

An exciting life of fluorescent proteins

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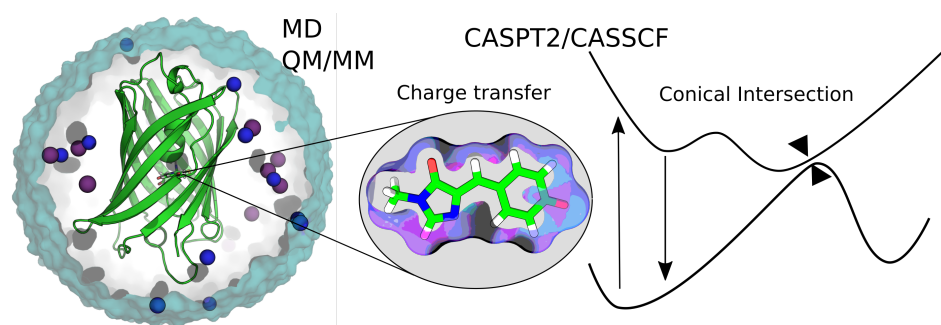
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Reversibly-switchable fluorescent proteins (RSFPs) are widely used in super-resolution microscopy. Fluorescence time decorrelation is used in order to break diffraction limit. In other words RSFPs should switch between fluorescent and non-fluorescent states on different timescales.

A rational approach to a study of an excited state reaction pathway is one of the key solution to understanding of their photo-switching mechanism. A set of five proteins based on Dronpa[1], one of the most commonly used RSFPs, was scrutinized in our study. Combination of MD simulations and QM/MM calculations was used to assess major reasons controlling the spectral tuning and photophysical properties of a consistent model set. On the basis of the RSFPs models, which are based on a CASPT2//CASSCF level of QM theory we reproduce an experimental absorption/emission trend. Then we show how protein environment controls chromophore's isomerization and spectral tuning. Furthermore, we identify how the conical intersection topography correlates with protein's photoswitching speed.



[1] Stiel et al, *Biochem. J.* **402**, 35 (2007)