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	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
2	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
3	Stable global tubular boron clusters in Na₂B₁₈ and Na₂B₁₈^{â^'}. RSC Advances, 2019, 9, 4665-4670.	3.6	18
4	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
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	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
7	Lithium doped tubular structure in LiB₂₀ and LiB₂₀^{â^'}: a viable global minimum. Physical Chemistry Chemical Physics, 2018, 20, 16202-16208.	2.8	32
8	The effect of hydrogen bonding on the nonadiabatic dynamics of a thymine-water cluster. Chemical Physics, 2018, 515, 472-479.	1.9	13
9	Tuning the Biradicaloid Nature of Polycyclic Aromatic Hydrocarbons: The Effect of Graphitic Nitrogen Doping in Zethrenes. ChemPhysChem, 2018, 19, 2492-2499.	2.1	11
10	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
11	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
12	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
13	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
14	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
15	Dressed Adiabatic and Diabatic Potentials To Study Topological Effects for F + H₂. Journal of Physical Chemistry A, 2014, 118, 6361-6366.	2.5	13
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	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
18	A tri-atomic Renner-Teller system entangled with Jahn-Teller conical intersections. Journal of Chemical Physics, 2013, 138, 024113.	3.0	16

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19	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
20	Dressed adiabatic and diabatic potentials to study conical intersections for F + H2. Journal of Chemical Physics, 2012, 136, 054104.	3.0	12
21	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
22	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
23	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
24	Derivation of diabatic potentials for F+H2 employing non-adiabatic coupling terms. Chemical Physics Letters, 2011, 517, 92-97.	2.6	10
25	Diabatization of the reactive F + H2 system employing rigorous Berry phases. European Physical Journal D, 2011, 65, 373-381.	1.3	9
26	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