Abstract (English)

In this thesis the applicability of the quantum mechanic simulation method *DFTB* (*Density Functional Theory with Tight Binding*) is tested for the reproduction of *STM*-image (*Scanning Tunneling Microscopy*). *STM* is a method for the generation of surface images at the atomic scale. The method maps a surface by screening it mechanically and measuring the tunneling current between an atomically sharp tip and the sample surface.
For the correct interpretation of an *STM*-image, additional information about the surface atoms is required. Simulations can help to verify the proposed interpretations regarding the underlying atomic structure. One method, that is used for these simulations is the classical *DFT* method. Because this method requires a high calculation time, the much faster *DFTB* method is tested for applicability and compared to *DFT*. As a model system two sample geometries are investigated. The unreconstructed $\mathbf{TiO_2}$-rutile surfaces: (110) and (001).
The results calculated by *DFTB* and *DFT* show good agreement for the two tested surfaces but only for individual signs of the bias voltage. The (110) surface shows good agreement when scanned for electronic states below the band gap (for a negative bias voltage). The (001) surface shows good agreement when scanned for states above the band gap (for a positive bias voltage).
The respectively opposite situation, however, leads to a disagreement between the results generated with *DFTB* and *DFT*. The largest deviation occurs in case of the (110) surface with a positive bias voltage. Here, the minima and maxima of the ISO-surface are inverted in height.
One possible cause is that electrons in *DFTB* are described by means of a orbital like basis, while *DFT* employs a plane wave basis set. As a possible improvement it is proposed to decrease the wave compression used in the *DFTB 'Slater-Koster'* files, which contain the parameterized pre-calculated electron basis. First calculations for this approach are presented at the end of this thesis, however no final conclusion can be drawn yet.