Md Mehboob Alam

List of Publications by Year
in descending order

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45	717	516215 16	552369 26
papers	citations	h-index	g-index

45	45	45	769
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Cd(ii) based metalâ€“organic framework behaving as a Schottky barrier diode. Chemical Communications, 2014, 50, 7858.	2.2	80
2	Solvent induced channel interference in the two-photon absorption processâ€”a theoretical study with a generalized few-state-model in three dimensions. Physical Chemistry Chemical Physics, 2012, 14, 1156-1165.	1.3	72
3	Chemical Control of Channel Interference in Two-Photon Absorption Processes. Accounts of Chemical Research, 2014, 47, 1604-1612.	7.6	59
4	Benchmarking the Performance of Exchange-Correlation Functionals for Predicting Two-Photon Absorption Strengths. Journal of Chemical Theory and Computation, 2018, 14, 3677-3685.	2.3	56
5	High-Polarity Solvents Decreasing the Two-Photon Transition Probability of Through-Space Charge-Transfer Systems â€” A Surprising In Silico Observation. Journal of Physical Chemistry Letters, 2012, 3, 961-966.	2.1	38
6	Ï€-Extended diketopyrrolopyrroleâ€“porphyrin arrays: one- and two-photon photophysical investigations and theoretical studies. Physical Chemistry Chemical Physics, 2016, 18, 21954-21965.	1.3	30
7	Choosing Bad versus Worse: Predictions of Two-Photon-Absorption Strengths Based on Popular Density Functional Approximations. Journal of Chemical Theory and Computation, 2022, 18, 1046-1060.	2.3	26
8	Electrostatic Spin Crossover and Concomitant Electrically Operated Spin Switch Action in a Ti-Based Endohedral Metallofullerene Polymer. Physical Review Letters, 2012, 109, 257204.	2.9	25
9	A critical theoretical study on the two-photon absorption properties of some selective triaryl borane-1-naphthylphenyl amine based charge transfer molecules. Physical Chemistry Chemical Physics, 2011, 13, 9285.	1.3	24
10	Tuning of hyperpolarizability, and one- and two-photon absorption of donorâ€“acceptor and donorâ€“acceptorâ€“acceptor-type intramolecular charge transfer-based sensors. Physical Chemistry Chemical Physics, 2019, 21, 17343-17355.	1.3	23
11	The role of relativity and dispersion controlled inter-chain interaction on the band gap of thiophene, selenophene, and tellurophene oligomers. Journal of Chemical Physics, 2012, 136, 094904.	1.2	22
12	New Design Strategy for the Two-Photon Active Material Based on Pushâˆ’Pull Substituted Bisanthene Molecule. Journal of Physical Chemistry A, 2011, 115, 2607-2614.	1.1	19
13	On the Origin of Large Two-Photon Activity of DANS Molecule. Journal of Physical Chemistry A, 2012, 116, 11034-11040.	1.1	18
14	Enhancement of Twist Angle Dependent Two-Photon Activity through the Proper Alignment of Ground to Excited State and Excited State Dipole Moment Vectors. Journal of Physical Chemistry A, 2012, 116, 8067-8073.	1.1	17
15	Ghost-interaction correction in ensemble density-functional theory for excited states with and without range separation. Physical Review A, 2016, 94, .	1.0	16
16	Channel interference in multiphoton absorption. Journal of Chemical Physics, 2017, 146, 244116.	1.2	16
17	Intersystem crossing rate dependent dual emission and phosphorescence from cyclometalated platinum complexes: a second order cumulant expansion based approach. Physical Chemistry Chemical Physics, 2018, 20, 23244-23251.	1.3	16
18	Combining linear interpolation with extrapolation methods in range-separated ensemble density functional theory. Molecular Physics, 2016, 114, 968-981.	0.8	15

