

Spin polarization of CuO nanowires

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Experimentally, the evidence of oxygen induced spin polarization in one dimensional Cu nanowires has been obtained [1,2]. In order to investigate the peculiar magnetic properties occurred in Cu nanowires, we have theoretically investigated if a 1D Cu nanowire can display spin polarized phase with the full potential linearized augmented plane wave (FLAPW). We found that the oxygen has substantial influence on the realization of ferromagnetism in 1D Cu atomic chain. It was found that the free standing Cu atomic chain has no magnetic phase. Nonetheless, the CuO diatomic chains maintained ferromagnetic state when the Cu-O inter atomic distance is large than the equilibrium one. We analyzed the m-resolved DOS features and discussed. Besides, the magnetic anisotropy calculation revealed that the direction of magnetization is perpendicular to the chain axis.

1. D.M Gillingham, C. Müller, and J.A.C Bland, *J. Phys: Condens. Mater.*, **15**, L291 (2003).

2. D.M Gillingham, C. Müller, and J.A.C Bland, *J. Appl. Phys.* **95**, 6995 (2004).