

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Sensitivity of dangling bonds to the presence of dopant atoms in hydrogen terminated silicon nanoclusters TORBJÖRN BLOMQUIST, GEORGE KIRCZENOW, Simon Fraser University — Dangling bonds on the surfaces of semiconductor nanoparticles are expected to play an important role in the self-assembly of hybrid molecule-semiconductor nanoelectronic devices[G.P. Lopinski, D. D. M. Wayner, and R. A. Wolkow, Nature 406, 48 (2000)] and should also directly impact the electronic and transport properties of such nanostructures. We have studied the dangling bond on hydrogen terminated silicon nanoparticles, both analytically in the effective mass approximation and using a self-consistent Poisson-Schrödinger model that we previously developed.[Phys. Rev. B, to be published] This model allows us to make calculations on silicon structures containing many hundreds of silicon atoms, enabling us to explore (doped) silicon nanoparticles with dangling bonds. A dangling bond on a hydrogen terminated silicon surface is shown to behave qualitatively as an electronic acceptor, its energy level however depends on the occupation of the dangling bond state which in turn depends on the the temperature and strongly on doping of the silicon. We will present energies and wave functions for dangling bond states on different (doped) hydrogen terminated silicon surfaces.

Torbjörn Blomquist
Simon Fraser University

Date submitted: 03 Dec 2004

Electronic form version 1.4