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Metal pulled-off effect: A unique explanation of different oxidation process on Cu and Al surfaces JUNYI ZHU, JOONGOO KANG, SU-HUAI WEI, National renewable Energy Lab — One interesting oxidation phenomenon is the difference of the oxidation of Cu and Al. Cu forms disordered domains, large surface reconstructions and oxide islands on the surface with some O atoms diffuse into inner layers to further oxidize inner Cu atoms. Al forms a dense oxide layer which protects the inner Al atoms from oxidation. In this talk, we demonstrate a possible electronic origin of this oxidation difference by using the first-principles method to calculate the initial oxidation of different metal surfaces and nanoclusters. On Cu 55 Icosahedron surface, we found that 2 O atoms at neighboring sites form a structure with a Cu atom in the middle pulled off from the surface. We also found the similar pull-offs on Cu, Pd, Zn surfaces, but not on Al surface, which is not a transition metal. This pulled off effect is explained by the strong metal d and O p coupling. We also checked different O concentration on Cu (111) surface and on Cu cluster surface and found that O atoms form chain or ring like structures. Our first principle molecular dynamic calculation confirms that these structures are stable. With this pull-off effect, additional O atoms can further oxidize inner Cu atoms and make Cu relative easy to oxidize. This finding enhances the scientific understanding of the initial oxidation of metallic nano-particles and surfaces, which may have important applications in catalysis, thermal storage and other surface science fields.

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