Structural Dynamics of Isolated Biological and Synthetic Photoswitches

E. Tan

SUMMARY

Over the past few decades, molecular photoswitches, as building blocks in pharmaceutical applications and molecular machines have contributed largely to the advances in nanotechnology. Observations on how nature uses simple molecules to execute higher order tasks give the inspiration of this PhD thesis. Eric Tan Meng Meng studied the biological chromophores and synthetic molecules that work on the principle of converting absorbed light into biological and mechanical functions. High-resolution laser spectroscopy and molecular beam were used to study those molecules under isolated conditions with techniques like REMPI, double-resonant depletion and pump-probe delayed ionization. Experimental results on the structural and dynamics of the molecules are accompanied by quantum-chemical calculations to investigate the primary processes of the molecules upon absorption of light, thus elucidating its *modus operandi* at the molecular scale.

Studies on the photoactive yellow protein (PYP) chromophores have revealed important aspects of the intrinsic properties including the conformational heterogeneity, excited state dynamics, and important barrier and decay channels in the excited states. Additionally, studies on *trans*-azobenzene led to groundbreaking results including the first high-resolution spectra recorded for the $S_1(n\pi^*)$ and $S_2(\pi\pi^*)$ states of *trans*-azobenzene that uncover the dynamics and *trans*-*cis* photoisomerization mechanism. By performing studies on clusters of molecules with water, specifically a UV-B filter commonly used in sunscreen products, Eric found out that the addition of water increases the effectiveness of sunscreen. The studies provide a route to a better future for sunscreens.