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Magnetism in Zigzag and Armchair CuO Nanoribbons: *Ab-Initio* Analysis

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Received: October 10, 2020

Revised: October 10, 2020

Accepted: October 16, 2020

The present work reports the magnetism analysis of zigzag and armchair forms of CuO nanoribbons by using density functional theory (DFT) based on *ab-initio* approach. The structural stability has been confirmed through the binding energy calculation. The electronic and magnetic properties have been analyzed as a function of varied width of CuO nanoribbons, interesting information for variety of applications. The metallic and ferromagnetic behaviors of CuO nanoribbons are observed, whereas its bulk counterpart shows a p-type semiconducting and antiferromagnetic nature. The computed magnetic moments for the zigzag and armchair forms of CuO nanoribbon are in the ranges of 0.19–0.61 μ_B and 0.24–0.97 μ_B , respectively. The computed spin polarizations confirms the half or full metallic ferromagnetic nature of these nanoribbons.

Keywords: CuO, nanoribbon, DFT + *U*, magnetic moment, ferromagnetism, spin polarization, band structure.