The effect of the pressure on electronic structure of the doped solid solutions ZnSeTe:T (T=Cr, Mn, Fe)

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INTRODUCTION

Transition metal doped II-VI chalcogenide laser materials offer a unique blend of physical, spectroscopic, and technological parameters that make them the gain media of choice for cost effective broadly tunable lasing in the mid-infrared [1] photon energy range. The II-VI semiconductor hosts provide a low phonon cut-off, broad infrared transparency, and high thermal conductivity. When doped with transition metal ions, the gain media feature a four-level energy structure, an absence of excited state absorption, broad absorption bands overlapping with many convenient fiber laser sources, a broad vibronic emission band enabling wide tunability, and high - close to 100 % quantum efficiency of fluorescence at room temperature [1].

RESULTS

The electronic structure of the ZnTSeTe solid solution, doped with T={Cr, Mn, Fe} 3d transition elements, was evaluated taking into account the strong correlations of 3d electrons. The electronic energy bands and density of states in the crystal supercell ZnTSeTe have been calculated with the hybrid exchange-correlation functional PBE0 [2]. Calculations were made by means of ABINIT code in the PAW formalism. The results obtained here are shown in Figures 1-3.

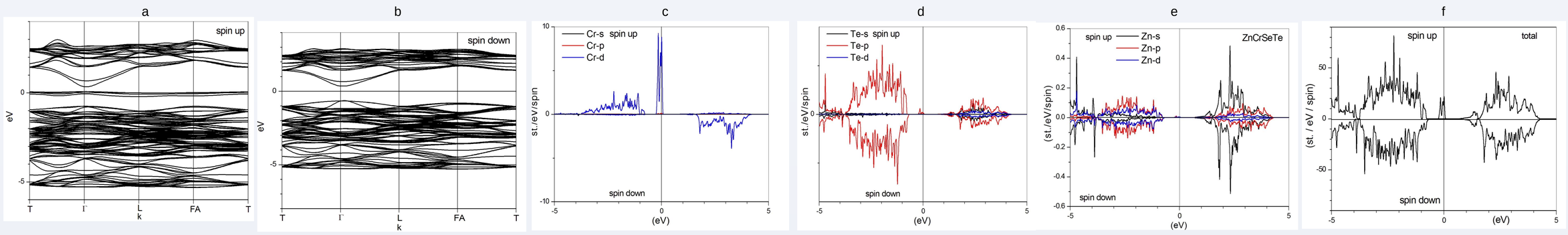

Fig. 1. Electronic energy bands of the crystal, evaluated by means of supercell Zn31Cr1Se8Te24: a – spin up; b – spin down; c and d – partial densities of electronic states on Cr and Te; e – total density of electronic states.

As can be seen from Figs 1 a, b, for the spin up states the crystal reveals metallic behaviour, and for opposite spins it is the direct band semiconductor. The Fig. 1 c shows the presence of the 3d Cr states at Fermi level. The 3d electrons are moving in narrow energy bands with a high density of states. So, here we are dealing with strongly correlated electrons, to which it is necessary to apply hybrid exchange-correlation functionals. In fig. 1d we find the dominance of the Te *p* states in the upper part of the valence band. The results shown in Fig. 1e, indicate a significant presence of s states of zinc in the conduction zone. The full density of electronic states is shown in Fig. 1 f. Its curves for opposite spins reveal a noticeable asymmetry, which indicates the existence of a non-zero magnetic moment of the supercell. The latter is equal to 4 Bohr magnetons.

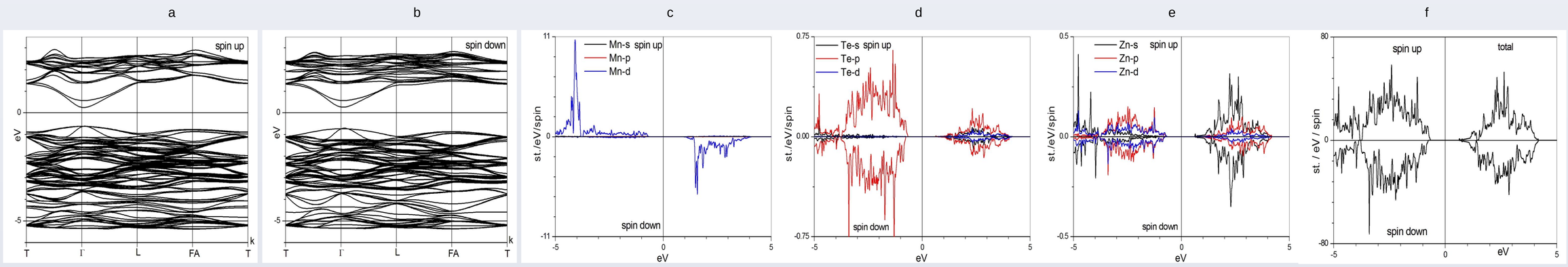

Fig. 2. Electronic energy bands of the crystal, evaluated by means of supercell Zn31Mn1Se8Te24: a – spin up; b – spin down; c, d and e – partial densities of electronic states on Cr, Te and Zn; f – total density of electronic states.

