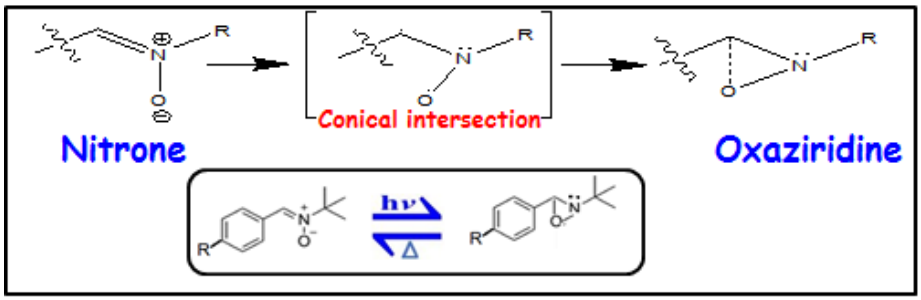
Research Page of Prof. Chattopadhyay

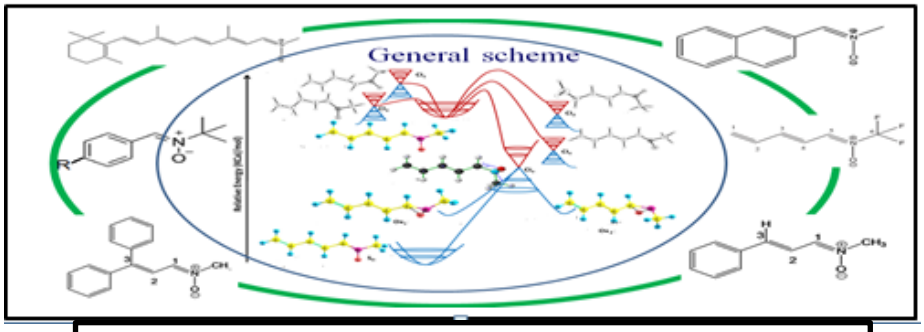
Computational Chemistry

Ultrafast **Photochemical Reactions (through Conical Intersections), Fluorescence & its quenching, Phosphorescence processes,**
ESPT, ESIPT, FRET, TICT, AIE, ISC, RISC, ROS

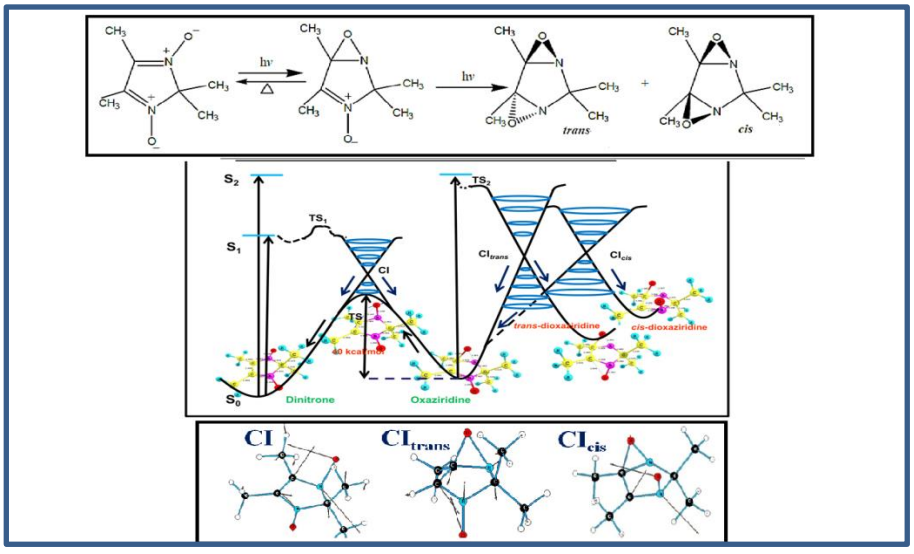
Nitrone (Cyclic & Acyclic) Photochemistry

