Molecular doping in Silicon Nanowires: an ab-initio study

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We present *ab-initio* calculations based on density functional theory (DFT) of the effects on the electronic bands structure, total and projected density of states of surface molecular adsorption onto hexagonal cross-section silicon nanowires (SiNWs) grown along the ⟨111⟩ direction.

Continuous miniaturization of microelectronic devices requires a corresponding reduction in feature size, and low-dimensional materials have become one of the most active research topics in recent years. In particular, SiNWs have attracted much attention due to their compatibility with conventional silicon-based integrated circuit technology allowing potential applications as building blocks in a variety of nano-scale devices such as field-effect transistors (FETs) [1], sensors [2], etc. Thus, advances in doping techniques are required that will allow the introduction of controlled amounts of dopants into nanowires (NWs) without degrading their electronic properties or morphology. Electrical doping for Si NWs has been achieved primarily through *in situ* doping, with the dopant introduced in the gaseous phase for incorporation during vapor-liquid-solid (VLS) growth, with metallic nanoparticles such as Au used as the catalytic growth seeds [3]. However, this in situ approach does not always give favorable results [4]. Enhanced surface doping during growth, for instance, competes with dopant introduction at the liquid-solid growth interface and can cause non-uniform doping along the NW length, with higher doping closer to the NW base. Electrical doping of NWs by *ex situ* techniques separates the doping step from the NW growth process and thus does not lead to sidewall-enhanced dopant variations along the NWs or changes in NW morphology [5]. *Ex situ* doping in a batch process also potentially allows for more uniform and controlled dopant concentrations over a large NW array, with the added possibility of spatial selectivity.

On the other hand, Fernández-Serra *et al.* [6] showed that in passivated NWs as large as few nanometers in diameter, a large proportion of dopants will be trapped and electrically neutralized at surface dangling bond defects, significantly reducing the carrier density. This inconvenience is shared by both conventional *in-situ* and *ex-situ* approaches. Here we explore the possibility of obtaining molecular doping of Si NWs. We show that a molecular-based *ex-situ* doping, where molecules are adsorbed at the sidewall of the NW, can be an alternative path to doping. We discuss the cases of both donors and acceptors.

We present some preliminary results for a Si NW doped with tetracyanoethylene [Fig. 1(c)], whose band structure is shown in Fig. 1(a). It can be seen that the adsorbed molecule contributes with a localized state (no dispersion) close to the conduction band edge, pinning the Fermi level. The molecular nature of this state is further supported by the total electronic density of states (DOS) and the projected DOS, where projections are made on every element [Fig.1(b)]. There it can be seen that the localized states is almost exclusively made up of C and N contribution, thus it is localized at the molecule adsorption site.
Finally in Figs. 1 (d-f) where the representation in real space of the corresponding wave functions iso-surfaces is shown; (d-e) and (f) iso-surfaces corresponding to top valence band two states and bottom conduction band one state respectively.

In larger nanowires, where the band gap is smaller due to a reduced quantum confinement, this state is expected to be shallow enough to be an active electron donor.

References:

[1] Y. Cui, Z.H. Zhong, D.L. Wang, W.U. Wang and C.M. Lieber, Nano Lett., **3** (2003) 149.
[2] Y. Cui, Q.Q. Wei, H.K. Park and C.M. Lieber, Science, **293** (2001) 1289.
[3] Y. Wang, K. K. Lew, T. T. Ho, L. Pan, S. W. Novak, E. C. Dickey, J. M. Redwing, and T. S. Mayer, Nano Lett., **5** (2005) 2139.
[4] L. Pan, K.-K. Lew, J. M. Redwing, and E. C. Dickey, J. Cryst. Growth, **277** (2005) 428.
[5] K. Byon, D. Tham, J. E. Fischer, and A. T. Johnson, Appl. Phys. Lett., **87** (2005) 193104.
[6] M.V. Fernández-Serra, Ch. Adessi, and X. Blase, Phys. Rev. Lett., **96** (2006) 166805.

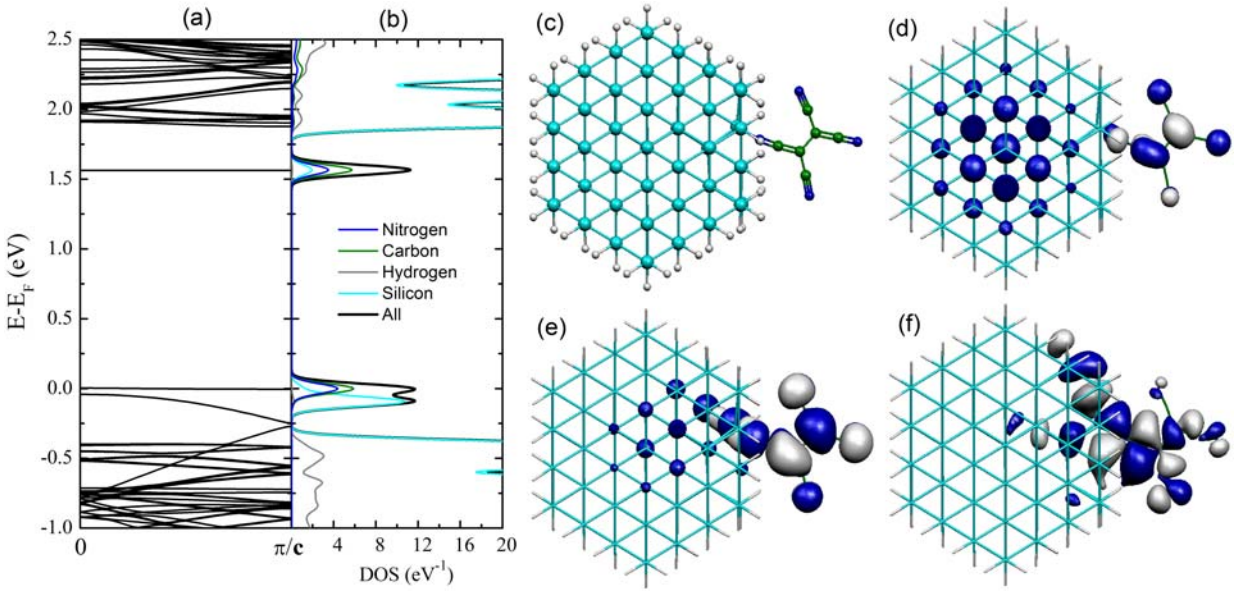

Figure 1. (a) The electronic band structure of the SiNW. One state have the Fermi level, the wave vector *k* in the first half of the Brillouin zone. (b) The total and projected electronic density of states of the SiNW, (c) Tetracyanoethylene doped on Silicon nanowire. The wave function iso-surfaces of the three states (d-f) of the SiNW.