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Thermal Disorder Effect on the DNA Electronic Structure

ALEXANDER BALAEFF, Duke University, ELIZABETH HATCHER, University of Maryland, Baltimore, SHAHAR KEINAN, RAVINDRA VENKATRAMANI, DAVID BERATAN, Duke University — We address the effect of the thermal dynamics of DNA structure on the energy and localization of the DNA electronic orbitals. Structural ensembles are generated for several DNA sequences by molecular dynamics simulations employing CHARMM and AMBER force fields. In the shortest sequences studied (CATG, GAAG, GATG, GAG), the highest occupied molecular orbitals (HOMOs) expectedly reside on the guanines (Gs), yet in a significant number of the structures the orbitals are observed to be delocalized between the Gs and the bridging adenines (As). Adding more Gs to the ends of the sequence expectedly shifts the orbitals toward the G clusters, yet the amount of orbital delocalization to the bridge is still significant. These observations suggest that a) contrary to the predominant view in the field, G-to-A thermal hopping may contribute significantly to the charge transfer in DNA even in the short-distance range, and b) the contribution of DNA structural fluctuations to triggering the charge transfer is as significant as that resulting from the ion gating mechanism.

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