

The puzzling case of Pt(111): Spin texture of the prototypical L -gap surface state

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This year, we celebrate the 50th anniversary of the first experimental detection of a metallic surface state [1]: the prototypical Shockley-type L -gap surface state on Cu(111). Already in the very first paper by Shockley on the occurrence of surface states associated with a periodic potential [2], it became clear that the energetic position of such states depends critically on the interatomic distance, i.e., on the lattice constant. Detailed studies on various other fcc(111) surfaces revealed, among other things, the influence of spin-dependent interactions, namely exchange and spin-orbit interaction. While the surface state becomes exchange-split for Ni, contributing to the surface magnetic moment [3], the spin degeneracy is lifted by the Rashba effect for the heavy element Au, leading to a \mathbf{k} -dependent spin splitting [4].

The equivalent surface state on Pt(111) had been slighted so far. Only one scanning-tunneling-spectroscopy study reported on the energy vs momentum dispersion [5]. Theoretical predictions based on DFT vary depending on the particular functionals used. To clarify this issue, we investigated the atomic structure of Pt(111) by low-energy electron diffraction and the unoccupied electronic structure by spin- and angle-resolved inverse photoemission [6]. The experimental results are backed by theoretical studies using different functionals, which show that the characteristics of the surface band depend critically on the lattice constant. We found that the surface resonance at Pt(111) is a showcase for a delicate interplay of atomic structure, hybridization with d bands, and the influence of spin-orbit interaction.

Keywords: Two-dimensional electron states, surface states, exchange interaction, spin-orbit interaction, spin-resolved (inverse) photoemission.

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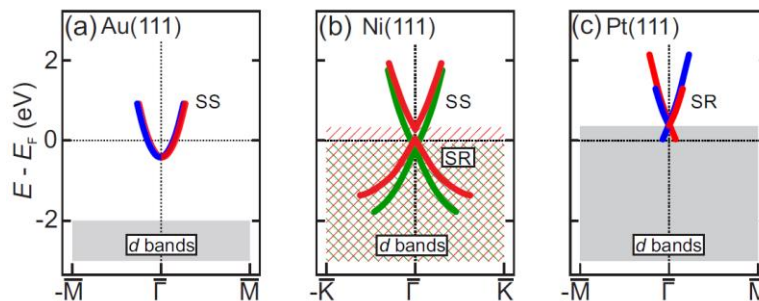


Figure 1. Simplified sketches of the L -gap surface states and d bands at (a) Au(111), (b) Ni(111), and (c) Pt(111).