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First-principles study of Berry curvature and intrinsic anomalous Hall conductivity in ferromagnetic materials using Maximally localized Wannier function

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Abstract

Electronic properties for bcc Fe and hcp Co in bulk state and also Fe-Co alloy were calculated by quantum calculation based on density functional theory and pseudopotential method. Combination of Wannier function and Berry phase theory was used for calculation of anomalous Hall conductivity in above structures. It was seen that split of band by the spin orbit interaction, lying on the Fermi level, has a major role in Berry curvature. Acquired results agree with experimental ones and thus it seems that conductivity in bulk state is intrinsic.

Keywords: Maximally localized Wannier function, Fe, Co, Fe-Co alloy, Berry curvature, intrinsic anomalous Hall conductivity

For full article, refer to the Persian section