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Structural and electronic modeling of Cuprum Oxide

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Abstract:

Recently, the Copper Oxide (Cu_2O) has been used in the fabrication of photovoltaics diodes devices and in the preparation of high sensibility gas sensors. These applications is due to its great characteristics of electrical rectification, photovoltaic performance and the good interaction of the experimental surface of the Cu_2O with gases [1-2]. The Cu_2O has a simple cubic structure (space group Pn-3m) and a band gap about 2.0 eV, a fact the helps to explain its electrical properties [3]. Figure 1 presents the unitcell of the studied Cu_2O.

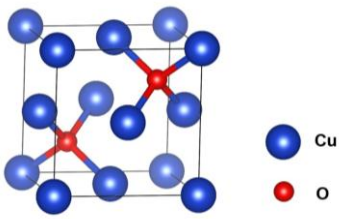

Figure 1: unitcell of the Cu_2O

This work consisted in a quantum computational study applied in the Cu_2O system in order to provide electronic information allowing the explanation of experimental properties. The calculations have been carried out according the DFT method implemented in the CRYSTAL package [4]. Two hybrid functionals, B3LYP e HSE06, and a set of copper Gaussian basis[5–7] were used to define the best theoretical conditions in order to compare with the experimental systems. The oxygen orbitals were described according to the 6-2111d1G basis [8]. All the calculations were performed as open-shell and the initial unitcell parameters were set according the experimental information found in ICSD 52043 card [9].

The gap energy and vibrational frequencies of the optimized structure indicated that the B3LYP functional associated to the base functions provide a better rapprochement when compared with the experimental result. Table 1 depict the structural parameters and the gap energy of the calculations.

Table 1: Structural parameters (*a*, Å) and band gap energy (E gap , eV) of the Cu_2O.

Functional	E_{gap}	*Lattice parameter (a)*
B3LYP	2,18	4,26
HSE06	2,12	4,21
Experimental result	2,20	4,27

The best combination functional and basis was used to elaborate a detailed study of density of states and electronic band transitions.

Keywords: Cu_2O, DFT, Theoretical modeling.

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