

DEPARTMENT OF INORGANIC AND PHYSICAL CHEMISTRY INDIAN INSTITUTE OF SCIENCE, BANGALORE

CURRENT RESEARCH

The Department of Inorganic and Physical Chemistry, one of the founding departments of the Indian Institute of Science, is devoted to advanced research and teaching in chemistry. The department has distinguished itself as a Centre for innovative and pioneering research in a wide range of areas in Inorganic and Physical Chemistry. It was elevated to the status of a UGC Centre of Advanced Study (CAS) in 1980 in recognition of its achievements and to the status of a DST-FIST Sponsored Department in the year 2000.

The research activities in the Department can be broadly classified under three disciplines:

(a) Inorganic Chemistry/Bio-inorganic Chemistry/Chemical Biology (b) Physical Chemistry/Polymers /Materials and (c) Theoretical Chemistry. Significant amounts of cross disciplinary efforts exist. The research scope is broad with faculty interested in both fundamental and applied aspects of science. The department ventures into many research fields which include but are not limited to novel inorganic molecules, materials, electrochemistry and spectroscopy with their applications to challenges in biology, medicine, catalysis and energy conversion and storage. A more detailed list follows.

a) Inorganic Chemistry

- Main Group, Coordination and Organometallic Chemistry – Synthesis and reactivity of organometallic compounds and metal clusters; homogeneous catalysis; magnetic materials and supramolecular chemistry; materials chemistry.
 - Chemistry in molecular nano-vessels, catalysis using organic nano-cages and coordination cage compounds.
 - Bioinorganic Chemistry – Mimicking natural evolution in metalloproteins through synthetic strategies; artificial nucleases; medically important zinc hydrolases; metal-based drugs.
 - Metalloenzymes-Biochemical investigation of activity, kinetics and mechanism of metalloenzymes; identification of reactive reaction intermediates; metalloenzymes for alkane biosynthesis with potential in biofuel applications; enzymes for biofilm dispersion with potential in therapeutics; metalloenzymes in bioremediation; protein engineering to improve properties of enzymes.
- Micellar catalysis: use of water for synthesis, green & Sustainable catalysis, heterogenous asymmetric catalysis.

b) Physical Chemistry

- Spectroscopy: Biospectroscopy and Ultrafast Raman spectroscopy; Application of in situ Raman and Mass Spectroscopy towards electrochemical energy conversion and storage.
- Photoelectron Spectroscopy: Investigation of ultrafast chemical processes and photocatalytic reaction dynamics.
- Molecular Beam Microwave Spectroscopy: Microwave spectroscopic studies in supersonic jets; spectroscopic studies on hydrogen bonded and van der Waals complexes.
- Chemical Kinetics: Liquid – protein/DNA interactions; shock tube kinetics for modeling combustion and atmospheric chemistry.
- Non-linear Optics with Molecules and Materials: Non-linear optical properties of molecules and materials/metal nanoparticles studied by laser light scattering.

- Light-matter interactions: Photophysics of molecules and materials under light-matter strong coupling; Chemical reactivity and charge transport under vibrational strong coupling; Interaction of chiral matter with chiral light.
- Electrochemistry: Electroanalytical chemistry; electrochemical biosensors; energy conversion and storage; batteries, fuel cells and supercapacitors, conducting polymers.
- Electrocatalysis: H₂ production from water, CO₂ conversion to synthetic fuels, oxidation of alcohols.
- Polymer Chemistry: Polymer synthesis; conducting polymers; foldamers; functional polymers with well-defined molecular architecture.
- Materials Chemistry – Nanostructured materials; functionalized nanoparticles; metallic nanoparticles – syntheses, properties, catalysis; organic thin films – self-assembly; Langmuir – Blodgett films; NLO properties.
- X-ray Crystallography: Small molecule crystallography - Metal-Nucleotide interactions, biological activity studies - anti cancer drugs.
- NMR spectroscopy and Imaging: Spin hyperpolarization; reaction monitoring; catalysis and synthesis of novel inorganic complexes; para-hydrogen; metabolic studies, Earth's field MRI.
- Single molecular studies: Single molecular electronics; single molecular spintronics; single particle electrochemistry, study of electromechanical properties under active conditions – From single molecule to single cell studies; development of novel methodologies and instrumentation for single molecular electronics applications (sensors).
- Surface Chemistry: In situ scanning probe techniques (EC-STM, EC-AFM); self- assembled monolayers; 2D nanoparticle networks; large area molecular junctions for molecular electronics and plasmonics applications (CP-AFM and E Gain molecular junctions)
- Chiral Spectroscopy and Dynamics: Femtosecond circular dichroism spectroscopy; Harnessing quantum dynamics for spintronics applications; Ultrafast dynamics in chiral exciton-plasmon systems; Femtosecond structural biology; Development of novel chiroptical techniques and computational spectroscopy.

c) Theoretical Chemistry

- Theoretical problems in classical and quantum dynamics; soft condensed matter; theoretical/computational chemistry; quantum chemistry; statistical mechanics of polymers.
- Non-linear laser Raman Spectroscopy, experiment; theory and simulations.
- Non-equilibrium electron transport, fluctuations and many-body interactions in quantum junctions.
- Modeling excited state electronic surfaces and photoprocesses; mixed quantum-classical simulations; nuclear quantum effects in small molecular systems.