

Abstract: Doped layers of crystalline silicon are currently the main driver of conventional photovoltaic devices. Direct introduction of group III and V atoms into the silicon matrix is still the mainstream of mass production of doped silicon. In this thesis, we are interested in non-invasive ways of doping of silicon wafers through the adsorption of molecules with a large intrinsic dipole moment on the semiconductor surface. These molecules, namely carboranedithiols, create a self-assembled monolayer accompanied by the surface dipole formation. In order to stabilise the dipole layer, an interfacial charge transfer can occur between the adsorbate and the substrate, modifying the density of accumulated charge carriers just below the silicon surface. These are the fundamental features of the surface transfer doping of the silicon substrate where we employ the carboranedithiol molecules as mediators of adsorbing dipole layer. Regarding the structure of the thesis, we first test the carboranedithiol molecules on gold, and then we move on to the issue of silicon-molecule junctions. We characterise the geometry and the electronic properties of the carboranedithiol molecules on both of these substrates by means of atomistic simulations based on a density functional theory.