EXPLORING MOLECULAR PROPERTIES OF AZOBENZENE-CONTAINING SYSTEMS USING COMPUTER MODELLING

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The incorporation of azobenzene-containing photosensitive compounds into macromolecular systems allows for the optical manipulation of the thin film morphology, the photoinduced motions at nanoscale and the photoactuation of various liquid-crystalline and biological macromolecules. Discovering the functional mechanisms of such light-induced phenomena frequently requires information that challenges the spatial and temporal resolution limits of current experimental techniques.

In this talk, I will present the perspective on the theoretical insights that a scientist might garner by complementing experiments with atomistic molecular dynamics simulations and quantum chemical calculations to capture the nanometer resolution behaviour of azobenzene (azo) system of interest.

To illustrate this perspective, I will consider the structural and optical characteristics of mono- and multiphotochromic azo systems used as photosensibilizers of polymeric films and brushes in the experiments conducted at the Department of Experimental Physics, University of Potsdam.

In the first example, several push-pull para-disubstituted azobenzenes will be considered for the investigation of the effects of functional groups on their optical properties. Other objects, namely azobenzene-containing cationic surfactants and polyamines having one azo fragment in their chemical structure represent convenient systems for the description of hydrophilicity/hydrophobicity of *trans*- and *cis*-isomers, as well for the validation of theoretical methods applied.

In the second example, the multiphotochromic azo star consisting of three azo units conjugated to a central benzene node serves as an object for the study of connectivity effects on the photochromic character of azobenzenes.

Finally, I will touch on the simulations of polymeric chains with ionically or covalently attached azo groups that exemplify the system where the coupling between the polymer backbone and the azo side chains comes into play.

At the end, I will consider the strengths and limitations of simulation methods and discuss the advances that such simulations may enable in the near future for the successful realization of the joint project with the Department of Experimental Physics, University of Potsdam.