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DFT Analysis of Ferromagnetism in Zigzag and Armchair CuO Nanosheets

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We report the structural, electronic, and magnetic properties of „zigzag“ and „armchair“ CuO nanosheets. The density function theory (DFT)-based *ab-initio* approach has been applied through revised Perdew, Burke, and Ernzerhof (rPBE) parameterized spin generalized-gradient approximation (SGGA) + mean-field Hubbard correction (U) exchange-correlation functional. In comparison to the semiconducting bulk CuO, the other forms of CuO nanosheets show metallic behavior and their structural stabilities have been analysed through binding energy estimation. Using SGGA, the computed magnetic moment per atom of zigzag CuO nanosheet varies irregularly between 0.66 and 1.19 μ_B, whereas for armchair CuO, between 0.59 and 1.53 μ_B. The addition of U changes this variation from 0.68 to 0.76 μ_B in zigzag and from 0.62 to 1.29 μ_B in armchair nanosheets, respectively. The computed spin polarization as unity or less than unity identifies the ferromagnetism in these materials. Obtained results of CuO nanosheets defend them as a potential candidate for a variety of electronic devices like gas sensors, electrodes, energy storage devices, etc.

Keywords: CuO, nanosheet, DFT, electronic properties, magnetic moment, SGGA.