Dinadayalane Tandabany
Associate Professor

Faculty member since 2014
Specialty: Chemistry (Computational and Materials)
Telephone: 404 880-6969 Fax 404 880-68909
Email: dtndabany@cau.edu
Chemistry Department
223 James P. Brawley Drive
Atlanta, Georgia 30314

Thomas W. Cole Jr. Research Center for Science and Technology
Room 2033-G

EDUCATION

Ph.D., Chemistry, April 2005 Pondicherry University, Puducherry, India
M. Sc. Chemical Sciences, May 2000 Pondicherry University, Puducherry, India
B. Sc., Chemistry, May 1998 Pondicherry University, Puducherry, India

POSITIONS

Department of Chemistry, Clark Atlanta University
Associate Professor 01/2014 - Present
Department of Chemistry and Biochemistry Jackson State University, Jackson, MS
Research Professor 04/2013 - 01/2014
Postdoctoral Research Associate 05/2005 - 03/2013
Research Assistant 08/2004 - 05/2005

PUBLICATIONS

https://scholar.google.com/citations?user=Y9MAIjUAAAAJ&hl=en

1. Dhandapani, P.; Balan, B.; Dinadayalane, T.; Angaiah, S. "In-situ grown of $FeCo_2O_4$ onto 2D - Carbyne coated nickel foam - A newer nanohybrid electrode for high performance supercapacitors", *New J. Chem.* **2022**
2. Cahill, K.; Akli, L.; **Dinadayalane, T.**; Gonzalez, A.; Isokpehi, R. D.; Nkwanta, A.; Vincent-Finley, R.; Rivera, L.; Tannouri, A. "Building a Computational and Data Science Workforce", *Comput. Sci. Ed.* **2022**, *13*, 27-31. https://doi.org/10.22369/issn.2153-4136/13/1/5
3. Lazare, J.; Daggag, D.; **Dinadayalane, T.** "DFT study on binding of single and double methane with aromatic hydrocarbons and graphene: Stabilizing CH…HC interactions between two methane molecules", *Chem.* **2021**, *32*, 591-605. https://doi.org/10.1007/s11224-020-01657-y
4. Pierce, M.; Hayden, L.; Dey, C.; Akli, L.; **Dinadayalane, T.**; Isokpehi, R.; Gonzalez, A. C. "Identifying Opportunities and Needs for Science Gateways in Education at Minority Serving Institutions", Practice & Experience in Advanced Research Computing 2020 (PEARC20) conference, virtual, July 27 - 31, **2020**. (Peer-reviewed conference article)
5. Daggag, D.; Lazare, J.; **Dinadayalane, T.** "Data related to conformation dependence of tyrosine binding on the surface of graphene: Bent prefers over parallel orientation", *Data Brief* **2019**, *26*, 104420. https://doi.org/10.1016/j.dib.2019.104420 Daggag, D.; Dorlus, T.; **Dinadayalane, T.** "Binding of histidine and proline with graphene: DFT study", *Phys. Lett.* **2019**, *730*, 147-152. https://doi.org/10.1016/j.cplett.2019.05.043Links to an external site. (corresponding author) (Published this paper with an undergraduate student Taylor Dorlus)
6. Daggag, D.; Lazare, J.; **Dinadayalane, T.** "Conformation dependence of tyrosine binding on the surface of graphene: Bent prefers over parallel orientation", *Surf. Sci.* **2019**, *483*, 178-186. https://doi.org/10.1016/j.apsusc.2019.03.181Links to an external site. (corresponding author)
7. Herath, D.; Dinadayalane, T. Computational investigation of double nitrogen doping on graphene, *Mol. Model.*, **2018**, *24*, 26. https://doi.org/10.1007/s00894-017-3560-0
8. Mirchi, A.; Sizochenko, N.; **Dinadayalane, T.**; Leszczynski, J. "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", *Phys. Chem. A*, **2017**, *121*, 8927–8938. DOI: 10.1021/acs.jpca.7b08725Links to an external site. (corresponding author)
9. Liao, L.; Ingram, C. W.; Bacsa, J.; Zhang, Z. J.; **Dinadayalane, T.** "A hydrogen bonded Co(II) coordination complex and a triply interpenetrating 3-D Manganese(II) coordination polymer from a diaza crown ether with dibenzoate sidearms", *CrystEngComm* **2016**, *18*, 2425-2436.
10. Paytakov, G.; **Dinadayalane, T.**; Leszczynski, J. "Towards selection of efficient density functionals for van der Waals molecular complexes: Comparative study of C-H…π and N-H…π interactions", *Phys. Chem. A* **2015**, *119*, 1190-1200. (corresponding author)

