# Tandabany C Dinadayalane

List of Publications by Year
in descending order



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|---|---|---|---|
| 58 papers | 1,919 citations | 236833 25 h-index | 254106 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. Advanced Drug Delivery Reviews, 2012, 64, 1663-1693. | 6.6 | 186 |
| 2 | Remarkable diversity of carbonâ€“carbon bonds: structures and properties of fullerenes, carbon nanotubes, and graphene. Structural Chemistry, 2010, 21, 1155-1169. | 1.0 | 136 |
| 3 | Comprehensive Study on the Solvation of Mono- and Divalent Metal Cations: Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>, Be<sup>2+</sup>, Mg<sup>2+</sup> and Ca<sup>2+</sup>. Journal of Physical Chemistry A, 2008, 112, 12944-12953. | 1.1 | 127 |
| 4 | 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. | 2.3 | 126 |
| 5 | Dielsâ^'Alder Reactivity of Butadiene and Cyclic Five-Membered Dienes ((CH)4X, X = CH2, SiH2, O, NH, PH,) Tj ETQq1 1 0.784314 rgBT /O | 1.1 | 90 |
| 6 | 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. | 1.1 | 80 |
| 7 | Stoneâ€“Wales defects with two different orientations in (5, 5) single-walled carbon nanotubes: A theoretical study. Chemical Physics Letters, 2007, 434, 86-91. | 1.2 | 80 |
| 8 | Chemisorption of Hydrogen Atoms on the Sidewalls of Armchair Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2007, 111, 7376-7383. | 1.5 | 79 |
| 9 | Surface Reactivity for Chlorination on Chlorinated (5,5) Armchair SWCNT: A Computational Approach. Journal of Physical Chemistry C, 2012, 116, 22399-22410. | 1.5 | 62 |
| 10 | Comprehensive theoretical study towards the accurate proton affinity values of naturally occurring amino acids. International Journal of Quantum Chemistry, 2006, 106, 2920-2933. | 1.0 | 60 |
| 11 | Open and capped (5,5) armchair SWCNTs: A comparative study of DFT-based reactivity descriptors. Chemical Physics Letters, 2012, 541, 85-91. | 1.2 | 46 |
| 12 | Geometries and stabilities of various configurations of benzene dimer: details of novel V-shaped structure revealed. Structural Chemistry, 2009, 20, 11-20. | 1.0 | 42 |
| 13 | DFT-based reactivity study of (5,5) armchair boron nitride nanotube (BNNT). Chemical Physics Letters, 2013, 565, 69-73. | 1.2 | 39 |
| 14 | 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. | 1.7 | 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. International Journal of Quantum Chemistry, 2007, 107, 2211-2219. | 1.0 | 32 |
| 16 | Structures and Energetics of the Cationâ^'Ï€ Interactions of Li<sup>+</sup>, Na<sup>+</sup>, and K<sup>+</sup> with Cup-Shaped Molecules: Effect of Ring Addition to Benzene and Cavity Selectivity. Journal of Physical Chemistry A, 2008, 112, 7916-7924. | 1.1 | 32 |
| 17 | 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. | 1.0 | 31 |
| 18 | Comprehensive Study on the Dissociative Chemisorption of NH<sub>3</sub> on the Sidewalls of Stoneâ€“Wales Defective Armchair (5,5) Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 6012-6021. | 1.5 | 31 |

