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Thermal Fluctuations and Excitonic Interactions in Polyadenosine JOHN JEAN, Regis University — Interest in the electronic structure and photophysics of DNA has been sparked in recent years by increased awareness of the biological effects of non-ionizing UV radiation as well as the possibility of using short DNA oligomers as molecular conduits for efficient charge or energy transport in nanoscale devices. The optical properties of DNA in the near UV region are governed by dipole-allowed transitions localized on the aromatic bases, which have excited state lifetimes on the order of a few hundred femtoseconds. Recent time-resolved experiments on polyadenosine oligomers, however, provide clear evidence for stacking-induced long-lived, stacking-induced states and spectral shifts compared to those of the monomer bases. The origin of these states and their relation to stacking dynamics is still largely unknown. DNA is a highly dynamic structure undergoing large-amplitude structural fluctuations on timescales spanning many orders of magnitude and spatial correlation lengths, thus characterization of the excitonic states requires understanding how nearest-neighbor Coulombic and exchange interactions couple to picosecond motions of the bases. In this paper, we present results from hybrid QM/MD simulations of polyadenosine in solution that provide detailed insight into the time-dependent stacking interactions in these systems and the effects of dynamic disorder on the temporal and spatial properties of the low-lying excitons.

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