

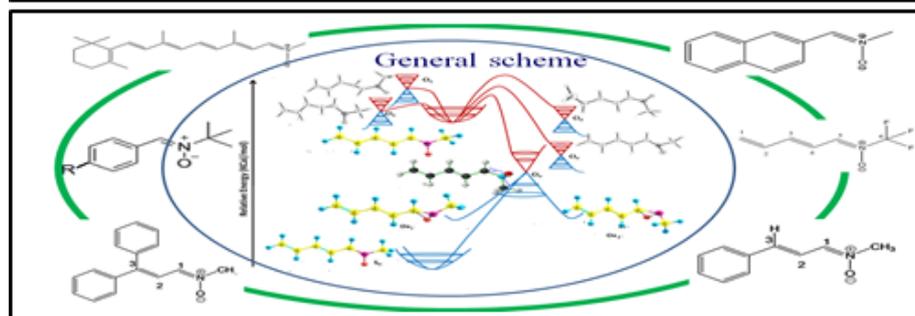
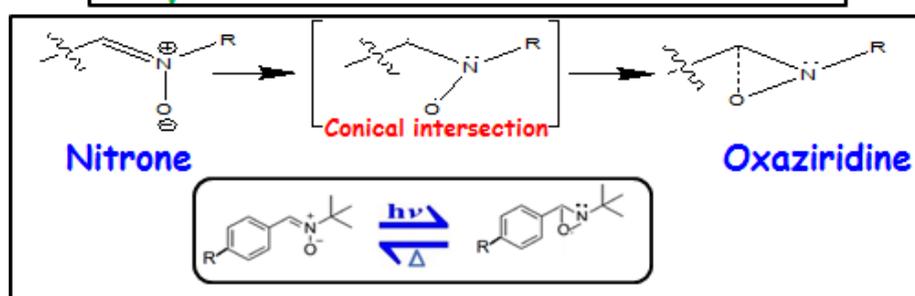


Computational Chemistry

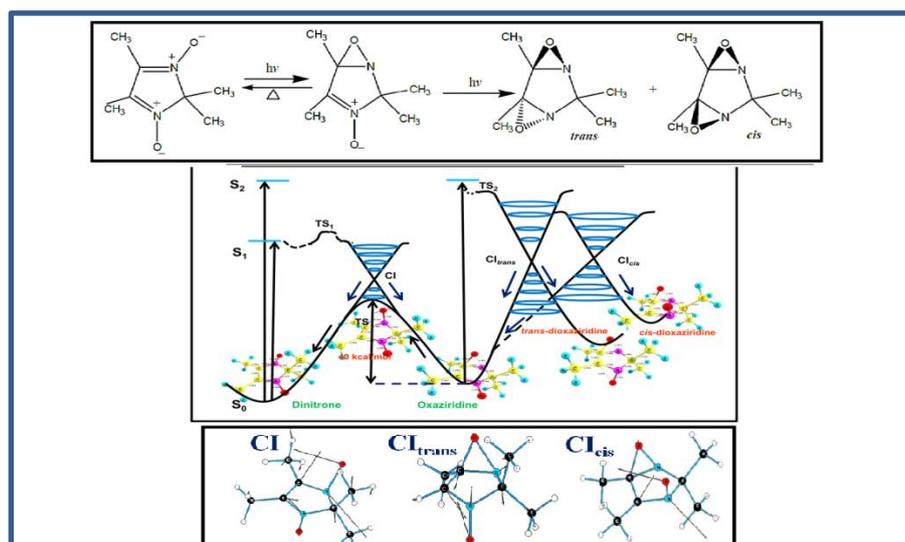
Ultrafast Photochemical Reactions (through Conical Intersections), Fluorescence & its quenching, Phosphorescence processes, ESPT, ESIPT, FRET, TICT, AIE, ISC, RISC, ROS

