Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Structural, electronic and magnetic properties of Mn-doped GaAs(110) surface ALESSANDRO STROPPA, MARIA PERESSI, Dep. of Theoretical Physics, University of Trieste and DEMOCRITOS National Simulation Center, Trieste (Italy) — First principles total-energy pseudopotential calculations have been performed to investigate structural, electronic—including scanning tunneling microscopy (STM) images—and magnetic properties of the (110) cross-sectional surface of Mn-doped GaAs. We have considered configurations with Mn in interstitial positions in the uppermost surface layers with Mn surrounded by As (Int_{As}) or Ga (Int_{Ga}) atoms. The presence of Mn on the GaAs(110) surface originates strong local distortion in the underlying crystal lattice, with variations of interatomic distances up to 8%. In both cases, Int_{As} and Int_{Ga}, the surface electronic structure is half-metallic (or *nearly* half metallic) with details strongly dependent on the local Mn environment. The atoms surrounding the Mn impurity show an induced polarization resulting in a ferromagnetic Mn–As and antiferromagnetic Mn–Ga configuration respectively in the two cases. The simulation of the STM images show very different patterns of the impurity region in the two cases, suggesting that they could be easily discerned by STM analysis. We have also simulated STM images of Mn interstitials pairs on surface. The comparison of the simulated images with recent experimental cross-sectional STM images of Mn δ-doped GaAs is discussed.

Gaetano Senatore
University of Trieste and DEMOCRITOS National Simulation Center, Trieste

Date submitted: 30 Nov 2005 Electronic form version 1.4