Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

First-principles method to study defect properties in semiconductor nanostructures BART PARTOENS, MOZHGAN AMINI, BOB SCHOETERS, ROLANDO SANIZ, DIRK LAMOEN, University of Antwerp - Department of Physics, CMT-EMAT COLLABORATION — The standard theoretical approach to examine the deep or shallow nature of defects in bulk crystals is through first-principles calculations of their (neutral and charged) formation energies. The character of a defect in a nanostructure might differ from its character in the bulk material and may vary with its position in the nanostructure. However, the standard method cannot be transferred directly to nanostructures. In calculations for a charged defect, a uniform background charge is considered. While this is well-defined for bulk calculations, the total energy of a charged nanostructure depends on the vacuum width. Therefore, total energies of charged nanostructures cannot be used to calculate defect formation energies. Here we propose a solution to this problem and present a first-principles method to determine formation energies for defects in different charge states in a nanostructure, together with the transition levels. As example, we focus on V_O in ZnO slabs and Si_{Ga} in GaAs slabs. Their preferential position as function of the distance to the surface is determined, together with the evolution of their optical and thermal ionization energies. This new method allows to study the character of a wide range of intrinsic and extrinsic defects in nanostructures.

Bart Partoens
University of Antwerp - Department of Physics

Date submitted: 13 Nov 2013 Electronic form version 1.4