

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Monolayered copper based film. Experimental observation and theoretical investigation.¹ PAVEL SOROKIN, Nat'l Univ., of Science and Tech., MISiS; Emanuel Institute of Biochemical Physics of RAS, EMI KANO, Univ., of Tsukuba; Nat'l Institute for Materials Science, DMITRY KVASHNIN, Nat'l Univ., of Science and Technology MISiS; Emanuel Institute of Biochemical Physics of RAS, LEONID CHERNOZATONSKII, Emanuel Institute of Biochemical Physics of RAS, SEIJI SAKAI, Advanced Science Research Center, AYAKO HASHIMOTO, MASAKI TAKEGUCHI, Univ., of Tsukuba; Nat'l Institute for Materials Science — Here we present the report of existence of novel two-dimensional phase of copper oxide studied by experimental and theoretical methods. Using *in situ* scanning transmission electron microscopy it was observed 2D CuO on graphene as well as in the graphene pore with principally different structure from the former reports Density functional theory allowed to elucidate the nature of the stability of observed CuO nanofilms. 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 CuO crystal 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.

¹P.B.S. acknowledges the nancial support of the Ministry of Education and Science of the Russian Federation in the framework of Increase Competitiveness Program of NUST "MISiS" No. 2-2015-033 and RFBR 16-32-60138 mol a dk Pavel Sorokin
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Date submitted: 13 Nov 2016

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