Photoemission Studies of Layered Materials and Alkali Metal Intercalation

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Abstact

The major part of this thesis is devoted to layered transition metal dichalcogenides (TMDCs), which are quasi-2D solids whose electronic structures can be manipulated through alkali metal intercalation. Photoelectron spectroscopy (PES) and low energy electron diffraction (LEED) have been used for studies of the following alkali/TMDC systems: Cs/$4H_b$-TaS_2, Rb/$1T$-$TaSe_2$, Rb/$TiTe_2$ and Rb/$TiSe_2$. In the Cs/$4H_b$-TaS_2 study, a photoelectron microscope (PEM) was used, to follow the intercalation process during successive Cs depositions. This kind of measurements on alkali/TMDC systems have not been done before, and gives valuable insight about the essence of intercalation. In the Rb/$1T$-$TaSe_2$ study, angle-resolved PES (ARPES) was used, and evidence for Rb intercalation was found. In addition, an interesting behaviour of the charge density wave (CDW) during intercalation was also found. The Rb/$TiTe_2$ and Rb/$TiSe_2$ systems have been studied both at room temperature and at 100 K. At room temperature, ARPES together with LAPW calculations reveals that Rb easily intercalates in both compounds. At 100 K, the clear majority of the deposited Rb atoms remains on the surface. At low concentrations they are in a dispersed phase, which condense at into a metallic phase at higher concentration. Further Rb deposition leads to growth of several Rb layers, which are clearly resolvable with high-resolution PES through different chemical shifts. Apart from the TMDC studies, this thesis presents high resolution PES spectra from core levels and valence bands in the layered ceramic Ti_3SiC_2.

keywords: layered materials, transition metal dichacogenides, $4H_b$-TaS_2, $1T$-$TaSe_2$, $TiTe_2$, $TiSe_2$, Ti_3SiC_2, alkali metal, Cs, Rb, angle-resolved photoelectron spectroscopy, photoelectron microscopy, intercalation, overlayers, low temperature, core level shifts, valence band.