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On the internal photorelaxation mechanism of DNA ERIC BITTNER, University of Houston — We propose a model for the photo-deactivation mechanism for DNA based upon accurate quantum chemical and molecular dynamical evaluations of model Watson/Crick nucleoside pairs and stacked pairs. Our results corroborate recent ultrafast experimental studies on DNA oligonucleotides and suggest that following photo-excitation to a local $\pi - \pi^*$ state, the excitation is rapidly delocalized over several (3-4) bases on an ultrafast time-scale. However, this delocalized state is unstable with respect to the motions of the protons involved in hydrogen-bonding between Watson/Crick pairs and rapidly re-localizes to a charge-transfer state on a longer time-scale ranging from 10 to 100 ps. This state, too, is unstable and relaxes via a conical intersection with the ground state near the geometry of the enol- and imino-tautomeric form. We suggest that this internal deactivation mechanism is responsible for the intrinsic photostability of DNA.

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