Arun K Manna

List of Publications by Year
in descending order

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28	2,533	516710 16	526287 27
papers	citations	h-index	g-index

28	28	28	5155
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Origins of Large Stokes Shifts in a Pyreneâ€“Styrene-Based Pushâ€“Pull Organic Molecular Dyad in Polar Solvents and Large Electron Mobility in the Crystalline State: A Theoretical Perspective. Journal of Physical Chemistry C, 2022, 126, 423-433.	3.1	15
2	Understanding High Fluorescence Quantum Yield and Simultaneous Large Stokes Shift in Phenyl Bridged Donorâ"Ï€â€“Acceptor Dyads with Varied Bridge Lengths in Polar Solvents. Journal of Physical Chemistry A, 2022, 126, 4221-4229.	2.5	11
3	Theoretical insights on tunable optoelectronics and charge mobilities in cyano-perylenediimides: interplays between â€“CN numbers and positions. Physical Chemistry Chemical Physics, 2021, 23, 14687-14698.	2.8	10
4	Magnetic properties of the S = 52 anisotropic triangular chain compound Bi3FeMo2O12. Physical Review B, 2021, 104, .	3.2	6
5	Molecular-scale engineering of the charge-transfer excited states in non-covalently bound Znâ€“porphyrin and carbon fullerene based donorâ€“acceptor complex. Physical Chemistry Chemical Physics, 2020, 22, 14822-14831.	2.8	8
6	Structural, Electronic, and Spectral Properties of Metal Dimethylglyoximato [M(DMG)₂; M = Ni²⁺, Cu²⁺] Complexes: A Comparative Theoretical Study. Journal of Physical Chemistry A, 2019, 123, 9166-9174.	2.5	8
7	Quantitative Prediction of Optical Absorption in Molecular Solids from an Optimally Tuned Screened Range-Separated Hybrid Functional. Journal of Chemical Theory and Computation, 2018, 14, 2919-2929.	5.3	51
8	Covalently Assembled Monolayers of Homoâ€•and Heteroleptic Fe^{II}â€Terpyridyl Complexes on SiO_x and ITOâ€Coated Glass Substrates: An Experimental and Theoretical Study. ChemPhysChem, 2017, 18, 3407-3415.	2.1	8
9	Photoinduced Homolytic Bond Cleavage of the Central Siâ€“C Bond in Porphyrin Macrocycles Is a Charge Polarization Driven Process. Journal of Physical Chemistry A, 2016, 120, 7634-7640.	2.5	6
10	Unraveling the Mechanism of Photoinduced Charge Transfer in Carotenoidâ€“Porphyrinâ€“C₆₀ Molecular Triad. Journal of Physical Chemistry Letters, 2015, 6, 1231-1237.	4.6	48
11	Calculating High Energy Charge Transfer States Using Optimally Tuned Range-Separated Hybrid Functionals. Journal of Chemical Theory and Computation, 2015, 11, 1110-1117.	5.3	51
12	Communication: Charge-transfer rate constants in zinc-porphyrin-porphyrin-derived dyads: A Fermi golden rule first-principles-based study. Journal of Chemical Physics, 2014, 141, 121102.	3.0	31
13	Molecular Structure, Spectroscopy, and Photoinduced Kinetics in Trinuclear Cyanide Bridged Complex in Solution: A First-Principles Perspective. Journal of the American Chemical Society, 2014, 136, 16954-16957.	13.7	13
14	BN-decorated graphene nanoflakes with tunable opto-electronic and charge transport properties. Journal of Materials Chemistry C, 2014, 2, 2918-2928.	5.5	35
15	Functional Corannulene: Diverse Structures, Enhanced Charge Transport, and Tunable Optoelectronic Properties. ChemPhysChem, 2014, 15, 885-893.	2.1	27
16	Stability and electronic structure of carbon capsules with superior gas storage properties: A theoretical study. Chemical Physics, 2013, 426, 23-30.	1.9	8
17	Stabilization of diketo tautomer of curcumin by premicellar anionic surfactants: UVâ€“Visible, fluorescence, tensiometric and TD-DFT evidences. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 104, 150-157.	3.9	41
18	Computational Studies on Nonâ€covalent Interactions of Carbon and Boron Fullerenes with Graphene. ChemPhysChem, 2013, 14, 1844-1852.	2.1	25

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19	Computational studies on structural and optical properties of single-stranded DNA encapsulated silver/gold clusters. Journal of Materials Chemistry, 2012, 22, 6774.	6.7	20
20	Beyond the FÃ¶rster formulation for resonance energy transfer: the role of dark states. Physical Chemistry Chemical Physics, 2011, 13, 12734.	2.8	18
21	Tunable Electronic and Magnetic Properties in B_xN_yC_z Nanohybrids: Effect of Domain Segregation. Journal of Physical Chemistry C, 2011, 115, 10842-10850.	3.1	97
22	Interaction of Inorganic Nanoparticles with Graphene. ChemPhysChem, 2011, 12, 937-943.	2.1	72
23	Inside Cover: Interaction of Inorganic Nanoparticles with Graphene (ChemPhysChem 5/2011). ChemPhysChem, 2011, 12, 882-882.	2.1	0
24	Visibleâ€“Nearâ€Infrared and Fluorescent Copper Sensors Based on Julolidine Conjugates: Selective Detection and Fluorescence Imaging in Living Cells. Chemistry - A European Journal, 2011, 17, 11152-11161.	3.3	173
25	MoS₂ and WS₂ Analogues of Graphene. Angewandte Chemie - International Edition, 2010, 49, 4059-4062.	13.8	1,417
26	A study of graphene decorated with metal nanoparticles. Chemical Physics Letters, 2010, 497, 70-75.	2.6	286
27	Doping single-walled carbon nanotubes through molecular charge-transfer: a theoretical study. Nanoscale, 2010, 2, 1190.	5.6	34
28	The role of H bonding and dipole-dipole interactions on the electrical polarizations and charge mobilities in linear arrays of urea, thiourea, and their derivatives. Journal of Chemical Physics, 2008, 129, 204301.	3.0	14