

Debdutta Chakraborty

List of Publications by Year in descending order

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22
papers

417
citations

840776

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752698

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27
all docs

27
docs citations

27
times ranked

304
citing authors

#	ARTICLE	IF	CITATIONS
1	Direct dynamics simulation of the thermal O(³ P) + dimethylamine reaction in the triplet surface. I. Rate constant and product branching. Journal of Physical Organic Chemistry, 2023, 36, .	1.9	3
2	Conceptual density functional theory based electronic structure principles. Chemical Science, 2021, 12, 6264-6279.	7.4	96
3	Dynamics of Pyrene-Dimer Association and Ensuing Pyrene-Dimer Dissociation. Journal of Physical Chemistry A, 2020, 124, 8907-8917.	2.5	17
4	Bonding, Reactivity, and Dynamics in Confined Systems. Journal of Physical Chemistry A, 2019, 123, 4513-4531.	2.5	48
5	Reactions involving some gas molecules through sequestration on Al ₁₂ Be cluster: An electron density based study. Journal of Computational Chemistry, 2018, 39, 535-545.	3.3	5
6	Host-guest interactions between octa acid and cations/nucleobases. Journal of Computational Chemistry, 2018, 39, 161-175.	3.3	12
7	Confinement induced thermodynamic and kinetic facilitation of some Diels-Alder reactions inside a CB[7] cavitand. Journal of Computational Chemistry, 2018, 39, 151-160.	3.3	34
8	Confinement induced catalytic activity in a Diels-Alder reaction: comparison among various CB[n], n=6, 8, cavitands. Journal of Molecular Modeling, 2018, 24, 228.	1.8	7
9	Does Confinement Always Lead to Thermodynamically and/or Kinetically Favorable Reactions? A Case Study using Diels-Alder Reactions within ExBox ⁴ and CB[7]. ChemPhysChem, 2017, 18, 2162-2170.	2.1	24
10	Effect of functionalization of boron nitride flakes by main group metal clusters on their optoelectronic properties. Journal of Physics Condensed Matter, 2017, 29, 425201.	1.8	6
11	Change in optoelectronic properties of ExBox ⁴ on functionalization and guest encapsulation. Physical Chemistry Chemical Physics, 2017, 19, 23373-23385.	2.8	10
12	Does Confinement Always Lead to Thermodynamically and/or Kinetically Favorable Reactions? A Case Study using Diels-Alder Reactions within ExBox ⁴ and CB[7]. ChemPhysChem, 2017, 18, 2136-2136.	2.1	0
13	Possible sequestration of polar gas molecules by superhalogen supported aluminum nitride nanoflakes. Journal of Molecular Modeling, 2016, 22, 271.	1.8	3
14	Sequestration and Activation of Small Gas Molecules on BN-Flakes and the Effect of Various Metal Oxide Molecules therein. Journal of Physical Chemistry C, 2016, 120, 27782-27799.	3.1	9
15	Encapsulation of small gas molecules and rare gas atoms inside the octa acid cavitand. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	29
16	Optical response and gas sequestration properties of metal cluster supported graphene nanoflakes. Physical Chemistry Chemical Physics, 2016, 18, 18811-18827.	2.8	26
17	Orbital free DFT versus single density equation: a perspective through quantum domain behavior of a classically chaotic system. Physical Chemistry Chemical Physics, 2015, 17, 31516-31529.	2.8	13
18	Confinement induced binding in noble gas atoms within a BN-doped carbon nanotube. Chemical Physics Letters, 2015, 621, 29-34.	2.6	33

#	ARTICLE	IF	CITATIONS
19	In Quest of a Superhalogen Supported Covalent Bond Involving a Noble Gas Atom. Journal of Physical Chemistry A, 2015, 119, 3064-3074.	2.5	23
20	Interaction of BN- and BP-doped graphene nanoflakes with some representative neutral molecules and anions. Molecular Physics, 2015, 113, 2916-2929.	1.7	0
21	Quantum equivalence of a driven triple-well Van der Pol oscillator: A QTM study. Chemical Physics, 2014, 438, 7-15.	1.9	7
22	Density dynamics in some quantum systems. International Journal of Quantum Chemistry, 2013, 113, 1747-1771.	2.0	7