ELECTRONIC STRUCTURE OF TRANSITION METAL OXIDE INTERFACES: AN AB INITIO STUDY

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The aim of this thesis is to achieve an understanding of the new physics that is emerging in transition metal oxide (TMO) heterostructures. The computational approach will be based on large scale density functional theory calculations for ground state properties, treatment of dynamic correlations that arise in single particle excitations, transport calculations for nanostructures, and calculations of magneto-optical spectra that allow direct contact with experiment. The most commonly studied systems are SrTiO3 (STO), LaAlO3 (LAO), and LaTiO3 (LTO). Characterization probes, including some with sub-nanoscopic resolution, recently have revealed totally unanticipated behavior that reflects new states of matter at oxide interfaces. These developments (1) pose fundamental new questions about how electrons respond to new environments that do not occur in naturally occurring materials, and (2) provide a novel type of behavior that could be important for next generation spintronics-type applications, a spin current might be carried by a single atomic layer. Recent experimental studies of oxide interfaces [1] have uncovered other kinds of altered symmetry and dramatically changed behavior. A conducting layer may appear between two insulators, magnetism may appear between non-magnetic materials; superconductivity even has been observed between two insulators [2]. Calculations [3] indicate that strong interactions typical of transition metal oxides often will lead to new broken symmetry states that at times may be only one atomic layer thick: charge order is probable, magnetic order may appear [2] and orbital order may remove the last portion of the entropy before the ground state is reached.

The goal of this thesis is to bring new understanding of the novel behavior observed in oxide nanostructures by applying the most relevant theoretical and computational techniques, with close connections with experimental groups that are synthesizing and characterizing the materials. It is imperative first to obtain the correct ground state at the interface, including structural relaxation, and magnetic and orbital order where it occurs. Thermodynamic, magnetization, transport, and optical data will be confronted by calculating the corresponding excited states in the interface region. Having a microscopic description will allow us to study many issues; for example, (1) how does the variation in the occupation of the open shell across the interface influence the electronic properties, (2) what interactions determine the charge state at the interface? or (3) in what cases is atomic relaxation at the interface a determining factor in its properties, and how is the lattice coupled to the spin and orbital degrees of freedom?

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