

Tandabany C Dinadayalane

List of Publications by Year in descending order

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58
papers

1,919
citations

236925

25
h-index

254184

43
g-index

60
all docs

60
docs citations

60
times ranked

1908
citing authors

#	ARTICLE	IF	CITATIONS
1	Advancing risk assessment of engineered nanomaterials: Application of computational approaches. <i>Advanced Drug Delivery Reviews</i> , 2012, 64, 1663-1693.	13.7	186
2	Remarkable diversity of carbon-carbon bonds: structures and properties of fullerenes, carbon nanotubes, and graphene. <i>Structural Chemistry</i> , 2010, 21, 1155-1169.	2.0	136
3	Comprehensive Study on the Solvation of Mono- and Divalent Metal Cations: Li^+ , Na^+ , K^+ , Be^{2+} , Mg^{2+} and Ca^{2+} . <i>Journal of Physical Chemistry A</i> , 2008, 112, 12944-12953.	2.5	127
4	Reactivities of Sites on (5,5) Single-Walled Carbon Nanotubes with and without a Stone-Wales Defect. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1351-1357.	5.3	126
5	Diels-Alder Reactivity of Butadiene and Cyclic Five-Membered Dienes ((CH) ₄ X, X = CH ₂ , SiH ₂ , O, NH, PH). <i>J. Phys. Chem. A</i> , 2004, 108, 11433-11448.	2.5	90
6	Exploration of C ₆ H ₆ Potential Energy Surface: A Computational Effort to Unravel the Relative Stabilities and Synthetic Feasibility of New Benzene Isomers. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11433-11448.	2.5	80
7	Stone-Wales defects with two different orientations in (5, 5) single-walled carbon nanotubes: A theoretical study. <i>Chemical Physics Letters</i> , 2007, 434, 86-91.	2.6	80
8	Chemisorption of Hydrogen Atoms on the Sidewalls of Armchair Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2007, 111, 7376-7383.	3.1	79
9	Surface Reactivity for Chlorination on Chlorinated (5,5) Armchair SWCNT: A Computational Approach. <i>Journal of Physical Chemistry C</i> , 2012, 116, 22399-22410.	3.1	62
10	Comprehensive theoretical study towards the accurate proton affinity values of naturally occurring amino acids. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2920-2933.	2.0	60
11	Open and capped (5,5) armchair SWCNTs: A comparative study of DFT-based reactivity descriptors. <i>Chemical Physics Letters</i> , 2012, 541, 85-91.	2.6	46
12	Geometries and stabilities of various configurations of benzene dimer: details of novel V-shaped structure revealed. <i>Structural Chemistry</i> , 2009, 20, 11-20.	2.0	42
13	DFT-based reactivity study of (5,5) armchair boron nitride nanotube (BNNT). <i>Chemical Physics Letters</i> , 2013, 565, 69-73.	2.6	39
14	Density Functional Theory Study on the Effect of Substitution and Ring Annulation to the Rim of Corannulene. <i>Journal of Organic Chemistry</i> , 2004, 69, 8111-8114.	3.2	32
15	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. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 2211-2219.	2.0	32
16	Structures and Energetics of the Cation Interactions of Li^+ , Na^+ , and K^+ with Cup-Shaped Molecules: Effect of Ring Addition to Benzene and Cavity Selectivity. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7916-7924.	2.5	32
17	Cumulative interaction triggers unusually high stabilization of linear hydrocarbons inside the single-walled carbon nanotube. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 2204-2210.	2.0	31
18	Comprehensive Study on the Dissociative Chemisorption of NH_3 on the Sidewalls of Stone-Wales Defective Armchair (5,5) Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 6012-6021.	3.1	31