11. Hassan, A.; **Dinadayalane, T. C.**; Grabowski, S. J.; Leszczynski, J. "Structural, energetic, spectroscopic and QTAIM analyses of cation-p interactions involving mono- and bi-cyclic ring fused benzene systems", *Chem. Chem. Phys.* **2013**, *15*, 20839-20856. (corresponding author)
12. **Dinadayalane, T. C.**; Leszczynski, J. "Comparative theoretical study on the positional preference for functionalization of two OH and SH groups with (5,5) armchair SWCNT", *Phys. Chem. C* **2013**, *117*, 14441-14450. (corresponding author)
13. **Dinadayalane, T. C.**; Paytakov, G.; Leszczynski, J. "Computational study on C-H…p interactions of acetylene with benzene, 1,3,5-trifluorobenzene and coronene", *Mol. Model.* **2013**, *19*, 2855-2864. (corresponding author)
14. Saha, S.; **Dinadayalane, T. C.**; Leszczynska, D.; Leszczynski, J. "DFT-based reactivity study of (5,5) armchair boron nitride nanotube (BNNT)", *Phys. Lett.* **2013**, *565*, 69-73. (corresponding author)
15. Gajewicz, A.; Rasulev, B.; **Dinadayalane, T. C.**; Urbaszek, P.; Puzyn, T.; Leszczynska, D.; Leszczynski, J. "Advancing risk assessment of engineered nanomaterials: application of computational approaches", *Drug Delivery Rev.* **2012**, *64*, 1663-1693. (**Review article**)
16. Saha, S.; **Dinadayalane, T. C.**; Murray, J. S.; Leszczynska, D.; Leszczynski, J. "Surface reactivity for chlorination on chlorinated (5,5) armchair SWCNT: A computational approach", *Phys. Chem. C* **2012**, *116*, 22399-22410. (corresponding author)
17. Furmanchuk, A.; Isayev, O.; **Dinadayalane, T. C.**; Leszczynska, D.; Leszczynski, J. "Recent advances in mechanical properties of silicon nanowires", *WIREs Comput. Mol. Sci.* **2012**, *2*, 817-828. (**Review article**)
18. Saha, S.; **Dinadayalane, T. C.**; Leszczynska, D.; Leszczynski, J. "Open and capped (5,5) armchair SWCNTs: A comparative study of DFT based reactivity descriptors", *Phys. Lett.* **2012**, *541*, 85-91. (corresponding author)
19. Turabekova, M. A.; **Dinadayalane, T. C.**; Leszczynska, D.; Leszczynski, J. "Comprehensive study on the dissociative chemisorption of NH_3 on the sidewalls of Stone-Wales defective armchair (5,5) single-walled carbon nanotubes", *Phys. Chem. C* **2012**, *116*, 6012-6021. (corresponding author)
20. **Dinadayalane, T. C.**; Hassan, A.; Leszczynski, J. "A theoretical study of cation-p interactions: Li^+, Na^+, K^+, Be^{2+}, Mg^{2+} and Ca^{2+} complexation with mono- and bi-cyclic ring fused benzene derivatives", *Chem. Acc.* **2012**, *131*, 1131.
21. Wu, J.; Hagelberg, F.; **Dinadayalane, T. C.**; Leszczynska, D.; Leszczynski, J. "Do Stone-Wales defects alter the magnetic and transport properties of single-walled carbon nanotubes?", *Phys. Chem. C* **2011**, *115*, 22232-22241.
22. Furmanchuk, A.; Isayev, O.; **Dinadayalane, T. C.**; Leszczynski, J. "Car-Parrinello molecular dynamics simulations of tensile tests in Si <001> nanowires", *Phys. Chem. C* **2011**, *115*, 12283-12292.
23. **Dinadayalane, T. C.**; Leszczynski, J. "Remarkable diversity of carbon–carbon bonds: structures and properties of fullerenes, carbon nanotubes, and graphene", *Chem.* **2010**, *21*, 1155-1169. (**Review article**) (**artwork selected for the issue's Cover Figure**)
24. **Dinadayalane, T. C.**; Hassan, A.; Leszczynski, J. "The effect of ring-annelation to benzene on cation-p interactions: DFT study", *Mol. Struct.* **2010**, *976*, 320-323.
25. **Dinadayalane, T. C.**; Murray, J. S.; Concha, M. C.; Politzer, P.; Leszczynski, J. "Reactivities of Sites on (5,5) Single-walled carbon nanotubes with and without a Stone-Wales defect", *Chem. Theory Comput.* **2010**, *6*, 1351-1357.

