

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Donor Wave Functions Delocalization in Silicon Nanowires ALBERTO DEBERNARDI, CNR-IMM, MDM laboratory Agrate Brianza, GUIDO PETRETTO, CEA Saclay, SRMP - CNR-IMM, MDM laboratory Agrate Brianza, MARCO FANCIULLI, CNR-IMM, MDM laboratory Agrate Brianza — The localization of the donor electron wave function can be of key importance in various silicon application, since it determines the interactions between neighboring donors and influences the charge density close to the donor atom. This is important in light of applications like nuclear spin qubits [1] or for determining the critical density of metal-insulator transitions [2]. In particular the delocalization is a critical feature when dealing with nanostructures, where the confinement induces a squeezing of the donor wave function. Using ab-initio calculations, we have studied the delocalization of the donor electron wave function along the axis of a nanowire with different orientations for P and Se donors[3]. We show that the shape and delocalization is greatly influenced by the orientation of the nanowire and that it considerably larger for [011] oriented nanowires, compared to [001] and [111] orientations. We also demonstrate that its value can be controlled by applying a compressive or tensile uniaxial strain. We also show the effect of the delocalization on the hyperfine parameters. [1] B. E. Kane, Nature 393, 133 (1998) [2] D. Belitz, T. R. Kirkpatrick, Rev. Mod. Phys. 66, 261 (1994) [3] G. Petretto, A. Debernardi, M. Fanciulli, Nano Letters 13, 4963 (2013)

Fabien Bruneval
CEA Saclay, SRMP

Date submitted: 15 Nov 2013

Electronic form version 1.4