

Abstract Submitted  
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**Tight binding study of single ion magnetic anisotropy of  $\text{Mn}^{2+}$  in  $\text{Ga}(\text{Mn})\text{As}$** <sup>1</sup> HEMACHANDER SUBRAMANIAN, JONG HAN, University at Buffalo, State University of New York — Bulk uni-axial magnetic anisotropy of  $\text{Ga}(\text{Mn})\text{As}$  observed in experiments has not been well understood as much as cubic magnetic anisotropy in the same material. We propose that the uni-axial anisotropy arises due to the coupling of local lattice distortions around  $\text{Mn}^{2+}$  impurity ion to its spin state through spin-orbit coupling of holes bound to the impurity ion. We model the coupling using nearest-neighbor tight-binding and many-body perturbation theory. The model includes intra-atomic Coulomb interaction inside  $\text{Mn}^{2+}$  ion, spin-orbit interaction of holes at the  $\Gamma$  point,  $p-d$  hopping interaction between  $\text{Mn}^{2+}$  ion  $d$  orbitals and As ion  $p$  orbitals, and strain due to local lattice distortions. We observe breaking of tetrahedral symmetry around the  $\text{Mn}^{2+}$  ion when the system is paramagnetic. We explore the effect of this broken symmetry in stabilizing certain magnetization directions through spin-orbit coupling in the ferromagnetic regime.

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