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Anisotropic spin-spin interactions of Mn-Mn pairs in III-V semiconductors¹ JIAN-MING TANG, MICHAEL E. FLATTÉ, University of Iowa — We calculate the energy splitting of acceptor states of Mn pairs in GaAs [1]. The calculated splittings show crystalline anisotropy that is in good agreement with recent scanning tunneling measurements [2]. The splitting is large when the pair axis is along the $\langle 110 \rangle$ axis and smaller when along the $\langle 100 \rangle$ axis. This anisotropy can be understood from the overlap of two Mn acceptor wavefunctions that have the approximate cubic symmetry [3]. Within a double exchange model, the splitting can be linked to the energy difference between parallel and antiparallel Mn spins. Our results show that the parallel configurations always have the lower energy. This exchange coupling energy follows the same crystalline anisotropy for the splitting because the anisotropy is predominately determined by the lowest hole state. The rotational symmetry of the total spin of Mn pairs is weakly broken by the spin-orbit interaction. [1] J.-M. Tang and M. E. Flatté, Phys. Rev. Lett. 92, 047201 (2004) [2] D. Kitchen, et al., Nature 442, 436 (2006) [3] A. M. Yakunin, et al., Phys. Rev. Lett. 95, 256402 (2005)

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