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Review

Key ingredients of the alkali atom – metal surface interaction: Chemical bonding versus spectral properties



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ABSTRACT

The interaction of alkali atoms with metal surfaces is reviewed. The peculiar electronic configuration of such atoms, with only one valence electron participating in the bond formation, suggested simple pictures to describe their interaction with a metal surface. But it was early evident that the adsorption properties depend on many aspects, related to the electronic structure of constituents, leading, for example, to different degrees of ionicity/covalency of the alkali atom-metal bond. Sophisticated theoretical modeling tried to shed light on this aspect. The spectral properties are the ultimate features in determining how the systems interact with each other. In this review the electronic and spectral properties are discussed focusing on different theoretical representations of the physical system and on their consequences. Surface projected energy gaps of the substrate as well as the substrate continuous spectrum are key aspects in determining the nature of the interaction and bonding with alkali adsorbates.

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1. Introduction

The presence of only one valence electron per atom in alkali metals, available to form bonds, makes these atoms good candidates to study, in a simple way, the adsorption phenomenon on different substrates. Nevertheless the scientific investigation extended along last decades demonstrated that an immediate interpretation is not easy. In fact, this class of adsorbates induces peculiar electronic properties, with implications in technology, and a variety of spectral features upon adsorption, displaying also a non trivial coverage dependence.

Since the early studies of low coverage Cs adlayers on W, Ni, and Mo [1–3] it was clear that the most evident aspect of alkali adsorption consists in the lowering of the work function Φ of the system: increasing the Cs coverage, the work function of the substrate takes a minimum before reaching a saturation value. The same behavior was observed for all alkalis on many metal substrates [4–13] as well as on semiconductors [14,15]. The work function change as a function of the Li, Na, K, Rb, and Cs coverage [4,5,12] on the Cu(001) surface is reported in Fig. 1 [16]. Here the coverage θ is defined as the ratio between the number of alkali atoms and that of Cu atoms in the first surface layer.

The initial lowering of Φ is explained by the classical picture of Langmuir and Kingdon [2] as the effect of the induced surface dipole μ due to ionization of the alkali atom upon adsorption, according to the relationship:

$$\Delta\Phi(\theta) = \frac{4\pi}{A} \theta \mu(\theta), \quad (1)$$

where A is the area attributed to a single substrate atom. A complete charge transfer from the adatom to the substrate, i.e. the adsorption of the alkali as a positive ion, was assumed, because the ionization

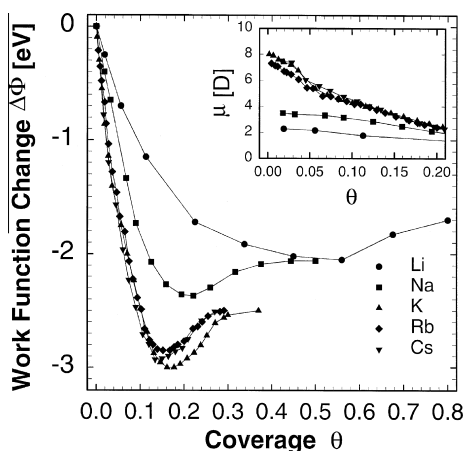


Fig. 1. Cu(001) work function change $\Delta\Phi$ and surface dipole moment as a function of alkali coverage (from Ref. [16]).

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