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2D COPPER OXIDE. EXPERIMENTAL EVIDENCE ON GRAPHENE AND THEORETICAL INVESTIGATIONS

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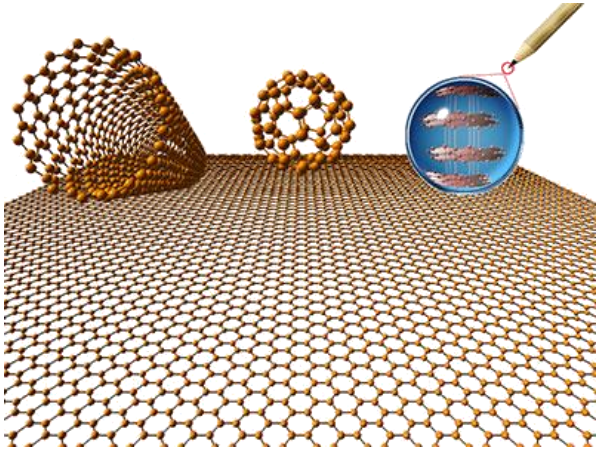
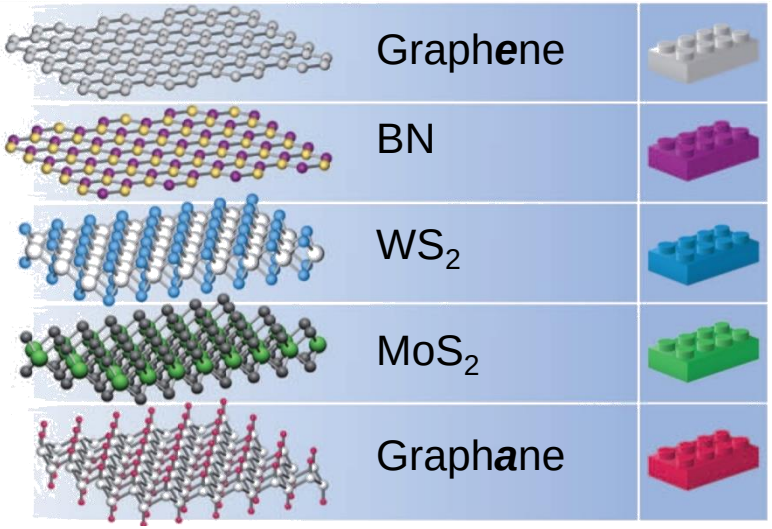
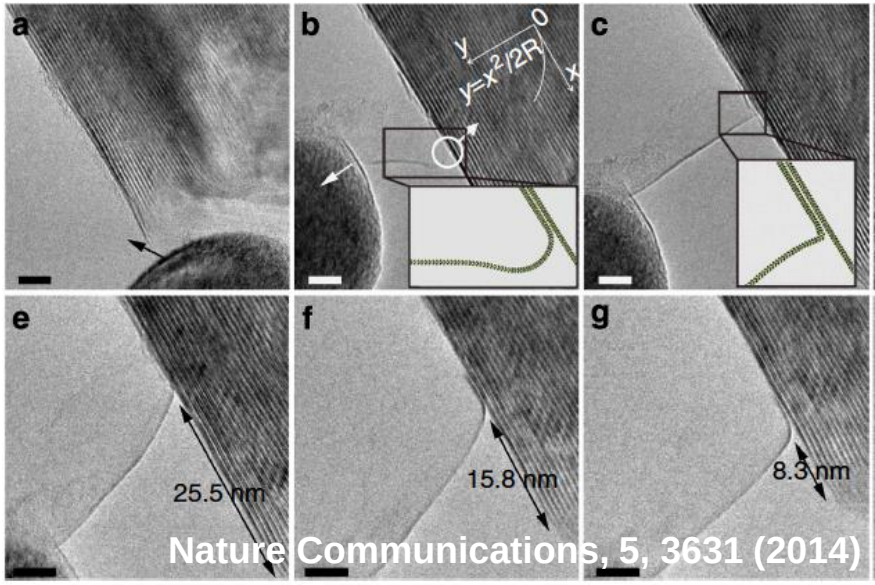
Introduction





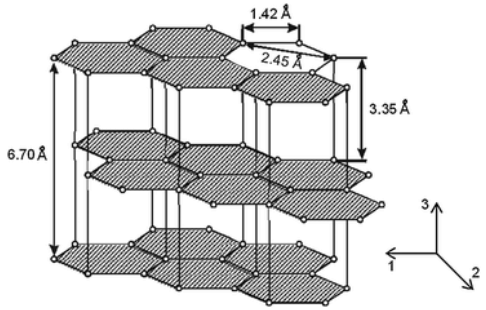
“Down to up”

“Up to down”



