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Chemical Identification in the Cu_3Au (100) Surface Using STM and DFT RODRIGO B. CAPAZ, UFRJ and Inmetro, Brazil, LUIS G. DIAS, Inmetro, Brazil, ALEXANDRE A. LEITÃO, UFJF and Inmetro, Brazil, RALF-PETER BLUM, HORST NIEHUS, Humboldt University, Germany, CARLOS A. ACHETE, UFRJ and Inmetro, Brazil — We describe the structure, energetics and electronic structure of the Cu_3Au (100) surface using a combination of scanning tunneling microscopy (STM) and first-principles calculations based on density functional theory (DFT). Our calculations show that the CuAu termination is the one with lower surface energy, in agreement with experiments. The well-known surface atomic rippling is also well reproduced by the calculations. Atomically-resolved STM images show an interesting voltage dependence, showing both types of atoms in the surface unit cell for lower voltages but just one type for higher voltages. Comparisons with theoretically-simulated STM images and cross- sectional electronic density profiles allows for an unambiguous assignment of Au atoms as the one appearing in higher voltage images, thus providing chemical identification at the surface.

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