Tandabany C Dinadayalane

List of Publications by Year
in descending order

58	1,919	236925 25	254184 43
papers	citations	h-index	g-index

60	60	60	1908
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Structures, properties, and applications of nitrogen-doped graphene. Theoretical and Computational Chemistry, 2022, , 211-248.	0.4	3
2	DFT study on binding of single and double methane with aromatic hydrocarbons and graphene: stabilizing CHâ€¦HC interactions between two methane molecules. Structural Chemistry, 2021, 32, 591-605.	2.0	7
3	Data related to conformation dependence of tyrosine binding on the surface of graphene: Bent prefers over parallel orientation. Data in Brief, 2019, 26, 104420.	1.0	4
4	Binding of histidine and proline with graphene: DFT study. Chemical Physics Letters, 2019, 730, 147-152.	2.6	11
5	Conformation dependence of tyrosine binding on the surface of graphene: Bent prefers over parallel orientation. Applied Surface Science, 2019, 483, 178-186.	6.1	10
6	Computational Chemistry and Biology Courses for Undergraduates at an HBCU: Cultivating a Diverse Computational Science Community. ACS Symposium Series, 2019, , 67-81.	0.5	1
7	Computational investigation of double nitrogen doping on graphene. Journal of Molecular Modeling, 2018, 24, 26.	1.8	9
8	Binding of Alkali Metal Ions with 1,3,5-Tri(phenyl)benzene and 1,3,5-Tri(naphthyl)benzene: The Effect of Phenyl and Naphthyl Ring Substitution on Cationâ^'Ï€ Interactions Revealed by DFT Study. Journal of Physical Chemistry A, 2017, 121, 8927-8938.	2.5	5
9	A hydrogen bonded Co(ii) coordination complex and a triply interpenetrating 3-D manganese(ii) coordination polymer from diaza crown ether with dibenzoate sidearms. CrystEngComm, 2016, 18, 2425-2436.	2.6	4
10	Toward Selection of Efficient Density Functionals for van der Waals Molecular Complexes: Comparative Study of Câ€“HÂ·Â·Â·Ï€ and Nâ€“HÂ·Â·Â·Ï€ Interactions. Journal of Physical Chemistry A, 2015, 119, 1190-1200.	2.5	22
11	Computational study on Câ^'Hâ€¦Ï€ interactions of acetylene with benzene, 1,3,5-trifluorobenzene and coronene. Journal of Molecular Modeling, 2013, 19, 2855-2864.	1.8	30
12	Structural, energetic, spectroscopic and QTAIM analyses of cationâ€“Ï€ interactions involving mono- and bi-cyclic ring fused benzene systems. Physical Chemistry Chemical Physics, 2013, 15, 20839.	2.8	21
13	Comparative Theoretical Study on the Positional Preference for Functionalization of Two OH and SH Groups with (5,5) Armchair SWCNT. Journal of Physical Chemistry C, 2013, 117, 14441-14450.	3.1	10
14	DFT-based reactivity study of (5,5) armchair boron nitride nanotube (BNNT). Chemical Physics Letters, 2013, 565, 69-73.	2.6	39
15	Comprehensive Study on the Dissociative Chemisorption of NH₃ on the Sidewalls of Stoneâ€“Wales Defective Armchair (5,5) Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 6012-6021.	3.1	31
16	Chapter 1. Graphene: Properties, Biomedical Applications and Toxicity. RSC Nanoscience and Nanotechnology, 2012, , 1-26.	0.2	2
17	Open and capped (5,5) armchair SWCNTs: A comparative study of DFT-based reactivity descriptors. Chemical Physics Letters, 2012, 541, 85-91.	2.6	46
18	Advancing risk assessment of engineered nanomaterials: Application of computational approaches. Advanced Drug Delivery Reviews, 2012, 64, 1663-1693.	13.7	186

