

Beulah S. Narendrapurapu

EDUCATION

University of Georgia, Athens, GA

Ph.D., Computational Chemistry

May 2013

GPA: 3.70/4.00

Indian Institute of Technology Bombay, Mumbai, India

M.Sc., Chemistry

July. 2006 - May 2008

CPI: 8.49/10.00

St. Ann's College, Osmania University, Hyderabad, India

B.Sc., Chemistry, Physics and Mathematics

June. 2003 - May 2006

CP: 82.0/100.0

TEACHING EXPERIENCE

- **Georgia Southern University**

Visiting Instructor

Statesboro, GA

since August 2013

– Courses taught:

- * Principles of Chemistry I

- * Principles of Chemistry II

- **North Georgia College and State University**

Temporary Instructor

Watkinsville, GA

June 2013 - July 2013

– Courses taught:

- * Survey of Chemistry I

- * Survey of Chemistry II

- **South Georgia State College**

Chemistry Instructor

Douglas, GA

Aug. 2011 - May 2012

– Courses taught:

- * Principles of Chemistry I

- * Principles of Chemistry II

- * Organic Chemistry I

- * Organic Chemistry II

- **University of Georgia**

Teaching Assistant

Athens, GA

Aug. 2008 - Dec. 2009

- **Center for Computational Quantum Chemistry**

Summer Research Mentor

Athens, GA

2011 & 2012

RESEARCH INTERESTS

- Chemistry education.
- Using highly accurate *ab initio* coupled cluster methods for geometries, vibrational properties and barrier heights of chemical systems and reactions.
- Using density functional theory to compute molecular properties of catalytic systems involving transition metals.

RESEARCH EXPERIENCE

• Center for Computational Quantum Chemistry

Athens, GA

Advisor: Prof. Henry F. Schaefer III

Aug. 2008 - Present

- Thesis title: "Quantum chemistry in bio-inorganic and combustion studies: Applying density functional theory and high accuracy *ab-initio* methods".
- Computed accurate energetics of molecules using high level coupled cluster computations with basis set extrapolation techniques.
- Collaborated with synthetic inorganic chemists; Employed natural charges on atoms, nuclear electrostatic potentials and molecular orbital analysis and investigated the role of hydrogen bonding in small molecular analogues of Nickel Superoxide Dismutase enzyme's active site.
- Utilized time dependent density functional theory to address fluorescence enhancement in a zinc dansyl-thiolate chemosensor.
- Currently investigating vanadium-catalyzed oxidation mechanisms, excited states of tritopic carbenes and the role of basis-set size on metal-metal bond distances in transition metal carbonyls.

• Indian Institute of Technology Bombay

Mumbai, India

Advisor: Prof. B. L. Tembe

2007-2008

- Thesis title: "System-size dependance of solvation structures of nacl in water-dmsol mixtures: A molecular dynamics study".
- Investigated how the dimension of simulation cell affects the solvation structure and dynamics of sodium chloride solute in a mixed solvent of dimethyl sulfoxide and water.
- Utilized Monte Carlo energy minimization procedures.

• Jawaharlal Nehru Center for Advanced Scientific Research

Bangalore, India

Summer Research

2004, 2005 & 2006

- Synthesized mesoporous silica material.
- Characterized copper ion impregnated bacterial cellulose using Infra-red spectroscopy and electron microscopy.
- Worked on green synthesis of semi-conductor nano-particles.

SKILLS

Programming/Scripting Languages: C/C++, Perl, Python, Mathematica, \LaTeX , Shell (TCSH/BASH) and Fortran.

Operating Systems: Linux (SuSE/Ubuntu), MacOS X, and Windows.

Applications: Gaussian, Psi4, QChem, CFOUR, Molpro, NWChem and ORCA.

Web tools: Blackboard, ConnectED.

SCIENTIFIC PUBLICATIONS

1. "Combustion Chemistry: Important Features of the C_3H_5 Potential Energy Surface, Including Allyl Radical, Propargyl + H_2 , Allene + H, and Eight Transition States", B. S. Narendrapurapu, A. C. Simmonett and H. F. Schaefer, *J. Phys. Chem. A*, **115**, 14209 (2011).
2. "Exploring the Effects of H-Bonding in Synthetic Analogues of Nickel Superoxide Dismutase (Ni-SOD): Experimental and Theoretical Implications for Protection of the Ni-SCys Bond", E. M. Gale, B. S. Narendrapurapu, A. C. Simmonett, H. F. Schaefer and T. C. Harrop, *Inorg. Chem.*, **49**, 7080 (2010).
3. "Metal-metal and metal-ligand bond distances in transition metal carbonyls: Investigating the effect of basis sets on the geometries of bi and tri metallic carbonyl compounds utilizing 35 DFT functionals", B. S. Narendrapurapu, N. A. Richardson, A. Copan, M. Estep, Y. Zheyue and H. F. Schaefer (*submitted to Journal of Chemical Theory and Computation on 03/25/2013*).

POSTER PRESENTATIONS

South Eastern Theoretical Chemistry Association (Duke University, NC)	2009
Molecular Quantum Mechanics (University of California, Berkeley, CA)	2010
South Eastern Theoretical Chemistry Association (University of Georgia, GA)	2012

AWARDS AND ACCOMPLISHMENTS

Gold medal in Chemistry (St. Ann's College, Hyderabad, India)	2006
Gold medal in Physics (St. Ann's College, Hyderabad, India)	2006
Secured 39th rank in Joint Admission to M.Sc., an All-India entrance exam for the Indian Institutes of Technology (IITs)	2006
Best Summer Research Fellow Award (JNCASR, Bangalore, India)	2005

COMMUNITY ACTIVITIES

Judge, Georgia Science and Engineering Fair (Douglas, GA)	2012
Judge, Science Olympiad (Douglas, GA)	2012
Member, American Chemical Society	2012
Judge, Georgia Science and Engineering Fair (Athens, GA)	2011
Executive member, Indian Student Association (University of Georgia, GA)	2009-2010

