Chinthaka Nadun Ratnaweera

CONTACT INFORMATION

Institute of Chemistry Ceylon
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RESEARCH INTERESTS

Ab initio calculations, statistical thermodynamics, molecular dynamics, computational chemistry programming

EDUCATION

Mississippi State University, Mississippi State, MS, USA

Ph.D., Physical/Theoretical Chemistry, May, 2015

- Dissertation Topic: "Entropy of the internal rotations"
- Adviser: Dr. Steven R. Gwaltney

University of Kelaniya, Kelaniya, Sri Lanka

M.S., Management and Information Technology, March, 2009

- Thesis Topic: "Utilization of information technology for science education in Sri lanka"
- Adviser: Dr. Ruwan Wickramarachchi

University of Colombo, Colombo, Sri Lanka

B.Sc., Special degree in Chemistry with second class upper, January, 2004

WORK AND TEACHING EXPERIENCE

Institute of Chemistry Ceylon, College of Chemical Sciences, Rajagiriya, Sri Lanka

- **Senior Lecturer (Full time) - June 2015 - present**
  - Currently teaching quantum chemistry (level 3), quantum mechanics (optional course), spectroscopy, statistical thermodynamics, and mathematics for chemists.
  - Supervise and coordinate the advanced physical chemistry laboratory course (Section-B), designed an experiment on computational chemistry
  - Conduct theory/practical course titled "IT for chemists" in November 2015
  - Coordinator of the research projects and research laboratory
  - Conducted a seminar on "IT applications for chemists"

Mississippi State University, Mississippi State, MS, USA

- **Graduate research assistant - January 2014 - May 2015**
- **Graduate teaching assistant - August 2009 - December 2013**
  - Taught two general chemistry Labs per semester of up to 24 students.
  - Tutored general chemistry for undergraduates.

National Science Foundation of Sri Lanka, Colombo, Sri Lanka

- **Scientific officer - May 2005 - June 2009**
  - Disseminated science and technology information to general public and school children in collaboration with local and international scientists.
  - Coordinated the NSF school science society program and conducted lectures for teachers and school children to popularize science.
  - Contributed to organize the Sri Lanka Science and Engineering Fair, 2007 - 2009

University of Colombo and **Open University of Sri Lanka**

- **Demonstrator - Feb 2004 - May 2005**

- Demonstrated and taught lab experiments in general chemistry and physical chemistry labs.
- Conducted tutoring sessions for physical chemistry and quantum chemistry.

Scientific Profile

- ***Ab initio* calculations** - DFT, MP2, and other electronic structure calculations using Q-Chem program, construct Z-matrixes to obtain high symmetry structures, anharmonic corrections, transition state searches and reaction paths.
- **Molecular dynamics (MD)** - MD atomistic simulations using Amber 12, molecular docking using Autodock4 and Autodock Vina, building protein structure models using Modeller, VMD, Pymol, and Spartan
- **Computational chemistry coding** - Developed a new method and code for correcting the entropy of internal rotations for the Q-Chem electronic structure program. Experience in compiling, building, and debugging Q-Chem source code.
- **Programming languages** - Fluent in FORTRAN, and Python and knowledgeable in C/C++, Mathematica, and MATLAB.
- **Computer platforms** - Ability to work in Unix-like OS, shell scripting, and experience working with GPU's and high performance computing.
- **Other applications** - Proficient in Gnu-plot, Xmgrace, Microsoft Excel, and LaTeX(for documents, slides, and posters)