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19	Solvent effects on static polarizability, static first hyperpolarizability and one- and two-photon absorption properties of functionalized triply twisted MÃ¶bius annulenes: a DFT study. Physical Chemistry Chemical Physics, 2016, 18, 21833-21842.	1.3	13
20	Metallophilic interactions in A-frame molecules [S(MPH3)2] (M=Cu, Ag, Au) from range-separated density-functional perturbation theory. Chemical Physics Letters, 2012, 554, 37-42.	1.2	12
21	Interplay of twist angle and solvents with two-photon optical channel interference in aryl-substituted BODIPY dyes. Physical Chemistry Chemical Physics, 2017, 19, 29461-29471.	1.3	11
22	Combining extrapolation with ghost interaction correction in range-separated ensemble density functional theory for excited states. Journal of Chemical Physics, 2017, 147, 204105.	1.2	11
23	On the microscopic origin of bending of graphene nanoribbons in the presence of a perpendicular electric field. Physical Chemistry Chemical Physics, 2012, 14, 9439.	1.3	9
24	Triply twisted MÃ¶bius annulene: a new class of two-photon active material â€“ a computational study. Physical Chemistry Chemical Physics, 2015, 17, 6827-6833.	1.3	9
25	Effect of donorâ€“acceptor orientation on solvent-dependent three-photon activity in through-space charge-transfer systems â€“ case study of [2,2]-paracyclophane derivatives. Physical Chemistry Chemical Physics, 2013, 15, 17570.	1.3	7
26	On the origin of the very strong two-photon activity of squaraine dyes â€“ a standard/damped response theory study. Physical Chemistry Chemical Physics, 2014, 16, 8030-8035.	1.3	7
27	A generalized few-state model for the first hyperpolarizability. Journal of Chemical Physics, 2020, 152, 244106.	1.2	7
28	Computational design of two-photon active organic molecules for infrared responsive materials. Journal of Materials Chemistry C, 2020, 8, 9867-9873.	2.7	7
29	Chemical control of a molecular spin switch in the presence of a gate. RSC Advances, 2013, 3, 19894.	1.7	6
30	Donors contribute more than acceptors to increase the two-photon activity â€“ a case study with cyclopenta[b]naphthalene based molecules. Physical Chemistry Chemical Physics, 2014, 16, 26342-26347.	1.3	6
31	Ultrafast, green and recyclable photoRDRP in an ionic liquid towards multi-stimuli responsive amphiphilic copolymers. Polymer Chemistry, 2021, 12, 4954-4960.	1.9	6
32	Two-Photon Absorption Activity of BOPHY Derivatives: Insights from Theory. Journal of Physical Chemistry A, 2021, 125, 2581-2587.	1.1	5
33	Electrically Controlled Eightâ€Spinâ€Qubit Entangledâ€State Generation in a Molecular Break Junction. ChemPhysChem, 2014, 15, 1747-1751.	1.0	4
34	On site coulomb repulsion dominates over the non-local Hartree-Fock exchange in determining the band gap of polymers. Journal of Physics and Chemistry of Solids, 2014, 75, 212-223.	1.9	4
35	Donor's position-specific channel interference in substituted biphenyl molecules. Physical Chemistry Chemical Physics, 2015, 17, 17571-17576.	1.3	4
36	One- and two-photon activity of diketopyrrolopyrrole-Zn-porphyrin conjugates: linear and quadratic density functional response theory applied to model systems. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	4

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37	Two-photon absorption in host-guest complexes. Molecular Physics, 2020, 118, e1777335.	0.8	3
38	Much of a Muchness: On the Origins of Two- and Three-Photon Absorption Activity of Dipolar Y-Shaped Chromophores. Journal of Physical Chemistry A, 2022, 126, 752-759.	1.1	3
39	Ultrafast and green ionic liquid-mediated controlled cationic polymerization towards amphiphilic diblock copolymers. Polymer Chemistry, 2022, 13, 517-526.	1.9	3
40	Ab initio study of solvent-dependent one-, two- and three-photon absorption properties of PRODAN-based chemo-sensors. Journal of Chemical Sciences, 2014, 126, 1217-1226.	0.7	2
41	Effect of relative position of donor and acceptor groups on linear and non-linear optical properties of quinoline system. Chemical Physics Letters, 2020, 754, 137582.	1.2	1
42	Designing curcumin-based non-linear optically active compounds. Molecular Physics, 2021, 119, e1876265.	0.8	1
43	Spatial spin-charge separation in neutral endohedral metallofullerene: A combined restricted open-shell MP2 and Carâ€“Parrinello molecular dynamics study. Chemical Physics Letters, 2013, 557, 71-75.	1.2	0
44	A Theoretical Study of One- and Two-Photon Activity of D-Luciferin. Computation, 2016, 4, 43.	1.0	0
45	Structure, Carbonyl Vibrational Frequencies, and Local Energy Decomposition of Binding Energy in Formaldehyde Clusters, (HCHO)n=1â€“10. Journal of Physical Chemistry A, 2022, 126, 416-423.	1.1	0