Simple Models for Complex Molecular Materials

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I will introduce some key concepts and approaches associated with modelling and understanding quantum dynamical processes in complex molecular materials, such as biomolecules. The following topics will be covered.
1. Examples of functional materials: optically active biomolecules, organic light emitting diodes and solar cells, enzymes, …
2. Examples of dynamical processes: charge separation, proton transfer, exciton transport, …
3. Partition of the system: discrete quantum system + environment (solvent or protein)
4. Form of Model Hamiltonians
5. Example: spin-boson model
6. Diabatic states and potential energy surfaces
7. Outstanding questions: quantum decoherence, sequential vs. co-operative processes, breakdown of Born-Oppenheimer approximation, ...
This provides background and motivation for understanding some of my work [1-3].

I will also describe my work on a simple model for the effect of quantum nuclear motion on hydrogen bonding in complex molecular materials. Most of chemistry can be understood by treating the atoms in molecules as classical particles. Quantum zero-point motion and tunnelling do not play an essential role. An exception is molecules involving hydrogen bonding, including water [4], proton sponges, and some biomolecules [5]. Quantum nuclear effects are revealed by isotope substitution experiments where hydrogen is replaced by deuterium. A simple model, based on two diabatic states, gives potential energy surfaces that can be used to calculate the quantum vibrational states of the shared proton/deuterium. The model gives a quantitative description of experimental data for bond lengths, vibrational frequencies, infra-red absorption intensities, and isotope effects for a diverse range of chemical compounds [2], including photoactive biomolecules [5]. The model can be extended to double proton transfer [3].

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