Acyclic Nitrones Photochemical Path

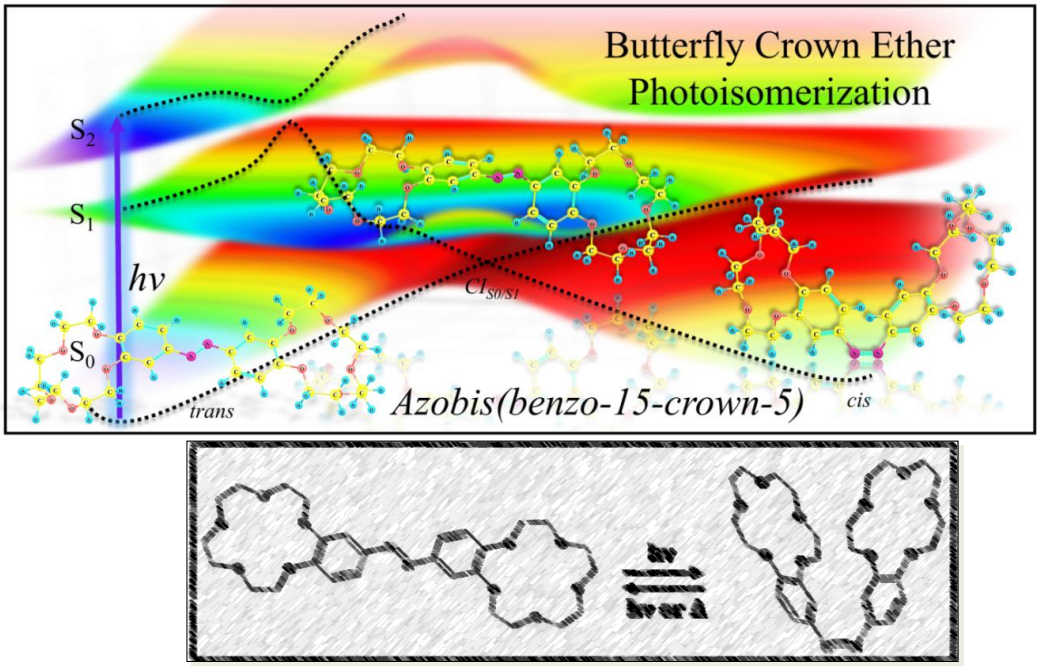




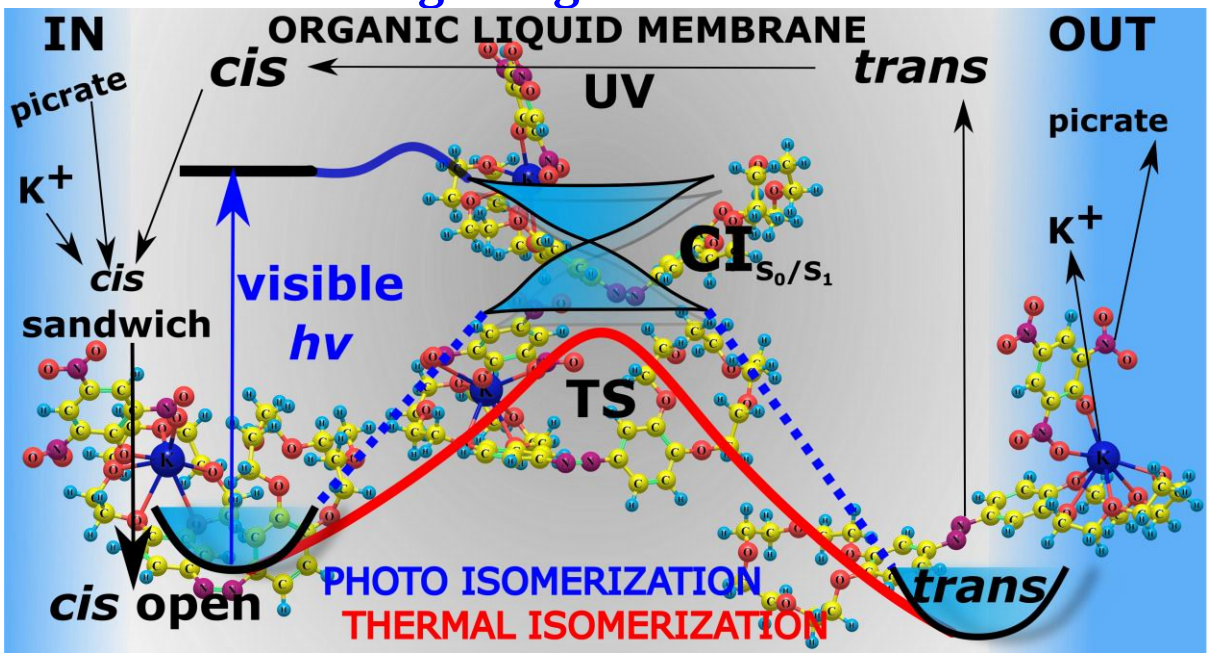
Cyclic Nitrones Photochemical Path



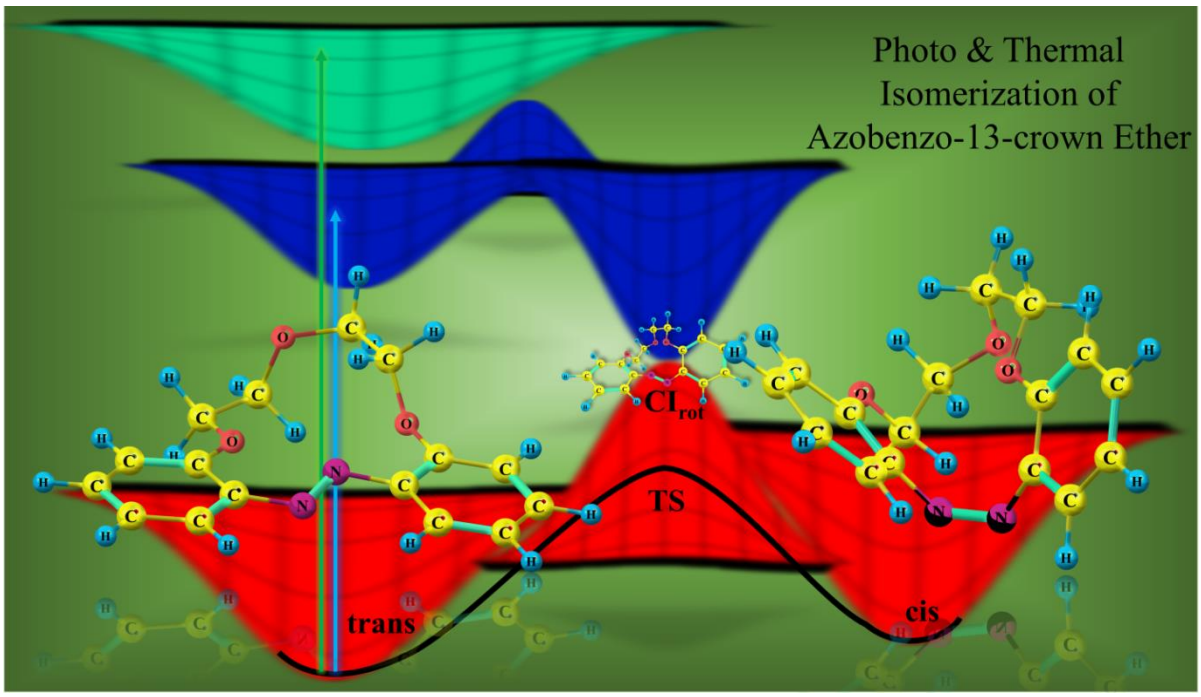
