Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Conductance, surface traps and passivation in doped Silicon Nanowires MARIVI FERNANDEZ-SERRA, CECAM ENS-Lyon, CHRISTOPHE ADESSI, LPMCN Universite Lyon 1, XAVIER BLASE, CNRS et LPMCN Universite Lyon 1 — By means of *ab initio* total energy and conductance calculations within the Landauer Formalism we investigate the structural, electronic and transport properties of doped silicon nanowires (SiNWs). We find that impurities always segregate at the surface of unpassivated wires, reducing dramatically the conductance of the surface states. Upon passivation, we show that for wires as large as a few nanometers in diameter, a large proportion of dopants will be trapped and electrically neutralized at surface dangling bond defects, significantly reducing the density of carriers. Impurities located in the core of the wire induce a strong resonant backscattering at the impurity bound state energies. Surface dangling bond defects have hardly any direct effect on conductance. Upon surface trapping, impurities become transparent to transport, as they are both electrically inactive and do not induce any resonant backscattering.

- M. V. Fernández-Serra, Ch. Adessi and Xavier Blase, Phys. Rev. Lett. **96**, 166805 (2006).
- M. V. Fernández-Serra, Ch. Adessi and Xavier Blase, NanoLetters. (In press) **12**, (2006)

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Date submitted: 28 Nov 2006 Electronic form version 1.4