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Oxidic copper on the Au(111) surface:A theoretical surface science approach TAEHUN LEE, Yonsei University, YONGHYUK LEE, KISUNG KANG, ALOYSIUS SOON, Department of Materials Science and Engineering, Yonsei University — Recently, via reactive Cu deposition in an oxygen ambience, high quality gold-supported cuprous oxide (Cu_2O) ultrathin nanofilms [1] have been prepared as a model system to further such catalytic studies. Nonetheless, an accurate atomic picture of these ultrathin Cu_2O nanofilms, which largely depends on its immediate oxygen environment, is currently lacking. In this work, we perform density-functional theory (DFT) calculations using the Vienna ab initio Simulation Package in combination with *ab initio* atomistic thermodynamics [2] to investigate stability of Cu_2O thin films on Au(111) as a function of oxygen chemical potential. Our results indeed show that some of the surface structures suggested in Ref. [1] are energetically more stable than the traditional copper oxide thin film structures on copper substrate, and elucidated the electronic structure of these ultrathin copper oxide films on gold, in comparison with available experimental data. [1] H. Sträer et al., J. Phys. Chem. C 119, 5975 (2015); [2] A. Soon et al., Phys. Rev. B 73, 165424 (2006)

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