Ab initio calculations of magnetic properties of wurtzite $Al_{0.9375}TM_{0.0625}N$, (TM=V, Cr, Mn, Fe, Co, Ni)

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9.7 cm

The electronic and magnetic properties of $Al_{1-x}Mn_xN$ in zinc-blende phase were studied recently [1, 2]. In this work we have analyzed the influence of six transition metals from V to Ni on the electronic and magnetic properties of wurtzite AlN. We applied an ab initio method based on density functional theory within generalized gradient approximation (GGA) and the pseudopotential method [3]. The spin polarized self-consistent calculations were made for the supercell of 32 atoms. The transition metal was substituted in the place of Al.

In case of Co, Cr and Mn the electronic states at the Fermi level are 100% spin polarized. In other cases we obtain zero density of states at Fermi level.

References

[1] R. de Paiva et al., J. Appl. Phys. **96**, 6565 (2004)

[2] M.B. Konoun et al., J. Phys. D Appl. Phys. **38**, 1853 (2005)

[3] S. Baroni, A. Dal Corso, S. de Gironcoli, P. Giannozzi et al., www.pwscf.org

13.4 cm

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