Anita Das

List of Publications by Year in descending order

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26 papers	458 citations	687363 13 h-index	713466 21 g-index
26 all docs	26 docs citations	26 times ranked	450 citing authors

#	Article	IF	Citations
1	Polyradical Character of Triangular Non-KekulÃ© Structures, Zethrenes, p-Quinodimethane-Linked Bisphenalenyl, and the Clar Goblet in Comparison: An Extended Multireference Study. Journal of Physical Chemistry A, 2016, 120, 1625-1636.	2.5	91
2	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
3	Lithium doped tubular structure in LiB₂₀ and LiB₂₀^{â^'}: a viable global minimum. Physical Chemistry Chemical Physics, 2018, 20, 16202-16208.	2.8	32
4	Rennerâ€“Teller intersections along the collinear axes of polyatomic molecules: H2CN as a case study. Journal of Chemical Physics, 2010, 133, 084107.	3.0	28
5	Kinetics of the Strain-Promoted Oxidation-Controlled Cycloalkyne-1,2-quinone Cycloaddition: Experimental and Theoretical Studies. Journal of Organic Chemistry, 2018, 83, 244-252.	3.2	24
6	Evaluation of the quasi correlated tight-binding (QCTB) model for describing polyradical character in polycyclic hydrocarbons. Journal of Chemical Physics, 2017, 146, 064106.	3.0	21
7	Stable global tubular boron clusters in Na₂B₁₈ and Na₂B₁₈^{â^'}. RSC Advances, 2019, 9, 4665-4670.	3.6	18
8	Structural and electronic properties of MB₂₂^{â^'} (M = Na, K) clusters: tubular boron versus quasi-planar boron forms. New Journal of Chemistry, 2019, 43, 6507-6512.	2.8	17
9	A tri-atomic Renner-Teller system entangled with Jahn-Teller conical intersections. Journal of Chemical Physics, 2013, 138, 024113.	3.0	16
10	Jahnâ€“Teller Intersections Induced by Introduction of Bending in Linear Polyatomics: Study with HCNH, a Selected Molecular System. Journal of Physical Chemistry A, 2012, 116, 1774-1785.	2.5	15
11	The adiabaticâ€toâ€diabatic transformation angle and the berry phase for coupled jahnâ€“teller/rennerâ€“teller systems: The F + H₂ as a case study. International Journal of Quantum Chemistry, 2012, 112, 2561-2570.	2.0	15
12	Dressed Adiabatic and Diabatic Potentials To Study Topological Effects for F + H₂. Journal of Physical Chemistry A, 2014, 118, 6361-6366.	2.5	13
13	Local Electron Correlation Treatment in Extended Multireference Calculations: Effect of Acceptorâ€“Donor Substituents on the Biradical Character of the Polycyclic Aromatic Hydrocarbon Heptazethrene. Journal of Chemical Theory and Computation, 2017, 13, 2612-2622.	5.3	13
14	The effect of hydrogen bonding on the nonadiabatic dynamics of a thymine-water cluster. Chemical Physics, 2018, 515, 472-479.	1.9	13
15	Dressed adiabatic and diabatic potentials to study conical intersections for F + H2. Journal of Chemical Physics, 2012, 136, 054104.	3.0	12
16	Jahnâ€“Teller intersections involving excited states of the F+H2 system: Identification and influence on the reaction system. Chemical Physics, 2013, 412, 51-57.	1.9	11
17	Tuning the Biradicaloid Nature of Polycyclic Aromatic Hydrocarbons: The Effect of Graphitic Nitrogen Doping in Zethrenes. ChemPhysChem, 2018, 19, 2492-2499.	2.1	11
18	Derivation of diabatic potentials for F+H2 employing non-adiabatic coupling terms. Chemical Physics Letters, 2011, 517, 92-97.	2.6	10

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19	Diabatization of the reactive F + H2 system employing rigorous Berry phases. European Physical Journal D, 2011, 65, 373-381.	1.3	9
20	Study of Nonadiabatic Effects in Low-Lying Electronic States of HCNH with Implication in Its Dissociation to HCN and HNC. Journal of Physical Chemistry A, 2013, 117, 8680-8690.	2.5	9
21	Dressed Adiabatic and Diabatic Potentials for the Rennerâ€“Teller/Jahnâ€“Teller F + H₂ System. Journal of Physical Chemistry A, 2013, 117, 8497-8505.	2.5	9
22	Single and double carbon vacancies in pyrene as first models for graphene defects: A survey of the chemical reactivity toward hydrogen. Chemical Physics, 2017, 482, 346-354.	1.9	9
23	Investigation of plausible mechanistic pathways in hydrogenation of Î·5-(C5H5)2Ta(H)=CH2: an analysis using DFT and AIM techniques. Journal of Molecular Modeling, 2014, 20, 2132.	1.8	7
24	Interplay between Aromaticity and Radicaloid Character in Nitrogen-Doped Oligoacenes Revealed by High-Level Multireference Methods. Journal of Physical Chemistry A, 2018, 122, 9464-9473.	2.5	6
25	The adiabaticâ€toâ€diabatic transformation angle and topological phases for strongly interacting states: Solution with four states. International Journal of Quantum Chemistry, 2012, 112, 2767-2774.	2.0	5
26	Topological effects in low-lying electronic states of linear N₂H₂⁺ and HBNH⁺ associated with onset of bending. Molecular Physics, 2018, 116, 2642-2651.	1.7	2