

Theoretical studies of photoinitiated processes in biologically relevant molecules

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3:00 p.m. Room 8335



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The theoretical description of photophysical and photochemical processes in molecules is challenging, since it requires accurate description of excited states and their potential energy surfaces away from equilibrium. Nonadiabatic events are also essential for the description of photoinitiated processes. Great progress has been made in this field, and we can now use quantum mechanics to provide insight in photoinitiated processes in biological chromophores. This talk will present our contributions to studies of photoinitiated processes in nucleobases, the basic DNA chromophores. This work provides insight into DNA photostability and can also be useful in developing efficient fluorescent probes to be incorporated in DNA.