First-principles calculations on the adsorption of prototype organic semiconductors on metal surfaces for organic electronics.

The aim of the present thesis is to perform first-principles calculations based on density functional theory (DFT), in order to reveal the atomic mechanisms of the adsorption of water on the clean metal surfaces, as well as to study the structural details and probe the electronic properties of a prototype donor-acceptor system in organic photovoltaics (OPVs), upon adsorption on a clean Ag surface. Firstly, we study the stability and work functions of the most exposed stable surfaces of prototype metals related to OPV-devices (i.e. aluminum and silver). We also address effects of water on these surfaces and associate the adsorption with the work function. Furthermore, we identify different stable configurations for the adsorption of $PC_{60}BM$ on Ag surfaces with different orientation of the molecules with respect to the interface and the most stable configuration of P3HT and we investigate the work function modification upon adsorption. As a last step we calculate the charge density difference at the interface due to adsorption, in order to investigate the formed interfacial dipole. These results, help clarify the interaction between prototype OPV materials and the Ag surface and may aid towards the increase of the performance of such materials on OPV devices.