Responsable :
Fabien BRUNEVAL
01 69 08 43 49

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Confinement and hyperfine structure in chalcogen doped silicon nanowires

Guido Petretto, A. Debernardi and M. Fanciulli

Laboratorio MDM - IMM - CNR - Agrate Brianza
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Dipartimento di Scienza dei Materiali, Universita degli Studi di Milano-Bicocca, Italy

Silicon nanowires are promising candidates for future nanodevices and for quantum information applications. In light of these possible applications we have performed ab initio simulations to obtain informations about the electronic properties when dimensions reduce to nanometric scale.

We have studied the electronic properties and hyperfine structure of substitutional chalcogens in silicon nanowires using plane-wave pseudopotential techniques. We simulated hydrogen passivated nanowires with various orientations and diameter up to 2 nm, analyzing the effect of quantum confinement on the defect formation energy and on the hyperfine parameters as a function of the diameter and of the defect position. We show that substitutional Se in silicon has favourable configurations for positions near the surface with possible formation of chalcogen-hydrogen complexes. We also show that hyperfine interactions increase at small diameters, as long as the nanowire is large enough to prevent surface distortion which modifies the symmetry of the donor wavefunction. Moreover, surface effects lead to strong differences in the hyperfine parameters depending on the Se location inside the nanowire, allowing the identification of impurity site on the basis of the EPR spectra.

Mardi 14 février 2012 à 10h30

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