FROM ENERGETIC CONTROL TO THERMALLY INDUCED HOPPING

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Abstract

Molecular wires constitute nanostructures whose spatial configuration, energetics, nuclear and electron dynamics promote long-range charge transport. DNA-based molecular electronics devices are expected to utilize the unique features of recognition, assembly and specific binding properties of nucleobases, with the DNA duplexes serving as building blocks or templates for the assembly and function of electronically active nanoelements. Neat, undoped DNA constitutes a 'vibronic molecular wire', where charge hopping between localized states prevails. The charge hopping mechanism in DNA is described in terms of the quantum mechanical nonadiabatic electron transfer theory, with the ingredients of electronic (direct exchange or superexchange) coupling, and nuclear coupling with low-frequency intermolecular and medium modes, together with high-frequency modes. Individual hole hopping processes, based on the concept of energetic control, involve unistep superexchange mediated hopping and thermally induced hopping, which provide the conceptual framework for bridge specificity of very long-range hole transport in DNA on the basis of our 'molecular polaron' model.

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