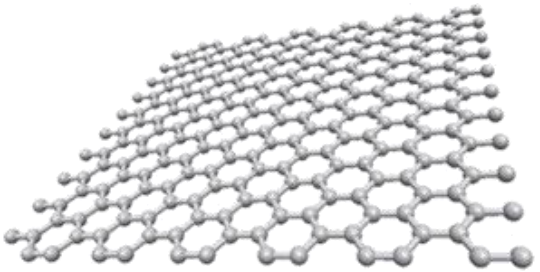
Nature Communications, 5, 3631 (2014)

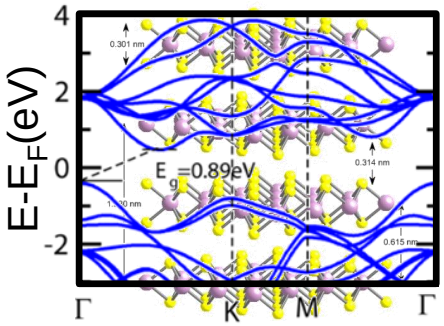
Introduction



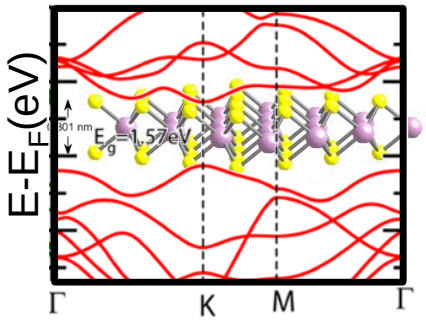
3D 2D

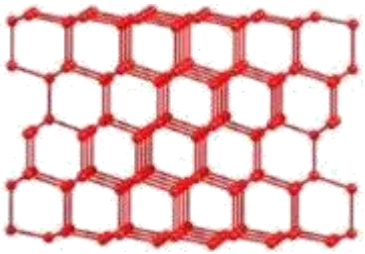
Graphite
(Graphene)



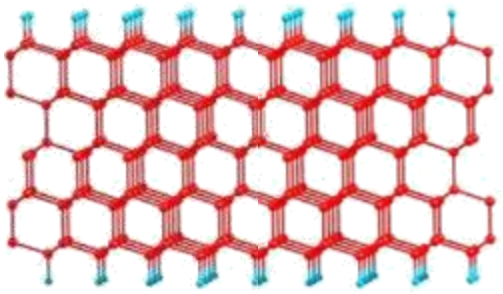


MoS_2





Diamond
(Diamane)



Graphene, 3, 52 (2014); J. Phys. Chem Lett., 5, 541 (2014)

