Noncollinear magnetism on UFe_xAl_{12-x} series: ab-initio calculations

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9.7 cm

The UFe_xAl_{12-x} series has been the object of a systematic experimental study in single crystals with different compositions [1]. Several measurements technics were used in Ref. [1] to suggest a magnetic phase diagram of the system. Three different ranges of composition were found to have different magnetic behavior: $x < 4 + \delta_1$, $4 + \delta_1 < x < 5 - \delta_2$, and $x > 5 - \delta_2$. The UFe_4Al_8 and UFe_5Al_7 compounds belong to two different regions of the phase diagram. DFT calculations and symmetry analysis for these two compounds [2, 3] contributed to the understanding of the origin of the complex magnetic behavior of the series. In order to complete the systematic study of the series we report calculations of the magnetic properties of $UFe_{4.5}Al_{7.5}$. The latter compound belongs to the third and the most interesting region of the phase diagram with two magnetic phase transitions. The symmetry analysis determines a magnetic structure with two noncollinear sublattices which is different from that proposed in Ref. [1] This is confirmed by the calculations which yield a magnetic moment in fair agreement with experimental data. We also discuss the phase diagram of the series based on both the experimental and the ab-initio studies.

[1] M. Kuznietz et al., Phys. Rev.B, 60 9494 (1999).

[2] C. Cardoso et al., Phys. Rev. B, 65, (2002) 94413-94417

[3] L.M. Sandratskii and J. Kübler, Phys. Rev. B, 60 (1999) R6961.

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