Nitron (Cyclic & Acyclic) Photochemistry

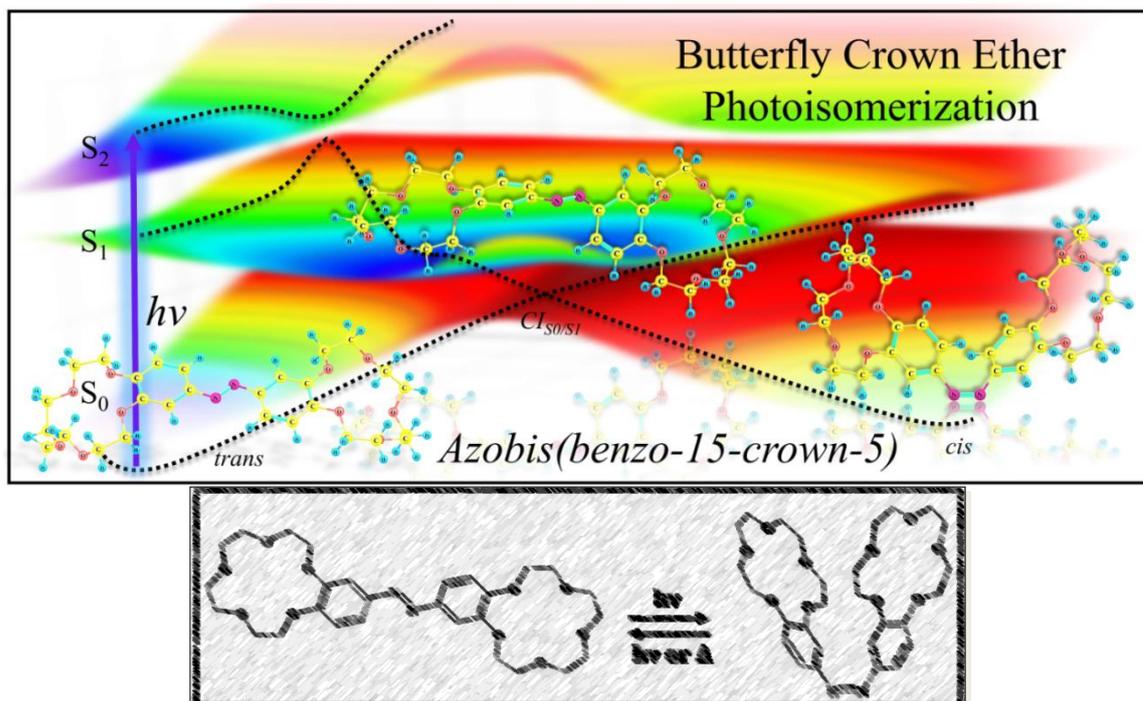
Acyclic Nitrones Photochemical Path



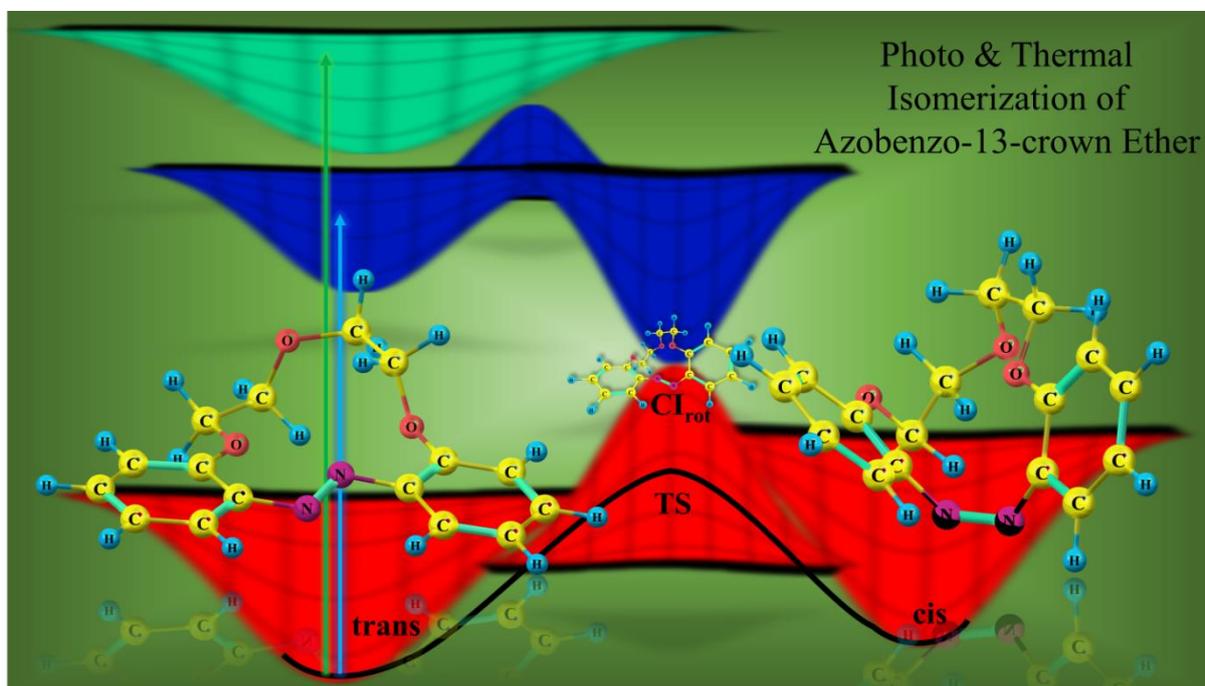
Cyclic Nitrones Photochemical Path



Butterfly Crown Photo-isomerization



