

DR.G. KRISHNA CHAITANYA PROFILE * * * *

Dr. G. K. Chaitanya

Lecturer

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Personal Information

Date of Birth	: 12-04-1981
Qualification	: M.Sc., NET, CSIR-SRF, Ph.D.
Specialization	: Physical Chemistry, Computational Chemistry
Teaching Experience	: 6 months PG Teaching Experience (Subjects Taught: Industrial Chemistry, Physical Chemistry, Molecular Spectroscopy and Computer applications in Chemistry)

Research Information

My research is focused on computational chemistry area which deals with the theoretical characterization of the molecular materials like near-infrared (NIR) dyes, dye sensitized solar cells (DSSC), Nano materials, Optical Materials and Hard Materials through high level *ab-initio* and DFT methodologies. Here the characterization involved in the study of ground and excited states of molecules (through methods like CIS, CCSD and SAC-CI) in both vacuum and solvent phases. Further extension of my research work at molecular level to bulk level like surface adsorption studies and solvent-solute interactions is under progress.

Research Area	: Computational Chemistry
Papers in Journals	: 10
M.Sc. Projects Guided	: 04

**Representative
Publications**

- *J. Phys. Chem. A*, **2005**, 109, 2614-2622.
- *J. Phys. Chem. A*, **2005**, 109, 8604-8616.
- *J. Phys. Chem. A*, **2006**, 110, 11717-11729.
- *Inorganic Chemistry*, **2006**, 45, 7600-7611.
- *J. Org. Chem.*, **2008**, 73, 9443-9446

Conferences

Conferences Conducted : --

Conferences Attended : 02