

FIRST-PRINCIPLES CALCULATIONS OF MANGANITE SURFACES AND INTERFACES FOR SPINTRONICSEmilio Artacho[§]*Department of Earth Sciences, University of Cambridge, Cambridge CB2 3EQ, UK*

Lanthanum-strontium manganites, $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ (LSMO), are materials that display an enormously rich phase diagram by varying temperature and composition, x , with phases displaying behaviours as interesting as colossal magnetoresistance. For $x \sim 1/3$ the material behaves as a ferromagnetic half metal, that is, with the Fermi level within a gap in the minority-spin density of states, and thus total spin polarisation of carriers at the Fermi level. It is an attractive material for spintronics, where the spin degree of freedom of the electrons is manipulated. Any such manipulation involves interfacing this material with others, which is the topic of this talk. In particular, an experimental group at Cambridge built nano-magnetoresistive devices by bridging a carbon nanotube (CNT) between two LSMO electrodes, and obtained remarkable magnetoresistance characteristics [1]. LSMO used as source and drain of electrons allow a much higher conduction through the device when both electrodes have their magnetisations aligned, while the conductance drops very substantially if they are counter-aligned. The electrons injected into the CNT have a high degree of spin polarisation, which barely alters when travelling along the CNT, given the very low spin-flip probability in the tube. If the drain electrode presents a gap for these carriers the resistance is high. The relative magnetisation orientation can be controlled easily with an external magnetic field, giving the desired magnetoresistive coupling.

The electronic characterisation of the LSMO-CNT interface prompted by these experiments, and performed by first-principles simulations [1], offered intriguing results, which made us turn back to the bare LSMO surface [2]. A detailed study has been performed on the MnO_2 -terminated (001) surface by means of density-functional calculations, showing clear indications of a latent ferroelastic phase, of a ferrodistorive kind analogous to the ferroelectric phase in BaTiO_3 . This phase is stabilised close to the surface, triggered by a surface buckling of Mn atoms outwards at the surface layer. This buckling is a canonical instability originated by the high density of states induced by a surface state, and thus hardly surprising. It is the subsurface propagation of the Mn off-centering in the respective O octahedra which is remarkable. It amounts to $\sim 0.1 \text{ \AA}$ close to the surface. Its decay length into the bulk cannot be determined from the calculations, except that it is longer than $\sim 10 \text{ \AA}$, determined by the thickness of the slab used in the calculations. The off-centring order parameter competes with the octahedral tilting order parameter in the bulk of the material, as shown by a suppression of the tilt towards the surface. The characterisation of this phase and its possible implications for this and other interfaces will be discussed.

[§]Work done in collaboration with JM Pruneda, V Ferrari, R Rurali, PB Littlewood and NA Spaldin.

[1] LE Hueso, JM Pruneda, V Ferrari, G Burnell, JP Valdés-Herrera, BD Simons, PB Littlewood, E Artacho, A Fert & ND Mathur, *Nature* **445**, 410 (2007).

[2] JM Pruneda, V Ferrari, R Rurali, PB Littlewood, NA Spaldin and E Artacho, *Phys. Rev. Lett.* **99**, 226101 (2007).