Debdutta Chakraborty

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3625811/publications.pdf

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22	417	840776	752698
papers	citations	11 h-index	20 g-index

27	27	27	304
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Conceptual density functional theory based electronic structure principles. Chemical Science, 2021, 12, 6264-6279.	7.4	96
2	Bonding, Reactivity, and Dynamics in Confined Systems. Journal of Physical Chemistry A, 2019, 123, 4513-4531.	2.5	48
3	Confinement induced thermodynamic and kinetic facilitation of some Dielsâ€“Alder reactions inside a CB[7] cavitand. Journal of Computational Chemistry, 2018, 39, 151-160.	3.3	34
4	Confinement induced binding in noble gas atoms within a BN-doped carbon nanotube. Chemical Physics Letters, 2015, 621, 29-34.	2.6	33
5	Encapsulation of small gas molecules and rare gas atoms inside the octa acid cavitand. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	29
6	Optical response and gas sequestration properties of metal cluster supported graphene nanoflakes. Physical Chemistry Chemical Physics, 2016, 18, 18811-18827.	2.8	26
7	Does Confinement Always Lead to Thermodynamically and/or Kinetically Favorable Reactions? A Case Study using Dielsâ€“Alder Reactions within ExBox⁺⁴ and CB[7]. ChemPhysChem, 2017, 18, 2162-2170.	2.1	24
8	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
9	Dynamics of Pyrene-Dimer Association and Ensuing Pyrene-Dimer Dissociation. Journal of Physical Chemistry A, 2020, 124, 8907-8917.	2.5	17
10	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
11	Hostâ€“guest interactions between octa acid and cations/nucleobases. Journal of Computational Chemistry, 2018, 39, 161-175.	3.3	12
12	Change in optoelectronic properties of ExBox⁺⁴ on functionalization and guest encapsulation. Physical Chemistry Chemical Physics, 2017, 19, 23373-23385.	2.8	10
13	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
14	Density dynamics in some quantum systems. International Journal of Quantum Chemistry, 2013, 113, 1747-1771.	2.0	7
15	Quantum equivalence of a driven triple-well Van der Pol oscillator: A QTM study. Chemical Physics, 2014, 438, 7-15.	1.9	7
16	Confinement induced catalytic activity in a Diels-Alder reaction: comparison among various CB[n], nâ€‰=â€‰6â€“8, cavitands. Journal of Molecular Modeling, 2018, 24, 228.	1.8	7
17	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
18	Reactions involving some gas molecules through sequestration on Al₁₂Be cluster: An electron density based study. Journal of Computational Chemistry, 2018, 39, 535-545.	3.3	5

#	Article	IF	Citations
19	Possible sequestration of polar gas molecules by superhalogen supported aluminum nitride nanoflakes. Journal of Molecular Modeling, 2016, 22, 271.	1.8	3
20	Direct dynamics simulation of the thermal O(³P)â€‰+â€‰dimethylamine reaction in the triplet surface. I. Rate constant and product branching. Journal of Physical Organic Chemistry, 2023, 36, .	1.9	3
21	Interaction of BN- and BP-doped graphene nanoflakes with some representative neutral molecules and anions. Molecular Physics, 2015, 113, 2916-2929.	1.7	0
22	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