TDDFT CALCULATIONS OF TRANSIENT IR SPECTRA OF DNA

RYAN M. RICHARD, JOHN M. HERBERT, *Department of Chemistry, The Ohio State University, Columbus, OH 43210.*

Establishment of ultraviolet radiation's role in DNA mutation has led to an increasing interest in understanding the electronic excited state dynamics of DNA. It is known that upon excitation of the ground state, the DNA bases are excited to an optically bright $\pi\pi^*$ state that then quickly decays back to the ground state; however, further investigations have shown that there are long-lived states within the excited state manifolds, which may be able to influence the excited state dynamics. The goal of our study is to calculate, with the aid of time-dependent density functional theory, several transient infrared spectra of double stranded and single stranded DNA in both gas phase and in solution, in order to help sort out the exact role of these states in the relaxation processes of DNA by comparison to available experimental data.