The electronic structure of doped crystals Si<B, T> (T=Mn, Cr, V)

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INTRODUCTION

Investigation of semiconductors with transition metal impurities has attracted a lot of attention in the few last years. For example, in the paper [1] the magnetoresistance of Si whiskers, doped with Ni and B elements, has been studied. The electronic structure of Si crystal with transition metal impurities has been evaluated within the GGA approach on PAW basis states [2]. Here we evaluate the electronic structure taking into account the strong correlated 3d electrons of transition elements, namely Mn, Cr, V.

RESULTS

The electronic structure of the co-doped silicon was evaluated taking into account the strong correlations of 3d electrons. The electronic energy bands and density of states in the crystal supercells $Si_{14}B_1Mn_1$, $Si_{14}B_1Cr_1$ and $Si_{14}B_1V_1$ have been calculated by means of the hybrid exchange-correlation functional PBE0. Calculations were made by means of ABINIT code in the PAW formalism. The results obtained here are shown in Figures 1-3.

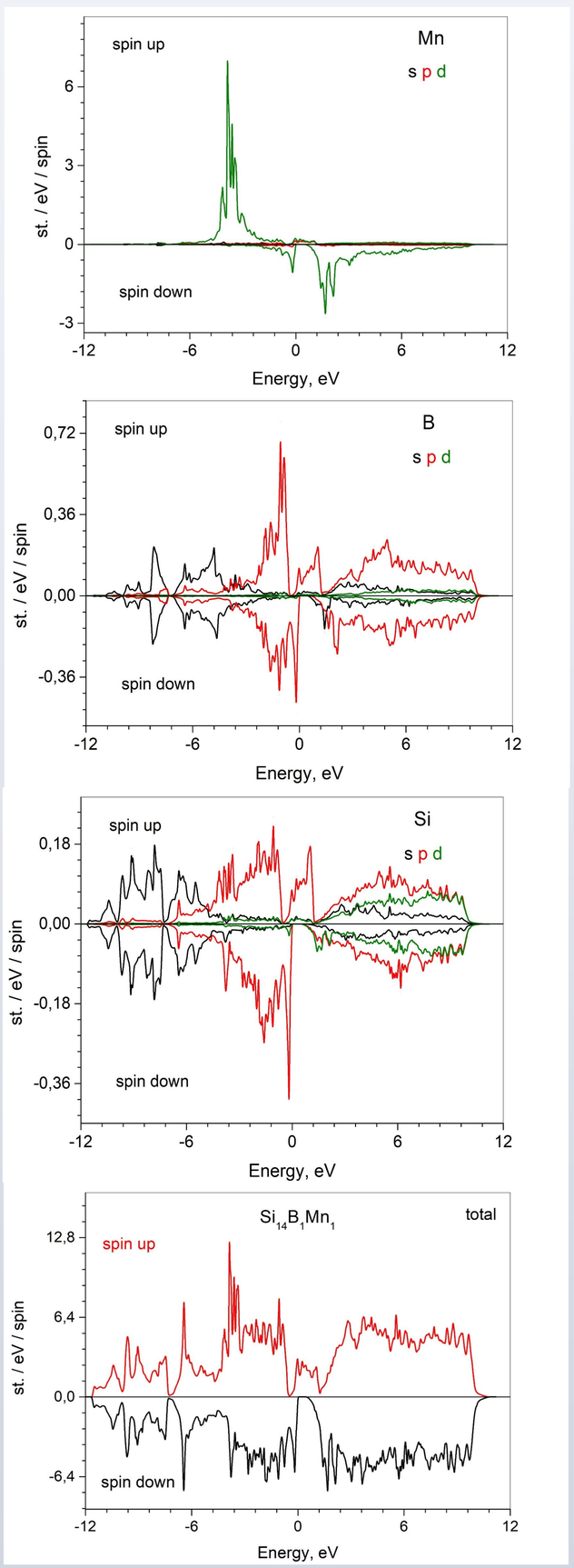

Fig. 1. The crystal $Si_{14}B_1Mn_1$: the partial density of electron states on an Mn (a), B (b), Si (c) atoms and the full density of electronic states in the crystal (d) with the orientation of the spin up and down.