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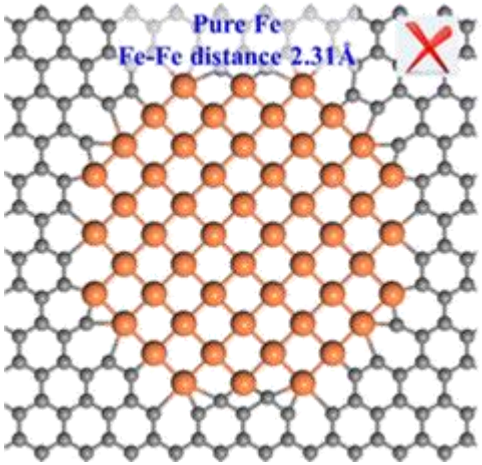
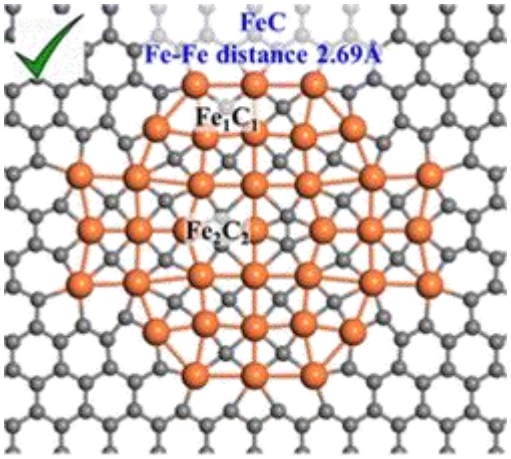
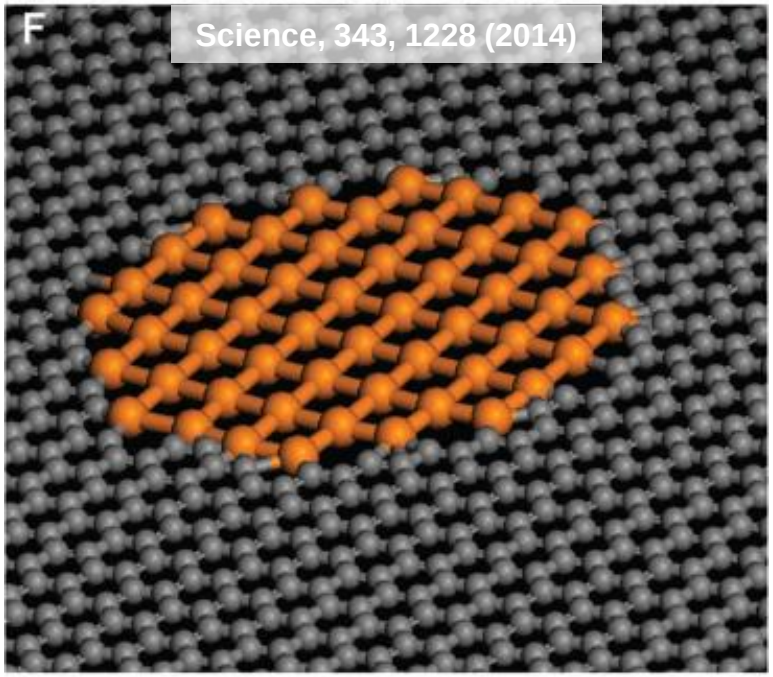
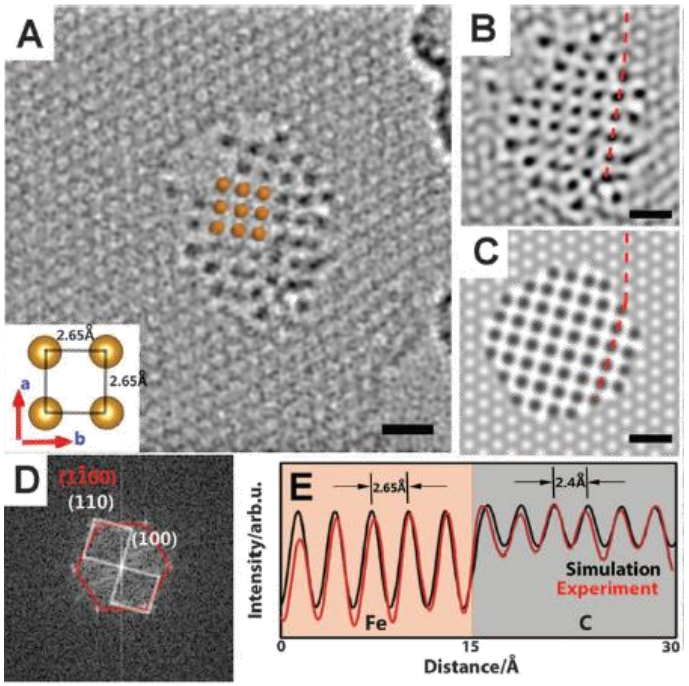
J. Phys. Chem. C, 119, 22954 (2015)

