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**Chemical trend of exchange coupling in II-VI diluted magnetic semiconductors** THOMAS CHANIER, University of Iowa, Iowa City, Iowa, USA, ROLAND HAYN, FRANÇOIS VIROT, IM2NP, Marseille, France — We present an ab-initio study of the magnetic couplings in Mn- and Co-doped II-VI DMS ZnA (A=O,S,Se,Te). We show the necessity of taking into account the strong electron correlation on the transition metal (TM) 3d level to reproduce correctly the experimental chemical trend. Within the LSDA+U (local spin density approximation with a Hubbard-type correction to TM 3d electrons), we find (i) the d-d exchange couplings between nearest-neighbor magnetic ions to be antiferromagnetic (AFM) of the order of -1 meV and (ii) the sp-d exchange constants between magnetic ions and conduction (valence) band electrons (holes) N$\alpha$ (N$\beta$) to be FM (AFM) of the order of 0.1 eV (-1 eV). In ZnMnO and ZnCoO, the strong p-d hybridisation leads to the presence of a bound state above the valence band, the failure of the commonly-used Larson perturbation theory formulae for p-d and d-d exchange interactions [1] and prevents high-Tc ferromagnetism [2].
[1] B. Larson *et al.* , PRB 37, 4137 (1988)
[2] T. Chanier *et al.* , PRB 79, 205204 (2009)

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