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Ab initio study of substitutional doping of III-V nanowires BOB SCHOETERS, University of Antwerp and IMEC, GEOFFREY POURTOIS, IMEC and University of Antwerp, BART PARTOENS, University of Antwerp — Using *ab initio* calculations we study the impact of substitutional dopants in thin III-V nanowires. In this study we focus on 4 different technologically relevant III-V nanowires: GaAs, InSb, InP and InGaAs, doped with either C, Si, Ge, Be, Mg or Zn. We determine the energetically most favorable positions for these dopants by looking at their formation energies. These preferred locations indicate whether a dopant will segregate to the surface or the center of the nanowire. This can have a large impact on the electronic properties, since it will lead to an inhomogeneous doping distribution. We can explain the preferential positions as a competition between a chemical and a relaxation effect. However, in reality these nanowires contain several defects, such as antisites, vacancies, dangling bonds at the nanowire surface, ... Therefore we also investigate the impact of these defects on the localization of the dopants. Finally we study the impact of these dopants on the electronic structure.

Bob Schoeters
University of Antwerp

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