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19	Structure–Energy Relationships in Curved Polycyclic Aromatic Hydrocarbons: Study of Benzocorannulenes. <i>Journal of Organic Chemistry</i> , 2002, 67, 4605-4607.	3.2	30
20	A theoretical study of cation–π interactions: Li+, Na+, K+, Be2+, Mg2+ and Ca2+ complexation with mono- and bicyclic ring-fused benzene derivatives. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	30
21	Computational study on C–H···π interactions of acetylene with benzene, 1,3,5-trifluorobenzene and coronene. <i>Journal of Molecular Modeling</i> , 2013, 19, 2855-2864.	1.8	30
22	Ab Initio and Density Functional Theory (DFT) Study on [1,5] Sigmatropic Rearrangements in Pyrroles, Phospholes, and Siloles and Their Diels–Alder Reactivities,. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5479-5487.	2.5	28
23	Do Stone–Wales Defects Alter the Magnetic and Transport Properties of Single-Walled Carbon Nanotubes?. <i>Journal of Physical Chemistry C</i> , 2011, 115, 22232-22241.	3.1	28
24	Isolated pentagon rule in buckybowls: a computational study on thermodynamic stabilities and bowl-to-bowl inversion barriers. <i>Tetrahedron</i> , 2003, 59, 8347-8351.	1.9	27
25	Theoretical studies on the effect of sequential benzannulation to corannulene. <i>Computational and Theoretical Chemistry</i> , 2001, 543, 1-10.	1.5	26
26	Effect of ring annelation on Li+–benzene interaction: A computational study. <i>Chemical Physics Letters</i> , 2007, 443, 205-210.	2.6	26
27	In the pursuit of small δ -cored shift of C–H stretching vibrational frequency of C–H···π interactions for benzene dimer: How to amend MP2 calculations to reproduce the experimental results. <i>Journal of Chemical Physics</i> , 2009, 130, 081101.	3.0	26
28	A computational study of the valence isomers of benzene and their group V hetero analogs. <i>New Journal of Chemistry</i> , 2002, 26, 347-353.	2.8	25
29	Toward Selection of Efficient Density Functionals for van der Waals Molecular Complexes: Comparative Study of C–H···π and N–H···π Interactions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1190-1200.	2.5	22
30	Structural, energetic, spectroscopic and QTAIM analyses of cation–π interactions involving mono- and bi-cyclic ring fused benzene systems. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 20839.	2.8	21
31	Is peri hydrogen repulsion responsible for flattening buckybowls? The effect of ring annelation to the rim of corannulene. <i>Tetrahedron Letters</i> , 2003, 44, 4527-4529.	1.4	20
32	Competitive Diels–Alder Reactions: Cyclopentadiene and Phospholes with Butadiene. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9310-9323.	2.5	20
33	Diels–Alder reactions between cyclic five-membered dienes and acetylene. <i>Computational and Theoretical Chemistry</i> , 2002, 589-590, 291-299.	1.5	19
34	An ab initio and DFT study of the valence isomers of pyridine. <i>Chemical Physics Letters</i> , 2001, 337, 361-367.	2.6	17
35	Fundamental Structural, Electronic, and Chemical Properties of Carbon Nanostructures: Graphene, Fullerenes, Carbon Nanotubes, and Their Derivatives. , 2012, , 793-867.		17
36	The effect of ring annelation to benzene on cation–π interactions: DFT study. <i>Journal of Molecular Structure</i> , 2010, 976, 320-323.	3.6	16

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37	Density Functional Theory Study on Dimerizations of Phospholes. <i>Organometallics</i> , 2003, 22, 5526-5533.	2.3	15
38	Synthetic strategies toward buckybowls and C60: benzannulation is remarkably facile compared to cyclopentannulation. <i>Tetrahedron Letters</i> , 2001, 42, 6421-6423.	1.4	14
39	Structures, energetics and vibrational spectra of the valence isomers of phosphinine. An ab initio and DFT study. <i>Chemical Physics Letters</i> , 2001, 336, 343-348.	2.6	14
40	Chapter 7 Toward nanomaterials: Structural, energetic and reactivity aspects of single-walled carbon nanotubes. <i>Theoretical and Computational Chemistry</i> , 2007, 18, 167-199.	0.4	13
41	Mechanical properties of silicon nanowires. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 817-828.	14.6	12
42	Binding of histidine and proline with graphene: DFT study. <i>Chemical Physics Letters</i> , 2019, 730, 147-152.	2.6	11
43	An assessment of semiempirical (MNDO, AM1 and PM3) methods to model buckybowls. <i>Computational and Theoretical Chemistry</i> , 2002, 579, 63-72.	1.5	10
44	A theoretical study on cycloaddition reactions between [c]-annelated heterocyclic five-membered dienes and acetylene. <i>Computational and Theoretical Chemistry</i> , 2003, 626, 247-262.	1.5	10
45	Comparative Theoretical Study on the Positional Preference for Functionalization of Two OH and SH Groups with (5,5) Armchair SWCNT. <i>Journal of Physical Chemistry C</i> , 2013, 117, 14441-14450.	3.1	10
46	Conformation dependence of tyrosine binding on the surface of graphene: Bent prefers over parallel orientation. <i>Applied Surface Science</i> , 2019, 483, 178-186.	6.1	10
47	Computational investigation of double nitrogen doping on graphene. <i>Journal of Molecular Modeling</i> , 2018, 24, 26.	1.8	9
48	Density functional theory study of the Diels-Alder reactivities of [b]-annelated cyclic five-membered dienes. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 152-161.	1.9	8
49	Toward Understanding of Hydrogen Storage in Single-Walled Carbon Nanotubes by Investigations of Chemisorption Mechanism. , 2009, , 297-313.		7
50	DFT study on binding of single and double methane with aromatic hydrocarbons and graphene: stabilizing CH ₃ -HC interactions between two methane molecules. <i>Structural Chemistry</i> , 2021, 32, 591-605.	2.0	7
51	Modelling of the Stabilization of the Complex of a Single Walled (5,5) Carbon Nanotube C ₆₀ H ₂₀ with Cumulenic or Acetylenic Chain. <i>AIP Conference Proceedings</i> , 2005, , .	0.4	6
52	Car-Parrinello Molecular Dynamics Simulations of Tensile Tests on Si Nanowires. <i>Journal of Physical Chemistry C</i> , 2011, 115, 12283-12292.	3.1	5
53	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 Cation-π Interactions Revealed by DFT Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8927-8938.	2.5	5
54	A hydrogen bonded Co(ii) coordination complex and a triply interpenetrating 3-D manganese(ii) coordination polymer from diaza crown ether with dibenzoate sidearms. <i>CrystEngComm</i> , 2016, 18, 2425-2436.	2.6	4

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55	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
56	Structures, properties, and applications of nitrogen-doped graphene. Theoretical and Computational Chemistry, 2022, , 211-248.	0.4	3
57	Chapter 1. Graphene: Properties, Biomedical Applications and Toxicity. RSC Nanoscience and Nanotechnology, 2012, , 1-26.	0.2	2
58	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