Arun K Pal

List of Publications by Year
in descending order

19 papers	239 citations	1040056 9 h-index	996975 15 g-index
19 all docs	19 docs citations	19 times ranked	329 citing authors

#	Article	IF	Citations
1	The Tripletâ€“Singlet Gap in the m-Xylylene Radical: A Not So Simple One. Journal of Chemical Theory and Computation, 2014, 10, 335-345.	5.3	56
2	On the Photomagnetism of Nitronyl Nitroxide, Imino Nitroxide, and Verdazyl-Substituted Azobenzene. Journal of Physical Chemistry A, 2012, 116, 3304-3311.	2.5	23
3	Calculation of linear and nonlinear optical properties of azobenzene derivatives with Kohnâ€“Sham and coupled-cluster methods. Physical Chemistry Chemical Physics, 2018, 20, 7303-7316.	2.8	23
4	Theoretical Investigation of Stilbene as Photochromic Spin Coupler. Journal of Physical Chemistry A, 2013, 117, 1773-1783.	2.5	22
5	Transition-State-like Planar Structures for Amine Inversion with Ultralong Câ€“C Bonds in Diamino-o-carborane and Diamino-o-dodecahedron. Journal of the American Chemical Society, 2020, 142, 5331-5337.	13.7	18
6	Polymorphism Dependent 9-Phosphoanthracene Derivative Exhibiting Thermally Activated Delayed Fluorescence: A Computational Investigation. Journal of Physical Chemistry A, 2020, 124, 11025-11037.	2.5	17
7	Theoretical and computational investigation of meta-phenylene as ferromagnetic coupler in nitronyl nitroxide diradicals. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	12
8	Ferrocene-based diradicals of imino nitroxide, nitronyl nitroxide and verdazyl, and their cations are possible SMM: A quantum chemical study. Chemical Physics Letters, 2017, 676, 70-76.	2.6	9
9	Remote Functionalization through Symmetric or Asymmetric Substitutions Control the Pathway of Intermolecular Singlet Fission. Journal of Chemical Theory and Computation, 2019, 15, 5014-5023.	5.3	9
10	Tuning of the optoelectronic properties of peptide-appended core-substituted naphthalenediimides: the role of self-assembly of two positional isomers. Soft Matter, 2021, 17, 7168-7176.	2.7	9
11	Theoretical Investigation of Photomagnetic Properties of Oxoverdazyl-Substituted Pyrenes. Journal of Physical Chemistry A, 2013, 117, 8609-8622.	2.5	8
12	Quantum Chemical Investigation of meta-Xylylene Based One-Dimensional Polymer Chain. Journal of Physical Chemistry A, 2015, 119, 2176-2185.	2.5	8
13	Quantum Chemical Investigation of Calix[4]arene-Based Radicals with Bis(biphenylene)methyl Linkers as Precursors of Spin Glass and Superparamagnets. Journal of Physical Chemistry C, 2014, 118, 27599-27610.	3.1	7
14	Harnessing Noncovalent Interactions for a Directed Evolution of a Six-Component Molecular Crystal. Journal of Physical Chemistry B, 2021, 125, 12584-12591.	2.6	6
15	Ferromagnetic Nature of Silicon-Substituted Meta-Xylylene Polyradicals. Journal of Physical Chemistry C, 2015, 119, 3754-3761.	3.1	4
16	Geometrical structure of meta-xylylene based symmetric polyradicals and their magnetic nature: A density functional study. Chemical Physics Letters, 2016, 648, 189-194.	2.6	3
17	Paradoxical design of a serendipitous pyrazolate bridging mode: a pragmatic strategy for inducing ineluctable ferromagnetic coupling. Dalton Transactions, 2020, 49, 13704-13716.	3.3	2
18	Understanding the Regioselectivity of Ion-Pair-Assisted Meta-Selective C(sp²)â€“H Activation in Conformationally Flexible Arylammonium Salts. Journal of Organic Chemistry, 2022, 87, 9222-9231.	3.2	2

#	Article	IF	Citations
19	Spin Alternation Rule in USCF for Through-Bond Magnetic Couplingâ”€A New Look: Why and When Does It Arise and How To See It. Journal of Physical Chemistry A, 2022, 126, 2309-2318.	2.5	1