

# Giant Spin Splitting Through Surface Alloying

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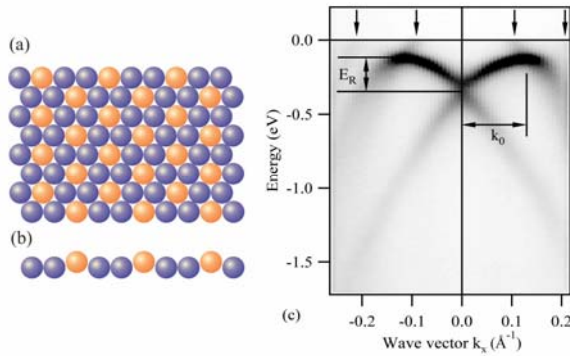
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In nonmagnetic solids, electronic states of opposite spin orientation are often implicitly taken to be degenerate (Kramers' degeneracy). However, spin degeneracy is a consequence of both time-reversal and inversion symmetry. If one of the latter is broken, the degeneracy can be lifted by, e.g., the spin-orbit (SO) interaction. This is, for example, the case in crystals that lack a center of inversion in the bulk (Dresselhaus effect). But also a structural inversion asymmetry, as it shows up at surfaces or interfaces, can lead to spin-split electronic states [Rashba-Bychkov (RB) effect]. In particular, clean surfaces of noble metals show spin-split surface states, where the splitting increases with the strength of the atomic SO coupling. The splitting can be further enhanced by adsorption of adatoms. Hence, using morphology and chemistry to tune the spin splitting of two-dimensional electronic states is a promising path to create a new class of nanoscale structures suitable for spintronic devices.

We have found a new class of materials that exhibits a giant spin splitting in the surface electronic structure. Using the concept of surface alloying, the Ag(111) ( $Z=47$ ) surface layer was doped with the heavy element Bi ( $Z=83$ ). The 2D band structure of the Bi/Ag(111) surface alloy was investigated by ARPES [at the EPFL in Lausanne, Switzerland, as well as at the SRC] and exhibits a spin splitting of unprecedented magnitude. It is shown in Figure 1.



**Figure 1**

scale (momentum offset  $k_0=0.13\text{\AA}^{-1}$ ) as well as an energy scale (Rashba energy  $E_R=200\text{meV}$ ), both of which are indicated in Fig. 1c. The four arrows indicate an additional spin-orbit split band with its band maximum in the unoccupied states.

The large spin-orbit splitting opens up new opportunities for investigation of SO split states. The RB model cannot explain the giant SO splitting in the surface alloy. To explain this the electronic structure of the Bi/Ag(111) surface alloy was calculated from first principles within the framework of the local spin-density approximation to density functional theory (DFT). The spin-splitting is the result of a sizable in-plane gradient of the potential that contributes to the splitting strength. The in-plane gradient manifests itself in the out-of-plane rotation of the spin polarization, as obtained from first-principles calculations, as well as in a hexagonal shape of the outer branches in the constant energy contours.

In Fig. 1a the structure of the surface alloy is shown. Each Bi atom (orange) is surrounded by six Ag atoms (blue), which results in a  $\sqrt{3} \times \sqrt{3} R30^\circ$  reconstruction. Fig. 1b shows a side view with the outward relaxation of the Bi atoms. The experimental band structure is shown in Fig. 1c. The characteristic band dispersion due to the spin-splitting showing two singly degenerate parabolic-like bands (with negative effective mass), whose maxima are shifted away from the high symmetry point, is clearly visible. The strength of the spin-orbit splitting can be projected onto a momentum