

XI - Plan Project Proposals : Radiation & Photochemistry Division

Proposals	Linkage
TP-28 <u>Energy Conversion</u> <u>XI-N-R&D-33</u> (S.K.Sarkar) 33.08 <u>Photochemistry at Surface and Interface</u> (H.Pal)	Part of Vision Document
■ Structure & Dynamics of Nano-Materials	ChD, DRDO
■ Single Molecule Multi-parameter Fluorescence	LPTD, BMG
■ Laser probing of Chemical Dynamics	TIFR, BMG
TP-29 <u>Radiation Effects in Biological Systems</u> <u>XI-N-R&D-34</u> (K.B.Sainis)	Part of Vision Document
34.06 <u>Free Radical Chemistry :Design & Application</u> (T.N.Das)	
■ Physico-Chemical basis of Radio-protection	BMG
■ Dielectric Barrier Discharge initiated Free Radical Chemistry	RTDS, MG
■ FRC in hydrogen generation & waste degradation	ChD, NRG
TP-04 <u>R&D in Back-End Processes</u> <u>XI-N-R&D-04</u> (P.K.Wattal)	
04.03 Development of Polymeric Extractant for radionuclides & toxic metals (M.Kumar)	BETD, NRG
TP-22 <u>Advanced Electromagnetic Technologies</u> <u>XI-N-R&D-26</u> (L.M.Gantayet)	Part of Vision Document
26.10 Coherent Control of Chemical Reactions (SKSarkar)	LPTD

Objectives / Deliverables

- 1. Photochemistry at Surface and Interface
- Structure & Dynamics of Nano-material

Investigation of chemical identity, orientation and conformation of adsorbed molecules & surface topography → Sum Frequency Generation (SFG) & Tip-Enhanced Raman Spectroscopic (TERS) techniques

Possible technological application → Catalysis, pollutant degradation on nanoparticles, targeting of biological cells, Environmental Chemistry

■ Single Molecule Multi-parameter Fluorescence

Address conformational / diffusion / transport dynamics in macromolecules, biomolecules, organized assemblies and supramolecular host-guest systems

Studies on Host-Guest Complexes → Aqueous Laser Dyes, sensors

Molecular Interactions and Bio-functionality → Enzyme-DNA, Molecular motor, switches

■ Laser steering of Chemical Dynamics



Develop ultrafast (<50 fs) time-resolved two-dimensional Infrared (2D IR) Spectrometer indigenously → Vibrational dynamics of simple system like H-bonding

Membrane Protein Structure & Role of lipid membranes in promoting pathological β -sheet structure → Protein mis-folding diseases (TIFR)


■ 2. Free Radical Chemistry : Design & Application

■ Physico-Chemical basis of Radio-protection


Identifying important phytochemicals, Herbal formulations etc. as potent

Radio-protector  Structural modifications to develop new target specific derivatives with high dose modification factor  in-vivo studies with BSG

■ Dielectric Barrier Discharge initiated Free Radical Chemistry

In-situ generation (with Dielectric Barrier Discharge) of varieties of free radicals and study their subsequent chemistry  Dispersed hydro- & liquid-meteor; Surface modification of materials via mono-functionalization

■ FRC in hydrogen generation & waste degradation

Feasibility of Radiolytic Hydrogen Generation  Controlled hydrolysis of borohydride & its regeneration by Radiolytic method (Utilization of radioactive waste as an energy source could be an economic driver)



Using excited uranyl photochemistry with peroxide  degrade the waste products like resins, solvents, extractants etc

■ 3. Development of Polymeric Extractant for radionuclides & toxic metals

Identify back-bone polymers & suitable functional groups for extraction especially in hostile environment of acid & radiation

 Testing of extraction capabilities, capacity, recycling effect with NRG

■ 4. Coherent control of chemical reactions

A properly shaped ultrashort pulse can cause a molecule to vibrate in such a way as to break the bond of our choice  Which control field to use & how to generate it ??  **Coherent Control : using a learning algorithm and Ultrashort pulse shaping equipment, the reaction control will be achieved**

Isotope Separation, Stereo-synthesis, and Photocatalysis