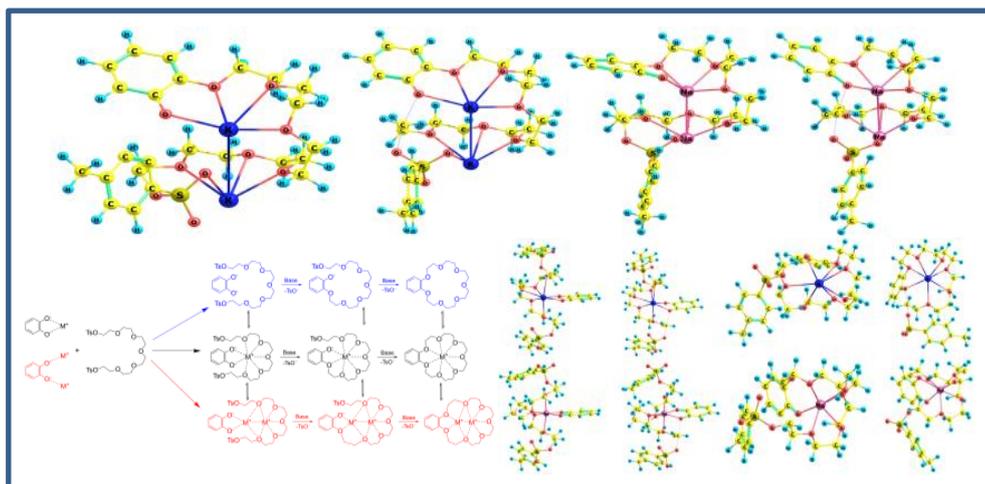
Strained Azo Crown Ether Photo-isomerization



Alkali metal ion Template Synthesis of Crown Ethers

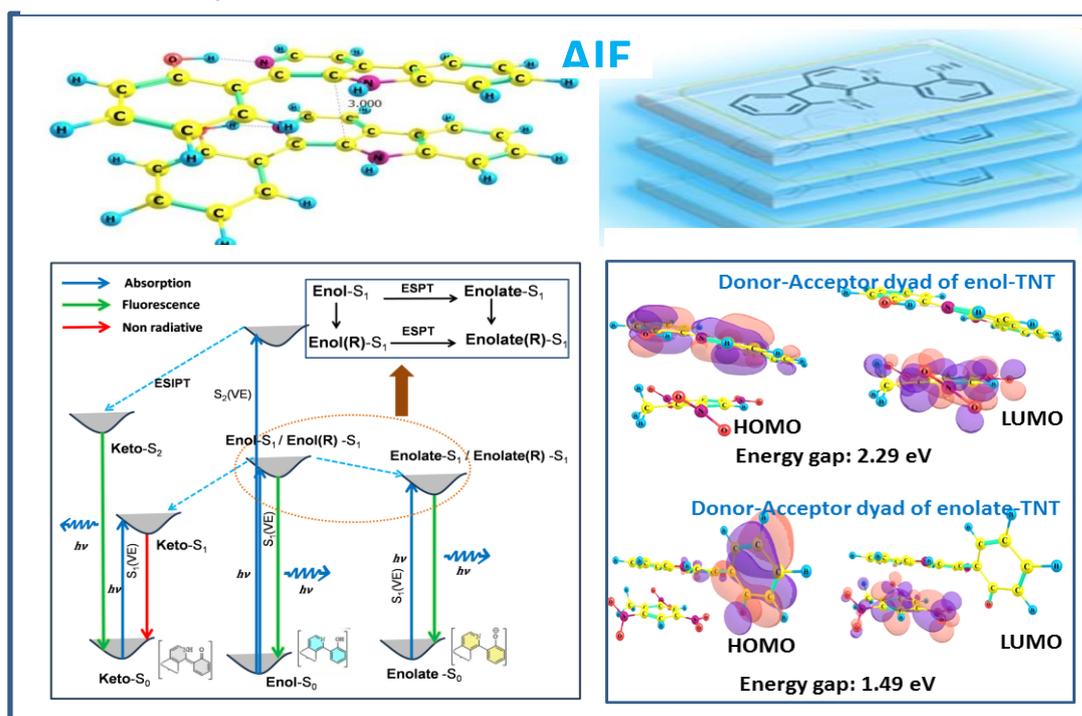
Template & Non-Template Synthesis Mechanisms of DB18C6 (Pedersen's Method)

