In this work I briefly described the basic ideas of density functional theory (DFT) for calculations of an electronic structure of molecules, solids and surfaces. I also summarized the fundamentals of DFT based Fireball code that was used for calculations of the atomic and electronic structures of several models. Further I described theory of scanning tunnelling microscopy (STM) and mentioned some approaches of simulating STM maps by means of results of DFT calculations. The studied models were reconstructions of a Si (111) surface, namely the 7×7, 2×1 *Pandey chain* and reconstructions with periodicity $\sqrt{3} \times \sqrt{3}$, where finding proper atomic structure, fitting to a new experimental observations, was required. I compared energetic favourableness of the reconstructions. I also studied an adsorption of benzene on 7×7. I have analysed the atomic and electronic structure of all the models and made STM simulations using STM code. I compared the results with experimental STM maps in literature and with results of the STM experiments made by RNDr. Pavel Kocán, Ph.D. (reconstruction v$\sqrt{3} \times \sqrt{3}$) and by Prof. Alastair McLean (benzene on 7×7). Probable model of observed metastable reconstruction $\sqrt{3} \times \sqrt{3}$ was found. The proof that benzene chamisorbate in so called di-σ-bridge position was also made.