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School on
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COHERENT ENERGY AND CHARGE TRANSPORT IN MOLECULAR SYSTEMS

1. Vibrational, Electronic and Excitonic Coherence

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Abstract:

In the first lecture, an introduction is given to quantum dynamical phenomena in molecular systems, including polyatomic molecules, molecule-solvent complexes, and molecular assemblies (polymers, DNA, light-harvesting systems) which reach into the nanoscale domain. Some focus is placed on photoinduced processes which are often ultrafast due to the presence of non-adiabatic (non-Born- Oppenheimer) effects. These processes typically evolve in a non-Markovian regime where the environment - e.g., the solvent - is neither static nor rapidly fluctuating. Quantum coherence plays an important role and can be surprisingly long-lived, in contrast to the conventional assumption that decoherence necessarily sets in within tens of femtoseconds. Against this background, the lecture presents typical classes of model Hamiltonians describing vibrational, electronic, and excitonic transfer phenomena, along with approaches to their dynamical treatment using wavefunction and density matrix propagation and/or reduced dynamics approaches.