KOUSIK SAMANTA

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HIGHLIGHT OF SKILLS

- **Theory/method development:**
  - ❖ Highly accurate and efficient single- and multi-reference wave-function based quantum chemistry methods to study small and large chemical systems (stable and metastable) relevant in atmospheric, biochemical and solid-state studies.
  - ❖ Methods based on quantum mechanical and semi-classical dynamics to investigate and predict the course of chemical reactions in the chemically relevant non-adiabatic realm.

- **Code development:**
  - ❖ Skilled in procedural as well as object-oriented programming using modern computer languages, e.g., C++, Python, Fortran, Perl.
  - ❖ Experienced in parallel programming using MPI and OpenMP.
  - ❖ Experienced in developing, modifying and maintaining large-scale scientific codes.
  - ❖ Worked as a part of the Gaussian® software development team.

- **Application:**
  - ❖ About 12 years of experience in molecular modeling and prediction of structures and properties of chemically and biochemically relevant systems in the ground and excited states using the mainstream quantum chemistry softwares, e.g., Gaussian®, Molpro®, Molcas®, Gamess®, Columbus®, Hyperchem®.
  - ❖ Experienced in the state-of-the-art wave-function based (CASSCF, CASPT2, MRCI, Coupled Cluster), density functional (DFT) based, semiempirical as well as hybrid QM/MM methods.

EDUCATION

- 05/2009 **Ph.D. / Chemistry, Texas A&M University, College Station, TX (**GPA: 3.48/4.0)
  Thesis: "Investigation of electron-atom/molecule scattering resonances using complex multiconfigurational self-consistent field method".
  Advisor: Prof. Danny L. Yeager

- 08/2003 **M.Sc. / Physical Chemistry, Indian Institute of Technology (IIT) Bombay, Mumbai, India**
  Thesis: "Treatment of resonances using dilated electron propagator".
  Advisor: Prof. Manoj K. Mishra

- 08/2001 **B.Sc. (Honours) / Chemistry, University of Calcutta, Kolkata, India**
  Major: Chemistry; **Minor:** Physics and Mathematics.

EMPLOYMENT

- 08/2012– present Assistant Professor, IIT Bhubaneswar, Orissa, India
- 09/2012–08/2014 Postdoctoral Researcher, University of Pennsylvania, Philadelphia, PA
- 08/2010–08/2012 **Postdoctoral Research Associate,** Rice University, Houston, TX
- 07/2009–07/2010 **Postdoctoral Fellow,** Johns Hopkins University, Baltimore, MD
- 08/2003–05/2009 **Graduate Assistant – Research & Teaching,** Texas A&M University, College Station, TX

TEACHING EXPERIENCE

- **General Chemistry Labs – I/II** (Freshman level): Texas A&M University
- **Physical chemistry** (Junior level): Texas A&M University
- **Introduction to Quantum Chemistry:** IIT Bhubaneswar

RESEARCH EXPERIENCE

09/2012-present **University of Pennsylvania, Philadelphia, PA** (Supervisor: Prof. Joseph Subotnik)
- Development of tools to study non-adiabatic chemical dynamics.
- Study of electron and charge transfer reactions.

08/2010–08/2012 **Rice University, Houston, TX** (Supervisor: Prof. Gustavo Scuseria)
- Application of symmetry projected Hartree-Fock theory to molecular systems.
- Development of symmetry projected quasiparticle theory under the periodic boundary condition for the accurate study of the periodic systems (theory and computer programs).
- Development of constrained unrestricted Hartree-Fock (CUHF) method under periodic boundary condition for the investigation of periodic systems and the incorporation of the same in the development version of Gaussian computer programs).

07/2009 – 07/2010 **Johns Hopkins University, Baltimore, MD** (Supervisor: Prof. David Yarkony)
- Investigation of non-adiabatic effects and the role of conical intersections in the photodissociation of some organic molecules and radicals that are important in the atmosphere (e.g., ethene, 1-hydroxyethyl radical).
- Investigation of the effects of the surrounding medium in the photodissociation reactions.