Butterfly Crown Photo-isomerization



Butterfly Crown Alkali Metal ion Transport Through Organic Membrane



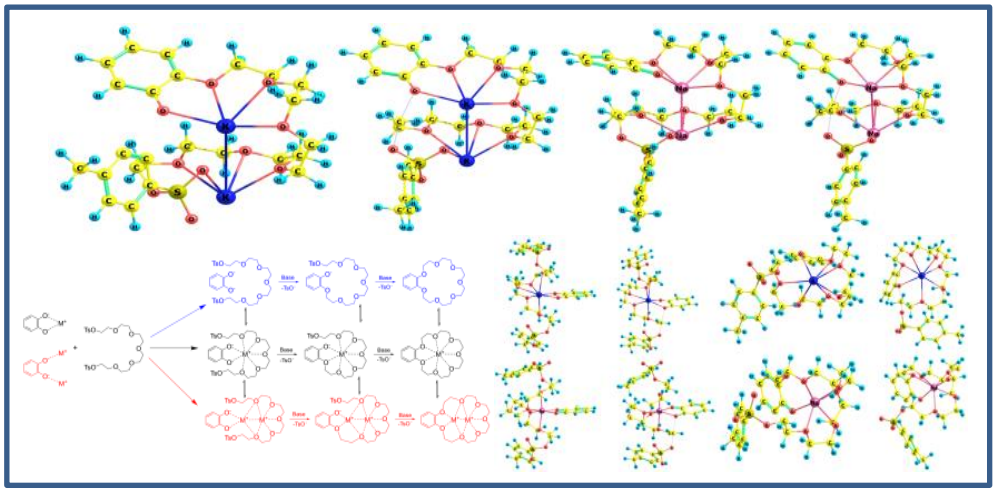
Strained Azo Crown Ether Photo-isomerization



