

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Excited State Dynamics of DNA and RNA bases¹ HANNELI HUDOCK, University of Illinois at Urbana-Champaign, Dept of Chemistry, BENJAMIN LEVINE, University of Illinois at Urbana-Champaign, Dept of Chemistry, TODD MARTINEZ, University of Illinois at Urbana-Champaign, Dept of Chemistry — Recent ultrafast spectroscopic experiments have reported excited state lifetimes for DNA and RNA bases and assigned these lifetimes to various electronic states. We have used theoretical and simulation methods to describe the excited state dynamics of these bases in an effort to provide a mechanistic explanation for the observed lifetimes. Our simulations are based on ab initio molecular dynamics, where the electronic and nuclear Schrodinger equations are solved simultaneously. The results are further verified by comparison to high-level ab initio electronic structure methods, including dynamic electron correlation effects through multireference perturbation theory, at important points along the dynamical pathways. Our results provide an explanation of the photochemical mechanism leading to nonradiative decay of the electronic excited states and some suggestions as to the origin of the different lifetimes. Comparisons between pyrimidines illustrate how chemical differences impact excited state dynamics and may play a role in explaining the propensity for dimer formation in thymine.

¹HH gratefully acknowledges the NIH Molecular Biophysics Training Grant at UIUC

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Date submitted: 20 Nov 2006

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