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Hybrid Hartree-Fock density functional study of transition-metal doped ZnO JESUAN BETANCOURT, ALAN KALITSOV, JULIAN VELEV, University of Puerto Rico — Dilute magnetic semiconductors (DMS) obtained by doping semiconductors with transition metals (TM) hold much promise for spintronics. Transition metal doped ZnO (ZnO:TM) has been investigated for a possible room-temperature DMS. Density functional theory gives incorrect prediction for the band gap of ZnO which leads to diverging interpretations for the magnetic behavior of ZnO:TM [1,2]. Here we report Heyd-Scuseria-Ernzerhof (HSE) hybrid functional study of the electronic structure of ZnO:TM (TM=Cu, Ni, Co, Fe, Mn). The hybrid functional corrects for both the bandgap problem on the host and the lack of correlation in the impurity, without the use of *ad-hoc* intra-atomic potentials. Our results show although the HSE opens the band gap of the host, the Hubbard splitting of the impurity levels makes the empty impurity levels reside in the host conduction band. This leaves open the possibility for spin polarized carriers. We discuss the validity of the results and explore their implications for the magnetic behavior of ZnO:TM. [1] H. Raebiger, S. Lany, and A. Zunger, Physical Review B 79, 165202 (2009). [2] P. Gopal and N. A. Spaldin, Phys.l Review B 74, 094418 (2006).

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