26. **Dinadayalane, T. C.**; Leszczynski, J. "In the pursuit of small red shift of C-H stretching vibrational frequency of C-H…p interactions for benzene dimer: How to amend MP2 calculations to reproduce the experimental results", *Chem. Phys.* **2009**, *130*, 081101-1/081101-4.
27. **Dinadayalane, T. C.**; Leszczynski, J. "Geometries and stabilities of various configurations of benzene dimer: Details of novel V-shaped structure revealed", *Chem.* **2009**, *20*, 11-20.
28. Rao, J. S.; **Dinadayalane, T. C.**; Leszczynski, J.; Sastry, G. N. "Comprehensive study on the solvation of mono- and divalent metal cations: Li^+, Na^+, K^+, Be^{2+}, Mg^{2+} and Ca^{2+}", *Phys. Chem. A* **2008**, *112*, 12944-12953.
29. **Dinadayalane, T. C.**; Afanasiev, D.; Leszczynski, J. "Structures and energetics of the cation-p interactions of Li^+, Na^+ and K^+ with cup-shaped molecules: Effect of ring addition to benzene and cavity selectivity", *Phys. Chem. A* **2008**, *112*, 7916-7924.
30. Hassan, A.; **Dinadayalane, T. C.**; Leszczynski, J. "Effect of ring annelation on Li^+-benzene interaction: A computational study", *Phys. Lett.* **2007**, *443*, 205-210.
31. **Dinadayalane, T. C.**; Kaczmarek, A.; Łukaszewicz, J.; Leszczynski, J. "Chemisorption of hydrogen atoms on the sidewalls of armchair single-walled carbon nanotubes", *Phys. Chem. C* **2007**, *111*, 7376-7383.
32. Kaczmarek, A.; **Dinadayalane, T. C.**; Łukaszewicz, J.; Leszczynski, J. "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" *J. Quantum Chem.* **2007**, *107*, 2211-2219.
33. **Dinadayalane, T. C.**; Gorb, L.; Simeon, T.; Dodziuk, H. "Cumulative p-p interaction triggers unusually high stabilization of linear hydrocarbon inside the single-walled carbon nanotube", *J. Quantum Chem.* **2007**, *107*, 2204-2210.
34. **Dinadayalane, T. C.**; Leszczynski, J. "Stone-Wales defects with two different orientations in (5,5) Single-Walled Carbon Nanotubes: A Theoretical Study", *Phys. Lett.* **2007**, *434*, 86-91.
35. **Dinadayalane, T. C.**; Sastry, G. N.; Leszczynski, J. "Comprehensive theoretical study towards the accurate proton affinity values of naturally occurring amino acids", *J. Quantum Chem.* **2006**, *106*, 2920-2933.
36. Panda, G.; Mishra, J. K.; Shagufta, **Dinadayalane, T. C.**; Sastry, G. N.; Negi, D. S. "Hard-soft acid-base (HSAB) principle and difference in d-orbital configurations of metals explain the regioselectivity of nucleophilic attack to a carbinol in Friedel-Crafts reaction catalyzed by Lewis and protonic acids", *Indian J. Chem.* **2006**, *45B*, 276-287.
37. **Dinadayalane, T. C.**; Gayatri, G.; Sastry, G. N.; Leszczynski, J. "Competitive Diels-Alder reactions: Cyclopentadiene and phospholes with butadiene", *Phys. Chem. A* **2005**, *109*, 9310-9323. (Highlighted as one of the best achievements in Mechanisms of Pericyclic Reactions in Chemistry in 2005, *Annu. Rep. Prog. Chem., Sect. B*, **2006**, *102*, 269-289)
38. **Dinadayalane, T. C.**; Gorb, L.; Dodziuk, H.; Leszczynski, J. "Modelling of the stabilization of the complex of a single walled (5,5) carbon nanotube $C_{60}H_{20}$ with cumulenic or acetylenic chain", *AIP Conf. Proc.* **2005**, *786*, 436-439.
39. **Dinadayalane, T. C.**; Priyakumar, U. D.; Sastry, G. N. "Exploration of C_6H_6 potential energy surface: A computational effort to unravel the relative stabilities and synthetic feasibility of new benzene isomers", *Phys. Chem. A* **2004**, *108*, 11433-11448.