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19	Surface Reactivity for Chlorination on Chlorinated (5,5) Armchair SWCNT: A Computational Approach. Journal of Physical Chemistry C, 2012, 116, 22399-22410.	3.1	62
20	Mechanical properties of silicon nanowires. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 817-828.	14.6	12
21	A theoretical study of cation-Ï€ interactions: Li+, Na+, K+, Be2+, Mg2+ and Ca2+ complexation with mono- and bicyclic ring-fused benzene derivatives. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	30
22	Fundamental Structural, Electronic, and Chemical Properties of Carbon Nanostructures: Graphene, Fullerenes, Carbon Nanotubes, and Their Derivatives. , 2012, , 793-867.		17
23	Carâ€“Parrinello Molecular Dynamics Simulations of Tensile Tests on SiâŸ·001âŸ© Nanowires. Journal of Physical Chemistry C, 2011, 115, 12283-12292.	3.1	5
24	Do Stoneâ€“Wales Defects Alter the Magnetic and Transport Properties of Single-Walled Carbon Nanotubes?. Journal of Physical Chemistry C, 2011, 115, 22232-22241.	3.1	28
25	The effect of ring annelation to benzene on cation-Ï€ interactions: DFT study. Journal of Molecular Structure, 2010, 976, 320-323.	3.6	16
26	Remarkable diversity of carbonâ€“carbon bonds: structures and properties of fullerenes, carbon nanotubes, and graphene. Structural Chemistry, 2010, 21, 1155-1169.	2.0	136
27	Reactivities of Sites on (5,5) Single-Walled Carbon Nanotubes with and without a Stone-Wales Defect. Journal of Chemical Theory and Computation, 2010, 6, 1351-1357.	5.3	126
28	In the pursuit of small â€œred shiftâ€•of Câ€“H stretching vibrational frequency of Câ€“Hâ‹¯Ï€ interactions for benzene dimer: How to amend MP2 calculations to reproduce the experimental results. Journal of Chemical Physics, 2009, 130, 081101.	3.0	26
29	Toward Understanding of Hydrogen Storage in Single-Walled Carbon Nanotubes by Investigations of Chemisorption Mechanism. , 2009, , 297-313.		7
30	Geometries and stabilities of various configurations of benzene dimer: details of novel V-shaped structure revealed. Structural Chemistry, 2009, 20, 11-20.	2.0	42
31	Structures and Energetics of the Cationâˆ’Ï€ Interactions of Li⁺, Na⁺, and K⁺ with Cup-Shaped Molecules: Effect of Ring Addition to Benzene and Cavity Selectivity. Journal of Physical Chemistry A, 2008, 112, 7916-7924.	2.5	32
32	Comprehensive Study on the Solvation of Mono- and Divalent Metal Cations: Li⁺, Na⁺, K⁺, Be²⁺, Mg²⁺ and Ca²⁺. Journal of Physical Chemistry A, 2008, 112, 12944-12953.	2.5	127
33	Chapter 7 Toward nanomaterials: Structural, energetic and reactivity aspects of single-walled carbon nanotubes. Theoretical and Computational Chemistry, 2007, 18, 167-199.	0.4	13
34	Chemisorption of Hydrogen Atoms on the Sidewalls of Armchair Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2007, 111, 7376-7383.	3.1	79
35	Stoneâ€“Wales defects with two different orientations in (5, 5) single-walled carbon nanotubes: A theoretical study. Chemical Physics Letters, 2007, 434, 86-91.	2.6	80
36	Effect of ring annelation on Li+â€“benzene interaction: A computational study. Chemical Physics Letters, 2007, 443, 205-210.	2.6	26

