Charge motion in bio-organic nanowires

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Abstract

We study nanowires. Their length is of the order of nm. Their width varies. We examine from atom-thick wires like cumulenic and polyynic carbynes (linear atom-thick carbon sequences ending at one or two or three hydrogens and cyclic carbynes that do not have hydrogens), dicyanopolyynes (linear atom-thick nitrogen, carbons, nitrogen sequences), small molecules, and so on, up to DNA sequences (which have a width of approximately 2 nm). We are interested in electronic structure, charge transfer and transport, optical properties etc. We use methods based on tight binding (TB) and methods based on density functional theory (DFT). In particular, the TB models that we use extend from coarse-grained models up to atomic-level models with many orbitals at each atom. All have advantages and disadvantages. Exempli gratia, concerning charge transfer, RT-TDDFT (real-time time-dependent DFT) is particularly time-consuming, so TB-based techniques have great usefulness. We study mainly coherent processes that dominate at short distances and low temperatures, but the study of thermal, incoherent processes is also possible with TB-based methods.