DEVELOPING A NEW EFFECTIVE MAGNETIC MODEL OF Fe_3GeTe_2 BASED ON AB-INITIO CALCULATIONS

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In our work we propose a new effective magnetic model for two-dimensional van der Waals ferromagnet Fe_3GeTe_2. To prove its correctness we conducted ab-initio calculations as well as compared Curie temperatures using Monte Carlo simulations with the obtained parameters.

Mermin-Wagner theorem prohibit intrinsic ferromagnetism in 2D materials. Recent papers reported that magnetocrystalline anisotropy is the key that opens up the possibility of intrinsic ferromagnetism in 2D [1-3]. To study magnetic properties of 2D Fe_3GeTe_2 we construct the spin model with isotropic exchange interactions between iron ions and single-ion anisotropy. In this material two types of iron atomic positions can be distinguished: Fe_1 and Fe_2. Two atoms of iron allocate position Fe_1 and another one allocate position Fe_2. Due to strong nearest neighbour ferromagnetic exchange between iron atoms in position Fe_1 ~ 114 meV we propose that we can consider two iron atoms in position Fe_1 as effective cluster.

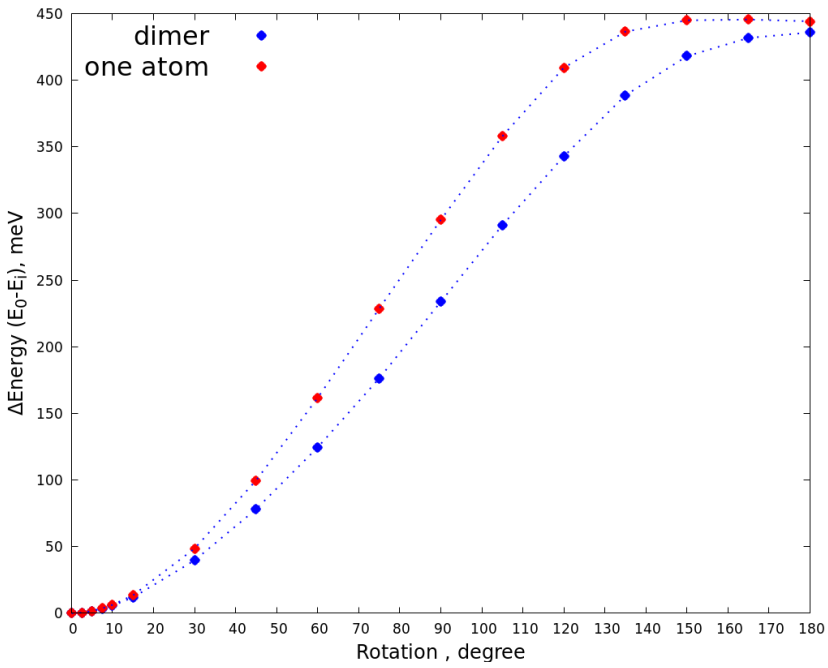

Рис. 1. Calculated energy difference between ferromagnetic ground state and energy with rotation of magnetic moments in one atom rotation scheme (red) and dimer rotation scheme (blue).

To prove this hypothesis we made calculations with rotation of magnetic moment of iron atoms position Fe_1 in two cases: rotation of one atom magnetic moment with constraining the others (one atom rotation scheme) and rotation of two iron atoms magnetic moments in position Fe_1 simultaneously as cluster with constraining the others (dimer rotation scheme). In our calculation we use Vienna Ab initio Simulation Package [5] that uses density functional theory. In our calculation we use 2x2 supercell with experimental crystal structure of bulk Fe3GeTe2 [4] with 16 angstrom additional space between layers to simulate monolayer structure. We calculate ground state energy for every 2.5 degree for small angles of rotation (less than 10 degree) and for every 15 degree for other angles. Our results demonstrate that rotation scheme with dimer cluster were more energy favorable. And both rotation cannot be fitted by simple (1-cos(alpha) function. Moreover, the obtained Curie temperature is in a good agreement with the one for the full model as well as with the results of other studies.

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