LMTO STUDY OF Al_6Mn: BAND-STRUCTURE CALCULATIONS AND THE CHARGE DISTRIBUTION

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9.7 cm

The crystalline Al_6Mn has the orthorhombic structure (Cmcm) and includes 28 atoms in a unit cell. The Mn atom is surrounded by ten Al atoms. From the experimental data the electron density distribution (EDD) maps were constructed and the number of valence electrons for each atom was estimated. The charge transfer from Al atoms to an Mn atom on the grounds of both an x-ray diffraction experiment and an analysis by the maximum-entropy method (MEM) was found. Results have shown strong covalent bonds beetween Al and Mn atoms and a strong ionic character of thes bonds [1].
In this comunication, we have studied the electron density distribution of Al_6Mn by the ab initio tight binding linearized muffin-tin orbital (TB-LMTO) method. The LMTO calculations have shown that the charge transfer from Al atoms to an Mn atom depends on the Wigner-Saitz radii. This method is used to construct the EDD maps in elementary cell and to calculate the photoemission spectrum.

[1] K. Yamamoto, Y. Matsuo, J. Phys.: Condens. Matter **12**, 2359 (2000)

13.4 cm

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