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



Photophysical Processes, Reaction Mechanisms (In Collaboration with experimental groups)

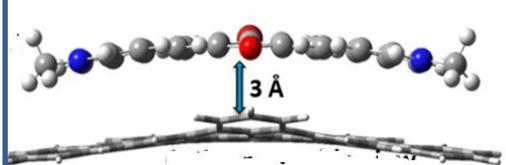
In collaboration with the experimental group of Prof. Anupam Bhattacharya (BITS-Pilani, Hyderabad)



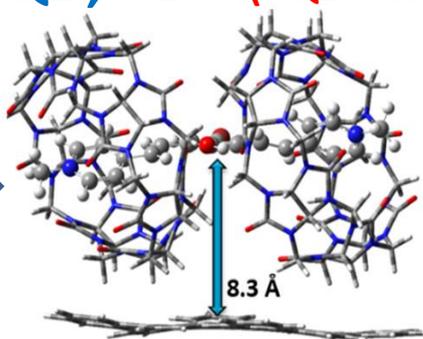
In collaboration with the experimental group of Prof. Mainak Banerjee (BITS-Pilani, Goa)

Donor-Acceptor Dye & GQD (GQD Fluorescence Quenched)

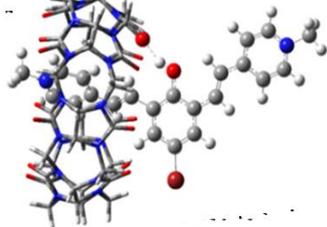
Donor-Acceptor Dye, GQD, CB-7 (GQD Fluorescence Back)



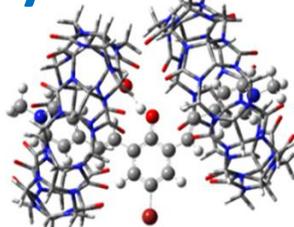
CB-7



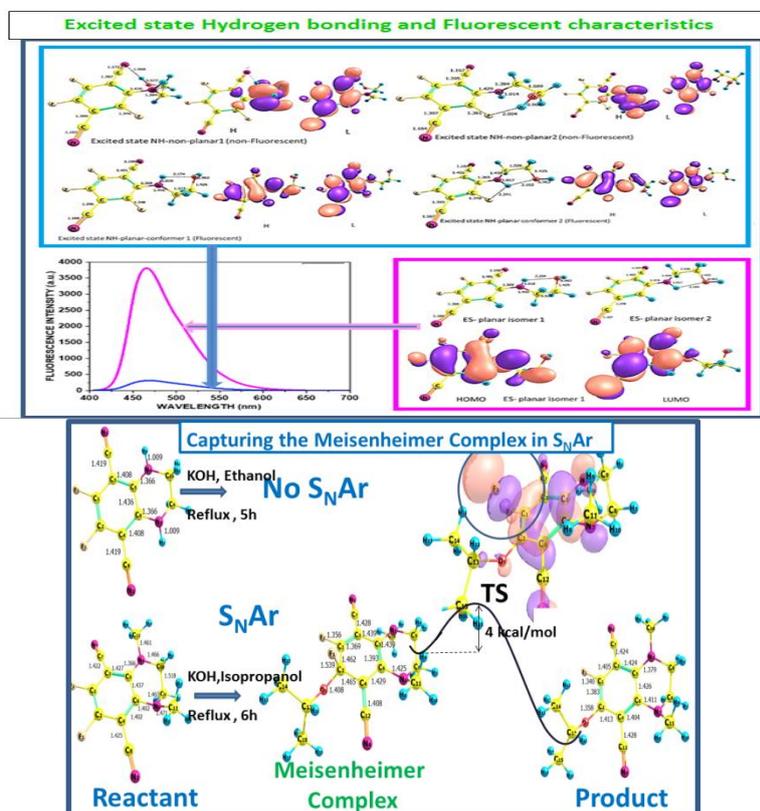
Dye : CB-7 → 1:1



Dye : CB-7 → 1:2



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 Exciplplex Laser systems

Ph.D Thesis guided (as Supervisor):

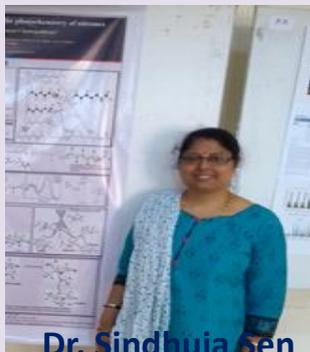
Dr. Praveen Saini (Year 2017)



Dr. Praveen Saini

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

Dr. Sindhuja Sen (Year 2020)



Dr. Sindhuja Sen

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