2003 Vol.40 No.4 pp.499-502 DOI:

First-Principles Studies for the Electronic Structures of Diluted Magnetic Semiconductors (Ga, Fe)As

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(Received: 2003-2-10; Revised:)

Abstract: First-principles LMTO-ASA band calculations are performed for $Ga_{1-x}Fe_xAs$ (x=1, 1/4, 1/8) by assuming supercell structures. It is found that the antiferromagnetic (AFM) state is stable for x=1/4. For x=1/8, ferromagnetic (FM) state is more stable than AFM state, and no stable magnetic state exists for x=1. In both the cases the magnetic moments of As and Ga atoms are parallel to those of the nearest Fe atoms due to the p-d hybridization. Further, the band structure shows rather localized Fe 3d state in the gap, and the parallel polarization is confined rather in the vicinity of Fe site.

PACS: 72.80.Ey, 75.50.Pp, 75.30.Hx, 75.50.Dd
Key words: diluted magnetic semiconductor, electronic band calculation, ferromagnetism

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