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Hole Transfer in Hydrated DNA Driven by Spatial Correlated Solvent Fluctuations

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We use a combination of computational approaches to address the transport properties of an electron hole in hydrated DNA. Molecular dynamics simulations are employed to study at the base level the nature and the strength of the solvent-induced electrostatic fluctuations. A hybrid first-principles/molecular-mechanics scheme designed for periodic calculations of biological systems is then used to determine the hole energy at DNA bases embedded in hydrated DNA chains. Thus, the combined effect of solvent fluctuations and sequence on energetics and transfer characteristics is addressed through the use of 1-D lattice models. In this study, we find that stacking and hydration introduce at each base normal energy deviations correlated in both space and time. Solvent-induced energy disorder yields localized hole states and supplies the driving force for transfer processes over distances exceeding the correlation length. Sequence, on the other hand, is found to determine the transfer rate across short DNA traits. Our investigation shows that correlated solvent fluctuations and sequence compete evenly to define hole energetics and transfer character in hydrated DNA.