Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

The role of d levels of substitutional magnetic impurities at the (110) GaAs surface M.R. MAHANI, ANNA PERTSOVA, FHOKRUL ISLAM, C.M. CANALI, Linnaeus University, Kalmar, Sweden — The study of the spin of individual transition-metal dopants in a semiconductor host is an emergent field known as magnetic solotronics, bearing exciting prospects for novel spintronics devices at the atomic scale. Advances in different STM based techniques allowed experimentalists to investigate substitutional dopants at a semiconductor surface with unprecedented accuracy and degree of details [1]. Theoretical studies based both on microscopic tight-binding (TB) models and DFT techniques have contributed in elucidating the experimental findings. In particular, for the case of Mn dopants on the (110) GaAs surface, TB models [2] have provided a quantitative description of the properties of the associated acceptor states. Most of these TB calculations ignore dealing explicitly with the Mn d-levels and treat the associated magnetic moment as a classical vector. However recent STM experiments [3] involving other TM impurities, such as Fe, reveal topographic features that might be related to electronic transitions within the d-level shell of the dopant. In this work we have included explicitly the d levels in the Hamiltonian. The parameters of the model have been extracted from DFT calculations. We have investigated the role that d levels play on the properties of the acceptor states of the doped GaAs(110) surface, and analyzed their implications for STM spectroscopy. [1] Yakunin et al., PRL 92, 216806 (2004), Kitchen et al., Nature 442, 436 (2006). [2] Tang et al., PRL 92, 047201 (2004), Strandberg et al., PRB 80, 024425 (2009). [3] J. Bocquel et al., arXiv:1203.6293v.1.

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Date submitted: 07 Nov 2012 Electronic form version 1.4