40. **Dinadayalane, T. C.**; Deepa, S.; Reddy, A. S.; Sastry, G. N. "Density functional theory study on the effect of substitution and ring annelation to the rim of corannulene", *Org. Chem.* **2004**, *69*, 8111-8114.
41. Punnagai, M.; **Dinadayalane, T. C.**; Sastry, G. N. "Density functional theory study of the Diels-Alder reactivities of [b]-annelated five-membered dienes", *Phys. Org. Chem.* **2004**, *17*, 152-161.
42. **Dinadayalane, T. C.**; Sastry, G. N. "Density functional theory study on dimerizations of phospholes", *Organometallics* **2003**, *22*, 5526-5533.
43. **Dinadayalane, T. C.**; Geetha, K.; Sastry, G. N. "Ab initio and density functional theory (DFT) study on [1,5] sigmatropic rearrangements in pyrroles, phospholes and siloles and their Diels-Alder reactivities", *Phys. Chem. A* **2003**, *107*, 5479-5487.
44. **Dinadayalane, T. C.**; Sastry, G. N. "Isolated pentagon rule in buckybowls: a computational study on thermodynamic stabilities and bowl-to-bowl inversion barriers", *Tetrahedron* **2003**, *59*, 8347-8351.
45. **Dinadayalane, T. C.**; Deepa, S.; Sastry, G. N. "Is peri hydrogen repulsion responsible for flattening buckybowls? The effect of ring annelation to the rim of corannulene", *Tetrahedron Lett.* **2003**, *44*, 4527-4529.
46. Geetha, K.; **Dinadayalane, T. C.**; Sastry, G. N. "Effect of methyl and vinyl substitution on the geometries, relative stabilities and Diels-Alder reactivities of phospholes: A DFT study", *Phys. Org. Chem.* **2003**, *16*, 298-305.
47. **Dinadayalane, T. C.**; Punnagai, M.; Sastry, G. N. "A Theoretical study on cycloaddition reactions between [c]-annelated heterocyclic five-membered dienes and acetylene", *Mol. Struct. (Theochem)* **2003**, *626*, 247-262.
48. **Dinadayalane, T. C.**; Sastry, G. N. "DFT study on the cycloaddition reactions of [c]-annelated carbo- and heterocyclic five-membered dienes with ethylene", *Chem. Soc., Perkin Trans. 2* **2002**, 1902-1908. (Highlighted as one of the best achievements in the field of computational organic chemistry in 2002, *Annu. Rep. Prog. Chem., Sect. B*, **2003**, *99*, 292-325)
49. Vijaya, R.; **Dinadayalane, T. C.**; Sastry, G. N. "Diels-Alder reactions between cyclic five-membered dienes and acetylene", *Mol. Struct. (Theochem)* **2002**, *589-590*, 291-299.
50. **Dinadayalane, T. C.**; Sastry, G. N. "Structure-energy relationships in curved polycyclic aromatic hydrocarbons: Study of benzocorannulenes", *Org. Chem.* **2002**, *67*, 4605-4607.
51. **Dinadayalane, T. C.**; Vijaya, R.; Smitha, A.; Sastry, G. N. "Diels-Alder reactivity of butadiene and cyclic five membered dienes ($(CH)_4X$, $X=CH_2$, SiH_2, O, NH, PH and S) with ethylene: A benchmark study", *Phys. Chem. A* **2002**, *106*, 1627-1633.
52. Priyakumar, U. D.; **Dinadayalane, T. C.**; Sastry, G. N. "A computational study of the valence isomers of benzene and their group V hetero analogs", *New J. Chem.* **2002**, *26*, 347-353.
53. **Dinadayalane, T. C.**; Priyakumar, U. D.; Sastry, G. N. "Ring closure synthetic strategies toward buckybowls: benzannulation versus cyclopentannulation", *Chem. Soc., Perkin Trans. 2* **2002**, 94-101.
54. **Dinadayalane, T. C.**; Sastry, G. N. "An assessment of semiempirical (MNDO, AM1 and PM3) methods to model buckybowls", *Mol. Struct. (Theochem)* **2002**, *579*, 63-72.
55. **Dinadayalane, T. C.**; Sastry, G. N. "Synthetic strategies toward buckybowls and C_{60}: Benzannulation is remarkably facile compared to cyclopentannulation", *Tetrahedron Lett.* **2001**, *42*, 6421-6423.

