Splitting?. Inorganic Chemistry, 2014, 53, 6386-6397.	4.0	126
9	Stacked antiaromatic porphyrins. Nature Communications, 2016, 7, 13620.	12.8	105
10	Hybridization of a Flexible Cyclooctatetraene Core and Rigid Aceneimide Wings for Multiluminescent Flapping Ï€ Systems. Chemistry - A European Journal, 2014, 20, 2193-2200.	3.3	82
11	Excitation energies and Stokes shifts from a restricted open-shell Kohn-Sham approach. Journal of Chemical Physics, 2013, 138, 164101.	3.0	78
12	Three-dimensional aromaticity in an antiaromatic cyclophane. Nature Communications, 2019, 10, 3576.	12.8	73
13	Fluorescence Quenching by Photoinduced Electron Transfer in the Zn²⁺ Sensor Zinpyr-1: A Computational Investigation. Journal of Physical Chemistry A, 2010, 114, 10427-10434.	2.5	71
14	Exceptional electron conduction in two-dimensional covalent organic frameworks. CheM, 2021, 7, 3309-3324.	11.7	41
15	Ab Initio Optical Rotatory Dispersion and Electronic Circular Dichroism Spectra of (S)-2-Chloropropionitrile. Journal of Physical Chemistry A, 2006, 110, 7649-7654.	2.5	39
16	Determinant Factors of Three-Dimensional Aromaticity in Antiaromatic Cyclophanes. Journal of the American Chemical Society, 2021, 143, 10676-10685.	13.7	38
17	A multireference perturbation method using non-orthogonal Hartree-Fock determinants for ground and excited states. Journal of Chemical Physics, 2013, 139, 174104.	3.0	29
18	Electronic Structure of Carbon Trioxide and Vibronic Interactions Involving Jahnâ˜Teller States. Journal of Physical Chemistry A, 2007, 111, 8271-8276.	2.5	28

#	Article	IF	Citations
19	Simulation of Solution Phase Electron Transfer in a Compact Donorâ€“Acceptor Dyad. Journal of Physical Chemistry B, 2011, 115, 12135-12144.	2.6	27
20	Hemilabile Proton Relays and Redox Activity Lead to {FeNO}^x and Significant Rate Enhancements in NO₂^{â€“} Reduction. Journal of the American Chemical Society, 2018, 140, 17040-17050.	13.7	24
21	Structure of Tm2 and Tm2C2 encapsulated in low-symmetry C82(Cs(6)) fullerene cage by single crystal X-ray diffraction. Chemical Physics Letters, 2014, 600, 38-42.	2.6	20
22	Acene-linked covalent organic frameworks as candidate materials for singlet fission. Journal of Materials Chemistry A, 2016, 4, 10500-10507.	10.3	12
23	Self-Consistent Optimization of Excited States within Density-Functional Tight-Binding. Journal of Chemical Theory and Computation, 2016, 12, 313-323.	5.3	11
24	Multifactor theoretical modeling of solar thermal fuels built on azobenzene and norbornadiene scaffolds. Sustainable Energy and Fuels, 2021, 5, 2335-2346.	4.9	10
25	Extension of Intramolecular Charge-Transfer State Lifetime by Encapsulation in Porous Frameworks. Journal of Physical Chemistry C, 2017, 121, 20673-20679.	3.1	8
26	How Parallel Are Excited State Potential Energy Surfaces from Time-Independent and Time-Dependent DFT? A BODIPY Dye Case Study. Journal of Physical Chemistry A, 2016, 120, 8160-8168.	2.5	6
27	Templating the 3D structure of conducting polymers with self-assembling peptides. Journal of Materials Chemistry B, 2017, 5, 4690-4696.	5.8	6
28	Chemoselective Carbonyl Allylations with Alkoxyallylsiletanes. Journal of Organic Chemistry, 2019, 84, 4421-4428.	3.2	6
29	Theoretical rationalization for reduced charge recombination in bulky carbazoleâ€based sensitizers in solar cells. Journal of Computational Chemistry, 2017, 38, 901-909.	3.3	2