ZERNIKE INSTITUTE COLLOQUIUM

Thursday, January 12th, 2012

16:00h, Lecture Hall: 5111.0080 **Coffee and cakes from 15:30h**

Spin-forbidden molecular excited-state processes

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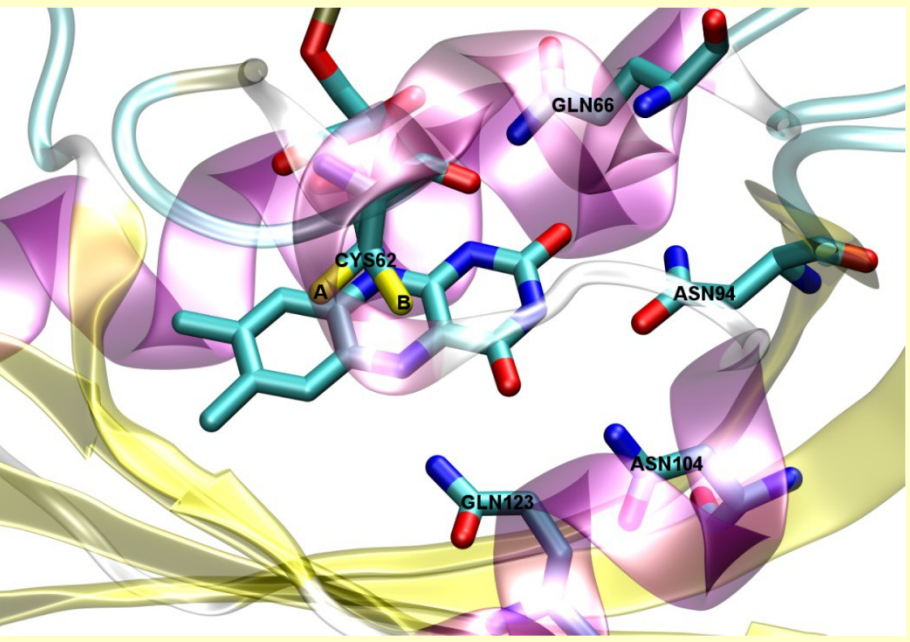
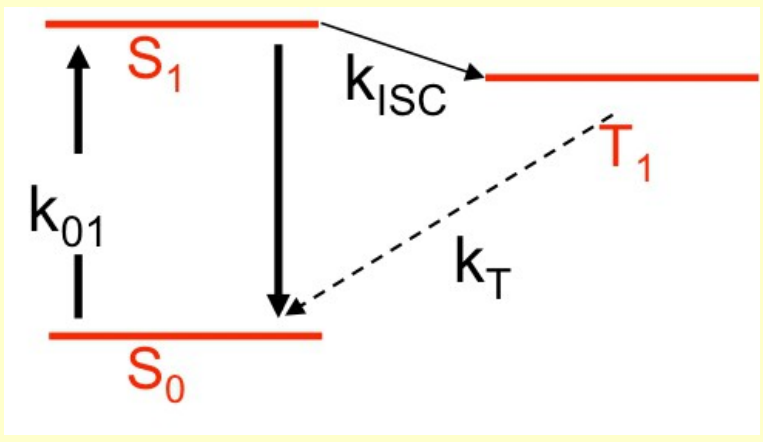
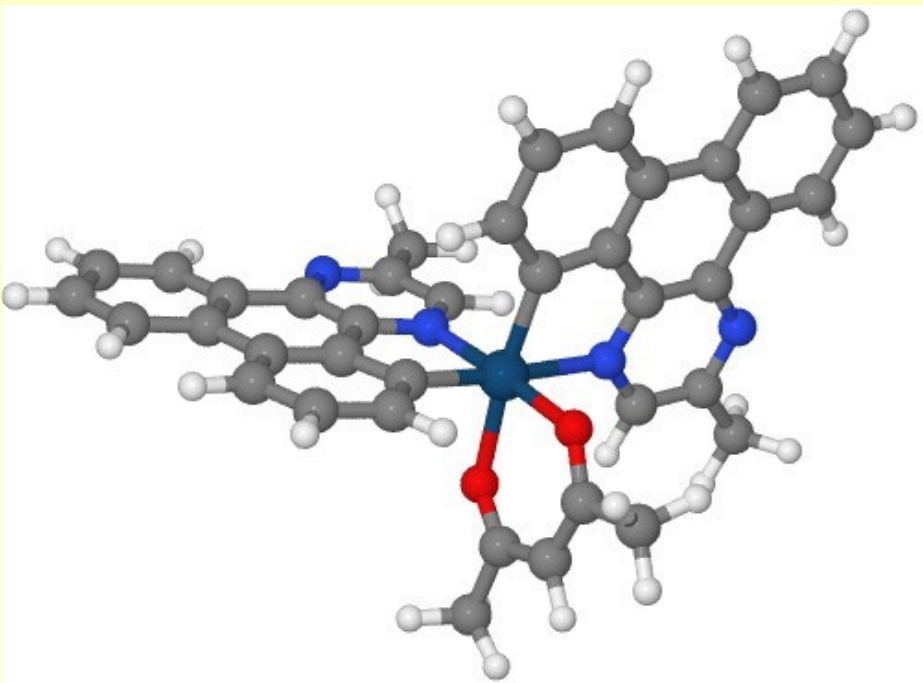
The rate at which radiative and radiationless excited-state processes occur is decisive for the functional properties of many chromophores. The importance of spin-forbidden transitions in photophysics, photochemistry, photobiology, and even medicine will be discussed addressing a few examples.



(i) Molecules with high triplet quantum yield and long triplet lifetime may serve as initiators of photochemical and transformations. In modeling these processes, environment effects have to be taken into account as they cannot only change the rates but also the mechanisms. A prominent example is the intersystem crossing of flavin in vacuum, aqueous solution, and in LOV domains of blue-light photoreceptors.



(ii) Molecules with efficiently deactivated triplets may function as triplet quenchers and can thus protect other substances from photodamage. For instance, in nature carotenoids have proven to possess outstanding photoprotective properties while short linear and cyclic polyenes increase the count rate of fluorescence dyes in single-molecule spectroscopy.



(iii) In organic light-emitting diodes (OLEDs) electric current is converted into visible light by means of phosphorescent emitters. The challenge for a computational treatment is to reliably predict the emission wavelength and phosphorescence lifetime and to give a realistic estimate of the triplet quantum yield. We have only recently started to study OLED dyes theoretically, but our first results are very promising.

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