Charge distribution in $YBa_2Cu_3O_7$ and $YBa_2Cu_4O_8$ by density functional theory

ABSTRACT

In this work, we analyze the electronic structure and charge distribution of the YBCO family compounds Y-123 and Y-124 bulk using the density functional theory. The band structures and the density of states of the compounds are shown. The charge transfers between the atoms in the two compounds are compared and discussed in detail. The lattice parameters obtained by Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm are compared with the experimental parameters. The critical differences of the charge distribution for these two compounds are discussed.

Keyword: Band structure; Charge distribution; Charge reservoir; Cooper pair; Density functional theory; Density of state; Y-123; Y-124; YBCO