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Abstract

Comparison of Band Structures of ErSb and ErNiSb Intermetallics from Ab Initio Calculations †

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Abstract: *R*NiSb intermetallics are composed of *R*-rare earth, T-transition metals, and X-p elements. This family of compounds demonstrates many outstanding properties and phenomena perspectives in functional applications. The intermetallic compounds are crystalized in the cubic half-Heusler structure (space group $F\bar{4}3$ m). Similar binary *R*Sb compounds with the same crystal structure are topological semimetals with unusual Dirac-cone-like states observed in ARPES studies. In this work, the band structure and magnetic properties of ErSb and ErNiSb compounds are investigated in the framework of the DFT+U method comprising the density functional theory and correction for strong electron correlations in Er 4f shell. The calculated magnetic properties of both alloys obtained, to be solely caused by the magnetic moments of the Er ions, provide good agreement with the experimental data. ErSb has the band structure of a topological semimetal. A narrow energy gap was found in the band structure of ErNiSb, i.e., this alloy is an indirect gap semiconductor. The energy gap in ErNiSb was calculated to be 0.25 eV due to the minority spin projection. The band structure exhibits the presence of occupied bands, which can form a hole pocket near Γ in the L-Γ-X and K-Γ directions. In the band structure of ErSb, one can find the hole pockets near the same k-point along L-Γ-X, K-Γ and an electron pocket along Γ-X-W. These bands form topological features in ErSb, in particular, and cause a semimetallic state.

Keywords: electronic structure; electronic correlations; topological materials; semimetal

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