Research projects

- **A simple approach to determine the entropy of low frequency internal rotations**
  Developed and tested two cost effective methods to determine the hindered rotor entropy of internal rotational modes. The proposed methods have been implemented in an experimental version of the Q-Chem electronic structure program and soon will be added to the standard Q-Chem code. Several subroutines were developed, including efficient code to calculate the reduced moment of inertia of the rotor. Implemented codes were written in Fortran, but some initial testing was performed using Python.
- **DFT studies on bis(tricarbonylchromium)dibenzo[a,e]-cyclooctatetraene**
  Conducted DFT studies to determine the minima and transition state structures and relative stabilities of its isomers to explain experimental findings. Proposed hindered rotor treatments were applied to the internal rotational modes of the *tricarbonylchromium* groups.
- **Effect of ethanol on Toll-like Receptor3 - RNA complex : A molecular dynamic study**
  This project involves modeling the mouse and human Toll-like Receptor (TLR3) dsRNA complex and studying its interaction with ethanol using molecular dynamics simulations. Apart from the standard Amber force fields (ff12SB), the latest GLYCAM force fields were used to simulate the sugar groups attached to the protein, and different concentrations of ethanol-water mixtures were included in the solvents. Results revealed no significant structural change upon the ethanol binding.
- **Determining the orientation of the human serum paraoxonase 1 (PON1) in lipid and study substrates binding**
  The PON1 is a calcium-dependant hydrolase bound to the HDL particles in the serum. I determined the correct orientation of the PON1 in lipid and currently analyzing of the molecular dynamic trajectories to study the changes to the active site upon the interaction with lipid molecules.
- **Reaction path of electrophilic nitration of mono-substituted benzene to understand the reaction mechanism**
  Determined the intermediates and transition states in the reaction path and relative energies using DFT to understand the significant regioselectivity of this reaction.

Publications

- Nilantha Bandara, Chinthaka N. Ratnaweera, Steven R. Gwaltney, William P. Henry, "Isolation and structure of the *anti,anti* isomer and a DFT study of it and the *syn,anti* isomer of bis(tricarbonylchromium) dibenzo[a,e]-cyclooctatetraene. Evidence for an attractive electrostaticinteraction between carbonyl oxygen atoms and $Cr(CO)_3$ -coordinated arene carbon atoms", *J. Organomet. Chem.* 2013, 86, 745.
- Chinthaka N. Ratnaweera, Steven R. Gwaltney, "The effects of a lipid layer on the structure and dynamics of human paraoxonase 1", *J. Chem. Phys.* (revisions needed)
- Chinthaka N. Ratnaweera, Manikanthan Bhavaraju, Steven R. Gwaltney, "The structure of human paraoxonase1 from molecular dynamic simulations", *Protein Sci.* (submitted)
- Nilantha Bandara, Chinthaka. N. Ratnaweera, Steven. R. Gwaltney, and W. P. Henry, "Anti vs. syn isomers in mononuclear 6-dibenzo[a,e]cyclooctatraene complexes of $Cr(CO)_3$ and $Mn(CO)^{3+}$: synthesis, structure, VT NMR spectroscopy, and theoretical calculations," *J. Organometallic. Chem.* (submitted)
- Chinthaka N. Ratnaweera, Steven R. Gwaltney, "Calculation of the gas phase entropy of n-alkanes using the approximate barrier height model", manuscript in preparation
- C.N. Ratnaweera New Era in Computational Chemistry- Graphic Processing Units (GPUs) to Accelerate Molecular Dynamics, Simulations, and Molecular Modeling, Chemistry in Sri Lanka, 2015, 32(3), 47-50.

Oral Presentations

- Invited talk on "Determine the structure of lipid-bound human paraoxonase1 and identify of its open and closed conformations and model Toll-like Receptor3 (TLR3) and determine its interaction with ethanol", Mississippi University for Women, Columbus MS, April, 29, 2015.
- "A simple approach to accurately determine the entropy of low frequency internal rotations", 66^{th} Southeastern Regional Meeting of the American Chemical Society (SERMACS) Nashville, TN, October, 16-19, 2014
- "Theoretical methods of calculation of entropy and their problems in producing accurate values", Structural Biology Interest Group (SBIG) meeting Mississippi State University, November 12, 2014
- "Accurate entropy of carbonyl rotations in bis(chromiumtricarbonyl) DBCOT using hindered rotor treatments", 4^{th} Annual Andrews Graduate Research Symposium, Mississippi State University, May 20 -21, 2014
- "A simple approach to accurately determine the entropy of low frequency internal rotations", Graduate student research symposium, Mississippi State University, MS, March 22, 2014
- "A theoretical investigation of the increased entropy in the transition state for inversion in bis(chromiumtricarbonyl) dibenzo[a,e]cyclooctatetraene (DBCOT)", The Southeastern Regional Meeting of the American Chemical Society (SERMACS), Raleigh, NC, November, 14-17, 2012
- "The reason for the increase in entropy at the transition state for inversion in bis(chromiumtricarbonyl) Dibenzo[a,e]cyclooctatetraene Complex.", 2^{nd} Annual Lester S. Andrews Graduate Research Symposium, Mississippi State University, MS, May 14-15, 2011 (First place)

