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**The spin polarized electronic structures and magnetic properties of Co doped and Ga codoped ZnO** M.-H. TSAI, T.-Y. JIANG, C.-Y. HUANG, National Sun Yat-Sen University — The understanding of the magnetic property of Co doped ZnO (ZnO:Co) has been inconclusive with confusing experimental observations. Here, spin-polarized first-principles calculations have been performed for ZnO:Co to better understand its magnetic property. Without O and Zn vacancies, the total energy per Co ion in ZnO:Co in the ferromagnetic (FM) state was found to be only 6meV lower than that in the antiferromagnetic (AFM) state, which suggests that at room or higher temperature ZnO:Co is in the spin glass state. O vacancies and co-doping with Ga ions were found to enhance Co-Co FM coupling by induced delocalized states in the vicinity of Co 3d bands. The O vacancy was found to have a greater effect of FM enhancement than the co-doped Ga ion. While Zn vacancies were found to lower the Fermi level and enhance hybridization between Co 3d and valence-band O 2p states, which enhances super-exchange coupling and renders ZnO:Co to be in the AFM state. The opposite effects of O and Zn vacancies imply that the magnetic property of ZnO:Co depends strongly on the relative concentrations of O and Zn vacancies.

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