Abstract

The search for new techniques, materials and ideas to improve and develop high efficient electrical devices is more relevant today as ever. In this doctorate thesis *ab-initio* density functional theory (DFT) is used to investigate two very different systems with very different properties. They have in common that they are low-dimensional (1D and 2D) and that spin-orbit coupling (SOC) is necessary for an accurate description. Therefore, at the beginning of this these, a new, high efficient relativistic approach is introduced which allows for an inclusion of SOC without pushing the computational limits.

The first explored system is given by indium-nanowires that self-organize on the silicon (111) surface. This quasi one-dimensional system is famous for its reversible temperature-induced phase transition from a (4×1) to a (8×2) structure. Although most properties are already studied intensively, the inclusion of SOC in the calculations unfolds a so far unknown but large Rashba splitting, located at the In-related bands, for both phases which is strongly anisotropic.

The second material investigated in this work is the bismuth (111) surface. The clean surface is a challenge itself as its electronic structure highly depends on the correct modelling. In contrast to the In-nanowires where most properties can be described without SOC, it is essential in the case of bismuth. Dramatic alterations in the band structure and Fermi surface are clearly the most obvious changes. The bismuth surface has spin-split surface states, a precondition for spintronics but a good understanding of controlled surface modification is useful for future applications. It is shown that transition metals (TMs) as well as noble metals occupy all the same sevenfold coordinated position within the first bismuth bilayer of the Bi(111) surface. Interestingly, the surface topography is unchanged. For the $3d$ TMs this incorporation even happens *barrier-free*, i.e. without thermal activation. By increasing the density of the adatoms, it is possible to create an energetically very stable δ-doping layer of $3d$ TMs which, while being invisible to scanning tunneling microscopy (STM), leads to changes of the electronic and magnetic surface properties.