

## Dr. Anoop Ayyappan

Department of Chemistry, Indian Institute of Technology Kharagpur, West Bengal, INDIA - 721 302  
Email: [anoop@chem.iitkgp.ernet.in](mailto:anoop@chem.iitkgp.ernet.in); Phone: +91 3222 283 316. Website: <http://anooplab.in>

---

### Professional Experience

#### Assistant Professor

- IIT Kharagpur (Since July 2010)

#### Post-Doctoral Fellow

- 2009–2010 - Institute for Physical and Theoretical Chemistry, University of Bonn with Prof. Frank Neese.
- 2006–2009 - Max-Planck Institut für Kohlenforschung, Mülheim a.d. Ruhr, Germany, with Prof. Walter Thiel.

### Teaching Experience

#### Courses taught

- 1<sup>st</sup> year UG Chemistry (PhysChem -Theory and Lab.
- Chemical Bonding and Reactivity (Elective)
- Computational Chemistry (Core, Elective and Lab)
- Molecular Photochemistry (Elective)

### Academic Qualification

- PhD (2005 University of Hyderabad)
- Supervisor: Prof. E. D. Jemmis

### Membership in professional bodies

- Chemical Research Society of India (CRSI)
- World Association of Theoretical and Computational Chemists (WATOC)

### Fellowships

- 2006-2009 - Max-Planck Fellowship
- 2002-2005 - UGC-CSIR SRF
- 1999-2002 - UGC-CSIR JRF

### Education

- 1996-1998 - MSc Chemistry at the School of Chemical Sciences, Mahatma Gandhi University, Kerala.
- 1993-1996 - BSc (Chemistry) at the Nirmala College, Muvattupuzha, Kerala

### Research Interests

- Computational study of Reaction Mechanism
- Structure and bonding in novel molecules, and clusters
- Developing methods to predict reaction & aggregation

### Publications

- From Kharagpur: 28
  - Angewandte Chemie Intl. Ed.: 3
  - Chemical Communication: 1
  - Chemistry - A European Journal: 1
  - Organic Letters : 1
  - The Journal of Organic Chemistry: 5
  - Physical Chemistry Chemical Physics: 3
  - RSC Advances: 2
  - Chemistry - An Asian Journal: 1
  - Journal of Physical Chemistry: 1
  - International. Journal of Quantum Chemistry: 2
- Others: 12

### Research Guidance

- 5 PhD students (2 completed; 3 ongoing)
- MSc Projects (12 completed, and 2 ongoing)

### External Funding

- DST Project “Effect of  $\pi$ - $\pi$  interaction in Chemical Reactions: Computational Study of Bergman Cyclisation.

### Collaborations

- Visited University of Muenster, Germany as a Visiting Professor during 2012 June-July.
- Published more than 25 articles in collaborations with in-house (>10), national (2), and international (2) partners.
- Facilitated exchange program with University of Muenster, in which faculties and students made exchange visits.