

Properties of photoinduced states in water covered Alkali atoms on a Cu(111) surface

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Time programmed desorption and work function measurements reveal that alkali atoms directly adsorbed on the metal Cu(111) substrate can be hydrated by surrounding water molecules. In addition, the electronic structure as a function of water coverage shows pronounced changes as the water coverage increases. The most striking effect is the appearance of a new state which can be attributed to excess electrons at the alkali-water-cluster, which are stabilized by response of the polar environment. The ability to bind such an electron depends on the type of alkali and increases with increasing dipole moment of the adsorbed alkali along the sequence Na, K, Cs.

By means of first-principles DFT modeling we will answer to the questions arising from the experimental observations on: (i) how the water molecules adsorb on the surface in presence of alkali atoms; (ii) how to probe the formation of a solvation shell of water molecules around the alkali ion as suggested by 2PPE measurements; (iii) how the water molecules affect the unoccupied alkali resonances.

We will show that the main experimental data can be accurately reproduced by combining configurational averages over the alkali-water clusters distribution at fixed overall water density and the structural averages at fixed number of water molecules within the cluster.