As can be seen from Figs 2 a, b, for both the spins the crystal reveals the direct band semiconductor behaviour. The Fig. 2 c shows the presence of the 3d Mn states, for up-spin states inside the valence band, and for opposite-spin states near the bottom of the conduction band. The 3d electrons are moving in narrow energy bands with a high density of states. So, here we are dealing with strongly correlated electrons, to which it is necessary to apply hybrid exchange-correlation functionals. In fig. 2d we find the dominance of the Te *p* states in the upper part of the valence band. The results shown in Fig. 1e, indicate a significant presence of s states of zinc in the conduction band. The full density of electronic states is shown in Fig. 2 f. Its curves for opposite spins reveal a noticeable asymmetry, which indicates the existence of a non-zero magnetic moment of the supercell. The latter is equal to 5 Bohr magnetons.

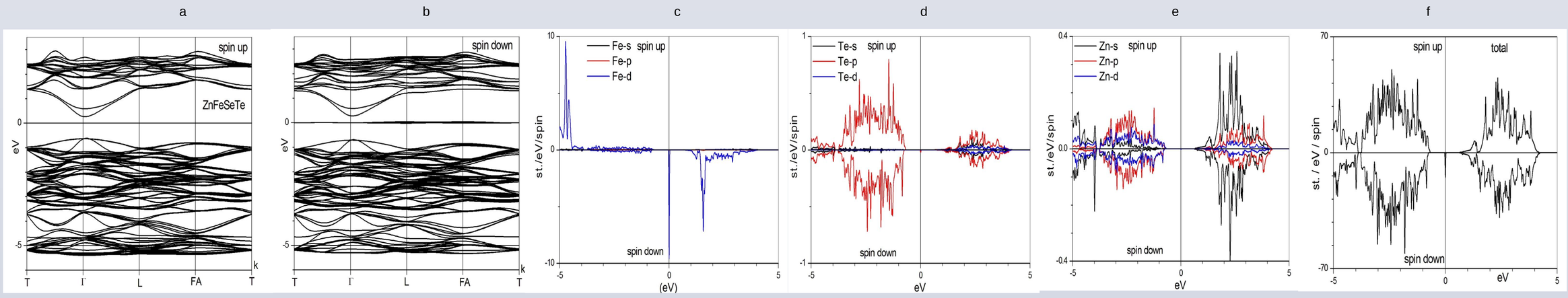

Fig. 3. Electronic energy bands of the crystal, evaluated by means of supercell Zn31Fe1Se8Te24: a – spin up; b – spin down; c, d and e – partial densities of electronic states on Cr, Te and Zn; f – total density of electronic states.

As can be seen from Figs 3 a, b, for both the spins the crystal reveals the direct band semiconductor behaviour. The Fig. 3 c shows the presence of the 3d Fe states, for up-spin states inside the valence band, and for opposite-spin states near the bottom of the conduction band. The 3d electrons are moving in narrow energy bands with a high density of states. So, here we are dealing with strongly correlated electrons, to which it is necessary to apply hybrid exchange-correlation functionals. In fig. 3d we find the dominance of the Te *p* states in the upper part of the valence band. The results shown in Fig. 3e, indicate a significant presence of s states of zinc in the conduction band. The full density of electronic states is shown in Fig. 3 f. Its curves for opposite spins reveal a noticeable asymmetry, which indicates the existence of a non-zero magnetic moment of the supercell. The latter is equal to 4 Bohr magnetons.

CONCLUSIONS

As can be seen from Figs. 1-3 the materials ZnCrSeTe and ZnFeSeTe exhibit semimetallic properties. The material ZnCrSeTe is a metal for spin-up electrons and a semiconductor for electrons with the opposite spin moment. The material ZnFeSeTe is a metal for spin-down electrons and a semiconductor for electrons with the opposite spin moment. But the ZnMnSeTe material is a semiconductor for electrons with two spin orientations. Comparing the partial densities of 3d electrons shown in Figures 1c - 3c, we conclude that the 3d electrons of Cr and Fe are present at the Fermi level, while the same electrons in the material ZnMnSeTe are localized in the valence and in the conduction band, respectively.

REFERENCES

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