Dr. Anoop Ayyappan

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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

- 1st 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
 - o Angewandte Chemie Intl. Ed.: 3
 - o Chemical Communication: 1
 - o Chemistry A European Journal: 1
 - o Organic Letters: 1
 - o The Journal of Organic Chemistry: 5
 - o Physical Chemistry Chemical Physics: 3
 - o RSC Advances: 2
 - o Chemistry An Asian Journal: 1
 - o Jounnal 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 π - π 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.