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First-principles Study on the Magnetic Interaction in ZnO-based Dilute Magnetic Semiconductors MASAYUKI TOYODA, The Institute of Scientific and Industrial Research, Osaka University, HISAZUMI AKAI, Graduate School of Science, Osaka University, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA, The Institute of Scientific and Industrial Research, Osaka University — Using first-principles calculations, we investigate the electronic structures and magnetic properties of dilute magnetic semiconductors (DMS). The electronic structures are calculated by using Korringa-Kohn-Rostoker method combined with the coherent potential approximation. Since the d electrons of the magnetic impurity in DMS are strongly localized, we apply self-interaction correction to the local density approximation for the exchange-correlation energy. From the first-principles results, we evaluate the magnetic exchange interaction J_{ij} between the pairs of magnetic impurities by using the Lichtenstein's formula. We found that the magnetic interaction in ZnO-based DMS is basically antiferromagnetic without any additional carrier because of large energy gaps between the occupied and unoccupied d states. We will also discuss about the carrier dependence of the magnetic interaction in ZnO-based DMS.

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