Alkali metal ion Template Synthesis of Crown Ethers

Template & Non-Template Synthesis Mechanisms of DB18C6 (Pedersen's Method)

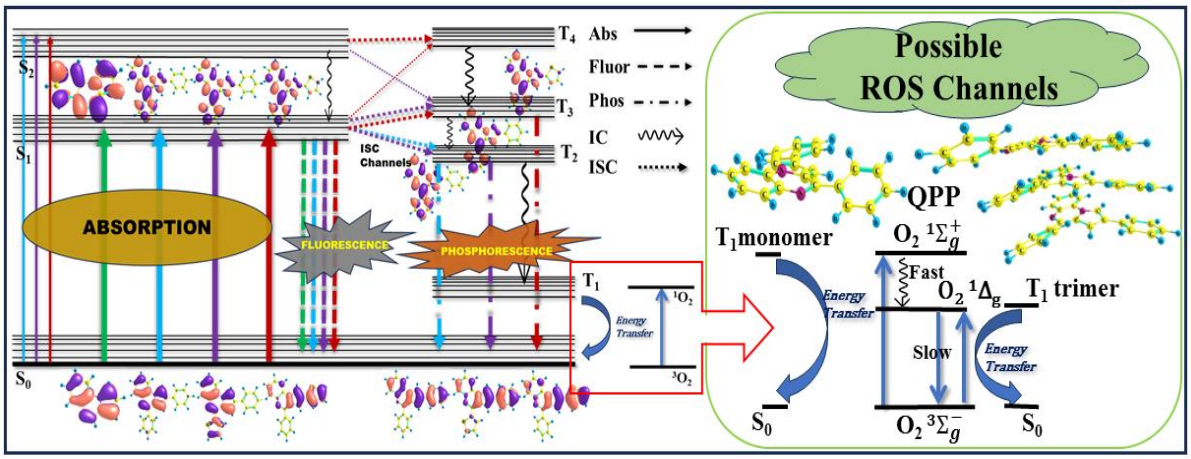
1:1 and 2:1 Template Synthesis Mechanisms of Crown ethers

