Quantum Transport In Post-CMOS Molecular Materials & Devices : Carbon Nanotubes & Semiconducting Nanowires

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ABSTRACT:

The downsizing limits of conventional CMOS technologies are requiring the development of advanced computational schemes and methodologies to support material and device engineering strategies. Bottom-up driven PostCMOS-molecular based nanodevices are envisioned as potential alternatives to circumvent CMOS limitations, including device performances, innovative architectures and enhanced functionalities (interconnects, molecular memories, bio-sensing capability, NEMS, etc..). Carbon nanotubes and semiconducting nanowires offer unique low-dimensional materials for improved quantum transport (including charge, spin, phonon and excitons), whose precise scaling properties need however to be ascertained, to allow these material to develop future mainstream technologies. Indeed, despite their spectacular physical properties, a large number of issues remain to be solved to clarify the intrinsic roadmap of POST-CMOS molecular nanodevices.

In this talk, I will discuss several topics concerning quantum transport in disordered carbon nanotubes or semiconducting nanowires, outlining novel properties and current directions of challenges. A hybrid methodology combining state of the art ab-initio calculations to sophisticated effective tight-binding models will be presented, and shown to able tackling with quantum transport in complex (doped, functionalized) systems (Kubo-Greenwood and Landauer-Büttiker frameworks) up to the mesoscopic scale (few microns). First chemically doped carbon nanotubes will be investigated with a characterization of basic scaling laws of elastic mean free paths and localization lengths in the coherent regime. The effect of surface roughness will be also addressed in silicon semiconducting nanowires.

In a second part we will discuss the effect of electron-phonon coupling on quantum transport considering low energy acoustic and weak localization regimes as well as high energy optic modes and current saturation in the high bias voltage regime.

Finally, some novel methodology to tackle with large complexity of carbon nanotubes based field effect transistors will be mentioned and first result presented.



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