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On the possibility of ferromagnetism in MgX (X = O, S, Se) with/without conventional magnetic atoms VAN AN DINH, ISIR, Osaka University, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA — We present a first principle study on the half-metallicity and ferromagnetism in rock salt MgZ (Z = O, S and Se) with and without conventional magnetic elements. The electronic structure, effective exchange coupling constant and chemical pair interaction are calculated within SIC-LSDA. The Curie temperature is predicted by performing Monte Carlo simulation. A possibility of spinodal decomposition is investigated and simulated. For transition-metal-doped MgO, our results reflect the observation in the experiment [1]. Without oxygen vacancy, Co- and Ni-doped MgO is anti-ferromagnetic. Except Ti and Cr, another transition metals cause the anti-ferromagnetic behavior in MgO. The ferromagnetism can be stabilized by oxygen vacancies. Oxygen vacancies also change the chemical interaction trend of transition metal atoms, and cause an inhomogeneous distribution in MgO. It is also found that N atoms which substitute for anions can introduce the half- metallic ground state and ferromagnetism in MgZ. Monte Carlo simulation shows the above room temperature ferromagnetism in $Mg_{0.8}N_{0.2}Z$. Nitrogen atoms in MgO and MgS have a tendency to create clusters, whereas the distribution of N atoms in MgSe is homogeneous at dilute regime. [1]. J. Narayan *et al.*, Appl. Phys. Lett. **93** (2008) 082507.

Van An Dinh
ISIR, Osaka University

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