

## Dr. Shiblee Ratan Barua

Email: [shibleeratan@gmail.com](mailto:shibleeratan@gmail.com) or [shiblee.barua@northsouth.edu](mailto:shiblee.barua@northsouth.edu)

### EDUCATION

**University of Georgia, Athens, GA (UGA)**  
PhD, *Computational Quantum Chemistry*

*Aug 2008 – May 2014*

**Berea College, Berea, KY**  
Bachelors, *Physics and Mathematics*

*Aug 2004 – May 2008*

### RESEARCH EXPERIENCE

**Center for Computational Quantum Chemistry, University of Georgia**

*Aug 2008 – May 2014*

Advisor: *Dr. Wesley D. Allen*

Thesis Title: *High-level ab initio quantum chemical studies of the competition between cumulenes, carbenes, and carbones.* (Online at: <http://athenaeum.libs.uga.edu/handle/10724/30293>)

- Evaluated relative energies utilizing high-level coupled cluster theory, basis-set extrapolation techniques, and highly accurate focal point analysis (FPA) method.
- Predicted experimental infrared spectra to excellent precision through anharmonic frequency computations by numerically evaluating the full quartic force field.
- Analyzed quantum tunneling processes by mapping out intrinsic reaction paths (IRPs) to study the interconversion between isomers at cryogenic temperatures.
- Utilized density functional theory (DFT) to investigate the topology and relative energetics of long-chain hydrocarbons and their oligomers.

**Department of Physics, University of Arkansas, Fayetteville, AR**

*May 2007 – July 2007*

Advisor: *Dr. Daniel Kennefick*

- Assisted in writing a FORTRAN code for the NASA funded project LISA (Laser Interferometer Space Antenna) aimed at detecting the existence of christodoulou memory of gravitational waves.

### SCIENTIFIC PUBLICATIONS

- 1) "Polytwistane", S. R. Barua, H. Quanz, M. Olbrich, P. R. Schreiner, D. Trauner and W. D. Allen, *Chem. Eur. J.* **2014**, *20*, 1638.  
Online at: <http://onlinelibrary.wiley.com/doi/10.1002/chem.201303081/abstract>
- 2) "Nearly Degenerate Isomers of C(BH)<sub>2</sub>: Cumulene, Carbene, or Carbone?", S. R. Barua, W. D. Allen, E. Kraka, P. Jerabek, R. Sure and G. Frenking, *Chem. Eur. J.* **2013**, *19*, 15941.  
Online at: <http://onlinelibrary.wiley.com/doi/10.1002/chem.201302181/abstract>
- 3) "Structures, Energetics, and Vibrational Spectra of C(AIH)<sub>2</sub>", S. R. Barua and W. D. Allen.  
Online at: <http://athenaeum.libs.uga.edu/handle/10724/30293>
- 4) "Quasilinearity in Fulminic Acid (HCNO) Molecule", S. R. Barua, C. -H. Wu and W. D. Allen.  
Online at: <http://athenaeum.libs.uga.edu/handle/10724/30293>

## TEACHING EXPERIENCE

### Department of Biology and Chemistry

North South University, Dhaka, Bangladesh (NSU)

*Assistant Professor of Chemistry*

- CHE 101 (General Chemistry I)
- CHE 201 (General Chemistry II)

*Jan 2016 – Present*

### Department of Chemistry and Biochemistry

California Polytechnic State University (Cal Poly SLO)

*Full-Time Lecturer*

- CHEM 111L (Chemistry for non-majors Lab)
- CHEM 127 (General Chemistry I)
- CHEM 128 (General Chemistry II)
- CHEM 129 (General Chemistry III)

*Sep 2014 – Jun 2015*

### Department of Chemistry, University of Georgia

*Graduate Teaching Assistant*

- Instructed General Chemistry I and II labs.
- Interacted with students in order to assist them with laboratory techniques, equipment, computerized data analyses, and lab reports.
- Tutored General Chemistry and Organic Chemistry students assisting them with homework assignments and course materials at the Chemistry Learning Center.

*Aug 2008 – May 2014*

### Departments of Physics, Mathematics, Berea College

*Undergraduate Teaching Assistant*

- Supervised weekly physics lab experiments and engaged students in discussions regarding laboratory techniques.
- Assisted students in solving homework problems at the departmental tutoring centers.
- Graded lab reports and homework assignments each week.

*Jan 2005 – May 2008*

## COMPUTER SKILLS

**Programming/Scripting:** Mathematica, Python, Perl, C++, Fortran.

**Operating Systems:** Windows, Linux (Ubuntu), Mac OS X.

**Quantum Chemistry Packages:** CFOUR, MOLPRO, GAMESS (US), QCHEM, PSI, GAUSSIAN.

**Teaching Software:** Moodle (Cal Poly), Blackboard (UGA).

## RESEARCH PRESENTATIONS

South Eastern Theoretical Chemistry Association (University of Georgia, GA)

*2012*

South Eastern Theoretical Chemistry Association (University of South Carolina, SC)

*2010*

Center for Space and Planetary Sciences REU Program (University of Arkansas, AR)

*2007*

## REFERENCES

**Dr. Wesley D. Allen**

*Associate Professor*

1004 Cedar Street

Center for Computational Quantum Chemistry

University of Georgia

Athens GA 30602-2556

*Email:* [wdallen@uga.edu](mailto:wdallen@uga.edu)

*Phone:* +1 (706) 542-7729

*Graduate Research Adviser*

**Dr. Henry F. Schaefer III**

*Graham Perdue Professor*

1004 Cedar Street

Center for Computational Quantum Chemistry

University of Georgia

Athens GA 30602-2556

*Email:* [ccq@uga.edu](mailto:ccq@uga.edu)

*Phone:* +1 (706) 542-2067

*Graduate Adviser*

**Dr. Alan Kiste**

*Assistant Professor*

1 Grand Avenue

Department of Chemistry and Biochemistry

California Polytechnic State University (Cal Poly SLO)

San Luis Obispo, CA 93407

*Email:* [akiste@calpoly.edu](mailto:akiste@calpoly.edu)

*Phone:* +1 (805) 756-1690

*Gen. Chem. Program Coordinator*

**Dr. Chia-Hua Wu**

*Postdoctoral Research Associate*

Department of Chemistry

University of Houston

Houston, TX 77204-5003

*Email:* [wujawa@gmail.com](mailto:wujawa@gmail.com)

*Phone:* +1 (706) 202-6423

*Graduate Research Collaborator*