56. Priyakumar, U. D.; **Dinadayalane, T. C.**; Sastry, G. N. "An ab initio and DFT study of the valence isomers of pyridine", *Phys. Lett.* **2001**, *337*, 361-367.
57. Priyakumar, U. D.; **Dinadayalane, T. C.**; Sastry, G. N. "Structures, energetics and vibrational spectra of the valence isomers of phosphinine. An *ab initio* and DFT study", *Phys. Lett.* **2001**, *336*, 343-348.
58. **Dinadayalane, T. C.**; Priyakumar, U. D.; Sastry, G. N. "Theoretical studies on the effect of sequential benzannulation to corannulene", *Mol. Struct. (Theochem)* **2001**, *543*, 1-10.

BOOK CHAPTERS

1. **Dinadayalane, T.**; Lazare, J.; Alzaaqi, N. F.; Herath, D.; Hill, B.; Campbell, A. E. "Structures, Properties and Applications of Nitrogen-Doped Graphene", In "*Properties and Functionalization of Graphene: A Computational Chemistry Approach*", Dinadayalane, T.; Hagelberg, F. (Eds.), Theoretical and Computational Chemistry, Elsevier, Amsterdam, The Netherlands, **2022**, 21, pp 211-248. (Book chapter – peer-reviewed)
2. **Dinadayalane, T.**; Hagelberg, F. "Preface", In "*Properties and Functionalization of Graphene: A Computational Chemistry Approach*", Dinadayalane, T.; Hagelberg, F. (Eds.), Theoretical and Computational Chemistry, Elsevier, Amsterdam, The Netherlands, **2022**, 21, pp ix-xiv.
3. **Dinadayalane, T.**; Bowen, N. J. "Computational Chemistry and Biology Courses for Undergraduates at an HBCU: Cultivating a Diverse Computational Science Community", In "*Growing Diverse STEM Communities: Methodology, Impact, and Evidence*", Winfield, L. L.; Gloria Thomas, G.; Watkins, L.; Wilson-Kennedy, Z. (Eds.), ACS Symposium Series; American Chemical Society: Washington, DC, **2019**, pp 67-81. (Book chapter – peer-reviewed)
4. **Dinadayalane, T. C.**; Leszczynski, J. "Fundamental structural, electronic and chemical properties of carbon nanostructures: Graphene, fullerenes, carbon nanotubes and their derivatives", In *Handbook of Computational Chemistry*, Leszczynski, J. (Ed.), Springer, Netherlands, **2016**, Edition 2, pp. 1-84. DOI: 10.1007/978-94-007-6169-8_22-2 (Book chapter – peer-reviewed) (corresponding author)
5. **Dinadayalane, T. C.**; Leszczynski, J. "Hydrogenated Graphene: Preparation, Properties and Applications", In *Graphene Science Handbook: Fabrication Methods*, M. Aliofkhazraei, M.; Ali, N.; Milne, W. I.; Ozkan, C. S.; Mitura, S.; Gervasoni J. L. (Eds.), CRC Press, Taylor & Francis Group, Boca Raton (USA), **2016**, 431-450. (Book chapter – peer-reviewed) (corresponding author)
