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The spin-resolved electronic energy bands of the CdMnTe solid solution evaluated with the hybrid exchange-correlation functional

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The spintronics is promising for discovering a new way of data storage media in the chip-producing industries [1]. This is a branch of science and technology which employs both the charge and the spin of the electron. This requires materials which exhibit both ferromagnetic and semiconductor properties in order to combine permanent magnetic storage and the conventional electronics of semiconductors in one device [2].

Here we present the results of the investigation of the electronic structure of zinc-blende solid solution $Cd_{1-x}Mn_xTe$ (x=0.25) that was carried out within the GGA and PBE0 approaches. All the calculations have been done by means of ABINIT code [3].

Let us consider briefly the results obtained in the GGA and PBE0 approaches. In the GGA approach the strong correlations of 4d (Cd) and 3d (Mn) electrons are not taken into account whereas in the approach PBE0 they are included in calculation scheme. The parameters of the electronic energy bands for the considered here CdMnTe solid solution, obtained within the GGA, are as follows. The examined material is the direct band semiconductor for both spin orientations. The minimum optical and fundamental gaps equal 1.33 eV for spin-up, and 1.69 eV for spin-down, and both are attributed to $\Gamma - \Gamma$ transition. In case of the approach PBE0, ie with the strong correlations, the minimum optical and fundamental gaps equal 1.47 eV for spin-up, and 2.14 eV for spin-down.

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