ELECTRONIC PROPERTIES OF $TM_3V_2O_8$ TM=Mn,Fe and Ni COMPOUNDS

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9.7 cm

$Mn_3V_2O_8$, $Fe_3V_2O_8$ and $Ni_3V_2O_8$ compounds are interesting magnetic materials that have a complex magnetic order in the kagome staircase. The magnetic and optical properties of $TM_3V_2O_8$ compounds were studied experimentally and theoretically in the last years [1-5]. In this work we present the electronic structure and magnetic properties of $TM_3V_2O_8$ for TM=Mn, Fe and Ni compounds calculated by full relativistic FPLO [6] method within in the local spin density approximation. In the LSD+U scheme the values of U parameters were assumed in the range from 5 eV to 7eV for TM elements.These compound have the orthorhombic (Cmca) crystal stucture [1]. The band calculations were performed for the experimental lattice parameters [1-5].

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13.4 cm

Subject category :

3. Magnetic Structure and Dynamics

Presentation mode :
poster

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