ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF $FeGe_2$

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The transition metal compounds with germanium and tin having the tetragonal C16-type crystal structure exhibit unusual magnetic, electrical and structural properties. These properties make them the subject of continuous experimental and theoretical investigations. $FeGe_2$ is an itinerant electron antiferromagnet, which has a second-order transition from a paramagnetic phase to an incommensurate phase at 289 K with a long-wavelength modulation in the basal plane, and the other first-order transition from an incommensurate to a commensurate antiferromagnetic phase at 263 K.

In our work we report results of theoretical calculations of electronic structure and magnetic properties of $FeGe_2$. *Ab initio* calculations of the volume dependent electronic structure and magnetic properties were performed by employing the full-potential LMTO and LAPW methods for paramagnetic and magnetic configurations of $FeGe_2$ compound. It is unambiguously established that the collinear antiferromagnetic configuration has clearly the lowest total energy so that it is the ground state of the bulk $FeGe_2$. The calculated magnetic moments of $FeGe_2$ appeared to be about 1.2 μ_B per formula unit and arise from the iron-derived 3*d* states. This is in agreement with neutron experiments, which reported the magnetic moments about 1.2 — 1.3 μ_B , and this clearly indicates the itinerant nature of antiferromagnetism in $FeGe_2$.

It is expected, that a pressure can provide drastic changes in electronic and magnetic properties. Therefore we studied a behavior of magnetic susceptibility χ under uniform and uniaxial pressures for the paramagnetic and antiferromagnetic phases. The spin and orbital Van Vleck contributions to χ and their volume dependences were calculated *ab initio* in an external magnetic field and were found in agreement with the available experimental data. It is appeared that the calculated $d\ln\chi / d\ln V$ derivative in the PM phase of $FeGe_2$ is large but somewhat lower than the corresponding derivatives in the PM compounds with highly enhanced spin susceptibility (e.g. $CeCo_2$, YCo_2, TiCo, Ni_3Al). Also, for the antiferromagnetic phase of $FeGe_2$ the substantially anisotropic and pressure dependent magnetic susceptibilities were evaluated *ab initio* , which allowed to shed light on results of recent experiments, including magnetostriction and uniaxial pressure effect on magnetic susceptibility.