

Reverse Monte Carlo CuO local structure studies across magnetic transitions (T = 10 - 300K) from EXAFS data

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CuO is a classical material with many interesting properties as catalyst, multiferroic, photovoltaics, and as a building block for superconductors with a rich phase diagram [1,2].

Here we look on the early results of refining what is called local structure from Cu *K*-edge x-ray absorption fine structure (XAFS) spectra applying reverse Monte Carlo combined with evolutionary algorithm (EvAX tool, developed by Jānis Timošenko) [3] extending our previous studies [4].

The essence of the x-ray absorption spectroscopy (XAS) is in the XAS technique is a measurement with an averaging time of less than 10^{-15} s where atoms are essentially static, so it measures the instantaneous local structure relative to instantaneous positions of the absorbing atom.

In this study we have a possibility to distinguish different Cu-O and Cu-Cu pairs and obtain information without any prior assumptions about structure and lattice dynamics model. We have also reconstructed radial distribution functions for Cu, visualizing the impact of correlation effects.

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