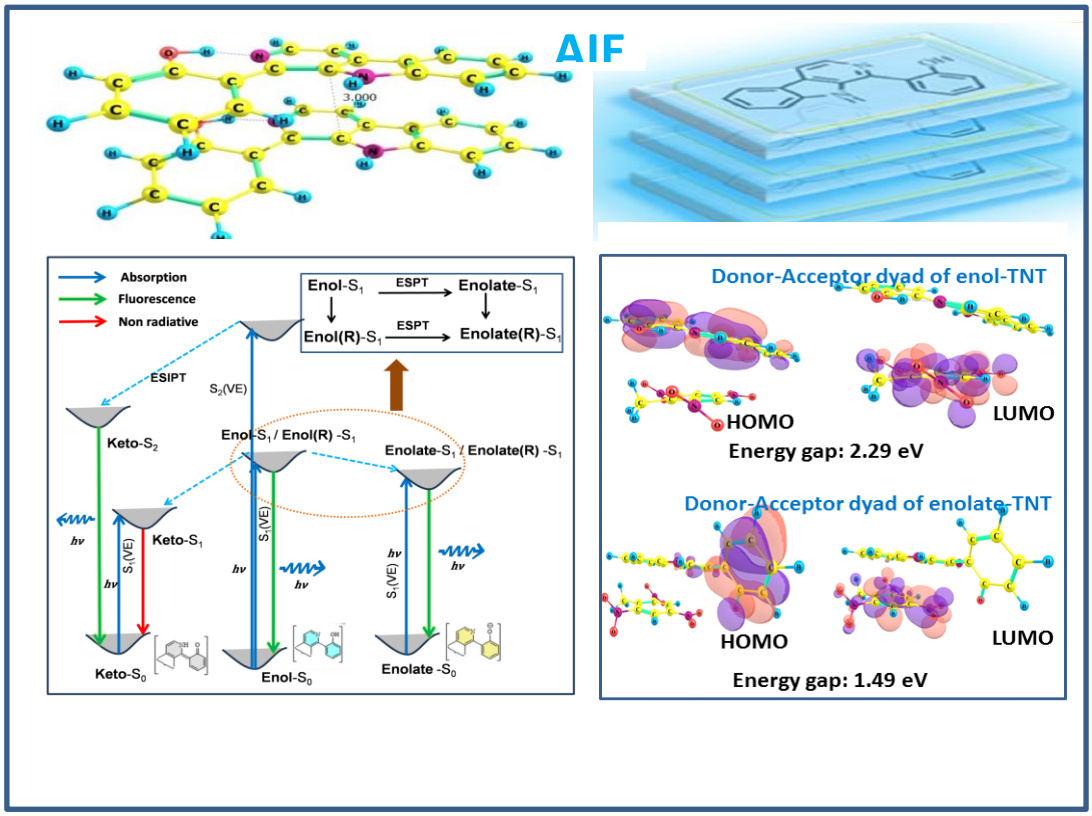


Photophysical Processes, Reaction Mechanisms

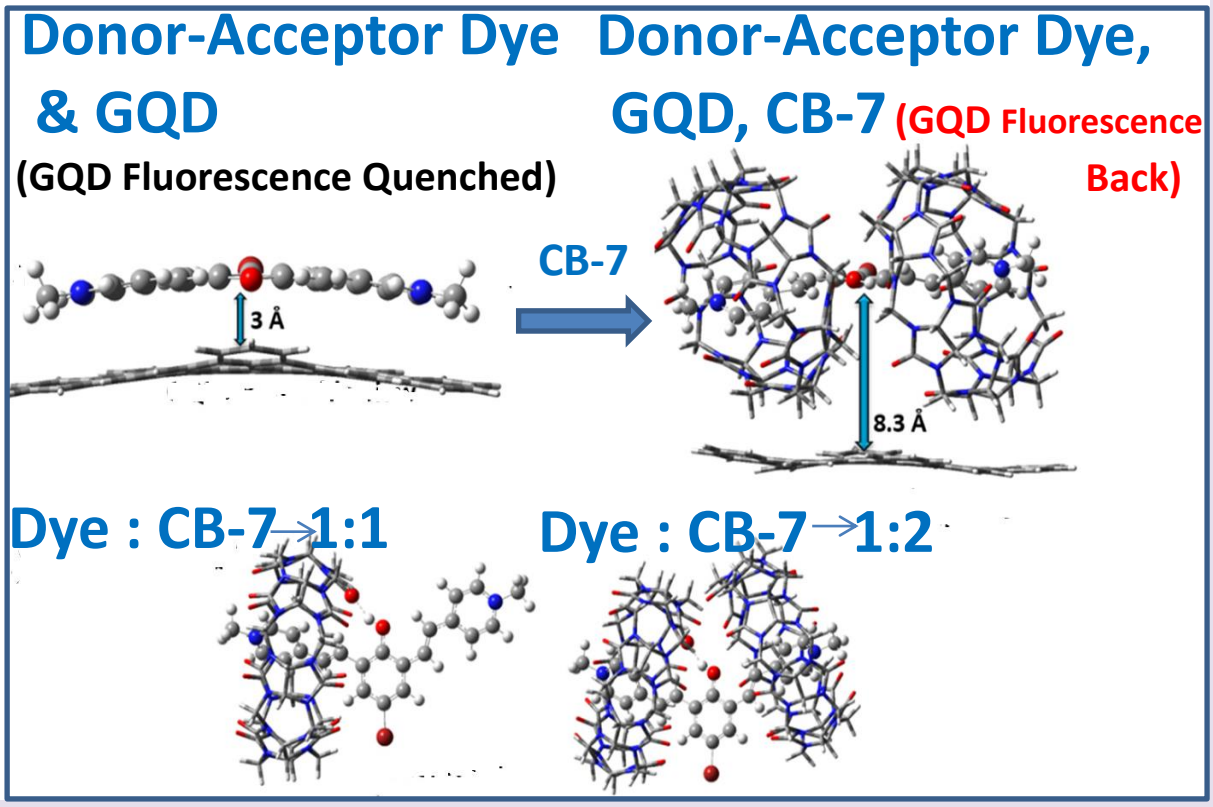
(In Collaboration with experimental groups)