08/2003–05/2009 **Texas A&M University, College Station, TX** (Supervisor: Prof. Danny Yeager)
- Development of Complex MCSCF theory and related computer programs.
- Application of Complex MCSCF theory to study electron-atom/molecule scattering resonances.

COMPUTER SKILLS

- **Quantum Chemistry tools:** Gaussian, Gamess, Molpro, Columbus, Hyperchem.
- **Mathematical tools:** Matlab, Mathematica, Octave, Gnuplot.
- **Visualization tools:** ChemDraw, Molden, Avogadro, Jmol, Xfig.
- **Publishing tools:** LaTeX, BibTeX, Microsoft Office, EndNote.
- **Programming and scripting languages:** C, C++, Fortran, Perl, Python, Shell (bash, csh/tcsh and zsh) scripting, parallel programming using message passing interface (MPI).
- **Operating systems:** Unix, GNU/Linux, Macintosh, Windows.

CONFERENCE ORGANIZATION

- Southwest Theoretical Chemistry Conference, College Station, TX (2007).

PROFESSIONAL AFFILIATIONS

- American Physical Society (APS).
- American Chemical Society (ACS).

REPRESENTATIVE PUBLICATIONS AND CONFERENCES

- "Investigation of ^{2}P Be$^-$ shape resonances using a quadratically convergent complex multiconfigurational self-consistent field method": Samanta, K.; Yeager, D. L. *J. Phys. Chem.* B **2008**, *112*, 16214–16219.
- "Obtaining resonance positions and widths of scattering resonances from a complex multiconfigurational self-consistent field state using the M_1 method": Samanta, K.; Yeager, D. L. *Int. J. Quantum Chem.* **2009**, *110*, 798–812.
- "On the role of conical intersections and their local topography in the photodissociation of the 1-hydroxyethyl radical": Samanta, K.; Yarkony, D. R. *Chem. Phys.* **2010**, *378*, 110–117.
- "Projected quasiparticle theory in molecular electronic structure": Scuseria, G. E.; Jiménez-Hoyos, C. A.; Henderson, T. M.; Samanta, K.; Ellis, J. K. *J. Chem. Phys.* **2011**, *135*, 124108.
- "Complex multiconfigurational self-consistent field based methods to investigate electron-atom/molecule scattering resonances": Samanta, K.; Yeager, D. L. *Adv. Chem. Phys.* **2012**, *150*, 103–142.
- "Exploring copper oxide cores using the projected Hartree-Fock theory": Samanta, K.; Jimenz-Hoyos, C, A., Scuseria, G. E. *J. Chem.Theor. Comput.* **2012**, *8*, 4944–4949 .
- Quantum dynamical investigation of the simplest Criegee intermediate, CH_2OO: Electronic spectroscopy and O-O dissociation channels": Samanta, K.; Beams, J. M., Lester, M. I.; and Subotnik, J. E. (under review):.
- "Investigation of electron-atom/molecule scattering resonances: two complex multiconfigurational self-consistent field approaches": Samanta, K.; Yeager, D. L. *Am. Inst. Phys. (AIP) Conf. Proc.* (in press).
- "The effects of higher angular momentum functions on shape resonances": Samanta, K.; Yeager, D. L. *Am. Inst. Phys. (AIP) Conf. Proc.* (in press).
- "The role of conical intersections in the photodissociation of 1-hydroxyethyl radical" (Poster): Samanta, K. *Gordon Research Conference, New London, NH (July 2010)*.
- "A complex multiconfigurational self-consistent field approach in the investigation of electron-atom/molecule scattering resonances" (oral): Samanta, K. *Southwest Theoretical Chemistry Conference, El Paso, TX (October 2008)*.

HONORS AND AWARDS

- Reviewer – Journal of Chemical Theory and Computation, ACS (2012-present).
- Freshman Chemistry Teaching Award, Texas A&M University (2008).
- Award for the best poster presentation, Southwest Theoretical Chemistry Conference (2007).
- Ranked *seventh* (99.76 percentile) in the nation-wide Graduate Aptitude Test in Engineering (GATE) conducted by the Department of Higher Education, Govt. of India (2003).
- College medal for excellence in B.Sc., R. K. Mission Vidyamandira, Calcutta University (2001).