

Quantum master equation for the study of electronic transport in organic systems.

Pedro David Manrique Charry
TU Dresden/ Material sciences
Dresden (Germany)

We calculate a non Markovian master equation for electronic transport through organic systems including the interaction of external bosonic degrees of freedom. Within this formalism we calculate the expression for the time dependent current (TDC) as the variation of the particle number of the electrodes (fermionic baths) at arbitrary temperatures. Some partial results for the TDC are shown for different values of boson coupling, in which we found significant changes at very short time evolution. In addition, for organic systems we calculate the total energy for different geometric configuration using density functional tight binding (DFTB) including the dispersion energy correction and contrasted the results with MP2 methods finding a very good agreement.