In collaboration with the experimental group of Prof. Anupam Bhattacharya (BITS-Pilani, Hyderabad)

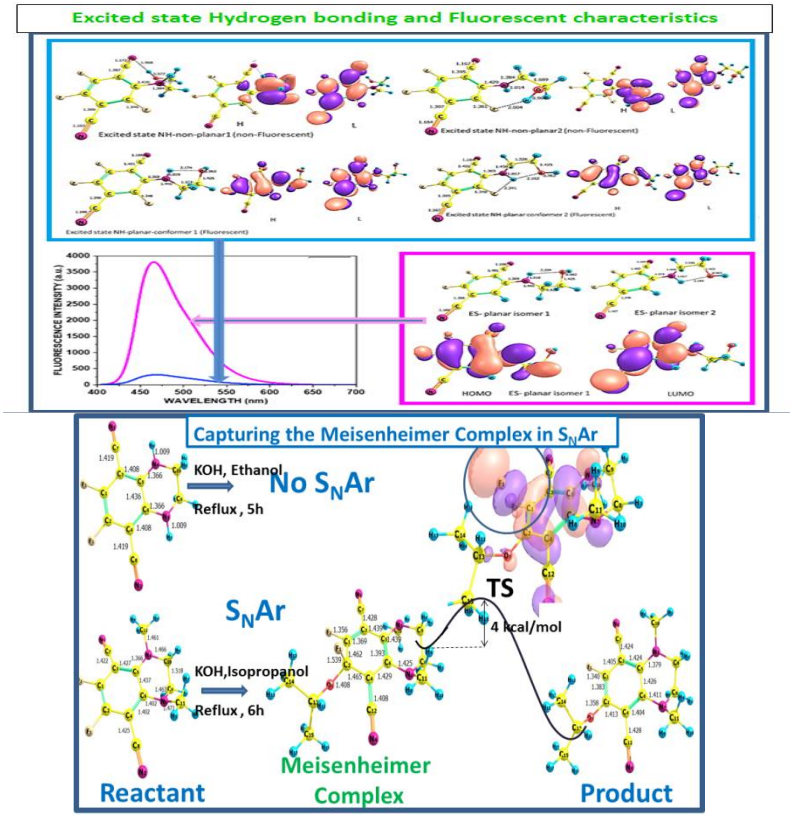




In collaboration with the experimental group of Prof. Mainak Banerjee (BITS-Pilani, Goa)



In collaboration with the experimental group of Prof. Subhadeep Banerjee (BITS-Pilani, Goa)

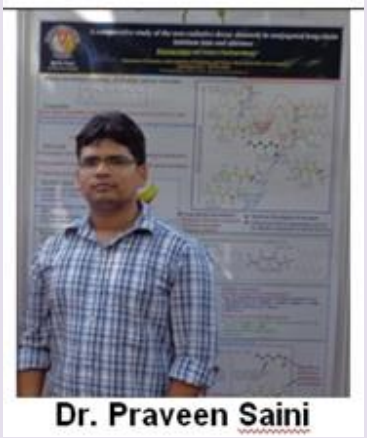


Other Significant Studies

Low-lying & High-lying Excited Electronic states of Alkali metal-Rare gas (van der Waals) molecules Potential Excliplex Laser systems

Ph.D Thesis guided (as Supervisor)

Dr. Praveen Saini (Year 2017)



Title of Thesis: A Computational Investigation of Oxaziridine Photoconversion and *E-Z* Isomerization Processes of Some Acyclic Nitrone Systems

Dr. Sindhuja Sen (Year 2020)

Title of Thesis:
A Computational Investigation of the Photochemical Oxaziridine Conversion and Subsequent Product Formation Pathways of Some Cyclic Nitrone Systems

Dr. Dilawar Singh Sisodiya (Year 2025)

Title of Thesis:
A Computational Investigation on the Mechanisms of Template Synthesis and Trans-Cis Isomerization Reactions of Some Selected Crown Ethers

Current Ph.D. Scholars

Ms. Rajeshwari Nikam

Ms. Anisha Mishra