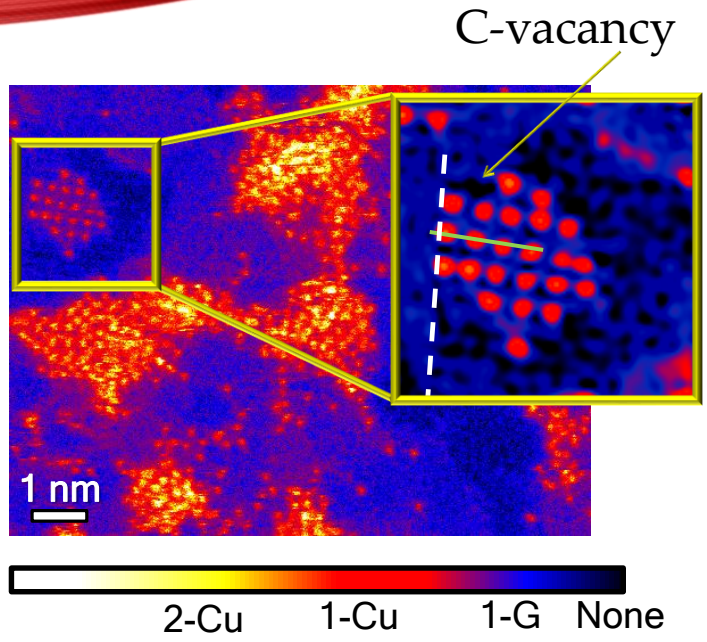






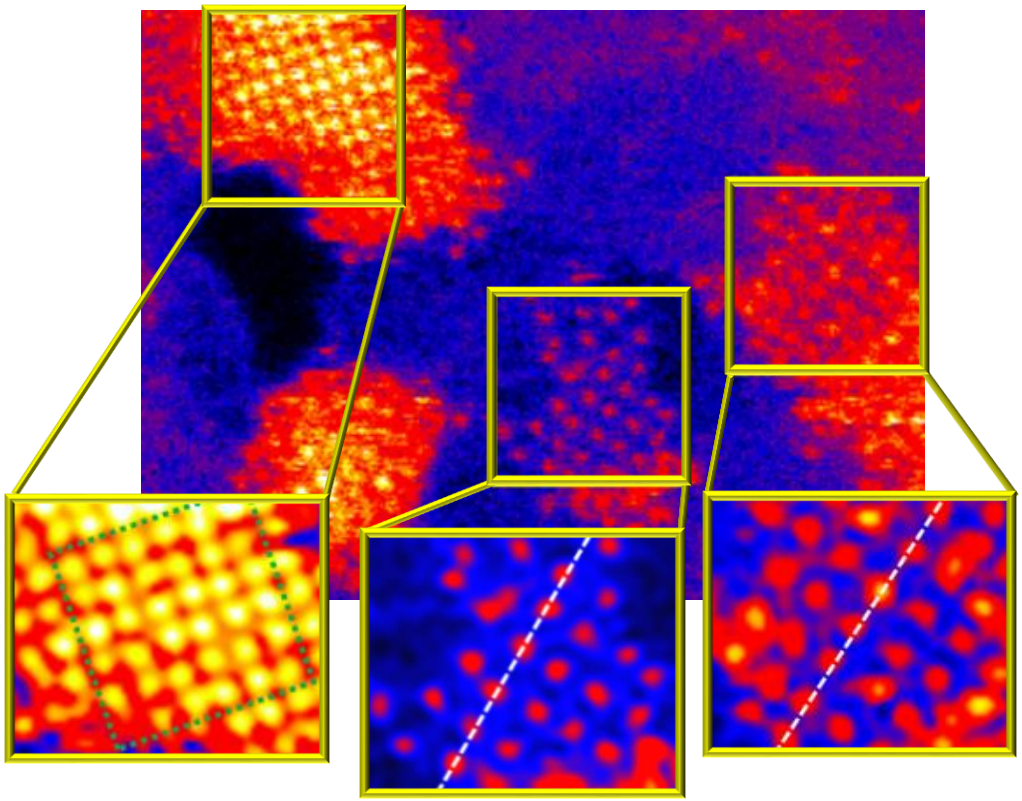


Experimental Observation



ADF-STEM image of the Cu cluster and atoms on graphene sheet.

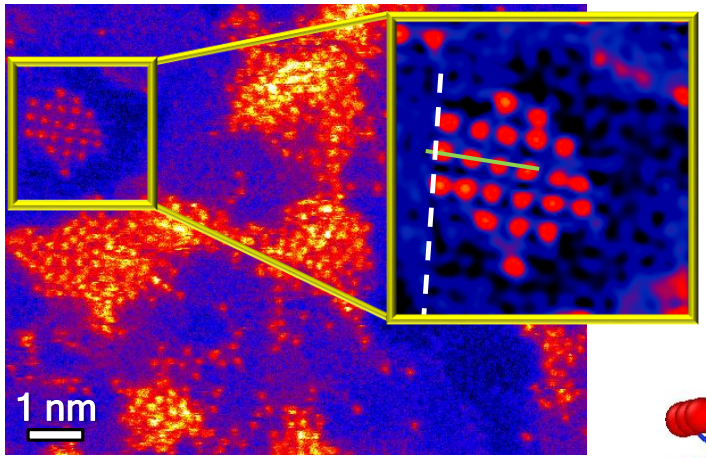
Beam-shower technique as room temperature was used to prevent both contamination and aggregation of Cu atoms.

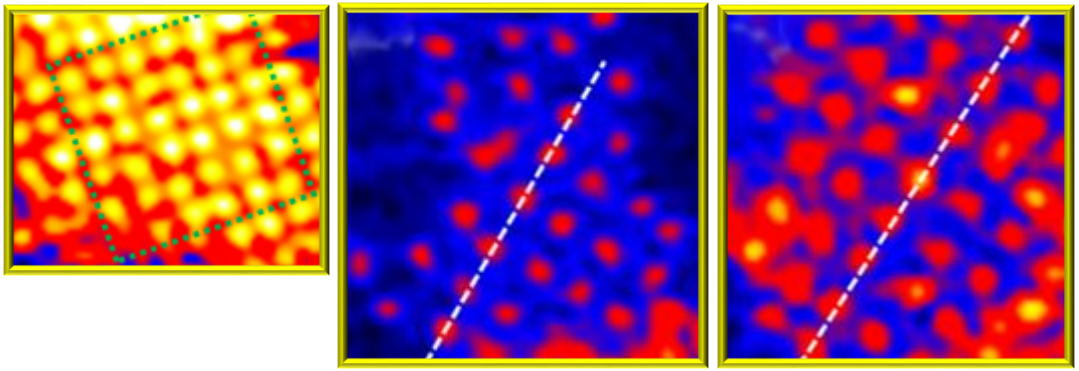


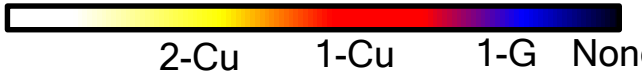
Sharp threshold peaks, so-called white lines, indicate a partial emptying of the Cu 3d band caused by the chemical bond with oxygen

