Atomistic treatment of nanotube-metal interfaces

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As silicon-based devices progressively move down towards atomistic dimensions, there is a lot of interest in assessing post-CMOS devices of the quantum wire and quantum dot flavor. Near-ballistic transport and unusually high mobilities have been reported in silicon nanowire and carbon nanotube devices. Under these conditions, transport is dominated mainly by the contact-device interface, making a thorough understanding of these interfaces essential. For carbon nanotube FETs in particular, experiments have typically demonstrated Schottky-barrier type behavior, although more recently ohmic contacts have been reported with palladium contacts. It is thus essential to develop an atomistic understanding of the nature of nanotube-metal contacts.

Understanding transport through nanotube-metal interfaces requires a combination of expertise belonging to different domains of research. One needs electronic structure calculations that do justice to the individual tube and metal bandstructures, surface physics calculations that describe the geometry and surface states of the relaxed metal-nanotube interfaces, quantum chemical codes that describe the bonding between the tube and metal atoms, electrostatic codes that describe charge and potential rearrangement driven by the workfunction difference between the tube and the metal, and quantum transport calculations that describe non-equilibrium transport through the interface under bias. In this article, we discuss how we can combine insights and techniques from these disparate disciplines into one unified formalism to generate an atomistic code for studying nanotube-metal interfaces. Such a natural partitioning is offered by the non-equilibrium Green's function (NEGF) treatment of transport where we model the device bandstructure within a suitable Hamiltonian, the self-consistent electrostatic potential separately using Poisson's equation, and the contact-induced shifting and broadening of the tube levels using self-energy matrices.

We adopt an unconventional treatment of nanotube-metal interfaces that might be more appropriate to its atomistic study. We adopt the chemists' viewpoint of atomistic structure, suitable for understanding charge transfer and bonding, and integrate it into our Poisson-NEGF treatment of transport. Specifically, we choose Extended-Huckel Theory (EHT) to describe atomistic properties of the tube and the metal. In contrast to tight-binding theories more familiar to device theorists, EHT has explicit basis sets, allowing us to formally mix and match entirely different theoretical descriptions developed in different domains, such as a physicist's basis set for bandstructure and a chemist's basis set for bonding, for instance. In the past, EHT has been successfully used to model both bandstructure and chemical properties using just a few fitting parameters, possible due to the non-orthogonality of its basis sets that describes chemistry through its overlap matrix. Furthermore, we have used it to describe surface states and reconstruction of open surfaces such as silicon substrates. We will show some of the results of our atomistic bandstructure simulations for metal contacts and nanotube devices using EHT. In addition to the bandstructure, the self-consistent potential profile is an important ingredient in determining the overall device properties. We use the complete-neglect of differential overlap (CNDO) approximation to solve the integral form of Poisson's equation in the non-orthogonal EHT basis. Finally, we show preliminary results obtained using these techniques.

A full journal publication of this work will be published in the Journal of Computational Electronics.

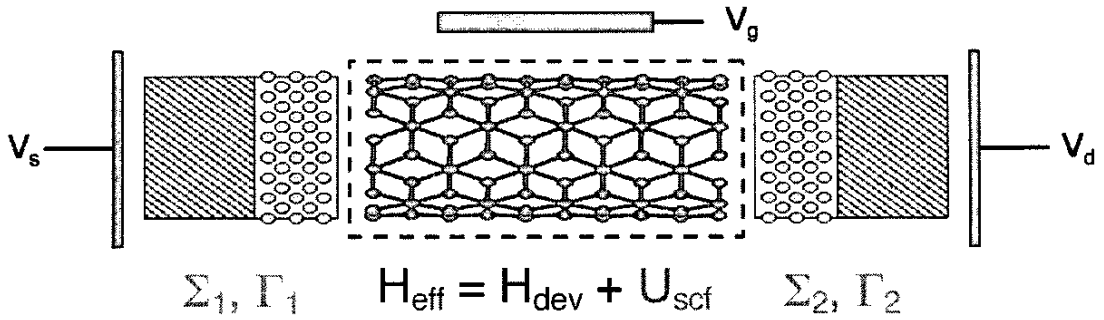

Figure 1: Sketch of a typical 3D-device geometry for a CNT connected to its left and right to metallic contacts, e,g. Gold in [111]-orientation. On top is the gate which is isolated from the tube. The effective device Hamiltonian consist of the Hamiltonian of the isolated device and the self-consistent calculated potential (Laplace + Poisson potential) complemented by energy-dependent contact self-energies $\Sigma_{1/2}(E)$. The self-energies account for the interaction of the device with its environment and are equivalent to boundary conditions for the device Green's function. The matrices $\Gamma_{1/2} = i(\Sigma_{1/2}-\Sigma_{1/2}^{+})$ cause a broadening of the deice levels due to the device-contact coupling. In general, the individual parts of the entire system (contacts, device, interface region) can be represented in different models, e.g. device in EHT, contacts in effective-mass theory, and the interface region in DFT, if necessary.

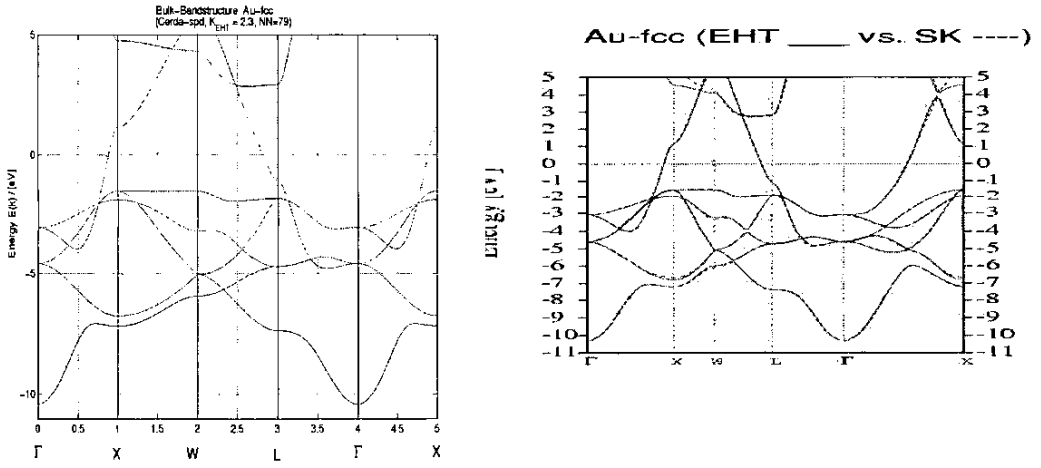

Figure 2: Calculated bandstructure for Gold. The left part shows the dispersion-relation E(k) for Gold modeled in Extended-Hueckel Theory, whereas the right part shows E(k) obtained from a ab-initio calculation using the DFT-package SIESTA as done by Cerda et.al..

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