

## Multiscale Modelling of the Photophysics of the Cyanobacteriochrome Protein Slr1393g3

Cyanobacteriochromes (CBCRs) are promising candidates for the use as photoswitches in biotechnological applications, owing to their photochromism, compactness and spectral diversity. In case of the CBCR Slr1393g3, one isomer absorbs red light ( $P_R$ ) and the other one green ( $P_G$ ). The two forms can be interconverted into each other by light illumination. Slr1393g3 binds phycocyanobilin as chromophore and the crystal structures of both forms have been obtained recently. In this talk, I will present results of hybrid QM/MM calculations of the  $P_R$  and  $P_G$  forms of Slr1393g3.

In order to understand the photophysical properties, thorough QM/MM studies starting from the crystal structures were performed. Firstly, the structures are optimized, followed by classical MD for thermalization and backbone relaxation. The snapshots for the excited state calculations are then generated via DFTB2+D/AMBER MD and the final spectrum is an average of the spectra from the different conformations of each form. The results of this approach are complemented by wave function analysis to obtain further insights into the spectral tuning on the molecular level.