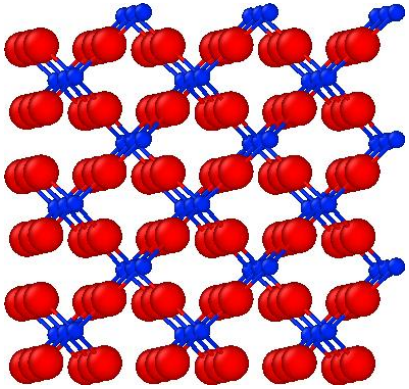
It was shown that after the annealing there are no formation of 2D structures

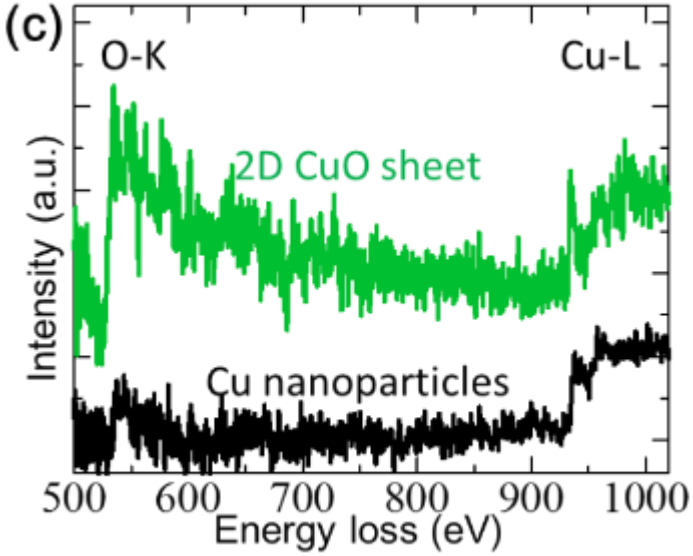
Experimental Observation

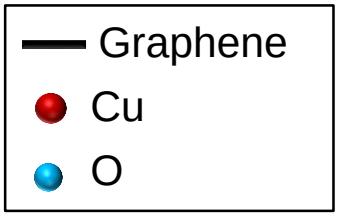


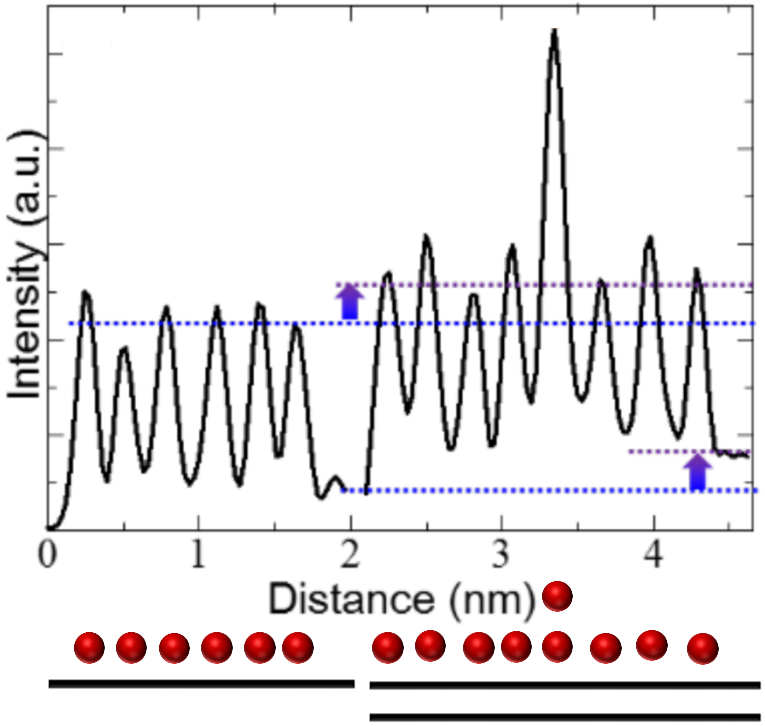






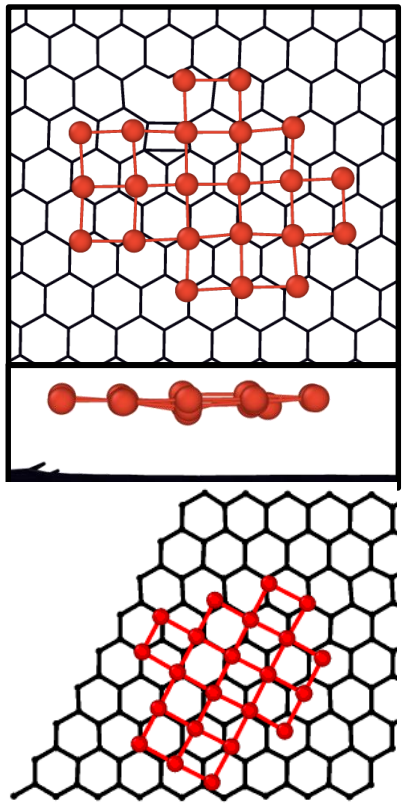


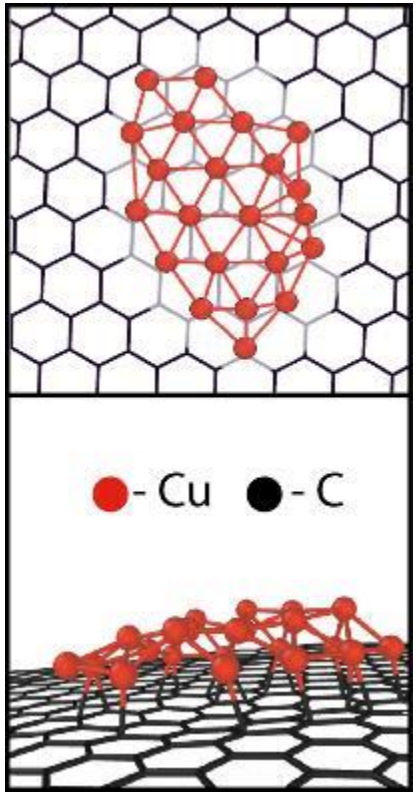




Theoretical Simulation

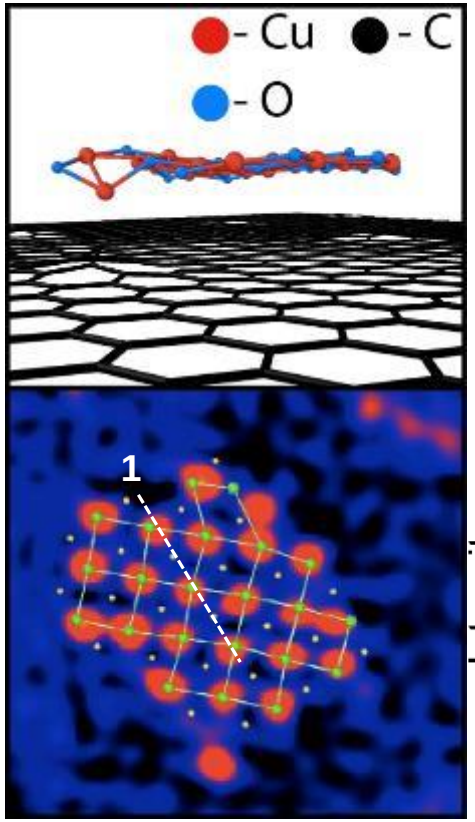
