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**Zinc Vacancy induced magnetism in ZnO thin films and nanowires**

QIAN WANG, Virginia Commonwealth University, QIANG SUN, Peking University, PURU JENA, Virginia Commonwealth University — Extensive theoretical studies based on first-principles have been carried out for the mechanism of magnetism in ZnO thin films and nanowires. It has been identified that the observed magnetism is introduced by Zn vacancy and is affected by its concentration. The main source of the magnetic moment comes from the unpaired 2p- electrons in oxygen sites around the Zn vacancy, instead of Zn 3d electrons. Moreover, Zn vacancy is more energetically favorable to reside on the surface, and its formation energy is found to be less than that of oxygen vacancy that does not introduce any magnetism. These findings suggest that the main vacancy species is Zn vacancy as expected by experiments. The present theoretical study not only provides some deep understandings for the experimentally observed magnetism in un-doped ZnO samples, but also suggests that introducing Zn vacancy is a natural and an effective way to fabricate magnetic ZnO structure for bio-magnetic applications.

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