

Abstract Submitted
for the TSF05 Meeting of
The American Physical Society

Electronic structure and dynamics of microhydrated DNA base clusters VALORIS SMITH, University of Texas at Austin, ELENA SAMOYLOVA, THOMAS SCHULTZ, HANS-HERMANN RITZE, I.V. HERTEL, Max Born Institute, Berlin — DNA and DNA bases emerged before the ozone layer was formed and therefore must have inherent properties protecting them upon irradiation with UV rays. These mechanisms might be ultrafast relaxation to the ground state via conical intersections or internal vibrational relaxation. Using gas-phase, femtosecond pump-probe methods, we try to determine which relaxation pathways are energetically favorable after excitation by a UV pump pulse. We also study the impact of microsolvation on the dynamics and electronic state character to bridge the gap between ab initio theory and biologically relevant liquid phase experiments.

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Date submitted: 15 Sep 2005

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