Based on experimental results the model of 2D Cu cluster on graphene surface with the same size was constructed.



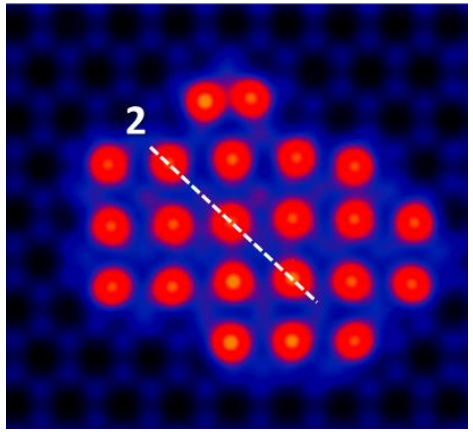


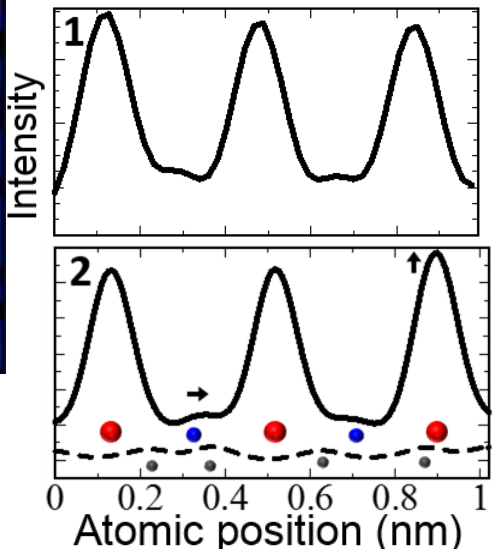
With the absence of oxygen impurities the 2D Cu cluster tends to curve and form 3D structure and binds with the graphene surface.

The oxygen impurity atoms placed in the centers of Cu rectangles play the major role in the stabilization of orthogonal lattice of 2D-Cu.