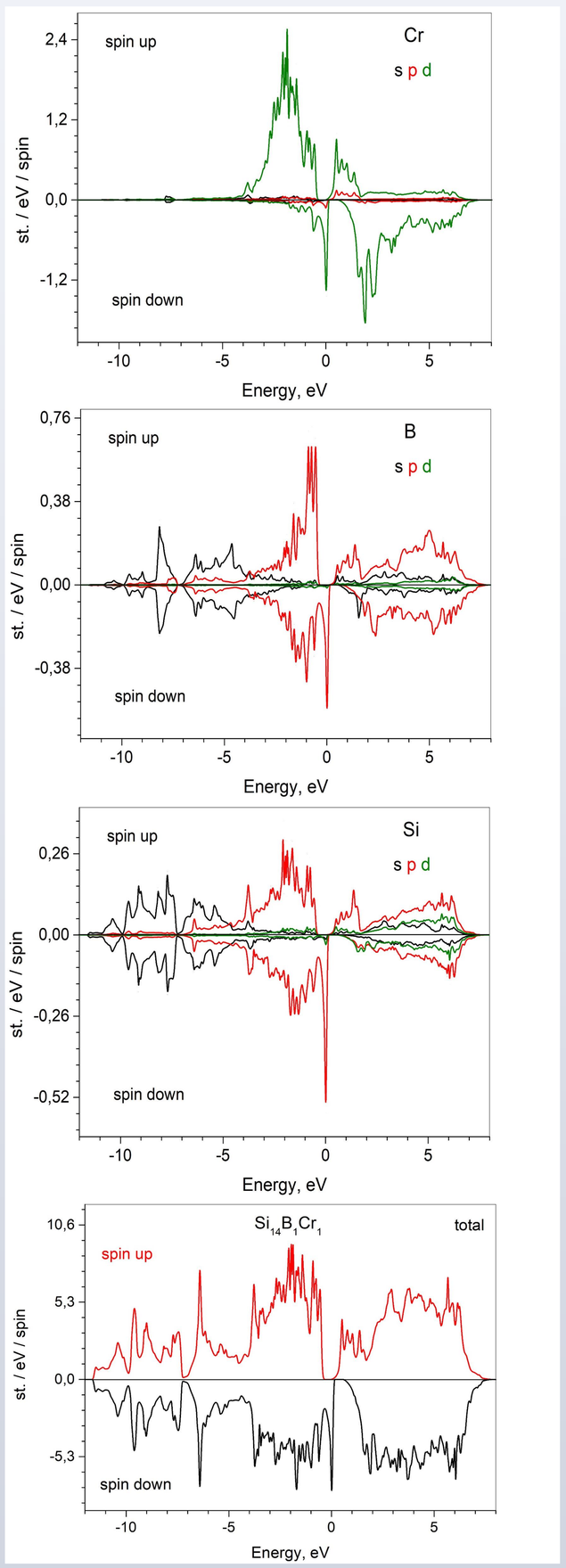

Fig. 2. The crystal $Si_{14}B_1Cr_1$: the partial density of electron states on an Cr (a), B (b), Si (c) atoms and the full density of electronic states in the crystal (d).

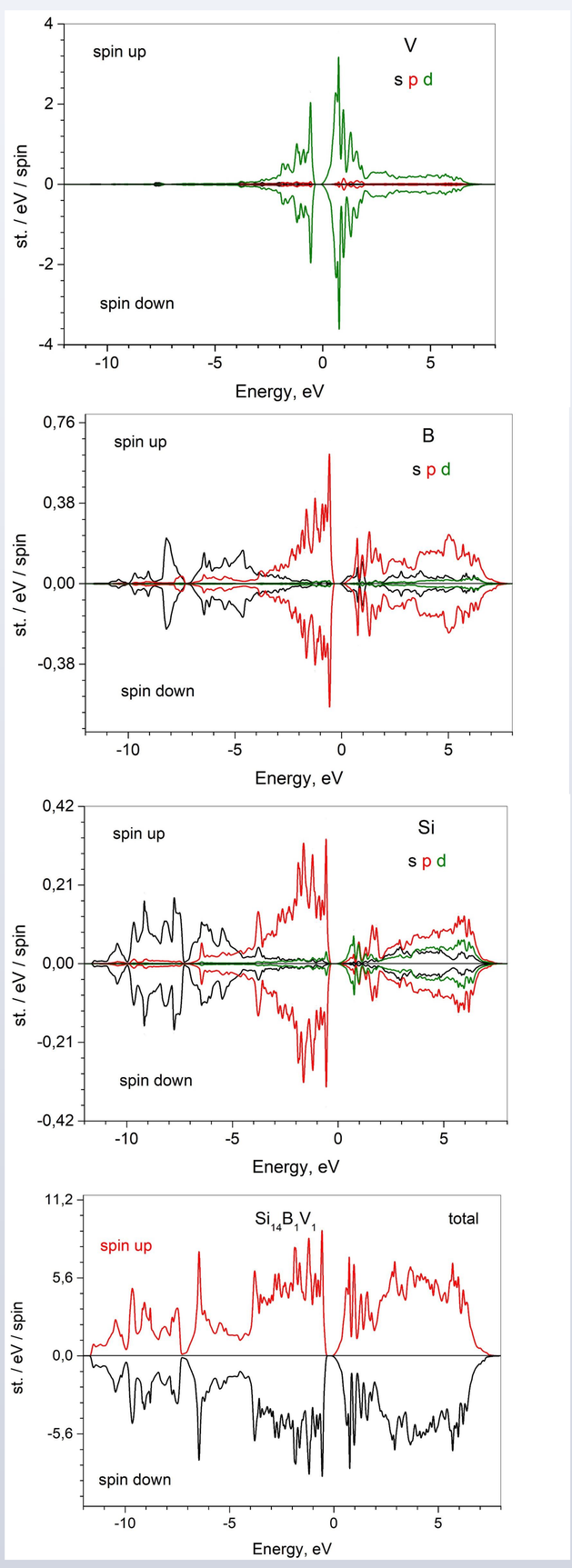

Fig. 3. The crystal $Si_{14}B_1V_1$: the partial density of electron states on an V (a), B (b), Si (c) atoms and the full density of electronic states in the crystal (d).

CONCLUSIONS

As can be seen from Fig. 1 the crystal $Si_{14}B_1Mn_1$ is a half-metal with band gap of 0.46 eV, for spin down states. Fig. 2 shows that the material $Si_{14}B_1Cr_1$ is a ferromagnetic semiconductor for both spins, and Eg=0.29 eV for spin up, and Eg=0.42 eV for spin down states, respectively. Fig. 3 confirm that the material $Si_{14}B_1V_1$ behaves like a nonmagnetic semiconductor, with Eg=0.21 eV for both spins.

REFERENCES

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2. *Zhang Z.Z., Portoens B., Kai Chang, Peeters F.M.,* First-principles study of transition metal impurities in Si // Phys. Rev. B. -2008.-**77**, 155201.-P. 1-8.