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	Determinant Factors of Three-Dimensional Aromaticity in Antiaromatic Cyclophanes. Journal of the American Chemical Society, 2021, 143, 10676-10685.	13.7	38
2	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
3	Exceptional electron conduction in two-dimensional covalent organic frameworks. CheM, 2021, 7, 3309-3324.	11.7	41
4	Multifactor theoretical modeling of solar thermal fuels built on azobenzene and norbornadiene scaffolds. Sustainable Energy and Fuels, 2021, 5, 2335-2346.	4.9	10
5	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	3.0	589
6	Three-dimensional aromaticity in an antiaromatic cyclophane. Nature Communications, 2019, 10, 3576.	12.8	73
7	Chemoselective Carbonyl Allylations with Alkoxyallylsiletanes. Journal of Organic Chemistry, 2019, 84, 4421-4428.	3.2	6
8	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
9	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
10	Templating the 3D structure of conducting polymers with self-assembling peptides. Journal of Materials Chemistry B, 2017, 5, 4690-4696.	5.8	6
11	Extension of Intramolecular Charge-Transfer State Lifetime by Encapsulation in Porous Frameworks. Journal of Physical Chemistry C, 2017, 121, 20673-20679.	3.1	8
12	Stacked antiaromatic porphyrins. Nature Communications, 2016, 7, 13620.	12.8	105
13	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
14	Acene-linked covalent organic frameworks as candidate materials for singlet fission. Journal of Materials Chemistry A, 2016, 4, 10500-10507.	10.3	12
15	Self-Consistent Optimization of Excited States within Density-Functional Tight-Binding. Journal of Chemical Theory and Computation, 2016, 12, 313-323.	5.3	11
16	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
17	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
18	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

#	Article	IF	Citations
19	What Can Density Functional Theory Tell Us about Artificial Catalytic Water Splitting?. Inorganic Chemistry, 2014, 53, 6386-6397.	4.0	126
20	Twoâ€Ðimensional Tetrathiafulvalene Covalent Organic Frameworks: Towards Latticed Conductive Organic Salts. Chemistry - A European Journal, 2014, 20, 14608-14613.	3.3	147
21	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
22	Excitation energies and Stokes shifts from a restricted open-shell Kohn-Sham approach. Journal of Chemical Physics, 2013, 138, 164101.	3.0	78
23	Constrained Density Functional Theory. Chemical Reviews, 2012, 112, 321-370.	47.7	454
24	Simulation of Solution Phase Electron Transfer in a Compact Donorâ€“Acceptor Dyad. Journal of Physical Chemistry B, 2011, 115, 12135-12144.	2.6	27
25	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
26	The Diabatic Picture of Electron Transfer, Reaction Barriers, and Molecular Dynamics. Annual Review of Physical Chemistry, 2010, 61, 149-170.	10.8	280
27	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
28	Electronic Structure of Carbon Trioxide and Vibronic Interactions Involving Jahnâ€Teller States. Journal of Physical Chemistry A, 2007, 111, 8271-8276.	2.5	28
29	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