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Interplay of strain and magnetism in manganese perovskites from first-principles calculations ALESSIO FILIPPETTI, CNR-INFM SLACS, GIUSEPPE COLIZZI, VINCENZO FIORENTINI — An exciting frontier for spintronic applications is the field of magnetic multilayered heterostructures capable of cleverly exploiting the coupling of strain and magnetism. A striking example is the piezoelectric/piezomagnetic heterojunction (e.g. $La_{1-x}Sr_xMnO_3$ (LSMO) grown on PZT) for which large resistance modulations have been observed. We have employed three different methodologies (GGA, GGA+U,and pSIC) to determine structural, electronic, and magnetic properties of LSMO at x=0.375 doping, and analyze a series of magnetic phase transitions caused by longitudinal strain applied on LSMO whose in-plane lattice constant is kept fixed at the value of several representative substrates. Overall we found LSMO quite sensitive to the applied strain, with highly anisotropic response in terms of both structural (i.e. Jahn-Teller) distortions and change in magnetization. In particular, the choice of two independent strain parameters (substrate and uniaxial strain) enables a nice tunability of the magnetic properties, which in turn, may dramatically alter the conductivity, even turning LSMO in insulator.

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