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Electron mediated ferromagnetism in cobalt doped ZnO[1] SU-HUAI WEI, ARON WALSH, JUAREZ L.F. DA SILVA, National Renewable Energy Laboratory — The potential to simultaneously tune both charge and spin in spintronic materials has lead to great interest in searching room temperature dilute ferromagnetic semiconductors. Among them, cobalt doped ZnO has become a focus of attention due to its reported high T_C and reversible cycling of FM ordering. Coupled with existing optical and electrical properties of ZnO, this makes it a potentially technologically essential material. However, the mechanism that leads to ferromagnetism in ZnO:Co is still under debate. Using band structure methods, we show that pure ZnO:Co has a weak preference for antiferromagnetic ordering. Stabilization of ferromagnetism is achieved only after the spin- down Co t_{2d} states are occupied through n-type doping. Our results are compared with available experimental data and results obtained from different levels of theoretical calculations. The limitations of the methods adopted in previous calculations are discussed.

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