Topological description of the half-metallic transition of MnAs

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Abstract
Topological analysis of the electronic charge density is introduced as a new tool for studying the electronic properties of the materials. In this method, the eigen values of the Hessian matrix of the electronic charge density as an scalar field are used to estimate the strength of the atomic bonds. We employ this method to study the half-metallic phase transition of MnAs in zinc blende structure. The results show that the topology of the electron density is preserved in this phase transition. So the total magnetization as the order parameter of the system changes continually and the phase transition is regarded as a second order transition. The geometrical changes observed in the electron density are interpreted by investigating the electronic structure.

Keywords: density functional theory, electronic structure, spintronics

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