

Pavel M Polestshuk

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	TWOF Code: An Efficient Tool for Explicit Partition of Coupled Cluster and Configuration Interaction Energies into Atomic and Diatomic Contributions. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3198-3207.	1.1	3
2	Interacting quantum atoms (IQA) energy partition: The employing exact response CCSD density to benchmark density matrix functional approximations. <i>Chemical Physics Letters</i> , 2019, 717, 136-140.	1.2	2
3	Control of triplet state generation in heavy atom-free BODIPY-anthracene dyads by media polarity and structural factors. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8016-8031.	1.3	96
4	BODIPY-Pyrene and Perylene Dyads as Heavy-Atom-Free Singlet Oxygen Sensitizers. <i>ChemPhotoChem</i> , 2018, 2, 606-615.	1.5	66
5	The Nature of Metal-Metal Interactions in Dimeric Hydrides and Halides of Group 11 Elements in the Light of High Level Relativistic Calculations. <i>Chemistry - A European Journal</i> , 2017, 23, 3257-3261.	1.7	7
6	Generation of Triplet Excited States via Photoinduced Electron Transfer in <i>meso</i> -anthra-BODIPY: Fluorogenic Response toward Singlet Oxygen in Solution and in Vitro. <i>Journal of the American Chemical Society</i> , 2017, 139, 6282-6285.	6.6	248
7	Reliability of interacting quantum atoms (IQA) data computed from post-HF densities: impact of the approximation used. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 16375-16386.	1.3	11
8	<i>Ad hoc</i> methods for accurate determination of Bader's atomic boundary. <i>Journal of Chemical Physics</i> , 2013, 139, 054108.	1.2	11
9	Accurate integration over atomic regions bounded by zero-flux surfaces. <i>Journal of Computational Chemistry</i> , 2013, 34, 206-219.	1.5	19
10	Forced Bonding and QTAIM Deficiencies: A Case Study of the Nature of Interactions in He@Adamantane and the Origin of the High Metastability. <i>Chemistry - A European Journal</i> , 2013, 19, 10945-10957.	1.7	22
11	A Bond Path and an Attractive Ehrenfest Force Do Not Necessarily Indicate Bonding Interactions: Case Study on M_2X_2 ($M=Li, Na, K; X=H, OH, F, Cl$). <i>Chemistry - A European Journal</i> , 2012, 18, 4982-4993.	1.7	72
12	Computational Exploration of the Mechanism of Alcohol Oxidation by Dioxygen Activated with Biquinoly-Containing Cu Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 3370-3386.	1.9	7
13	The electronic structure and energetics of V^+ -benzene half-sandwiches of different multiplicities: Comparative multireference and single-reference theoretical study. <i>Journal of Chemical Physics</i> , 2008, 129, 054307.	1.2	7