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On mechanism of influence of alkali adsorbates on the interaction of co-adsorbed molecules with metal surface[1] SERGEY STOLBOV, TALAT S. RAHMAN, Kansas State University — It is well known that adsorption of alkali atoms on metal surfaces dramatically changes their properties. Alkali adsorbates promote various chemical reactions on catalyst surfaces, form quantum wells at the Cu(111) surface, and substantially reduce vibration frequencies of co-adsorbed molecules. To understand the nature of these effects, we study the electronic structure of Cu and Pd surfaces adsorbed with alkalis and reveal groove-like or plateau-like features of surface potential formed upon the adsorption. These features are found to produce high density low-energy electronic excitations strongly delocalized toward vacuum with respect to the ground states. We find this phenomenon to be responsible for strong enhancement of the electronic polarizability in the vicinity of the surface that leads to dramatic softening of the vibration frequencies of co-adsorbed molecules. We also discuss the connection of this phenomenon to the promotion of surface reactivity and unusual optical properties of quantum wells formed at Cu(111) upon alkali adsorption.

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