Magnetic and electronic properties of selected rare-earth chromium germanides compounds

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The ternary rare-earth based systems exhibit interesting physical and structural properties. Lots of them, eg. chromium germanides were experimentally studied concerning their magnetic properties [1] and up to our knowledge they were never studied theoretically explaining nature of their magnetic behaviour. In the presented work the magnetic and electronic properties of $RCrGe_2$ and $RCr_{0.3}Ge_2$ (R=Tb, Dy, Ho or Er) were investigated theoretically applying plane-wave DFT/PBE methodology. The computational investigations were performed for the crystallographic structure with the space group Cmcm. The stoichiometry of the rare-earth chromium germanides compounds has also significant effect on the electronic properties of compounds. The theoretically obtained structural parameters are in good agreement to the data contained in work of Bie et al [2]. The theoretical predictions are compared to the experimentally obtained results.

References:

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