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First-principles study of the effect of vacancies on magnetic properties YOSHI KAWAZOE, Tohoku University, QIAN WANG, Virginia Commonwealth University, QIANG SUN, Peking University and Virginia Commonwealth University, PURU JENA, Virginia Commonwealth University — Due to the high solubility of Co in ZnO, the magnetic properties of Co-doped ZnO thin films have been extensively studied experimentally. Unfortunately, these results have led to diverse conclusions. To better understand the origin of the controversial experimental findings, we have carried out detailed theoretical studies, focusing on the role of concentration and distribution of Zn and O vacancies on the magnetism of Zn1-xCoxO thin films. We find that when Co atoms are substitutionally doped in ZnO thin films without any defects, the magnetic coupling between Co atoms is intrinsically anti-ferromagnetic. The coupling, however, changes to ferromagnetic when sufficient oxygen vacancies are introduced. On the other hand, Zn vacancies stabilize the anti-ferromagnetic coupling, in sharp contrast with that found in Zn1-xMnxO thin films. Our theoretical studies explain the origin of the different magnetic behavior observed experimentally.

Yoshi Kawazoe
Tohoku University

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