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Ab initio study of confinement effects and hyperfine structure in chalcogen doped Silicon nanostructures[1] ALBERTO DEBERNARDI, CNR-IMM, MDM laboratory Agrate Brianza, GUIDO PETRETTO, ANDREA MASSE, MARCO FANCIULLI, CNR-IMM, MDM laboratory Agrate Brianza, University Milano-Bicocca — In recent years, increasing interest has been focused on Si nanostructures as building blocks for ultra-scaled electronic devices where quantum mechanic effects are relevant. We have investigated the atomic and electronic structures of a single chalcogen donor in H passivated Si nanostructures of different size by means of the plane-wave pseudopotential techniques we used in Ref. [1] to study Se doped Si (001) nanowires (NW). Our results showed an increase in the gap with diminishing diameter of Si NW. We studied the size dependence of electronic properties and hyperfine constant of single substitutive chalcogen impurity in Si-NWs (001) and (111) oriented, and Si-dots and their dependence on the distance from the NW axis or the centre of the dot. We show that the hyperfine parameters are strongly dependent on the impurity position: we proved that surface effects can lead to strong differences in the hyperfine parameters depending on the chalcogen location inside the nanowire, suggesting a way to determine experimentally the position of the defect on the basis of electron paramagnatic resonance spectra. Preliminary results on chalcogen doped Ge nanowires complete the work. [1] G. Petretto, A.Debernardi, and M. Fanciulli, Nano Letters, Vol. 11, 4509 (2011).

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Alberto Debernardi
CNR-IMM, MDM laboratory Agrate Brianza

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