Curriculum Vitae

Dr. Abhijit Boruah

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EDUCATIONAL QUALIFICATION	• M. Sc., Ph.D.
AREA OF INTEREST	• Physical and Quantum Chemistry • Theoretical and Computational Chemistry • Density Functional Theory
ACADEMIC & RESEARCH ACHIEVEMENTS	• CSIR-Senior Research Fellowship (direct) for the session 2018-2020 • State Eligibility Test (North-East region) 2021
PROFESSIONAL EXPERIENCES	• Assistant Professor (Part-time) at Department of Chemistry, Jorhat Engineering College, Jorhat, Assam (March, 2021 – till date) • Guest faculty at Department of Chemistry, Madhabdev University, Narayanpur, Assam (November, 2020-February, 2021) • Teaching Assistant of Chemistry in Integrated M. Sc. Course at Department of Physics, Dibrugarh University, Assam (January, 2017- June 2018). • Project Assistant at Department of Chemistry, Dibrugarh University in a 3 Year research project entitled 'Development and Application of Long-range Corrected Density Functional' funded by DST-SERB, New Delhi, India (September, 2014- August 2017)

ACADEMICS

Qualification	Board/ University	Institution	Year
Ph.D.	Dibrugarh University	Department of Chemistry, Dibrugarh University	2020
M.Sc.	Dibrugarh University	Department of Chemistry, Dibrugarh University	2014
B.Sc.	Dibrugarh University	North Lakhimpur College	2012
HS	AHSEC	North Lakhimpur College	2009
HSLC	SEBA	B.B.C.M. Sankardev Vidya Nikaton, North Lakhimpur	2007

ABOUT Ph.D. RESEARCH

Ph.D. thesis title: ***A Theoretical Study on the Ground and Excited State Properties using the Long-range Corrected Density Functionals***

Supervisor: Dr. Rahul Kar, Department of Chemistry, Dibrugarh University

My Ph.D. research work focused on development and application of Long-range corrected density functionals. I have studied various ground and excited state properties such as vertical ionization energy, electron affinity, frontier orbital energies, HOMO-LUMO energy gap, excitation energies, optical gap etc. for a large variety of molecular systems using the range-separated density functionals. We have developed non-empirical tuning scheme which can accurately determine the orbital energy in solvent for a large set of molecules and clusters. These tuning schemes are applied extensively for some molecules which are suitable for organic photovoltaics. Apart from that, we have also designed a new class of sandwich organometallic complexes which may be used as ligands.

SOFTWARE SKILLS	• Gaussian 09 (Computational Chemistry Software) • General Atomic and Molecular Electronic Structure System (GAMESS) • Molecular and electronic structure processing program like GaussView, Molden
RESEARCH PAPAER PUBLISHED	1. **"**Switching of carbene spin states: effect of hydrogen bond donors", A. K. Guha, **A. Boruah**, M. Hazarika, S. Kaman; *Reports in Theoretical Chemistry* 3 (2015) 1–6. 2. "Ionisation potential theorem in the presence of the electric field: Assessment of range-separated functional in the reproduction of orbital and excitation energies", M. P. Borpuzari, **A. Boruah**, R. Kar, *The Journal of Chemical Physics* 144 (2016) 164113-164125**.** 3. **"**Assessment of range-separated functionals in the presence of implicit solvent: Computation of oxidation energy, reduction energy, and orbital energy", **A. Boruah**, M. P. Borpuzari, Y. Kawashima, K. Hirao, R. Kar, *The Journal of Chemical Physics* 146 (2017) 164102-164111. 4. "UV-Vis spectroscopy and density functional study of solvent effect on the charge transfer band of n→σ* complexes of 2-Methylpyridine and 2-Chloropyridine with molecular iodine" P. Gogoi, U. Mohan, M. P. Borpuzari, **A. Boruah,** S. K. Baruah, *Journal of Molecular Structure* 1131 (2017) 114-123. 5. "Iron sandwiched between group 13 analogues of N-Heterocyclic carbene: A theoretical investigation", **A. Boruah**, M. P. Borpuzari, R. Maity, R. Kar, *Journal of Organometallic Chemistry* 863 (2018) 54-59. 6. "Performance of Range Separated Density Functional in Solvent Continuum: Tuning Long-range Hartree-Fock Exchange for Improved Orbital Energies", **A. Boruah**, M. P. Borpuzari, R. Kar, *Journal of Computational Chemistry* 41 (2019) 295-304. 7. "UV-Visible spectroscopy and density functional study of solvent effect on halogen bonded charge-transfer complex of 2-Chloropyridine and iodine monochloride", P. Gogoi, U. Mohan, M. P. Borpuzari, **A. Boruah,** S. K. Baruah, *Arabian Journal of Chemistry* 12 (2019) 4522-4532.
BOOK CHAPTERS	**1. Book: Contemporary Research in Chemistry**, Reactivity Study of Group 13 and Group 14 Analogs of N-Heterocyclic Carbene by Using Conceptual DFT Tools (Chapter 9). **ISBN: 978-93-89840-85-8** **2. Book: An Era of Chemical Catalysis: A Theoretical and Experimental Perspective**, A Theoretical Study on Activation of Dihydrogen by NHeterocyclic Carbenes (Chapter 2). **ISBN: 978-81-949998-0-5**
SCHOOL ATTENDED	BRNS School on **"Computational Methodologies Across Length Scales"** from August 28 to September 09, 2017 at Bhabha Atomic Research Centre, Mumbai.

