Electronic and Magnetic Properties of CuO and Cu2O:Bulk to Nanosystems

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Abstract

The structural stability, electronic band structure and magnetic properties of zigzag ($4 \leq n \leq 12$) and armchair ($3 \leq n \leq 8$) copper oxide nanotubes and cuprous Oxide have been analyzed by employing a standard Density Functional Theory based ab-intio approach using spin polarized generalized gradient approximation with revised Perdew Burke Ernzerhoff type parameterization.

In case of CuO, the binding energy of both zigzag as well as armchair nanotubes are found to be increased with increasing diameter. Whereas, calculated total magnetic moment decreases with increasing diameter. Among the considered chiralities, (5, 5) armchair (diameter 9.08 Å) and (9, 0) zigzag (diameter 9.47 Å) CuO nanotubes show highest degree of spin polarization, however total magnetic moment is found to be highest for (4, 0) zigzag and (3, 3) armchair CuO nanotubes. The computed electronic properties of considered CuO Nanotube, confirms the metallic nature of these nanotubes. Further we have investigated temperature and size dependence magnetic moment of zigzag (n, 0) (n= 4, 6, 8, 10) copper oxide nanotubes (CuO NTs). Bond length, binding energy and total magnetic moment have been analysed and found to be that the bond length decreases with increasing size of the nanotube. Highest binding energy of (10, 0) confirms this as the most stable amongst all the NTs taken into consideration. From the calculation It is also found that magnetic moment of NTs (n,0) first increase up to room temperature (300K) and then decreases for all NTs except (8, 0).

Incase of Cu2O, the stability of Nanowires increases with increase in diameters. Nanowires exhibit half metallic with 100% spin polarization at fermi level contrast to bulk Cu2O is p type direct band gap Semiconductor.Half metallic and magnetic moments comes from strong hybridization between Cu-3d and O-2p. Nano wires of hexagonal cross sectional shows high magnetic moments per unit cell than square cross sectional for comparative diameters.

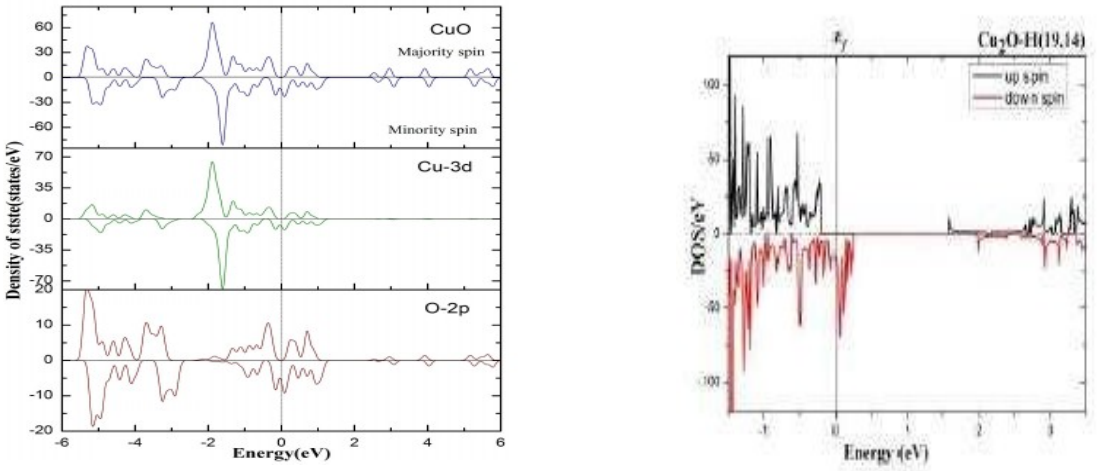


Fig1.Density of states for CuO (5,5) nanotubes and Cu2O(19,14) with hexagonal cross sectional Nanowire.

Recent Publications

1. Andrés A. , Chico L. , and Jaskólski W. (2008). *Phys. Rev. B*, 77(8):085435.
2. Miao J., Hu W., Guo N., Lu Z., XumingZou L., Liao S. S., et al. (2014). *ACS Nano* **8** (4): 3628–3635.
3. Paudel S., Dandeliya S., Chaurasiya R., Srivastava A., Kaphle, G. C. (2016). *J. Magn. and Magn. Mater.,406:8-14.*
4. Robertson J. (2004). *Mater. Today*, 7 (10): 46-52.
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Biography

Dr Gopi Chandra Kaphle is an Associate Professor of Central Department of Physics(CDP), TU. He has 16 years of experience in Physics research, teaching and training. To his credit, Dr Kaphle has published over 15 research articles.

His major contribution is on the Condensed Matter Physics, Material sciences as well as Science and Technology education in Nepal. He also has collaborative work in India and German related to research in Material sciences which ultimately help to developed the field of Science and Technology in Nepal. Dr Kaphle is an active member of several organization related to Science and Technology like Nepal Physical Society, Hydra Research and Policy center, IOST, TU, IEEE/EDS Nepal Chapter, Magnetic Society of India etc.

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