Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

A First-Principles Study of Zinc Oxide Honeycomb Structures

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We present a first-principles study of the atomic, electronic and magnetic properties of two dimensional (2D), single and bilayer ZnO in honeycomb structure and its armchair and zigzag nanoribbons. In order to reveal the dimensionality effects, our study includes also bulk ZnO in wurtzite, zincblende and hexagonal structures. The stability of 2D ZnO, its nanoribbons and flakes are analyzed by phonon frequency, as well as by finite temperature ab-initio MD simulations. 2D ZnO and its armchair nanoribbons are nonmagnetic semiconductors, but acquire net magnetic moment upon the creation of zinc vacancy defect. Zigzag ZnO nanoribbons are ferromagnetic metals with spins localized at the oxygen atoms at the edges and have high spin polarization at the Fermi level. However, they change to nonmagnetic metal upon termination of their edges with hydrogen atoms. Under tensile stress the nanoribbons are deformed elastically maintaining honeycomb like structure, but yield at high strains. Beyond yielding point honeycomb like structure undergo a structural change and deform plastically by forming large polygons. The variation of the electronic and magnetic properties of these nanoribbons have been examined under strain.

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Date submitted: 09 Dec 2009 Electronic form version 1.4