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First-principles studies of conformation and solution effects on DNA transport BIKAN TAN, MIROSLAV HODAK, WENCHANG LU, JERRY BERNHOLC, North Carolina State University — The electrical conductivity of DNA molecules is of fundamental interest in the life sciences. We use first-principles techniques combined with molecular dynamical (MD) simulations to calculate transport properties of B-DNA connected to carbon nanotubes via alkane linkers. The quantum transport properties are calculated for over a hundred of snapshots recorded in MD trajectories. We discover that the DNA conformation and especially the overlaps between sequential guanine bases play a critical role in electron transport. DNA charge transport is indeed governed by charge delocalization with wavefunctions extent controlled by geometrical overlaps. Solvent atoms also affect the conductivity, with counterions decreasing the conductance by a factor of 2-3. In addition, we find that water molecules around the double helix screen the negatively-charged phosphate groups suppressing the conductance of DNA. Comparing transport properties of 4-base-pair (BP) with 10-BP DNA, we find weak distance dependence of the conductivity. Finally, we discuss the effect of sequence on DNA conductivity.

Bikan Tan
North Carolina State University

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