

Ankur Kanti Guha



Assistant Professor

Department of Chemistry

Cotton College State University (CCSU)

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Academic Qualifications

Ph.D (Applied Theoretical Chemistry) : Tezpur University, Assam, India-784028

Title of the Ph.D Thesis : *Electronic Structure and Stability of Inorganic Ring Systems, Metallatranes, Carbon Bases and Mechanism of dinitrogen Reduction*

Thesis Supervisor : Prof. Ashwini K. Phukan

Tezpur University, Tezpur, Napaam, Assam, Inida-784028

M.Sc (Physical Chemistry) : Gauhati University, Assam, Inida

B.Sc (Chemistry) : B. N. College, Dhubri, Gauhati University

Employment History

(1) Assistant Professor in Chemistry, Cotton College State University, 2015-Present

(2) Assistant Professor in Chemistry (Ad-Hoc), Dibrugarh University, 2013-2014

(3) Adjunct Professor in Chemistry, Kaziranga University, 2014-2014 (4 Months)

Areas of Expertise

- Applied Theoretical (Computational Quantum) Chemistry
- Computational reaction mechanism
- Computational Spectroscopy

HONORS AND AWARDS

- Awarded the Senior Research Fellowship of CSIR, India in 2011.
- Awarded the UGC meritorious scholar Fellowship in 2008, Tezpur University.

Peer-Reviewed Research Publications

Hirsch (H) Index = 9

1. A. K. Phukan; **A. K. Guha**, B. Silvi, “*Is Delocalization a Prerequisite for Stability of Ring Systems? A Case Study of Some Inorganic Rings*” **Dalton Trans**, 2010, 39, 4126-4137.
2. **A. K. Guha**, S. Sarmah, A. K. Phukan “*Effect of Substituents at the Heteroatom on the Structure and ligating Properties of Heterocyclic Carbene, Silylene, Germylene and Abnormal Carbene: A Theoretical Study*” **Dalton Trans**, 2010, 39, 7374-7383.
3. **A. K. Guha**, A. K. Phukan, “*Theoretical Study on the Mechanism of Catalytic Reduction of Hydrazine to Ammonia Mediated by Vanadium (III) Thiolate Complexes*” **Inorg. Chim. Acta**, 2010, 363, 3270-3273.
4. A. K. Phukan, **A. K. Guha**, “*Nature of Transannular Intramolecular Interactions in Group 4 and 6 Metallatrane: A Combined Density Functional Theory and Atoms in Molecules Theory Study*” **Inorg. Chem**, 2010, 49, 9884-9890.
5. **A. K. Guha**, C. Das, A. K. Phukan, “*Heterocyclic carbenes of diverse flexibility: A theoretical insight*” **J. Organomet. Chem**, 2010, 696, 586-593.
6. A. K. Phukan, **A. K. Guha**, “*Nature of Intramolecular Transannular Interaction in Group 13 Atrane: A Theoretical Study*” **Inorg. Chem**, 2011, 50, 1361-1367.

7. **A. K. Guha**, A. K. Phukan, “*Why Vanadium Complexes Perform Poorly in Comparison to Related Molybdenum Complexes in the Catalytic Reduction of Dinitrogen to Ammonia (Schrock Cycle): A Theoretical Study*” **Inorg. Chem.**, 2011, 50, 8826-8833.
8. **A. K. Guha**, B. Konwar, S. Sarmah, A. K. Phukan, “*Effect of Substituents at the Heteroatoms on the Structure and Ligating Properties of Carbodicarbenes and Its Silicon Analog: A Theoretical Study*” **Theor. Chem. Acc.**, 2011, 131, 1134.
9. U. Gogoi, **A. K. Guha**, A. K. Phukan, “*Nature of Intramolecular Metal-Metal Interactions in Supported Group 4- Group 9 and Group 6- Group 9 Heterobimetallic Complexes: A Combined Density Functional and Topological Study*” **Organometallics**, 2011, 30, 5991.
10. **A. K. Guha**, A. K. Phukan, “*Do Carbenes have “Hidden” Carbon (0) Character? Revisiting the Electronic Structure of 2,2'-Bipyridyl Carbene*” **Chem. Eur. J.** 2012, 14, 4419-4425.
11. A. K. Phukan, **A. K. Guha**, “*Stabilization of cyclic and acyclic carbon(0) compounds by differential coordination of heterocyclic carbenes: A theoretical study*” **Dalton. Trans.** 2012, 41, 8973-8981.
12. S. Konwer, **A. K. Guha**, S. K. Dolui, “*Graphene oxide-filled conducting polyaniline composites as methanol-sensing materials*” **J. Mater Sci**, 2012 (in press).
13. S. Sarmah, **A. K. Guha**, A. K. Phukan, “*Donor Acceptor Complexes of N-Heterocyclic Carbene and Abnormal Carbene with Group 13 (B, Al, Ga) Elements: A Combined DFT and AIM Study*” **Eur. J. Inorg. Chem.**, 2013 (Accepted).
14. A. K. Phukan, **A. K. Guha**, S. Sarmah, “*Ligand Properties of Boron Substituted Five-, Six- and Seven-Membered Heterocyclic Carbenes: A Theoretical Study*” **Organometallics** 2013, 32, 3238-3248.
15. U. Gogoi, **A. K. Guha**, A. K. Phukan “*Tracing the Route to Ammonia: A Theoretical Study on the Possible Pathways for Dinitrogen Reduction Using Tripodal Complexes of Iron*” **Chem. Eur. J.** 2013, 19, 11077-11089.