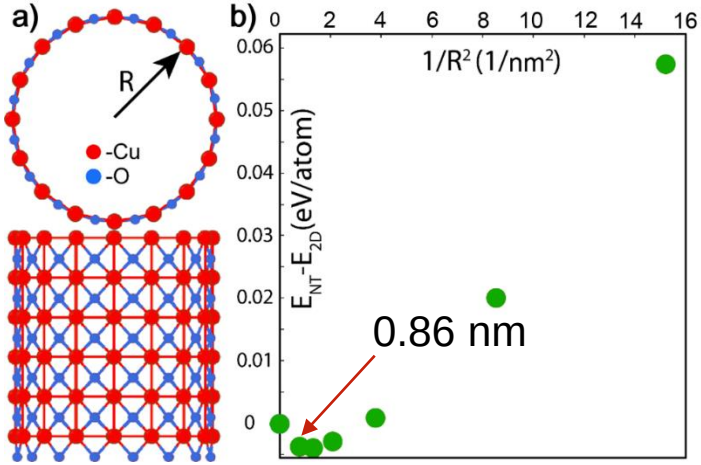


STEM image simulation totally confirmed the experimental observations





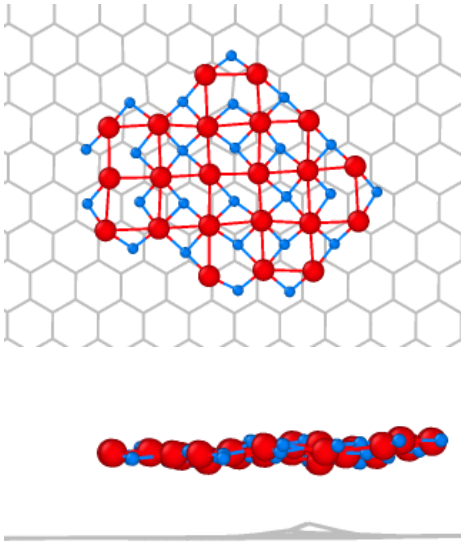
In-plane stability



Dependence of the energy difference between energy per atom of CuO nanotube (E_{NT}) and CuO monolayer (E_{2D}) on the inverse squared diameter of the tube

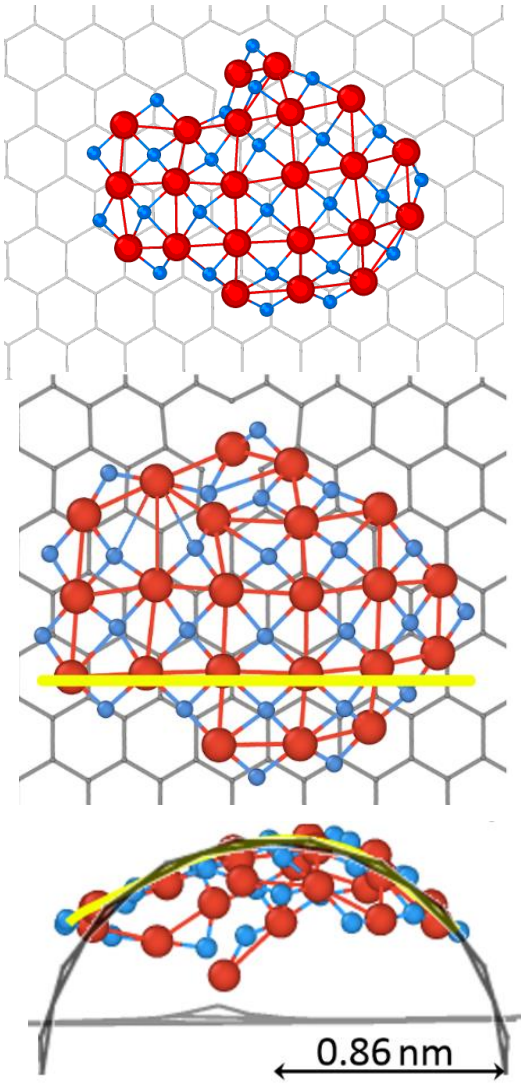
Our estimations of stability of freestanding CuO layers show that the flat 2D CuO structure will be unstable, in particular, it will be corrugated with bending radius ~5 nm

