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Optical capabilities in copper oxides, a density functional study

Copper oxides have attracted a lot of interest due to their photo-catalytic applications in solar cells, water splitting and CO 2 reduction. They are novel candidates to provision of clean renewable routes to fuels. These processes require that copper oxides should have a higher solar conversion efficiency which is to this date reported to be low for cost-effective applications. Previous studies hint the possibility of lattice distortions on Cu 2 O and CuO to boost their optical capabilities but details on their photo-absorption in the distorted regime are still unclear and thus limited applicability. The authors here in employ the state-of-the-art ab initio methods to study the photo-absorption in Cu 2 O, CuO and Cu 4 O 3 for solar cells applications. All the calculations will be done in the density functional theory (DFT) framework as implemented in the Quantum ESPRESSO package. Post-processing of the preliminary data will be done using the Yambo code that solves the Bethe-Salpeter equation to obtain the optical absorption spectra. The findings in this work are expected to enhance photo-response in copper oxides for solar cells applications.

Keywords

Key Key words: copper oxides, first-principles, Density functional theory.

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