THE STUDY OF SOME ELECTRICAL PROPERTIES OF Cu_2O COMPOUND BY *AB-INITIO* METHODS

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The cuprous oxide (Cu_2O) it is evidenced by high stability, natural abundance, non-toxicity, low production costs and remarkable electrical properties. All this makes possible a wide range of applications like gas sensor, catalyst, negative electrode for lithium batteries and solar cells. Considering the design of Cu_2O-based materials with improved electrical properties, a useful tool in this endeavor consists of a theoretical study based on *ab-intio* methods, possibly due to the development of specialized packages on cuanto-chemical calculations. A first stage consists in determining the calculation parameters for the original structures, a kind of calibration of them. So it is necessary to calculate the basic properties-such as the band structure, respectively the density of states of the original material.

Keywords: cuprous oxide, band structure, density of states.

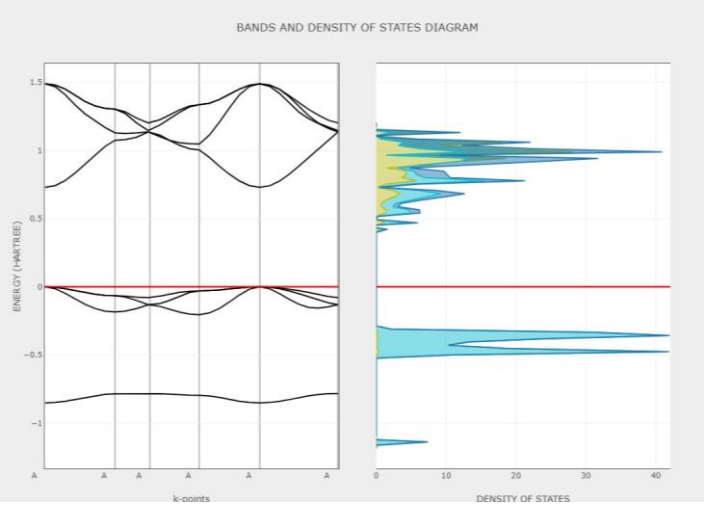

Fig.1 Band structure and density of states of Cu_2O

References

1. N-Type Conductivity of Cu_2O thin film prepared in basic aqueosus solution under hydrothermal conditions. Daniel Ursu, Nicolae Miclau, Marinela Miclau Electronic Materials Letters (2018) 14, 405-412
2. Investigation of the p-type dye-sensitized solar cell based on full Cu_2O electrodes. Daniel Ursu, Melinda Vajda, Marinela Miclau. Journal of Alloys and Compounds 802 (2019) 86-92.
3. First principle investigation of hydrogen behavior in M doped Cu2O (M= Na, Li and Ti)
   A.Larabi. A. Mahmoudi, M.Mebarki, M.Dergal. Condensed Matter Physics , 2019, vol.22, No.2 23702:1-11.