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Highly-biased photoswitching in molecular systems: origin, control and applications

Description for the general public

A possibility of utilizing molecular systems as functional devices working at the nanoscale has, over recent decades, inspired great number of scientists for ground-breaking and cross-disciplinary studies. Nowadays, molecular devices comprise rich range of functionalities, including switches, rotors, rectifiers, motors, elementary logic gates and many more. Individual and supra-molecular systems are employed in studies on cutting-edge technologies, such as silicone-free electronics, molecular information storage, photoresponsive materials, sensitizers in super-resolution imaging techniques, and remotely-controllable drug delivery and release units. In 2016, the exciting advances in the field of molecular devices were acknowledged with the Nobel prize in Chemistry. Amidst functional molecular systems, molecular photoswitches play special role as they can act as gating units controlling other moieties and, thus, constitute core for more advanced devices.

The proposed project concentrates on a phenomenon of highly-biased molecular photoswitching – a special kind of switching, in which one observes a large difference in efficiency and rate of transformations in the opposite directions. Such feature may be rationally employed in development of existing, and design of novel molecular technologies. In our investigation, we focus on photoswitching molecules belonging to a family of diarylethene compounds (DAE), whose strongly-biased switching characteristics is widely acknowledged. Recently, it has been experimentally observed that application of multi-color irradiation pulses – instantaneous or in a controlled sequence – may significantly alter the resulting photoswitching efficiency of model DAE systems. At the same time, the mechanism lying behind this effect remains unknown.

Our goal is to explain the effect of highly-biased photoswitching observed in the DAE family and to identify possible means of control of the switching efficiency in these systems through application of multi-color light irradiation protocols. Successful realization of our project would, on the one hand, provide explanation for the recent experimental results and, on the other hand, the acquired knowledge would support development of molecular technologies, such as photostabilizers (molecules and materials protecting their environment from damage caused by external electromagnetic irradiation), molecular memory (molecular setups for information storage that can be fully manipulated with use of two light colors only), and novel super-resolution imaging techniques (based on nonlinear interaction effects between the switches and neighbor fluorescent molecules).

The intended scientific investigation has a theoretical character and is based on quantum-chemical calculations, aiming at characterization of the single-and multi-photon photoswitching mechanism of model DAE molecules. We will apply rich spectrum of modeling approaches, including static techniques (such as calculation of potential energy profiles of occuring photoreactions) and dynamics simulations (allowing for real-time study on the ongoing processes). We also plan to design and implement a new software tool for multi-photon nonadiabatic molecular dynamics simulations.

We envision several directions of our project's scientific impact. Firstly, we believe, that the new perspective over the molecular photoswitching we propose will support systematic efficiency improvement in existing cutting-edge applications and will open a way for novel molecular technologies development. Secondly, we aim to provide explanation for the observed experimentally complex photophysics of DAE systems. Another impact direction we expect our project to contribute to, is the systematic investigation on, up to now, only hardly studied, high-excited-state photochemistry of molecular photoswitches. This is direction will be further explored in the context of development and examination of possible advanced, multi-photon protocols for control of switching in DAE systems, which would also constitute a new contribution in the field rational molecular photoswitches design. Finally, the design and implementation of a unique software tool for multi-photon NAMD simulations will directly provide means for photochemical simulations, which are not possible at the moment.