

Abstract Submitted
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Thermodynamic Stability and Structure of Oxidized Cu(110) Surfaces: The Critical Role of non-Local Interactions JOSEPH BAMIDELE, Dept. of Physics, King's College London, The Strand, London, U.K., JAN BRNDIAR, IVAN STICH, Inst. of Physics, Slovak Acad. of Sciences, 84511 Bratislava, Slovakia, LEV KANTOROVITCH, Dept. of Physics, King's College London, The Strand, London, U.K. — Thermodynamic stability of oxidized Cu(110) surface is studied using DFT techniques. At high oxygen exposures standard techniques predict more phases to be quasi-isoenergetic, whereas experiments observe only the $c(6 \times 2)$ phase at high oxygen exposures clearly indicating this phase to be the ground-state separated by considerable energy differences from other candidates. We show that this surface system is stabilized by a delicate coexistence and balance of chemi- and physi-sorption. Agreement with experiments is only achieved if the van der Waals interaction between the surface templates is accounted for in DFT thermodynamics. Moreover, van der Waals stabilization of the surface structure is anticipated to be a general feature present also in the cases of other related surfaces.

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