First Principle Calculations of Magnetic Anisotropy for Single and Pair of Mn Ions in GaN

K. Das[1], N. Gonzalez Szwacki[2], R. Hayn[3] and D. Sztenkiel[1]

[1] *Institute of Physics, Polish Academy of Sciences, Warsaw, Poland*
[2] *Faculty of Physics, University of Warsaw, Warsaw, Poland*
[3] *IM2NP, UMR 7334, Universite d'Aix-Marseille and CNRS, Marseille, France*

We investigate here a dilute ferromagnetic semiconductor, $Ga_{1-x}Mn_xN$, that merges semiconductor/insulator and magnetic properties. In this material, a single-ion magnetic anisotropy of Mn impurity can be controlled by an electric field through the inverse piezoelectric effect [1]. This holds promise for an experimental observation of precessional magnetization switching in $Ga_{1-x}Mn_xN$ by the application of sub-nanosecond electric pulses. To achieve this goal, it seems necessary to have a thorough understanding of the magnetic anisotropy in this material.

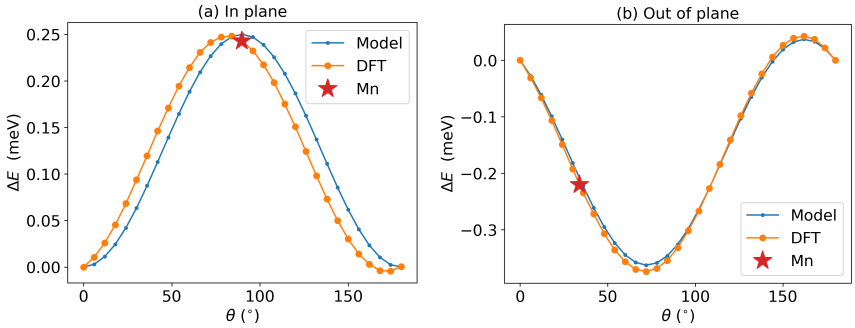

Figure 1: Comparison of DFT data with a simplified model $\mathcal{H} = -K^{tr}S_z^2 - K^p(\mathbf{S}\cdot\mathbf{e}^p)^2$, where K^{tr} and K^p are trigonal and paring anisotropy constants, respectively.

We employ the Vienna Ab initio Simulation Package (VASP) with the Projector Augmented Wave (PAW) method for an investigation of the magnetic anisotropy of isolated single and pair of Mn impurities in GaN supercell [2]. A series of ionic relaxations are conducted across supercells of varying sizes with a single Mn ion to simulate different impurity concentrations, $x = 0.02$–0.5. The obtained data reveal distinctive Jahn-Teller T_{2D} distortion in the preliminary results. Moreover, the findings exhibit a noteworthy dependency of magnetic anisotropy on the $\xi = \frac{c}{a} - \sqrt{\frac{8}{3}}$ ratio [1], where c and a are lattice parameters. Expanding our investigation, we introduce a second Mn ion in the nearest cation position in both in-plane and out-of-plane directions. Exploring magnetic energy E as a function of spherical angles $E(\theta, \phi)$ highlights the presence of an additional anisotropy along the Mn–Mn direction $\mathbf{e}^p$, elucidating nuanced magnetic behavior in response to the presence of nearest neighboring Mn ions. This investigation will add the missing puzzle in refining our theoretical framework used to simulate magnetic properties [3] including ferromagnetic resonance FMR studies in $Ga_{1-x}Mn_xN$ layers.

The work is supported by the National Science Centre, Poland, through projects DEC-2018/31/B/ST3/03438 and Centre de Calcul Intensif d'Aix-Marseille, France by high performance computing resources.

[1] D. Sztenkiel et al., *Nature Comm.* **7**, 13232 (2016).
[2] K. Das, et al., *to be published.*
[3] Y. K. Edathumkandy and D. Sztenkiel, *JMMM.* **562**, 169738 (2022).