Erratum: *Ab initio* electronic structure, magnetism, and magnetocrystalline anisotropy of UGa_2 [Phys. Rev. B 53, 9658 (1996)]

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In a recent publication,[1] we reported on a detailed theoretical study of the intermetallic compound UGa_2, including density-functional and crystal-field model calculations. One particular point in this study was the evaluation of the magnetocrystalline anisotropy energy (MAE) ΔE under three different model assumptions: itinerant U-5f states (the usual local spin-density approximation, LSDA, in a relativistic approach including spin-orbit coupling), localized $U\text{-}5f^2$ or $U\text{-}5f^3$ configurations. The MAE was found to be particularly large, $\Delta E = 564$ meV, if itinerant $5f$ behavior was assumed.

Latterly emerging new interest in the peculiar properties of UGa_2 (Refs. 2–6) led us to repeat the previous calculations with an updated version of the relativistic LCAO code (this version was also used to compute the MAE of YCo_5 and related compounds, Ref. 7). With one exception, the data published in Ref. 1 could be confirmed. The mentioned value of ΔE, however, has been found erroneous due to a wrong treatment of multicenter terms when rotating the spin quantization axis in the older version of the code. It should be replaced in Sec. III A and in Table IV of Ref. 1 by $\Delta E = -9$ meV (-100 K), now predicting an easy c axis of magnetization. The easy direction of magnetization found in different experiments (quoted in Ref. 1) is within the hexagonal plane. Thus, our previous conclusion that the itinerant LSDA approach does not describe the experimental MAE is still valid.

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