600K

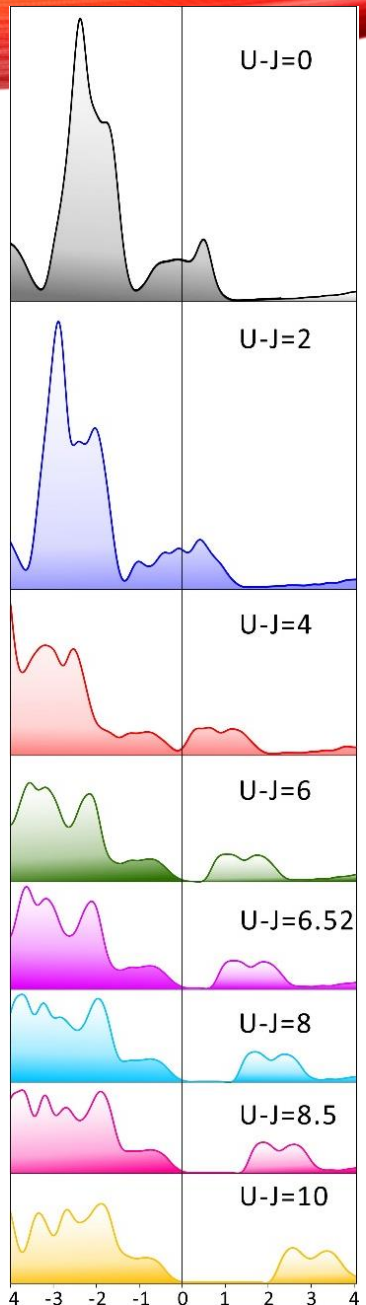


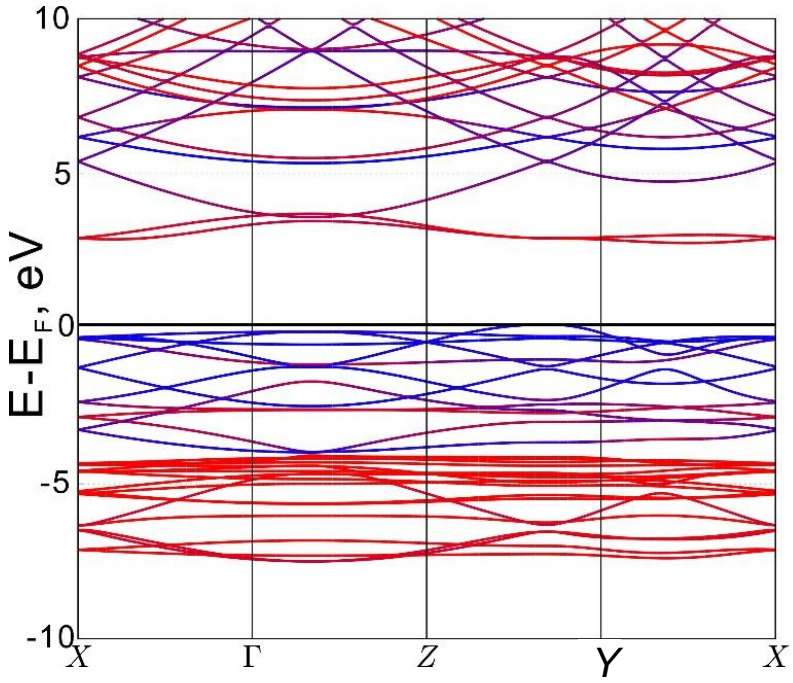
At 600K it was observed in-plane instability and structural instability as well

300K



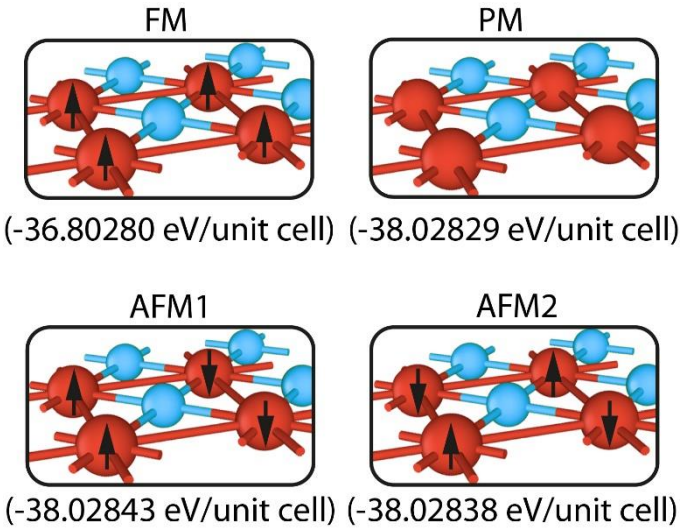
Electronic Properties (DFT+U)





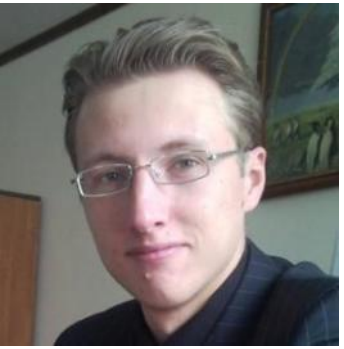
Obtained data allow to concluded that the studied structure is wide gap semiconductor, while 3D phase of CuO is a narrow gap semiconductor with the band gap about 1.5 eV .

Unlike the bulk phase of Cu and CuO which have a paramagnetic (PM) state as a ground state the 2D CuO has an antiferromagnetic (AFM) ground state with the energy difference between PM and AFM about ~-0.018 meV/atom.



Nanoscale, 9, 3980-3985 (2017)

Acknowledgments



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Thank you for your attention!

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SkolTech, Russia

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