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37	Effect of tube length on the chemisorptions of one and two hydrogen atoms on the sidewalls of (3,3) and (4,4) single-walled carbon nanotubes: A theoretical study. International Journal of Quantum Chemistry, 2007, 107, 2211-2219.	2.0	32
38	Cumulative Ï€-Ï€ interaction triggers unusually high stabilization of linear hydrocarbons inside the single-walled carbon nanotube. International Journal of Quantum Chemistry, 2007, 107, 2204-2210.	2.0	31
39	Comprehensive theoretical study towards the accurate proton affinity values of naturally occurring amino acids. International Journal of Quantum Chemistry, 2006, 106, 2920-2933.	2.0	60
40	Competitive Dielsâ^'Alder Reactions:â€‰ Cyclopentadiene and Phospholes with Butadiene. Journal of Physical Chemistry A, 2005, 109, 9310-9323.	2.5	20
41	Modelling of the Stabilization of the Complex of a Single Walled (5,5) Carbon Nanotube C60H20 with Cumulenic or Acetylenic Chain. AIP Conference Proceedings, 2005, , .	0.4	6
42	Density functional theory study of the Dielsâ€“Alder reactivities of[b]-annelated cyclic five-membered dienes. Journal of Physical Organic Chemistry, 2004, 17, 152-161.	1.9	8
43	Density Functional Theory Study on the Effect of Substitution and Ring Annelation to the Rim of Corannuleneâ€. Journal of Organic Chemistry, 2004, 69, 8111-8114.	3.2	32
44	Exploration of C6H6Potential Energy Surface:Â A Computational Effort to Unravel the Relative Stabilities and Synthetic Feasibility of New Benzene Isomersâ€. Journal of Physical Chemistry A, 2004, 108, 11433-11448.	2.5	80
45	Isolated pentagon rule in buckybowls: a computational study on thermodynamic stabilities and bowl-to-bowl inversion barriers. Tetrahedron, 2003, 59, 8347-8351.	1.9	27
46	Is peri hydrogen repulsion responsible for flattening buckybowls? The effect of ring annelation to the rim of corannulene. Tetrahedron Letters, 2003, 44, 4527-4529.	1.4	20
47	A theoretical study on cycloaddition reactions between [c]-annelated heterocyclic five-membered dienes and acetylene. Computational and Theoretical Chemistry, 2003, 626, 247-262.	1.5	10
48	Ab Initio and Density Functional Theory (DFT) Study on [1,5] Sigmatropic Rearrangements in Pyrroles, Phospholes, and Siloles and Their Dielsâ^'Alder Reactivities,. Journal of Physical Chemistry A, 2003, 107, 5479-5487.	2.5	28
49	Density Functional Theory Study on Dimerizations of Phospholesâ€. Organometallics, 2003, 22, 5526-5533.	2.3	15
50	Structureâ^'Energy Relationships in Curved Polycyclic Aromatic Hydrocarbons:â€‰ Study of Benzocorannulenes. Journal of Organic Chemistry, 2002, 67, 4605-4607.	3.2	30
51	Dielsâ^'Alder Reactivity of Butadiene and Cyclic Five-Membered Dienes ((CH)4X, X = CH2, SiH2, O, NH, PH,) Tj ETQq1 1 0.784314 rgBT	2.5	90
52	A computational study of the valence isomers of benzene and their group V hetero analogs. New Journal of Chemistry, 2002, 26, 347-353.	2.8	25
53	An assessment of semiempirical (MNDO, AM1 and PM3) methods to model buckybowls. Computational and Theoretical Chemistry, 2002, 579, 63-72.	1.5	10
54	Dielsâ€“Alder reactions between cyclic five-membered dienes and acetylene. Computational and Theoretical Chemistry, 2002, 589-590, 291-299.	1.5	19

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55	Synthetic strategies toward buckybowls and C60: benzannulation is remarkably facile compared to cyclopentannulation. Tetrahedron Letters, 2001, 42, 6421-6423.	1.4	14
56	Structures, energetics and vibrational spectra of the valence isomers of phosphinine. An ab initio and DFT study. Chemical Physics Letters, 2001, 336, 343-348.	2.6	14
57	An ab initio and DFT study of the valence isomers of pyridine. Chemical Physics Letters, 2001, 337, 361-367.	2.6	17
58	Theoretical studies on the effect of sequential benzannulation to corannulene. Computational and Theoretical Chemistry, 2001, 543, 1-10.	1.5	26