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Effect of As vacancies on the binding energy and exchange splitting of Mn impurities on a GaAs surface M.R. K. MAHANI, C.M. CANALI, Linnaeus University, Kalmar, Sweden, A.H. MACDONALD, University of Texas at Austin — State-of-the-art STM spectroscopy is nowadays able to manipulate and probe the magnetic properties of individual magnetic impurities located near the surface of a semiconductor. A recent advance of these technique employs the electric field generated by a As vacancy in GaAs to affect the environment surrounding substitutional Mn impurities in the host material [1]. Here we calculate the binding energy of a single Mn dopant in the presence of nearby As vacancies, by using a recently-introduced tight-binding method [2] that is able to capture the salient features of Mn impurities near the (110) GaAs surface. The As vacancies, modeled by the repulsive potential they produce, are expected to decrease the acceptor binding energy in agreement with experiment [1]. Within this theoretical model, we investigate the possible enhancement of the exchange splitting for a pair of ferromagnetically ordered Mn impurities, observed experimentally when As vacancies are present [3]. We also calculate the response of the Mn-impurity—As-vacancy complex to an external magnetic field.

[1] H. Lee and J. A. Gupta, Science, 1807-1810, (2010).

[2] T. O. Strandberg, C. M. Canali, A. H. MacDonald, Phys. Rev. B 80, 024425, (2009).

[3] J.A. Gupta, private communication.

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