Transport In Molecules And Nanowires From Density Functional Theory

Mads Brandbyge

Dept. of Micro and Nanotechnology (MIC)
Technical University of Denmark (DTU) build. 345, 2800 Kgs. Lyngby, Denmark
mbr@mic.dtu.dk

I will present our recent results of transport calculations on molecular and nanowire systems. Our approach use density functional theory (DFT) and non-equilibrium Greens functions (NEGF) [1]. We can treat the electron-phonon interaction using the self-consistent Born approximation (SCBA). However, recently we have shown how the rather demanding DFT-NEGF-SCBA accurately can be approximated by an efficient lowest order expansion (LOE) [2].

I will discuss three topics where we employ our method: (i) electron-phonon transport signals in molecular systems comparing our results of the inelastic electron tunnel spectra (IETS) with experimental data [3], (ii) preliminary results on transport in magnetic organometallic molecules [4], and finally (iii) recursive Greens function calculations of the mean-free path and localization length in Silicon nanowire systems [5]. In the latter case we compare the results with the Kubo-wavepacket approach of Roche [6].

References:

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