

## Curriculum Vitae

### Dr. Rupashree Shyama Ray

Lecturer

Department of Chemistry

Ravenshaw University

Ph. No: 7894322392

Email: [shyama.tum@gmail.com](mailto:shyama.tum@gmail.com)



### PROFESSIONAL EXPERIENCE:

**2010-continuing:** Lecturer in Chemistry, Ravenshaw University

**2009- 2010:** **Postdoctoral Researcher**

*Explicit (scalar)-relativistic first-principle molecular dynamics simulations in order to study solvent effects and heavy elements*

*Advisor:*

**Prof. Dr. Barbara Kirchner**, University of Leipzig, Germany

*Project synopsis:*

- Simulation of actinides with all-electron DKH method in AIMD (CP2K) framework
- Catalytic study of methane activation using novel palladium catalyst

**2004-2009** **Graduate Research Assistant**

*Dissertation:*

*A Relativistic density functional study of Uranyl Hydrolysis and Complexation by Carboxylic Acid in Aqueous Solution*

*Advisor:*

**Prof. Dr. h.c. Notker Rösch**, Technical University of Munich, Germany.

*Project synopsis:*

- Theoretical investigation of uranyl monohydroxide: Structure and Energetic
- Structure, coordination mode and energetic of uranyl monocarboxylates
- Ternary complexes of uranyl monocarboxylate: A density functional model study of uranyl-humate complexation

### EDUCATION:

**2009**

**Ph.D. in Theoretical Chemistry**

Technical University of Munich, Munich, Germany

**2004**

**Master of Science in Chemistry**

University of Hyderabad, Hyderabad, India

**2002**

**Bachelor of Science in Chemistry**

Ravenshaw College (Autonomous), Cuttack, India

### AREAS OF SPECIALIZATION:

**Computational Chemistry, Molecular Modeling**

Currently I am focusing on *ab initio* molecular dynamic simulations of actinides and biomolecules in aqueous solution in collaboration with Prof.

Barbara Kirchner, University of Leipzig and Juelich Supercomputer Center, Germany.

## PUBLICATIONS:

1. Schuster, O.; Monkowius, U.; Schmidbaur, H.; **Ray, R. S.**; Krüger, S.; Rösch, N. *Unexpected Structural Preference for Aggregates with Metallophilic Ag-Au Contacts in (Trimethylphosphine)silver(I) and -gold(I) Phenylethynyl Complexes: An Experimental and Theoretical Study*, **Organometallics**, **2006**, 25, 1004-1011.
2. Krüger, S.; Schlosser, F.; **Ray, R. S.**; Rösch, N. *Uranyl Complexation By Carboxylic Acids: A relativistic Density Functional model Study for Actinide Complexation by Humic Acids*, **Lecture series on Computer and Computational sciences**, **2006**, 7, 904-907.
3. **Ray, R. S.**; Krüger, S.; Rösch, N. *Uranyl monocarboxylates of aromatic acids: A density functional model study of uranyl-humate complexation* **Dalton Trans.**, **2009**, 3590-3598.
4. **Ray, R. S.**; Krüger, S.; Rösch, N. *Ternary Complexes of Uranyl monocarboxylate: Structure, Energetic and Stability Constant* **Inorg. Chim. Acta**, **2009**, 363, 263-269.
5. **Ray, R. S.**; Krüger, S.; Rösch, N. *Theoretical investigation of Uranyl monohydroxide: Structure and Energetic* (submitted to Inorganic Chemistry).
6. Schlosser, F.; **Ray, R. S.**; Krüger, S.; Rösch, N. *Uranyl monocarboxylates: mono- or bidentate coordination? A Relativistic density functional study* (submitted to Inorganic Chim Acta).
7. **Ray, R. S.**; Hutter, J.; Kirchner, B. *Relativistic AIMD simulation of uranyl in aqueous solution* (manuscript under preparation).

## CONFERENCE PRESENTATIONS:

### PROCEEDING ABSTRACTS:

- Krüger, S.; **Ray, R. S.**; Kremleva, A.; Zakhariyeva, O.; Schlosser, F.; Rösch, N. *"Density functional studies on uranyl complexes with organic ligands"* 11<sup>th</sup> International Conference on the Chemistry and Migration Behavior of Actinides and fission products in the Geosphere. Migration **2007**, Munich, Germany.
- Thar, J.; **Ray, R.S.**; Golze, D.; Weber, H.; Kirchner, B. *"Relativistic all-electron molecular dynamics simulations"* 2nd German-Indian Symposium on "Frontiers of Chemistry" **2009**, Leipzig, Germany.
- Thar, J.; **Ray, R.S.**; Golze, D.; Weber, H.; Kirchner, B. *"Relativistic all-electron molecular dynamics simulations"* International-Bunsen-Meeting-Discussion, **2009**, Leipzig, Germany.

#### POSTER PRESENTATIONS:

- **Ray, R. S.**; Krüger, S.; Kremleva, A.; Zakharieva, O.; Schlosser, F.; Rösch, N. “*Density functional studies on uranyl complexes with organic ligands*” 11<sup>th</sup> International Conference on the Chemistry and Migration Behavior of Actinides and fission products in the Geosphere. Migration **2007**, Munich, Germany.
- Schlosser, F.; Krüger, S.; Moskaleva, L.; **Ray, R. S.**; Kremleva, A.; Rösch, N. “*Relativistic density functional study on Actinide complexes in solution*” Actinides **2005**, Manchester, UK.
- Thar, J.; **Ray, R.S.**; Golze, D.; Weber, H.; Kirchner, B. “*Relativistic all-electron molecular dynamics simulations*” 2nd German-Indian Symposium on "Frontiers of Chemistry" **2009**, Leipzig, Germany.
- Thar, J.; **Ray, R.S.**; Golze, D.; Weber, H.; Kirchner, B. “*Relativistic all-electron molecular dynamics simulations*” International-Bunsen-Meeting-Discussion, **2009**, Leipzig, Germany.

#### WORKSHOP/CONFERENCE ORGANIZED:

- Organized workshop on ‘Migration of Radioactive Elements’ in Technical University of Munich, Germany in Technical University of Munich, Germany, **2008**
- Organized workshop on ‘Catalysis’ in Technical University of Munich, Germany, **2009**
- Organized School on Physics and Chemistry of Plasma Processing, Ravenshaw University, October, Cuttack, Orissa, **2010**.

#### HONORS AND ACADEMIC DISTINCTIONS:

- Gold medalist in B.Sc. (2002)
- Gold medalist in M.Sc. (2004)
- Qualified in Council of Scientific and Industrial Research (CSIR) examination for Junior Research Fellowship (Dec 2003)
- Qualified in Graduate Aptitude Test in Engineering (GATE) 2004
- Selected as a summer visiting student by the Indian Academy of Sciences and Jawaharlal Nehru Center for Advanced Scientific Research in 2003
- Awarded for securing 17<sup>th</sup> position in H.S.C Examination in state level and 26<sup>th</sup> position in I.C.S.E. exam in state level.
- Awarded National Merit Scholarship in Secondary and Higher Secondary examination (1997-2002).

#### MEMBERSHIP IN PROFESSIONAL BODIES

- Orissa Chemical Society (Life member)