6. Majumdar, D.; Roszak, S.; Wang, J.; **Dinadayalane, T. C.**; Rasulev, B.; Pinto, H.; Leszczynski, J. Advances in *In Silico* Research on Nerve Agents, *Practical Aspects of Computational Chemistry III*, Leszczynski, J.; Shukla, M. K. (Eds.), Springer, USA, **2014**, 283-322. (Book chapter – peer-reviewed)
7. **Dinadayalane, T. C.**; Leszczynska, D.; Leszczynski, J. "Graphene: Properties, biomedical applications and toxicity", In *Towards Efficient Designing of Safe*

Nanomaterials: Innovative Merge of Computational Approaches and Experimental Techniques, Leszczynski, J.; Puzyn, T. (Eds.), RSC Nanoscience & Nanotechnology, Royal Society of Chemistry, Cambridge, UK, **2012**, Vol. *25*, pp. 1-26. (**Artwork selected for the book's Cover Figure**) (Book chapter – peer-reviewed)

8. **Dinadayalane, T. C.**; Leszczynski, J. "Fundamental structural, electronic and chemical properties of carbon nanostructures: Graphene, fullerenes, carbon nanotubes and their derivatives", In *Handbook of Computational Chemistry*, Leszczynski, J. (Ed.), Springer, Netherlands, **2012**, pp. 793-867. (Book chapter – peer-reviewed)
9. **Dinadayalane, T. C.**; Leszczynski, J. "Toward understanding of hydrogen storage in single-walled carbon nanotubes by chemisorption mechanism", In *Practical Aspects of Computational Chemistry: Methods, Concepts and Applications*, Leszczynski, J.; Shukla, M. K. (Eds.), Springer, New York, **2009**, pp. 297-313. (Book chapter – peer-reviewed)
10. **Dinadayalane, T. C.**; Leszczynski, J. "Toward nanomaterials: Structural, energetic and reactivity aspects of single-walled carbon nanotubes." In *Nanomaterials: Design and Simulation*, Balbuena, P. B.; Seminario, J. M. (Eds.), Theoretical and Computational Chemistry, Elsevier, Amsterdam, The Netherlands, **2007**, Vol. 18, pp. 167-199. (Book chapter – peer-reviewed)
11. **Dinadayalane, T. C.**; Leszczynski, J. "A theoretical study on the cycloadditions of o-quinodimethane to the sidewalls of (5,5) armchair single-walled carbon nanotube", In *Proceedings of "Construction, Material Science, Machinery Construction*", Bolshakov, V. I. (Ed.), **2006**, Issue 36, part 1, Series: Starodub's Readings, pp. 58-67.
12. **Dinadayalane, T. C.**; Gorb, L.; Dodziuk, H.; Leszczynski, J. "Modelling of the stabilization of the complex of a single walled (5,5) carbon nanotube $C_{60}H_{20}$ with cumulenic or acetylenic chain", In *Electronic Properties of Novel Nanostructures: Proceedings: XIX International Winterschool/Euroconference*, **2005**, *1*, pp. 436-439. (Peer-reviewed)