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Theoretical studies of positron states and annihilation characteristics at the oxidized Cu(100) surface

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Abstract

In this work we present the results of theoretical studies of positron surface and bulk states and annihilation probabilities of surface-trapped positrons with relevant core electrons at the oxidized Cu(100) surface under conditions of high oxygen coverage. An ab-initio study of the electronic properties of the Cu(100) missing row reconstructed surface at various on surface and sub-surface oxygen coverages has been performed on the basis of the density functional theory (DFT) using the Dmol3 code and the generalized gradient approximation (GGA). Surface structures in calculations have been constructed by adding oxygen atoms to various surface hollow and sub-surface octahedral sites of the 0.5 monolayer (ML) missing row reconstructed phase of the Cu(100) surface with oxygen coverages ranging from 0.5 to 1.5 ML. The charge redistribution at the surface and variations in atomic structure and chemical composition of the topmost layers associated with oxidation and surface reconstruction have been found to affect the spatial extent and localization of the positron surface state wave function and annihilation probabilities of surface trapped positrons with relevant core electrons. Theoretical results are compared with experimental data obtained from studies of oxidation of the Cu(100) surface using positron annihilation induced Auger electron spectroscopy (PAES). It has been shown that positron annihilation probabilities with Cu 3s and 3p core electrons decrease when total (on-surface and sub-surface) oxygen coverage of the Cu(100) surface increases up to 1 ML. The calculations show that for high oxygen coverage when total oxygen coverage is 1. 5 ML the positron is not bound to the surface. © 2013 AIP Publishing LLC.

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Keywords

Adsorption, Annihilation, Copper, Oxidation, Oxygen, Positron, Reconstruction, Surface