The use of atomic-chain scaled Si nanowires to detect molecules

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Abstract - Inspired by the work of Lieber et al. [1], we present a general discussion of the possibility of using atomic-chain scaled Si nanowires to detect molecules. Surface-modified Si nanowires (NWs) were optimized by density functional theory (DFT) calculations. The electronic transport properties of the whole system, including Si NWs and adsorbed molecules, sandwiched between two gold electrodes are investigated by means of non-equilibrium Green's function (NEGF) formalism. However, the overall transport properties, including current-voltage (*I-V*) and conductance-voltage (*G-V*) characteristics hardly show adsorbate sensitivity. Interestingly, our results show that the conductance gap clearly varies with the different adsorbates. Therefore different molecules can cause differences in the conductance gap compared with the bare Si NWs. The results provide valuable information regarding the development of atomic-chain scaled molecular detectors.

Semiconductor NWs are emerging as a powerful and general class of ultrasensitive, electrical sensors for the direct detection of biological and chemical species [1]. The similarity in size of the NWs and biological and chemical species being sensed makes NWs an obvious choice for creating highly sensitive tools that can probe nanometer-sized systems. Semiconductor NWs, moreover, exhibit unique electrical and optical properties that can be exploited for sensing. These characteristics make semiconductor NWs one of the best defined and most versatile nanomaterial systems available today [2].

Lieber *et al*. [1] discussed representative examples of NWs nanosensors for ultrasensitive detection of proteins and individual virus particles as well as recording, stimulation, and inhibition of neuronal signals in NWs-neuron hybrid structures. The concepts underlying these experiments is as follows: When a single particle binds to a receptor linked to the surface of a NWs FET detector, it yields a conductance change due to the change in surface charge; when the particle subsequently unbinds, the conductance returns to baseline.

In this work, we tried to use the same method to detect molecules using ultra-thin Si NWs. The optimized Si NWs and Si NWs adsorbed different molecules or atom (H_2, H_2O, O_2 and Fe) have been obtained by DFT calculations (Figure 1). We also investigated the electronic transport properties of silicon NWs without and with adsorbate molecules using non-equilibrium Green's function (NEGF) formalism. Because of the presence of the adsorbate molecules, all of the electronic transport properties of the NWs are in principle different. However it becomes difficult to identify molecules from the overview of G-V curves. Interestingly, the conductance gap shows clear change in response to different adsorbates (Figure 2). So we suggest that Si NWs can be used as nanosensors for molecular detection by measuring the change of conductance gap.

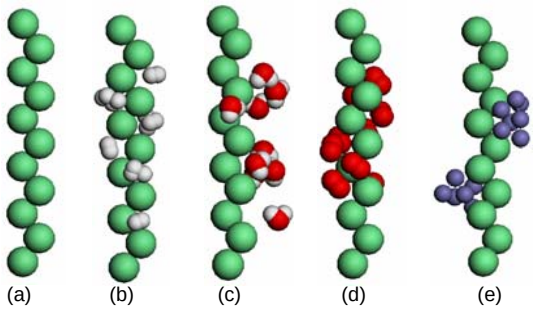

Figure 1. (a)Snapshots of Si_{11} chain, (b) Si_{11}&$9H_2$ (c) Si_{11}&$9H_2O$ (d) Si_{11}&$9O_2$ (e) Si_{11}&13Fe obtained from our calculations.

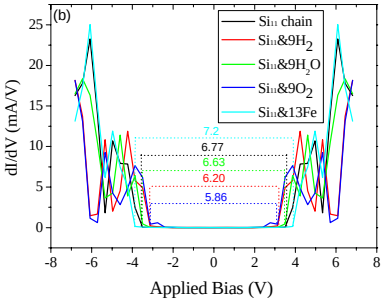

Figure 2. Conductance spectra of Si_{11} chain, Si_{11}&$9H_2$, Si_{11}&$9H_2O$, Si_{11}&$9O_2$ and Si_{11}&13Fe.

1. F. Patolsky, B.P. Timko, G. Zheng and C.M. Lieber, MRS Bull **32**, 142 (2007).
2. F. Patolsky and C.M. Lieber, Materials Today **8**, 20-28 (2005).