Toward the two dimensional layered metals. Experimental observation and theoretical investigation of 2D Cu-based monolayers

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The high interest to atomically thin films initiated by investigation of graphene 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. 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 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 electronic and magnetic properties were investigated. First-principles calculations explained the origin of the 2D phase formation and confirms the experimentally observed structures. Authors acknowledge the financial support of the Ministry of Education and Science of the Russian Federation in the framework of Increase Competitiveness Program of NUST "MISIS"(No. K2-2015-033). P.B.S. acknowledges the Grant of President of Russian Federation for government support of young PhD scientists MK-6218.2015.2 (project ID 14.Z56.15.6218-MK).