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Carrier-mediated Ferromagnetism in N Co-doped (Zn, Mn)O (10 0) Thin Film SUN QIANG, QIAN WANG, PURU JENA, Virginia Commonwealth University, YOSHI KAWAZOE, Tohoku University — Considerable experimental work is available on the (Zn, Mn)O system. However, the results have been rather controversial. While some groups have reported ferromagnetism in (Zn, Mn)O systems, others report observations of anti-ferromagnetic or spin-glass behavior. Using first principles calculations based on the density functional theory and generalized gradient approximation we show that the ground state of Mn doped ZnO $(10\bar{1}0)$ thin film changes from antiferromagnetic to ferromagnetic when co-doped with N. The ferromagnetic coupling between Mn spins arises due to the overlap between N 2p and Mn 3d electrons in the spin up band, rendering the system half-metallic character.

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