Crossroads electronic structure of MnS, MnSe, and MnTe*

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Using the LDA+U method, we have investigated the electronic structures of MnB^{VI} (B^{VI}=S,Se,Te) which are end-point materials for wide gap semiconductors, $A^{II}_{1-x}Mn_xB^{VI}$(A^{II}=Zn,Cd,Hg) using parameters calculated by the so called solid atom method. All these MnB^{VI} compounds have semiconducting electronic structures in the antiferromagnetic phase. The character of each energy gap is on the crossroads between charge transfer type insulators and band insulators. The LDA+U method yields enhanced energy gaps and magnetic moments, as compared to those of the LDA method in agreement with experimental values. Based on the LDA+U total energy results, we have identified the character of peaks observed in photoemission experiments, and have derived an understanding of the tendency of Neel temperatures in MnB^{VI} to increase with anionic atomic number.

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