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Magnetism of IV-VI compound based DMS HITOSHI FUJII, TETSUYA FUKUSHIMA, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — The electronic structure and the magnetic properties of Mn doped GeTe, which is IV-VI compound semiconductor based dilute magnetic semiconductors (DMS), are calculated from first principles. Although the ferromagnetism was discovered in GeMnTe before III-V compound DMS systems [1], IV-VI DMS have not been so popular in DMS community due to the low Curie temperature and the incompatibility with present electronic materials. However, the carrier concentration and hence the magnetic properties can be controlled easily by forming Ge vacancies. In this work, in order to discuss potentiality of IV-VI DMS systems as semiconductor spintronics materials, the electronic structure are calculated based on the local density approximation and we use the Korringa-Kohn-Rostoker coherent potential approximation method [2]. The magnetic exchange interactions between Mn impurities are calculated by using the Lichitenstein's method [3]. Based on the calculation results, we will also discuss the Curie temperature by using Monte Carlo simulations.

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