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|---|---|---|---|
| 19 | Structureâ^'Energy Relationships in Curved Polycyclic Aromatic Hydrocarbons:â€‰ Study of Benzocorannulenes. Journal of Organic Chemistry, 2002, 67, 4605-4607. | 1.7 | 30 |
| 20 | 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. | 0.5 | 30 |
| 21 | 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. | 0.8 | 30 |
| 22 | 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. | 1.1 | 28 |
| 23 | Do Stoneâ€“Wales Defects Alter the Magnetic and Transport Properties of Single-Walled Carbon Nanotubes?. Journal of Physical Chemistry C, 2011, 115, 22232-22241. | 1.5 | 28 |
| 24 | Isolated pentagon rule in buckybowls: a computational study on thermodynamic stabilities and bowl-to-bowl inversion barriers. Tetrahedron, 2003, 59, 8347-8351. | 1.0 | 27 |
| 25 | Theoretical studies on the effect of sequential benzannulation to corannulene. Computational and Theoretical Chemistry, 2001, 543, 1-10. | 1.5 | 26 |
| 26 | Effect of ring annelation on Li+â€“benzene interaction: A computational study. Chemical Physics Letters, 2007, 443, 205-210. | 1.2 | 26 |
| 27 | 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. | 1.2 | 26 |
| 28 | A computational study of the valence isomers of benzene and their group V hetero analogs. New Journal of Chemistry, 2002, 26, 347-353. | 1.4 | 25 |
| 29 | 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. | 1.1 | 22 |
| 30 | 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. | 1.3 | 21 |
| 31 | Is peri hydrogen repulsion responsible for flattening buckybowls? The effect of ring annelation to the rim of corannulene. Tetrahedron Letters, 2003, 44, 4527-4529. | 0.7 | 20 |
| 32 | Competitive Dielsâ^'Alder Reactions:â€‰ Cyclopentadiene and Phospholes with Butadiene. Journal of Physical Chemistry A, 2005, 109, 9310-9323. | 1.1 | 20 |
| 33 | Dielsâ€“Alder reactions between cyclic five-membered dienes and acetylene. Computational and Theoretical Chemistry, 2002, 589-590, 291-299. | 1.5 | 19 |
| 34 | An ab initio and DFT study of the valence isomers of pyridine. Chemical Physics Letters, 2001, 337, 361-367. | 1.2 | 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-Ï€ interactions: DFT study. Journal of Molecular Structure, 2010, 976, 320-323. | 1.8 | 16 |

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| 37 | Density Functional Theory Study on Dimerizations of Phospholesâ€. Organometallics, 2003, 22, 5526-5533. | 1.1 | 15 |
| 38 | Synthetic strategies toward buckybowls and C60: benzannulation is remarkably facile compared to cyclopentannulation. Tetrahedron Letters, 2001, 42, 6421-6423. | 0.7 | 14 |
| 39 | Structures, energetics and vibrational spectra of the valence isomers of phosphinine. An ab initio and DFT study. Chemical Physics Letters, 2001, 336, 343-348. | 1.2 | 14 |
| 40 | Chapter 7 Toward nanomaterials: Structural, energetic and reactivity aspects of single-walled carbon nanotubes. Theoretical and Computational Chemistry, 2007, 18, 167-199. | 0.2 | 13 |
| 41 | Mechanical properties of silicon nanowires. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 817-828. | 6.2 | 12 |
| 42 | Binding of histidine and proline with graphene: DFT study. Chemical Physics Letters, 2019, 730, 147-152. | 1.2 | 11 |
| 43 | An assessment of semiempirical (MNDO, AM1 and PM3) methods to model buckybowls. Computational and Theoretical Chemistry, 2002, 579, 63-72. | 1.5 | 10 |
| 44 | 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 |
| 45 | 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. | 1.5 | 10 |
| 46 | Conformation dependence of tyrosine binding on the surface of graphene: Bent prefers over parallel orientation. Applied Surface Science, 2019, 483, 178-186. | 3.1 | 10 |
| 47 | Computational investigation of double nitrogen doping on graphene. Journal of Molecular Modeling, 2018, 24, 26. | 0.8 | 9 |
| 48 | 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. | 0.9 | 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 CHâ€¦HC interactions between two methane molecules. Structural Chemistry, 2021, 32, 591-605. | 1.0 | 7 |
| 51 | 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, , . | 0.3 | 6 |
| 52 | Carâ€“Parrinello Molecular Dynamics Simulations of Tensile Tests on SiâŸ001âŸ© Nanowires. Journal of Physical Chemistry C, 2011, 115, 12283-12292. | 1.5 | 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 Cationâ^Ï€ Interactions Revealed by DFT Study. Journal of Physical Chemistry A, 2017, 121, 8927-8938. | 1.1 | 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. CrystEngComm, 2016, 18, 2425-2436. | 1.3 | 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. | 0.5 | 4 |
| 56 | Structures, properties, and applications of nitrogen-doped graphene. Theoretical and Computational Chemistry, 2022, , 211-248. | 0.2 | 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 |