In this work I briefly summarized *ab-initio* methods for computation an atomic and an electronic structure of molecules, solid states and their surfaces; particularly I pursued a density functional theory. Then I described the method of Fireball simulation package here, which is based on the density functional theory. With Fireball I made computations of the electronic structure of Silicon bulk and computations of the atomic and the electronic structure of reconstructions 2×1, p(2×2) and c(4×4) of Si (100) surface. I compared my results with previously made and published computations and experiments here. Subsequently I performed STM simulations of these reconstructions, which I also compared with the experimental data.