A theoretical study of surface reconstructed silicon nanowires

R. Rurali and N. Lorente

Laboratoire Collisions, Agrégats, Réactivité,

IRSAMC, Université Paul Sabatier,

118 route de Narbonne, 31062 Toulouse cedex, France

Abstract

One-dimensional nanostructures are attracting a great interest for their potentially high impact in future molecular electronics applications, such as nanoswitches and nanocontacts.

Silicon nanowires (SiNWs) appear to be a special appealing alternative, due to the ideal interface compatibility with conventional Si-based technology and to the possibility to tune their conductive properties by means of electrical doping.

While it has been extensively demonstrated that in H-terminated SiNWs quantum confinement induces a gap-broadening effect[1], very little is known about surface reconstruction of non-passivate wires and their electronic structure features. We present a theoretical study based on density-functional calculations of realistic $\langle 100 \rangle$ SiNWs[2], with a bulk Si core and a diameter of $\sim$ 1.5 nm. Particularly, we focus our attention on the features of the electronic properties of the wire as determined by the different possible lateral surface reconstruction. We find two competing geometries for the $\{100\}$ facets. One of them shows a semi-metallic behavior with one state approaching the Fermi level at the zone boundary, while the other has four metallic states. These states show a great degree of surface localization. Therefore, current flow is almost entirely sustained by the outer layers of the SiNW[3].

The possibility to obtain one-dimensional metallic Si nanostructures opens up the way to a wide range of novel nanoscience applications that require stout and atomic-scale contacts. Metallic SiNWs are a promising path to usher Si in nanotechnology applications.

Preliminary results of non-equilibrium electron transport calculations will also be presented[4].

---

[1] B. Delley and E. F. Steigmeier, Appl. Phys. Lett., **67**, 2370 (1995).

[2] D. D. D. Ma, C. S. Lee, F. C. K. Au, S. Y. Tong and S. T. Lee, Science, **299**, 1874 (2003).

[3] R. Rurali and N. Lorente, Phys. Rev. Lett. **94**, 026805 (2005); R. Rurali and N. Lorente, cond-mat/0412236.

[4] M. Brandbyge, J.-L. Mozos, P. Ordejón, J. Taylor, and K. Stokbro, Phys. Rev. B **65**, 165401 (2002).