

Magnetism of Ag_2Se : a first principles study

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Silver chalcogenide Ag_2Se is well-known to exhibit unusual magnetoresistance: large and linear magnetoresistance for a magnetic field up to 6 Tesla in temperature range from 5 to 500 K [1]. Origin of this behavior is still unclear. Ferromagnetism of Ag_2Se is observed in a recent SQUID measurement at room temperature. In this study, by using the density functional theory, we investigate effects of intrinsic defects on the magnetic properties of Ag_2Se . It is found that the intrinsic defects such as silver (V_{Ag}) and selenium (V_{Se}) vacancy do not show any magnetism both in bulk and thin films. However, with a certain combination of intrinsic defects in the thin film, magnetism was observed, which suggests that a defect cluster may induce the magnetism. Detailed electronic structure of the system is provided to discuss the magnetism.

Reference

- [1] R. Xu, A. Husmann, T. F. Rosenbaum, M.-L. Saboungi, J. E. Enderby, and P. B. Littlewood, *Nature* **390**, 57 (1997)

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