

Molecular electronics: a computational approach

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Molecular electronics has been an important area of research for the last few decades. It consists of using single molecules as the active units of devices. Due to the continuous presence of a organic/inorganic interface, this area overlaps with another intensive area of research, namely, surface science. From the theoretical point of view, important developments have been made in order to better understand molecular break junction experiments, light-induced effects and electron transport properties of molecular junctions. In this talk, we give a overview of how we perform computational simulations of electronic devices such as molecular junctions, organic photovoltaics as well as how we deal with the important problem of energy level alignment of the organic/inorganic interfaces. We present a combination of *ab-initio* approaches based on density functional theory (DFT), non-equilibrium Green's Function formalism (NEGF) and also model Hamiltonians. We further compare our electron transport calculations results with experimental measurements for the long-standing problem of Au-benzene-dithiol molecular junctions.

References:

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