MAGNETIC ORDERING IN WEAKLY COUPLED VAN DER WAALS SYSTEMS, WITH APPLICATION TO VI_3

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Magnetic van der Waals (vdW) materials exhibit promising potential for high-tech magnetic, magneto-electric and magneto-optic applications in nanostructures [1]. Due to their intrinsic magnetocrystalline anisotropy, several vdW magnets could be thinned down to nanoscale thickness while overcoming the consequences of Mermin-Wagner theorem and still maintaining magnetic order. A prominent example of such materials are transition metal trihalides, in particular CrI_3, a first atomically thin ferromagnet, realized in 2017 [2].

In van der Waals materials exchange coupling between layers is rather weak and can be relatively easily modified. Regime of weak interlayer coupling represents a transition between the more explored cases of isotropic bulk-like exchange and the ideal 2D (monolayer) limit [3]. Here we examine general features of finite temperature magnetic order in this regime by atomistic spin dynamics methods. The method is applied to a particularly interesting system from this class, VI_3. It is a quasi 2D ferromagnetic semiconductor with $T_C = 50$ K, and a rather unusual magnetic anisotropy [4]. The anisotropy was reproduced by first-principles calculations only if lattice distortions present at its low temperature phases were taken into account [5]. The calculations also revealed an exceptionally large orbital momentum on V atoms, showing that the effect of spin-orbit interaction is more important than the crystal field in this case. Employing calculated exchange interactions we study how is the Curie temperature affected by interlayer coupling of this system and how much this solution differs from the mean-field model results. We also predict a possibility of magnetic order with parallel aligned spins inside layers that are magnetically decoupled from each other. This phase may occur at some temperatures above T_C in case that magnetic anisotropy and specific exchange interactions fall within a certain range of values.

References

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