Copper-oxide thin films: Morphology and water adsorption

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A direct band gap of 2.1 eV makes cuprous oxide a promising material for photocatalytic water splitting. To understand associated processes, copper-oxide model systems have been prepared by reactive Cu deposition on Au(111) and investigated with scanning tunneling microscopy and density functional theory [1]. Depending on Cu coverage and thermal treatment, either 1D oxide stripes with Au[112] or Au[110] orientation or planar (2×2) Cu-O networks with specific domain structures can be prepared. The latter are identified as Cu_3O_2 honeycomb lattice with oxygen ions alternatingly located in surface and interface positions. Strain minimization and a thermodynamic preference for Cu-rich edges lead to the formation of structurally well-defined domain boundaries.

D_2O exposure to the Cu_3O_2 surface gives rise to apparently amorphous water islands of monolayer height [2]. Closer inspection reveals local hexagonal ordering of the molecules with 6Å periodicity, indicating a weak template effect of the oxide support. Combined with a thermal desorption peak at 175 K, the observed behavior is compatible with water physisorption to an oxygen-terminated surface, in agreement with theoretical findings. More reactive surfaces, exposing low-coordinated Cu_{Cus} ions, can be produced by preparing thicker films at oxygen-lean conditions.

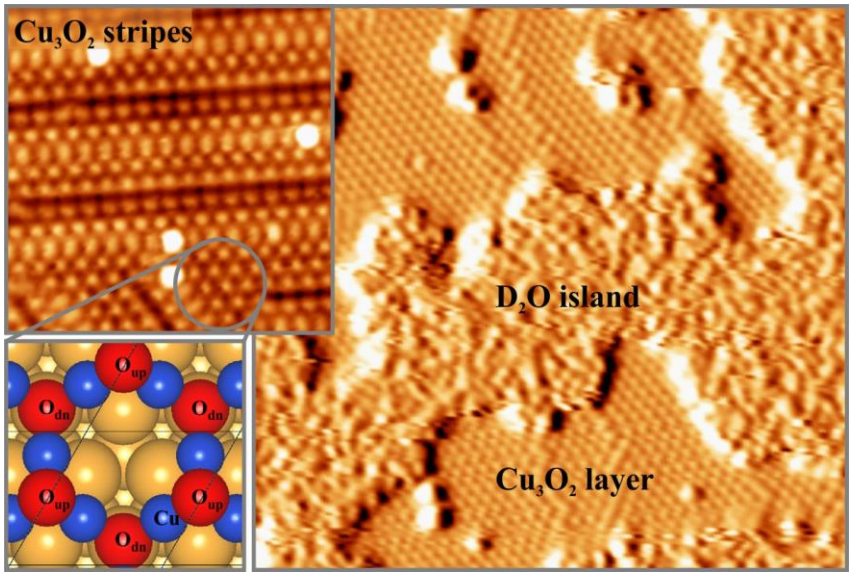

Figure: STM image of a Cu_3O_2 film on Au(111) and ball model of the underlying honeycomb structure (10×10 nm^2, left). Similar surface after water exposure (25×25 nm^2, right).

[1] C. Möller, H. Fedderwitz, C. Noguera, J. Goniakowski, N. Nilius, Phys. Chem. Chem. Phys. 2018, DOI: 10.1039/C7CP08387D.
[2] C. Möller, N. Nilius, J. Phys. Chem. C 121 (2017) 20877–20881.