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Topology of the band structure and magnetic properties of RSb and RNiSb materials with R = Gd, Tb, Dy

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Ternary RNiSb and binary RSb materials with R = Gd, Tb, Dy were investigated in terms of their electronic properties and band structures using density functional theory DFT+U method. This method is used to take into account strong electron correlations in the 4f shell of the rare earth metals. Our calculations showed that the considered ternary RNiSb materials are semiconductors with an indirect band gap of 0.26, 0.21, and 0.21 eV for GdNiSb, TbNiSb, and DyNiSb, respectively. Additional calculations with spin-orbit coupling resulted in the slightly increased value of the band gap in GdNiSb to 0.38 eV. The calculations for the compressed cell of GdNiSb revealed a semiconductor-to-metal transition under pressure accompanied by transformation of the band gap unto a direct one and further overlap of a few bands. In our calculations, the binary RSb compounds with R = Gd, Tb, Dy were found to be semimetals with the hole and electron pockets near high-symmetry points Γ and X. Recent optical measurements for GdSb and TbSb confirmed the semimetallic state in these materials. Moreover, the experimental conductivity spectra were found in good agreement with the theoretical interband conductivity spectra obtained from these calculations [Yu.V. Knyazev, Yu.I. Kuz'min, S.T. Baidak, A.V Lukoyanov, Solid State Sci. 136, 107085 (2023)]. The magnetic moment of all considered compounds were shown to be fully determined by magnetic moments of the rare earth elements in agreement with previously published experimental results. The results of our study were published in several scientific articles [S.T. Baidak, A.V Lukoyanov, Materials 16, 242 (2023); S.T. Baidak, A.V. Lukoyanov, Int. J. Mol. Sci. 24, 8778 (2023); R.D. Mukhachev, S.T. Baidak, A.V. Lukoyanov, J. Magn. Magn. Mater. in press].
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