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Positron states and annihilation characteristics of surface-trapped positrons at the oxidized Cu(110) surface[1] N.G. FAZLEEV, ANTOINE OLENGA, A.H. WEISS, Department of Physics, University of Texas at Arlington — The process by which oxide layers are formed on metal surfaces is still not well understood. In this work we present the results of theoretical studies of positron states and annihilation characteristics of surface-trapped positrons at the oxidized Cu(110) surface. An ab-initio investigation of stability and associated electronic properties of different adsorption phases of oxygen on Cu(110) has been performed on the basis of density functional theory and using DMOl3 code. The changes in the positron work function and the surface dipole moment when oxygen atoms occupy on-surface and sub-surface sites have been attributed to charge redistribution within the first two layers, buckling effects within each layer and interlayer expansion. The computed positron binding energy, positron surface state wave function, and annihilation probabilities of surface trapped positrons with relevant core electrons demonstrate their sensitivity to oxygen coverage, elemental content, atomic structure of the topmost layers of surfaces, and charge transfer effects. Theoretical results are compared with experimental data obtained from studies of oxidized transition metal surfaces using positron annihilation induced Auger electron spectroscopy.

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