Devashis Majumdar

List of Publications by Year
in descending order

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13	118	1307594 7	1281871 11
papers	citations	h-index	g-index

14	14	14	168
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	First-Principles Approach for Assessing Cold Electron Injection Efficiency of Dye-Sensitized Solar Cell: Elucidation of Mechanism of Charge Injection and Recombination. Journal of Physical Chemistry C, 2020, 124, 2817-2836.	3.1	25
2	Exploring Relative Thermodynamic Stabilities of Formic Acid and Formamide Dimers â€“ Role of Low-Frequency Hydrogen-Bond Vibrations. Journal of Chemical Theory and Computation, 2013, 9, 1016-1026.	5.3	17
3	Probing the Acetylcholinesterase Inhibition of Sarin:â€‰ A Comparative Interaction Study of the Inhibitor and Acetylcholine with a Model Enzyme Cavity. Journal of Physical Chemistry B, 2006, 110, 13597-13607.	2.6	16
4	Role of the Multipolar Electrostatic Interaction Energy Components in Strong and Weak Cationâˆ’Ï€ Interactions. Journal of Physical Chemistry A, 2013, 117, 7989-8000.	2.5	12
5	Density Functional Theory Based Studies on the Nature of Raman and Resonance Raman Scattering of Nerve Agent Bound to Gold and Oxide-Supported Gold Clusters: A Plausible Way of Detection. Journal of Physical Chemistry A, 2010, 114, 4340-4353.	2.5	10
6	Understanding the influence of low-frequency vibrations on the hydrogen bonds of acetic acid and acetamide dimers. Physical Chemistry Chemical Physics, 2017, 19, 24866-24878.	2.8	10
7	Do the low-energy conformers of nerve agents (NAs) really have cholinesterase inhibition properties? Investigations of the low-energy conformers of acetylcholine and the two NAs sarin and soman. Molecular Physics, 2007, 105, 2551-2564.	1.7	9
8	Theoretical investigations of the structure and bonding of several transition metal complexes to probe their carbon monoxide releasing properties. International Journal of Quantum Chemistry, 2009, 109, 2263-2272.	2.0	8
9	Conformational studies on parathion. International Journal of Quantum Chemistry, 2006, 106, 2356-2365.	2.0	3
10	In silico modeling of functionalized graphene oxide-metal cluster conjugates as Raman probe: Raman activity of pyridine. Structural Chemistry, 2017, 28, 379-389.	2.0	2
11	Jahn-Teller and Pseudo Jahn-Teller Effects: Influences on the Electronic Structures of Small Transition, Main Group and Mixed Metal Clusters. Structural Chemistry, 2020, 31, 7-23.	2.0	2
12	Another look at the structure of the (H2O)nâ€¢Ó¾ system: water anion vs. hydrated electron. Structural Chemistry, 2021, 32, 655-665.	2.0	2
13	First-Principles Modeling of Non-covalent Interactions in Molecular Systems and Extended Materials. , 2022, , 71-124.		0