16. A. K. Phukan, **A. K. Guha**, S. Sarmah, R. D. Dewhurst, "Electronic and Ligand Properties of Annelated Normal and Abnormal (Mesoionic) N-heterocyclic Carbene: A Theoretical Study" *J. Org. Chem.* 2013, 78, 11032.
17. **A. K. Guha**, U. Gogoi, A. K. Phukan, "Revisiting the Reactivity of Different Carbon Bases: A Theoretical Study" *Int. J. Quantum. Chem.*, 2013 (Accepted). (**Highlighted as one of the cover page**).
18. K. K. Bania, **A. K. Guha**, P. K. Bhattacharyya, S. Sinha, "Effect of Substituents and Solvent on Cation-pi Interaction in Benzene and Borazine: A Computational Study, *Dalton Trans*, 2013, DOI: 10.1039/C3DT52081A.
19. S. Sarmah, **A. K. Guha**, A. K. Phukan, A. Kumar, S. R. Gadre "Stabilization of Si(0) and Ge(0) Compounds by Different Silylenes and Germynes: A Density Functional and Molecular Electrostatic Study" *Dalton Trans*, 2013 (Accepted).
20. **A. K. Guha**, A. K. Phukan "A Theoretical Study on the Effect of Annelation and Carbonylation on the Electronic and Ligand Properties of N-Heterocyclic Silylenes and Germynes: Carbene Comparisons Begin to Break Down" *J. Org. Chem*, 2014 (Accepted).
21. S. Pratihar, P. Pegu, **A. K. Guha**, B. Sarma, "Pd (ii) coordinated deprotonated diphenyl phosphino amino pyridine: reactivity towards solvent, base, and acid" *Dalton Trans*. 2014, 43, 17136.
22. M. P. Borpuzari, **A. K. Guha**, R. Kar, "Structural, Electronic Reactivity Studies on Group 15 Analogues of N-Heterocyclic Carbenes" *Struct. Chem.* 2015, 26, 859.
23. R. Borgohain, **A. K. Guha**, S. Pratihar, J. G. Handique, "Antioxidant Activity of Some Phenolic Aldehydes and Their Diimine Derivatives: A DFT Study" *Comput. Theor. Chem*, 2015 (In press).
24. **A. K. Guha**, A. Boruah, M. Hazarika, S. Kaman, "Switching of Carbene Spin States: Effect of Hydrogen Bond Donors," *Reports in Theoretical Chemistry*, 2016 (in press).
25. **A. K. Guha**, "N-Heterocyclic Carbene: Computational Discovery of a Divalent Carbon(0) Compound" *Reports in Theoretical Chemistry*, 2016 (in press)

26. R. Pegu, R. Mandal, **A. K. Guha**, S. Pratihari, “*Selective ratiometric fluoride ion sensor with a (2, 4-dinitrophenyl) hydrazine derivative of bis (indolyl) methane and its mode of interaction*” *New J. Chem.* **2015**, 39, 5984.
27. R. Borgohain, J. G. Handique, **A. K. Guha**, S. Pratihari, “*A Theoretical Study on Antioxidant Activity of Ferulic Acid and its Ester Derivatives*” *J. Theor. Comput. Chem.* **2016** (Accepted, in press)

BOOK CHAPTERS

1. **A. K. Guha** “*New Era of Carbon: A Theoretical and Experimental Perspective*” in *Recent Advances in Biological and Chemical Sciences, Perspectives to North East India*, Edited by S. Roy and B. Baruah, Published by Global Publishing House, India, ISBN: 978-93-81563-41-0 (2014).

5. SCHOOL/WORKSHOP/SUMMER SCHOOL ATTENDED:

1. “**14th National Workshop on Catalysis, catalysis for Clean Environment and Sustainable Future**” Dec 21-23, 2009 held at Tezpur University, Assam, India.
2. “**DST Sponsored Summer School on Green Chemistry, June 2-22, 2009**” held at Tezpur University, Assam, India.
3. “**Frontier Lecture Series in Chemistry, Nov 20-22, 2009**” sponsored by JNCASR held at Tezpur University, Assam, India.
4. “**Frontiers in Chemical Sciences, Dec 3-4, 2010**” sponsored by Indian Institute of Technology (IIT), Guwahati, Assam, India.
5. “**International Seminar, Nov 2-5, 2011**” sponsored by Indian Institute of Chemical Technology (IICT), Hyderabad, India.