Selected Poster Presentations

- "A simple approach to accurately determine the entropy of low frequency internal rotations", 248^{th} ACS National Meeting and Exposition, San Francisco, CA, August 9-14, 2014 (PHYS & Sci-Mix)
- "A Simple Approach to Accurately Determine the Entropy of Low Frequency Internal Rotations", Southeastern Theoretical Chemistry Association (SETCA), Emory University, Atlanta, GA, May 15-17, 2014
- "A simple approach to accurately determine the entropy of low frequency internal rotations", Mississippi EPSCoR Annual State meeting, Mississippi State University, April 1, 2014
- "An approach to determine the entropy of low frequency internal rotations without knowing

transition states or rotational barriers" 22^{nd} International Conference on Current Trends in Computational Chemistry Conference, Jackson, MS, November 15-16, 2013 (First place)

- "Effect of ethanol on Toll-like receptor RNA complex: molecular dynamic Study", 245^{th} ACS National Meeting and Exposition, New Orleans, LA, April 7-11, 2013
- "Modeling human TLR3-dsRNA complex and effect of ethanol", Southeastern Theoretical Chemistry Association (SETCA), University of Auburn, AL, May 9-11, 2013
- "A theoretical investigation of the increased entropy in the transition state for inversion in bis(chromiumtricarbonyl) dibenzo[a,e]cyclooctatetraene (DBCOT)", 21st Conference on Current Trends in Computational Chemistry (CCTCC), Jackson, MS, November 9-10, 2012
- "The reason for the increase in entropy at the transition state for inversion in bis (chromiumtricarbonyl) DBCOT complexes" Southeastern Theoretical Chemistry Association (SETCA), Mississippi State University, MS, May 13-14, 2011
- "Electrophilic nitration of mono-substituted benzene: role of the intermediates and the transition States", Southeastern Theoretical Chemistry Association (SECTA), Columbia, SC, May 21-22, 2010

Awards and Prizes

- 1st place in poster presentation, 22^{nd} International Conference on Current Trends in Computational Chemistry Conference, Jackson, MS, November 15-16, 2013
- Best oral presentation, 2^{nd} Annual Lester S. Andrews Graduate Research Symposium, Mississippi State University, MS, May 14-15, 2011

Workshops

- "Hands-on" Workshop on Computational Biophysics (NIH sponsored workshop) at Georgia Institute of Technology, Atlanta, GA, November 3-7, 2014
- Training workshop on Exploring Opportunities in Nanoscience and Nanotechnology (Nanotech-2008) Kandy, Sri Lanka, June, 2-6, 2008
- Training of Trainers in Science Communication Colombo, Sri Lanka September 18-20, 2007

Certifications

- Occupational Safety and Health Administration (OSHA), Missisippi State University, May 2012
- Diploma in Quality Management, Sri Lanka Standard Institution, September 2005

Other Activities

- Visiting lecturer at the CINEC Maritime Campus, Malabe, SL
- Presided/moderated the Drug Discovery: Methodologies session on August 12, 2014 for the COMP division at the 248^{th} national ACS meeting in San Francisco, CA
- Wrote and published a book on Nanotechnology for school children in 2007
- Steering committee member of the Young Scientist Forum at NASTEC, Sri Lanka, 2008-2009
- Judge - Region V Mississippi Science Engineering Fair in 2011 and 2014
- Coordinator of the Sasnaka Sansada scholarship fund for school children 2004-2009
- Secretary of the Softball Cricket Club - Mississippi State University 2013-2014
- Won medals for Badminton at the International Games at MSU 2010-2013

Affiliations and Memberships

- Institute of Chemistry Ceylon (M.I .Chem. C.) - Life Member
- American Chemical Society (2013-2014)
- Chemistry Graduate Student Association - Mississippi State University (2009-2015)
- Sri Lanka Association for Advancement of Science - Life Member
- Old Anandian Association - Life Member

References

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