Abstract

Polarity discontinuities at the interfaces between different polar and non polar oxides is known to lead to nontrivial local atomic and electronic structure. If these polarity discontinuities can be atomi- cally controlled, unusual charge states that are not present in bulk materials could be found. These discontinuities are often found in naturally layered oxide structures. Oxide interfaces are of such a great interest because in many transition-metal compounds the electrons are strongly correlated: the motion of one carrier is related and depend crucially on the motion of all the others. Strongly correlated electron systems are known to support interesting and potentially useful effects, including magnetism with high Curie temperatures, superconductivity with high transition temperatures, metal–insulator transitions and multiferroicity. In this thesis we describe how polar discontinuities at the interface in- troduces large energy cost which corresponds to the surface termination along a polar plane without any surface charge reconstruction, result- ing in diverging potential energy. How the system responds to this energy cost is already known, we are just using a simple electrostatic model in our calculations to capture this response. We will also try to discuss LaNiO3/CaMnO3 interface, to understand how two different perovskites gives rise to interfacial ground states with totally different properties than the original perovskites. This interface has recently been studied where interfacial ferromagnetism is observed in the MnO2 layer. LaNiO3 shows metal-insulator transition which is thickness de- pendent. Also, this ferromagnetism is found to be coexistent with the metallic state of LaNiO3 . But it is still not clear, what are the ordering patterns present in nickel oxide layer. A recent study reveals a spiral state which is not commonly observed in metallic systems for superlat- tices with 2 adjacent LNO layers. We are using effective hamiltonian approach to study the interface of LaNiO3 and CaMnO3 . We are try- ing to understand the effect of interfacial doping on the NiO2 layer by modelling the system via a two dimensional Hubbard model on lieb lattice. We are using Hartree Fock self consistent method in mean-field approximation.