Molecular Doping on the Electronic Properties of Silicon Nanowires in the [112], [110], [100] and [111] directions

A. Miranda[1,3], X. Cartoixà[2], E. Canadell[1], R. Rurali[1]

[1] Institut de Ciència de Materiales de Barcelona (ICMAB–CSIC), Campus de Bellaterra, 08193 Bellaterra (Barcelona), Spain

[2] Departament d'Enginyeria Electrònica, Universitat Autònoma de Barcelona, Campus de Bellaterra, 08193 Bellaterra (Barcelona), Spain

[3] Instituto Politécnico Nacional, ESIME-Culhuacan, Av. Santa Ana 1000, 04430 México D.F., México

amiranda@icmab.es

We report *ab-initio* calculations on Silicon Nanowires (SiNWs) oriented along the [112], [110], [100] and [111] directions based on density functional theory (DFT). The influences of the molecular doping and quantum confinement on the electronic properties onto SiNWs are studied [1].

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 are especially attractive for their possible efficient integration in conventional Si-based microelectronics [2,3]; the interest is essentially related to the strong modifications of the basic properties of the material induced by space confinement, with remarkable effects on the optical properties.

The possibility that an adsorbed molecule could provide shallow electronic states that could be thermally excited have received less attention than substitutional impurities and could potentially have a high impact in the doping of SiNWs. With such an approach one would simultaneously get rid of two problems that bedevils SiNW doping: (i) the competition between catalyzed and uncatalyzed incorporation of the impurities, often leading to sizeable disuniformities in the dopant concentration [4]; however, this *in-situ* approach does not always give favorable results [5], (ii) the need to carry out demanding annealing cycle to promote diffusion in *ex-situ* doping [6,7].

This inconvenience is shared by both conventional *in-situ* and *ex-situ* approaches. Here we explore the possibility of obtaining molecular doping of SiNWs. 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 [8]. We discuss the cases of donors.

We present results for SiNWs with a diameter of 1.5 nm oriented along the [112], [110], [100] and [111] doped with NH_3, whose the band structure are shown in Figs. 1(a), 2(a), 3(a) and 4(a) respectively. It can be seen for all SiNWs that the adsorbed molecule contributes with a localized state close to the conduction band edge, where it pins the Fermi level. Therefore the adsorbed molecule is found to be an efficient donor, as carriers can be thermally excited into the conduction band. More specifically we have found that NH_3 requires less energy to adhere to {110} faces, regardless of the growth orientation of the SiNWs. The molecular nature of these states are further supported by the projected electronic density of states, where projections are made on nitrogen, hydrogen and silicon [Fig. 1(b), 2(b), 3(b) and 4(b)]. There it can be seen that the localized states is almost exclusively made up of N and H contribution, thus it is localized at the molecule adsorption site.

We acknowledge the financial support Funding under Contract Nos. TEC2009-06986, FIS2009-12721-C04-03, and CSD2007-00041 and Postdoctoral Abroad - Consejo Nacional de Ciencia y Tecnología, México.

References

[1] R. Rurali, Rev. Mod. Phys. **82** (2010) 427.
[2] J. Chen, Microelectron. J. **39** (2008) 50.
[3] W.M. Weber, L. Geelhaar, A.P. Graham, *et al.,* Nano Lett. **6** (2006) 2660.
[4] G. Imamura, T. Kawashima, M. Fujii, *et al*., Nano Lett. **8** (2008) 2620.
[5] L. Pan, K.-K. Lew, J.M. Redwing, and E.C. Dickey, J. Cryst. Growth, **277** (2005) 428.
[6] S. Ingole, P. Aella, P. Manandhar, S. *et al.*, J. Appl. Phys. **103** (2008) 104302.
[7] A. Colli, A. Fasoli, C. Ronning, S. Pisana, S. Piscanec, and A. C. Ferrari, Nano Lett. **8** (2008) 2188.
[8] A. Miranda-Durán, X. Cartoixà, M. Cruz-Irisson and Rurali, Nano Lett. **10** (2010) 3590.

