Abstract of Results

In this thesis, the quasiparticle band structure of thin silicon layers and the Si(001)-surface was calculated and analysed with a combination of DFT(LDA) and G_0W_0. The main interest was the position of surface states, surface resonance and the size of the band gap.

For the first time, an implementation of the G_0W_0-approximation has been proposed that, within the supercell approach, takes the directional dependence of the macroscopic dielectric tensor into account properly and in a transparent manner. Thereby, it is possible to describe non cubic systems and to calculate slabs, surfaces, molecules and quantum wires within a single numerical concept.

Within this implementation, a long ranged interaction between the slabs in the supercell approach has been observed. In this thesis, a detailed understanding of the interaction has been obtained. With the developed periodicity contribution it is possible to correct the long ranged interaction and to work with a small spacing between the slabs. Despite this improvement, it is pointed out that a decoupling of the slabs in the G_0W_0-calculation is still preferable, but this is left for future studies.

For the first time, the dependence of the quasiparticle band gap on the slab thickness of thin silicon slabs is calculated by first principles. As a result, it has been observed that the quasiparticle correction is proportional to the inverse of the slab thickness. By means of the first principle results, we have confirmed an electrostatic model that describes the thickness dependence of the quasiparticle correction for sufficiently sized slabs.

Surface states show a much smaller dependence on the slab thickness than bulk states. At 0.9 eV, the fully converged indirect quasiparticle band gap of the $p(2\times1)$-surface, calculated with the aforementioned implementation, is about 0.2 eV bigger than the value presented in the literature.

The discrepancy between theory and experiment concerning the occupied surface states of the $c(4\times2)$-surface in the work of Weinelt *et al.* has also been analysed. It was shown, that the theoretical band structure alone is not a proper basis for a comparison with experimental data. However, by calculating the locally projected density of states and of excitation spectra in the lowest unoccupied surface band, a better comparison with the experimental data is, in principle, possible.