Sharmin Akter

CONTACT INFORMATION

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RESEARCH INTERESTS

Density functional theory, Self interaction correction, FLOSIC

EDUCATION

The University of Texas at El Paso, TX, USA — December, 2022 (Expected)

Ph.D. Candidate, Computational Science

- Dissertation Topic: Density Functional Theory, Electronic Structure Calculation. Density Functional Theory (DFT) is one of the most successful and popular quantum mechanical approaches to understand material properties. Although in principle density functional theory is exact, it, however, relies on approximations for exchange-correlation energy functional. This approximate nature leading to the spurious self-interaction error in DFT. Our group is a part of FLOSIC (Fermi-Löwdin-orbital self-interaction correction) center is one of several Computational Chemical Sciences Centers funded by the U.S. Department of Energy in September 2017. We are developing and applying simulation software that can run FLOSIC calculations in density functional theory in predicting and developing materials with properties that meet sufficient, clean, sustainable, and efficient energy supply to our world.
- Advisor: Dr. Tunna Baruah
- Co-advisor: Dr. Rajendra Zope

The University of Texas at El Paso, TX, USA — December, 2017

M.S., Physics

- Thesis Topic: "Self-interaction corrected polarizabilities of small molecules"
- Advisor: Tunna Baruah, Ph.D
- Co-advisor: Rajendra Zope, Ph.D

University of Dhaka, Dhaka, Bangladesh — December, 2012

M.Sc., Physics

- Thesis Topic: "Study of structural and dielectric properties of $La_{0.75}Ca_{0.05}Sr_{0.20-x}Ba_xMnO_3$ (x=0.10 and 0.15) polycrystalline perovskite"
- Advisor: Sabina Hussain, Ph.D, Department of Physics, University of Dhaka, Dhaka, Bangladesh
- Co-advisor: A.K.M. Akther Hossain, Ph.D, Department of Physics, Bangladesh University of Engineering and Technology, Dhaka, Bangladesh

University of Dhaka, Dhaka, Bangladesh — December, 2011

B.Sc., Physics

ACADEMIC EXPERIENCE

The University of Texas at El Paso, El Paso, TX, USA

Research Assistant — January 2018 - Present

- Project: Polarizability is one of the properties that depends on the electron density which is the response of a system to an applied electric field. I design the electronic structures of different molecules and apply Perdew-Zunger self-interaction correction scheme and the recently developed local scaling of self-interaction-correction methods to examine the polarizabilities. I use several open source software packages in designing the electronic structures of the system then carry out simulations to determine the dipole moment, ground state energy,

highest occupied molecular orbital energy, polarizability etc, to see the effect of self-interaction correction methods in the presence or absence of electric field. I have already worked with different types of molecules and systematically examined the self-interaction error using different methods. The ultimate goal of my research group is to develop a self-interaction free method that allows efficient and predictive modeling of materials without unphysical effects of electron self-interaction, the major flaw present in existing methods. To this far, we have already developed locally scaled self-interaction correction method which is also known as LSIC method. I recently applied this method for different molecules and published my work which shows an excellent agreement with reference values. To understand the overall efficiency of this newly developed method for different systems, more applications and investigations are needed, for which I am currently working on. This work is directed by Dr. Tunna Baruah and Dr. Rajendra Zope.

Teaching Assistant January 2016 – Present

- Duties at various times have included office hours and leading weekly computer lab exercises.
- Helped students in several Physics, Math, Statistics, Astronomy, and Engineering classes (Both Lectures and corresponding Laboratories)
- Tutored students in the Math Resource center for student (MARCS) at UTEP.
- Students got highly motivated and realized significant improvement as reflected in their reviews.

Computer Skills

- Languages: C/C++, Python, R, Maxima, FORTRAN, Matlab, LaTeX, Unix shell scripts, MPI parallel processing library.
- Software: NRLMOL, FLOSIC, JMol, Origin, several plotting and visualization packages, common Windows database, spreadsheet, and presentation software
- Operating Systems: Unix/Linux, Windows

Publications

[1] **Sharmin Akter**, Jorge Vargas, Kamal Sharkas, Juan E Peralta, Koblar A Jackson, Tunna Baruah, and Rajendra R Zope. "How well do self-interaction corrections repair the over-estimation of molec-ular polarizabilities in density functional calculations?" *Physical Chemistry Chemical Physics*, 2021

[2] **Sharmin Akter**, Yoh Yamamoto, Rajendra R Zope, and Tunna Baruah. "Static dipole polarizabilities of polyacenes using self-interaction-corrected density functional approximations". *The Journal of Chemical Physics, 154.11*, p.114305, 2021

[3] **Sharmin Akter**, Yoh Yamamoto, Carlos M Diaz, Koblar A Jackson, Rajendra R Zope, and Tunna Baruah. "Study of self-interaction errors in density functional predictions of dipole polarizabilities and ionization energies of water clusters using Perdew–Zunger and locally scaled self-interaction corrected methods". *The Journal of Chemical Physics* , 153(16):164304, 2020