Figures

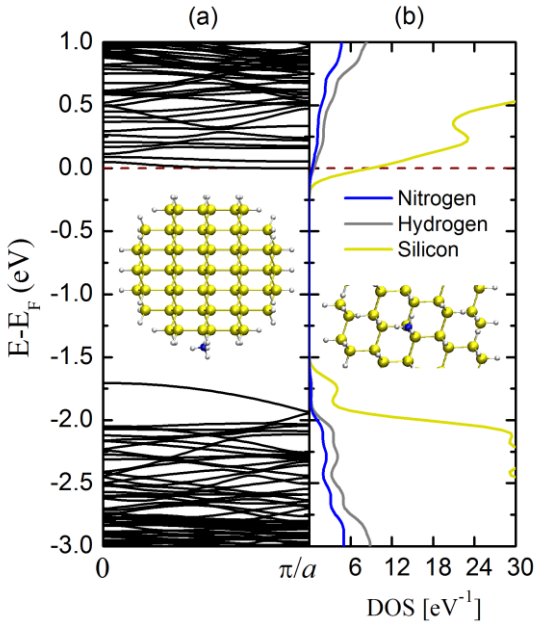

Figure 1. SiNW doped with NH_3 in the [112] direction (a) Electronic band structures, (b) Projected electronic density of states.

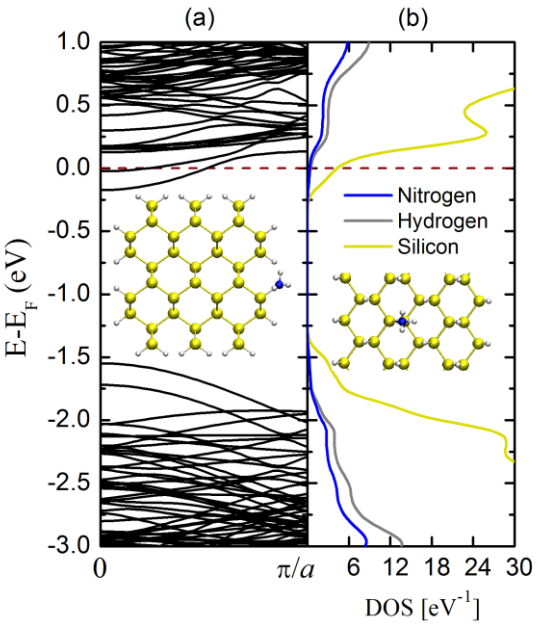

Figure 2. SiNW doped with NH_3 in the [110] direction (a) Electronic band structures, (b) Projected electronic density of states.

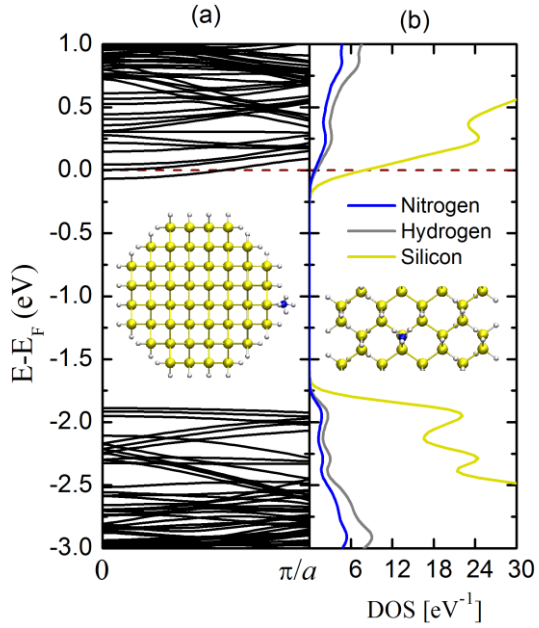

Figure 3. SiNW doped with NH_3 in the [100] direction (a) Electronic band structures, (b) Projected electronic density of states.

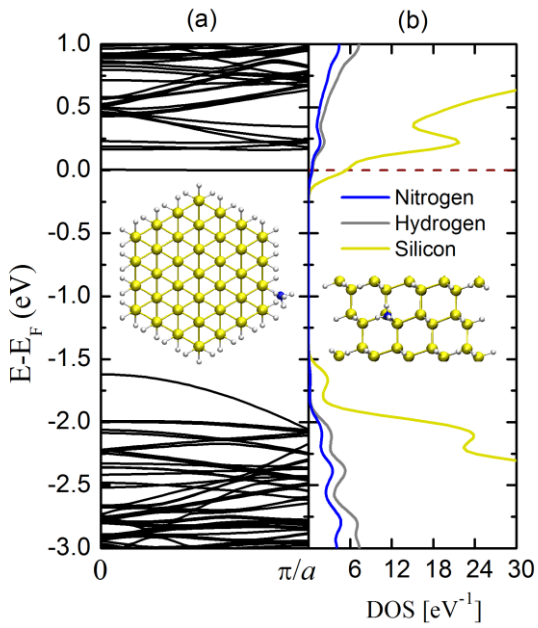

Figure 4. SiNW doped with NH_3 in the [111] direction (a) Electronic band structures, (b) Projected electronic density of states.