

Abstract

SOFT MOLECULAR MATERIALS FOR SENSING AND ACTUATION

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The thesis work titled "SOFT MOLECULAR MATERIALS FOR SENSING AND ACTUATION" focusses on developing soft molecular crystalline material that are mechanically responsive to light illumination. These materials are a class of smart materials that have exceptional ability to directly convert light energy into various types of mechanical response such as bending, shape change, jumping, cracking, volume expansion etc due to the photoinduced chemical transformation of the molecules in solid state. The molecular motion generated due to photoinduced reaction is amplified to macroscopic motion by cooperative mechanism which is manifested as actuation. The research work is divided in four chapters. First chapter includes literature survey on soft actuating materials.

In the second chapter, I have carried out the synthesis of a new green fluorescent organic compound (*E*-ArF₂) which display light controlled actuation and shape change in presence of 390 nm light. We have demonstrated that the direction of the motion of the solid crystals can be manipulated and steered by controlling the illumination direction.

In the third chapter, we reported the first example of two crystal solvatomorphs (solvates) of an anthracene-hydrazide based molecule (Ant) that display very distinct photo-responsive behaviour when 365 or 405 nm or visible light is illuminated. While one solvatomorph (**Ant-H₂O**) display an unique photo-puffing behaviour with large volume expansion that mimic the phenomenon of rice puffing (by heat treatment), the other solvatomorph (**Ant-DMF**) display photoinduced cracking, bending and jumping behaviour in presence of 405 nm light.

The last chapter discusses about the synthesis and distinct photo-responsive behaviour of two geometric isomers of a single molecule (NMe₂CNF₂) synthesis of a new green fluorescent organic compound (NMe₂CNF₂) by Knoevenagel condensation reaction. The single crystals of the *trans*- (*E*- NMe₂CNF₂) isomer display photo-actuation, and salient property in presence of 405 nm light, while the corresponding *cis*-isomer, *Z*-NMe₂CNF₂ is silent to light illumination. Our mechanistic investigation reveals that the distinct photo-response in solid state is rooted to their molecular configuration, packing and intermolecular interactions in solid state.

In summary, the work presented in my thesis demonstrate some novel photo-responsive systems that can perform direct energy transduction from light. These results have been published in various mainstream journals such as *Chemistry-A European Journal*, *Angew Chem. Int. Ed*, *CrystEngComm*, *Cryst Growth & Design* etc


SIGNATURE (with seal)
Dr. Manas Panda
Assistant Professor
Date Department of Chemistry
Jadavpur University
Kolkata - 700 032



(FULL SIGNATURE OF THE CANDIDATE)

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