DFT STUDY OF CHARGE AND SPIN INTERPLAY AT METAL-OXIDE SURFACES AND INTERFACES

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Metal oxide thin films and oxide heterojunctions form quasi-two-dimensional electronic phases which display a wealth of phenomena[1-6], including tunable metal-insulator-superconductor transitions, large magnetoresistance, ferromagnetism and superconductivity. The perovskite $SrTiO_3$ in particular is a substrate of choice[7,8] and is thus a workhorse in the emerging field of metal-oxide electronics.

Using density functional theory (DFT) within the spin generalized gradient approximation and a moderate Coulomb U we have investigated the structural, electronic and magnetic properties of metal oxide surfaces and interfaces, with a focus on $SrTiO_3$. We find surface and interface properties to be tunable functions of doping and of oxygen vacancies. We find that oxygen vacancies order in periodic arrays giving rise to surface magnetic moments and a quasi two-dimensional electron gas in the occupied Ti 3-d orbitals. The surface confinement and octahedra distortions create dispersive sub-bands which open a spin-gap due to oxygen vacancy ordering, thus creating an effective Zeeman field and spin-momentum correlations[9] in the occupied bands, which can then be modulated using an external field[10]. The presence of multiple tunable properties opens up interesting technological applications.

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Category: LD

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