- Public Abstract
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- Ph. D.
- Physics and Astronomy
- Theory of the Two-Dimensional Airy electron gas: Hartree-Fock and Density-functional studies
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Transition metal oxides are one of the most interesting and heavily researched materials in the field of condensed matter physics. They exhibit several unique properties, like the Colossal Magnetoresistance effect, which refers to the sharp drop in resistance with the application of a magnetic field, and high temperature superconductivity. Recently, there has been a breakthrough in the fabrication of superlattices of these materials, which consist of two different oxides, layers of which are stacked alternately. Similar superlattice systems have been fabricated using semiconductors for the past couple of decades and are now commonly used in a whole range of everyday electronics applications. What is really exciting about the oxide superlattices is that the quality of the fabricated superlattices is comparable to the semiconductor superlattices, which opens up the possibility of fabricating novel devices with unusual capabilities.

The thesis describes a theoretical study of the oxide superlattices using two methods - Hartree-Fock approximation and Density-functional theory. In particular, we study the interface in these superlattices, which show interesting properties, very different from the bulk materials constituting the superlattice. Among other properties, we examined the electron distribution at the interface and the effect of the dielectric constant of the medium, in which the electrons are embedded. We focus on a particular superlattice - the $(LaTiO_3)_1/(SrTiO_3)_n$ system, where one layer of $LaTiO_3$ is grown on n layers of $SrTiO_3$. An important feature of this system is that, the La atoms that form a plane at the interface, donate an electron and become positively charged. The stripped off electrons are however, confined to the vicinity of the La plane, though they spread out over several $SrTiO_3$ layers. The spread of these electrons has been experimentally measured by other authors using Electron energy loss spectroscopy. We calculated the spread of the electron distribution using density-functional theory and obtained results consistent with experiments.

Our work is an important first step in studying the novel two-dimensional electron gas found at the oxide superlattices, which are very promising materials from the point of view of device applications.

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