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Surface states and annihilation characteristics of positrons trapped 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. Oxidation of the Cu(100) surface has been studied by performing an ab-initio investigation of the stability and electronic structure of the Cu(100) missing row reconstructed surface at various on-surface and subsurface oxygen coverages ranging from 0.5 to 1.5 monolayers using density functional theory (DFT). All studied structures have been found to be energetically more favorable as compared to structures formed by purely on-surface oxygen adsorption. The observed decrease in the positron work function when oxygen atoms occupy on-surface and subsurface sites has been attributed to a significant charge redistribution within the first two layers, buckling effects within each layer and an interlayer expansion. The computed positron binding energy, positron surface state wave function, and annihilation probabilities of the surface trapped positrons with relevant core electrons demonstrate their sensitivity to oxygen coverage, atomic structure of the topmost layers of surfaces, and charge transfer effects. 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). The results presented provide an explanation for the changes observed in the probability of annihilation of surface trapped positrons with Cu 3p core-level electrons as a function of annealing temperature.

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