

One-atom-thick 2D material based on CuO. Experimental observations and theoretical study

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2D materials have attracted lots of attention since discovery of graphene which was found to exfoliate easily from bulk graphite. Increasing of such interest has recently triggered for the study of two-dimensional materials with nonlayered bulk like boron, zinc oxide, sodium chloride or iron. Among all these materials the latter one attracts special attention because the formation of two-dimension layered metal is unexpected and controversial due to the indirect nature of metallic bonds.

In this work we present the observation of novel two-dimensional one atom thick layer based on copper oxide studied by both experimental and theoretical methods.

Using *in situ* STEM it was observed special crystal lattice of 2D CuO on graphene which structure is principally different from the former reports. Structural parameters and chemical compounds of 2D cluster were determined.

Using DFT the stability and properties of observed CuO nanoclusters was studied. It was defined a critical role of the oxygen impurity atoms in the formation of stable 2D CuO cluster with unexpected orthogonal crystal lattice. Mechanical, electronic and magnetic properties were studied as well.

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Figures

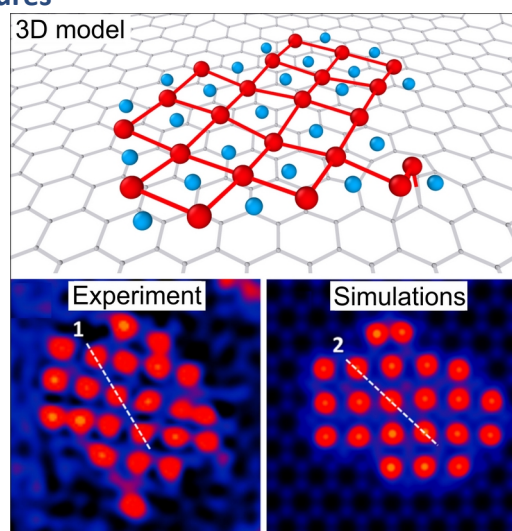


Figure 1. Atomic model of observed CuO cluster (top panel); STEM image in comparison with simulated STEM image of the sample (bottom panel)