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Selenium passivation of GaAs(001): a combined experimental and theoretical study

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Abstract. The chemical and electronic properties of selenium passivated GaAs(001)-2 × 1 surfaces were investigated by a combination of theoretical calculations and core level photoemission experiments. An anion exchange results in gallium-selenide like layers showing a 2 × 1 reconstruction in low energy electron diffraction (LEED). The analysis of the different components in the core level spectra of As 3d, Ga 3d and Se 3d limits the number of possible structural models. The Se/GaAs(001)-2 × 1 reconstruction has been also analysed by means of DFT-LDA calculations and theoretical STM currents. In a first step, different geometries are considered and the most stable one, from the point of view of the thermodynamic potential, is determined. Then, STM currents and the corresponding surface corrugation are calculated and compared with the experimental evidence. We conclude that the Se/GaAs(001)-2 × 1 reconstruction has a single Se atom in the last crystal layer, bonded to two Ga atoms of the second layer, and another Se layer replacing the third As layer of the crystal. These surfaces may be considered as chemically stable because they withstand considerable exposure to air. In terms of electronic passivation, i.e. the removal of any surface band bending, the selenium modification is not successful. Band bending on n-type doped samples is reduced while band bending on the p-type doped samples is further increased.

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