SEMINAR/ SYMPOSIUM/ CONFERENCES	1. Dr. A. K. Guha and **A. Boruah**, "Activation of Hydrogen Molecule by N-heterocyclic carbenes", presented at National Seminar on "Recent Trends in Fundamental and Applied Chemical Sciences" held at Dibrugarh University, during 19-21 November, 2014. 2. **A. Boruah** and R. Kar, **"**Range Separated Density Functionals in the Presence of External Electric Field: Computation of Orbital Energies**"** presented at National Conference on "Contemporary Developments in Chemical Sciences" held at Tezpur University during November 23 -24, 2015. 3. **A. Boruah** and R. Kar, **"**Range Separated Density Functionals: Orbital energies computed in solvent environment**"** presented at National Symposium on "Emerging Trends in Chemistry" held at NEHU, Shillong during March 28-29, 2016. 4. **A. Boruah** and R. Kar, "Range-Separated Functional under the Self Consistent Reaction Field: Computation of Orbital Energies" presented at National Seminar on "Recent Developments in Synthesis and Catalysis" held at Department of Chemistry, Dibrugarh University, Dibrugarh, Assam, India during March 10-11, 2017. 5. **A. Boruah** and R. Kar, "Novel sandwich organometallic complexes of iron: Prospect as Catalyst" presented at International Conference on "Emerging Trends Chemical Sciences" held at the Department of Chemistry, Dibrugarh University, Assam, India during February 26-28, 2018. 6. **A. Boruah** and R. Kar, "A novel class of sandwich compounds of Iron with the group 13 analogues of N-Heterocyclic carbene" presented at International Conference on "Frontiers in Chemical Sciences 2018" held at IIT Guwahati, Assam, India during 6-8 December, 2018. 7. **A. Boruah** and R. Kar, "A New Tuning Scheme of Range-Separated Functional for Computing Oxidation Energy in Solvent Environment" presented at International Conference on "Theoretical Chemistry Symposium 2019 (TCS-2019)" held at BITS, Pilani, Rajasthan during 13-16 February, 2019. 8. **A. Boruah** and R. Kar, "Accessibility of Non-empirically Tuned Range-separated Functional for the Molecules Relevant for Organic Photovoltaics", presented at International Conference on "Emerging Trends Chemical Sciences 2020 (ETCS 2020)" held at the Department of Chemistry, Gauhati University, Assam, India during 13-15 February, 2020.
SOCIAL RESPONSIBILITY	• Executive member of Dibrugarh University Research Scholar Association (DURSA) for the session 2016-17. • Executive member of Gaurav Sanmilito Samaj, a society with the aim of social, educational, economical and environmental development of Assam.