EXCITED STATES OF NON-ISOLATED CHROMOPHORES

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The photophysical and photochemical behavior of nucleobases is very important because of their biological role as the building blocks in DNA and RNA. Great progress has been made in understanding the excited-state properties of single bases. In order to understand the photophysical properties of nucleobases in complex environments we have investigated their excited states (a) in aqueous solutions and (b) as π-stacked dimers in DNA. The solvatochromic shifts of the excited states of pyrimidine nucleobases in aqueous solution have been investigated using a combined QM/MM procedure where the quantum mechanical solute is described using high level multireference configuration interaction methods while molecular dynamics simulations are used to obtain the structure of the solvent around the solute in an average way. The excited states of π-stacked nucleobases have also been investigated using various ab initio methods. The effect of the environment on the excited states and conical intersections is investigated.