[4] Kamal Sharkas, Kamal Wagle, Biswajit Santra, **Sharmin Akter**, Rajendra R Zope, Tunna Baruah, Koblar A Jackson, John P Perdew, and Juan E Peralta. "Self-interaction error overbinds water clusters but cancels in structural energy differences". *Proceedings of the National Academy of Sciences*, 117(21):11283–11288, 2020

[5] Kushantha P. K. Withanage, **Sharmin Akter**, Chandra Shahi, Rajendra P. Joshi, Carlos Diaz, Yoh Yamamoto, Rajendra Zope, Tunna Baruah, John P. Perdew, Juan E. Peralta, and Koblar A. Jackson. "Self-interaction-free electric dipole polarizabilities for atoms and their ions using the Fermi-Löwdin self-interaction correction". *Phys. Rev. A*, 100:012505, July, 2019

[6] **Sharmin Akter**, Rajendra R Zope, and Tunna Baruah. "Study on oxygen evolving complex (OEC) in photosystem II (PS-II) using DFT" (manuscript in preparation).

Conference Presentations

[7] Yoh Yamamoto, Carlos Diaz, Luis Basurto, Po Hao Chang, Prakash Mishra, Peter Ufondu, **Sharmin Akter**, Rajendra Zope, Tunna Baruah. "Self Interaction Correction for Improved Description of Molecular Properties". *US-Africa Initiative Workshop in Electronic Structure*, June, 2021.

[8] Kamal Sharkas , **Sharmin Akter**, Jorge A. Vargas , Juan E. Peralta , Koblar A. Jackson , Tunna Baruah and Rajendra R. Zope. "Improving density functional calculations of molecular polarizabilities using locally scaled self-interaction corrections". *American Physical Society*, March Meeting 2021.

[9] Jorge A. Vargas, **Sharmin Akter**,Kamal Sharkas , Juan E. Peralta , Koblar A. Jackson , Tunna Baruah and Rajendra R. Zope. "Improving density functional calculations of molecular polarizabilities using locally scaled self-interaciton corrections". *20th International Workshop on Computational Physics and Materials Science*, February 2021.

[10] **Sharmin Akter**, Yoh Yamamoto, Rajendra Zope, and Tunna Baruah. "Fermi-Löwdin orbital self-interaction corrections applied to water clusters: Polarizabilities, dipole moments, and ionization energies". *American Physical Society*, March Meeting 2020.

[11] **Sharmin Akter**, Yoh Yamamoto,Carlos M. Diaz, Koblar A. Jackson, Rajendra Zope, and Tunna Baruah. "Self-interaction-corrected polarizabilities of water clusters". *FLO-SIC Center all hands meeting*, July, 2020.

[12] **Sharmin Akter**, Yoh Yamamoto, Luis Basurto, Tunna Baruah, and Rajendra Zope. "Ionization potentials and static dipole polarizabilities of polyacenes using Fermi-Löwdin self-interaction corrected density functional approximation". *American Physical Society*, March Meeting 2019.

[13] Kushantha Withanage, **Sharmin Akter**, Chandra Shahi, Tunna Baruah, Rajendra Zope, John Perdew, Juan Peralta and Koblar Jackson. "Self-interaction corrected dipole polarizabilites of free atoms and their ions". *American Physical Society*, March Meeting 2019.

[14] **Sharmin Akter**, Yoh Yamamoto, Rajendra Zope, and Tunna Baruah. "FLOSIC applications on atomic and molecular properties". *FOMMS 2018 - Foundation of Molecular Modeling and Simulation*, Delavan, Wisconsin, July, 2018.

[15] **Sharmin Akter** and Tunna Baruah. "Self-interaction corrected polarizabilities of small molecules". *2017 Graduate Student Research Expo*, UTEP, El Paso, TX, 2017.

Honors and Awards

Research Assistantship Award January 2018 - Present
In part by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award No. DE-SC0002168, DE-SC0018331 and NSF (Grant No. TG-DMR090071) under Dr. Tunna Baruah.

Texas Public Educational Grant Program (TPEG) Award ($6K) Sept., 2019 - May, 2021

Grace Hopper Student Scholarship and Travel Awards September, 2018
Anitab.org

Travel Award ($1500) July, 2018
In part by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award No. DE-SC0002168 to present a poster at *FOMMS 2018*

Academic and Research Excellence Award December, 2017
University of Texas at El Paso, El Paso,TX

Shaon Memorial Scholarship January, 2010
University of Dhaka, Dhaka, Bangladesh

Higher Secondary School Certificate Scholarship January, 2005
Central Women's College, Dhaka, Bangladesh

Secondary School Tuition Waiver Scholarship January, 2003
Matuail Girls High School, Dhaka, Bangladesh

Professional Memberships

- American Physical Society (APS)
- The FLOSIC Center
- Society for Industrial and Applied Mathematics (SIAM)

Referees

Available on request.