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Theory of STM spectroscopy in Mn clusters on GaAs surfaces. TOR OLOF STRANDBERG, Lund University, ALAN MACDONALD, University of Texas at Austin, CARLO CANALI, Kalmar University — Small numbers of Mn atoms can be manipulated into arbitrary spatial arrangements on the $< 110 >$ surface of GaAs by means of a novel STM atom-by-atom substitution technique, which enables the replacement of individual Ga atoms by Mn [1]. The tunneling differential conductance over an isolated Mn atom reveals a large and broad resonance in the GaAs energy gap. For a Mn pair placed less than 1 nm apart, the resonance splits into two peaks, whose spacing is thought to be related to the exchange-energy interaction between Mn ions. We report on theoretical results for the local density of states and the Mn acceptor-level splittings for a Mn dimer, based on a tight-binding model of Mn substitutions on the $< 110 >$ GaAs surface. We compare our model with previous work which does not account for the surface. We then derive an effective quantum spin Hamiltonian for the Mn cluster, based on a Chern number theory developed recently, which includes Berry phase effects [2]. We study the transition from surface to bulk for the substitutional Mn impurity in GaAs as well as Mn-Mn interactions at the surface and in bulk at various distances and along different crystalline directions. [1] D. Kitchen et al., Nature 442, 436 (2006). [2] C.M. Canali, A. Cehovin and A.H. MacDonald, Phys. Rev. Lett. 91, 046805 (2003)

Tor Olof Strandberg
Lund University

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