

First-principles calculations on the adsorption of water molecules on the silver surface. Work function modification and effect on OPVs and OLEDs performance.

The purpose of the present thesis is to study from first-principles the adsorption of water molecules on the (111) surface of silver, in order to examine possible changes on the metal work function, a factor that affects energy level alignment and therefore the performance of organic electronic devices (OPVs and OLEDs). First principles calculations are based on density functional theory (DFT) and van der Waals interactions are taken into account by implementing DFT-D3 method of Grimme. As a first step, the clean (111) surface of silver is studied and important properties like surface energy and work function are calculated. As a next step, we study the adsorption of water molecules on the metal surface. The properties of the metal-water system have been addressed by modeling several water coverages on the Ag (111) surface and the obtained structures are structurally and energetically examined. The induced Ag (111) electrostatic potential change upon water adsorption is then calculated for all the systems modeled. In order to elucidate the origin of the observed electrostatic potential modification, we examine the contribution of the intrinsic water dipole and the interfacial dipole formed in water-metal interface. Finally, we identify the induced Ag (111) work function modification and demonstrate its effect on the performance of conventional and inverted organic photovoltaic devices and OLEDs.