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2D Copper Oxide. Experimental evidence on graphene and theoretical investigations

Nowadays 2D materials are the one of the attractive materials since discovery of graphene by means of micromechanical exfoliation technique (scotch-tape method) 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 [1,2]. Among all these materials the latter one attracts special attention because the formation of 2D layered metal is unexpected and controversial. 2D layer with metals is very difficult to form because metallic bonding leads to form 3D structures.

Here we present the report of existence of novel two-dimensional phase of copper studied by experimental and theoretical methods. Using in situ scanning transmission electron microscopy (STEM) it was observed special crystal lattice of 2D Cu on graphene which structure is principally different from the former reports.

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 density functional theory the stability of observed Cu nanoclusters was studied. It was defined a critical role of the oxygen impurity atoms in the formation of stable 2D Cu cluster with unexpected orthogonal crystal lattice. It was found that the structure and stability of 2D Cu clusters strongly depends on the concentration and relative arrangement of oxygen impurities. Number of oxygen configurations was analyzed and the stable configuration was found corresponded well with experimental data.

Additional to separated clusters, the periodic 2D Cu crystal with embedded oxygen atoms was studied in details. Relative stability, features of elastic, electronic and magnetic properties were investigated. First-principles calculations explained the origin of the 2D phase formation and confirms the experimentally observed structures.

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References

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Figures

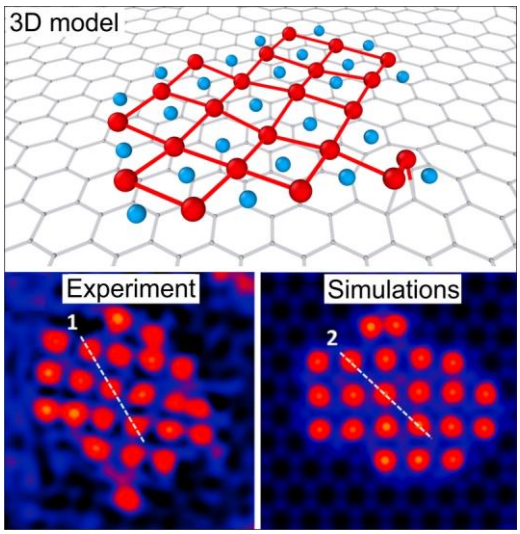

Figure 1: Atomic model of observed CuO cluster (top panel); STEM image in comparison with simulated STEM image of the sample (bottom panel)