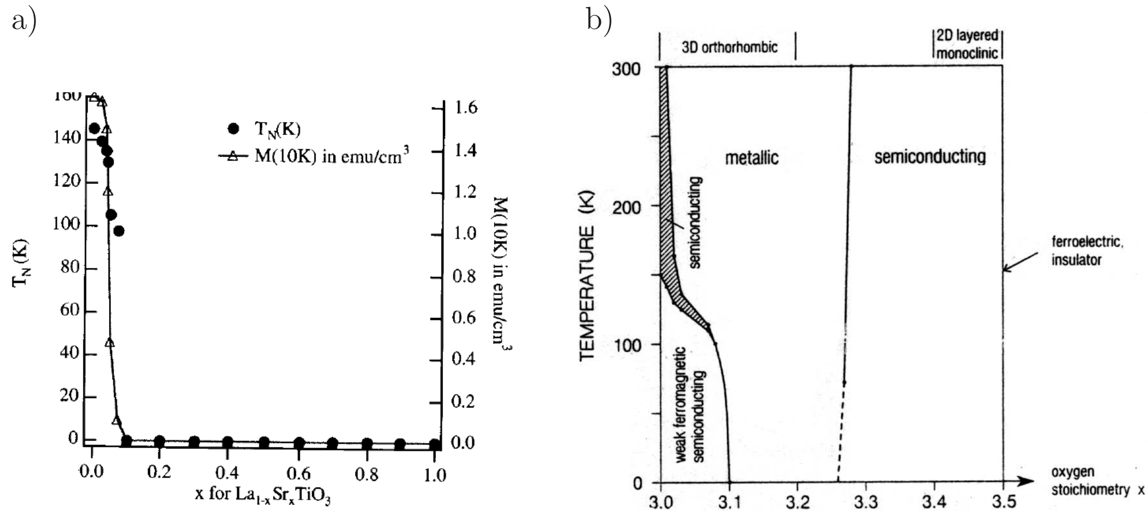

Figure 5.2: a) Néel temperature T_N and remanent magnetization at $T = 10$ K for $La_{1-x}Sr_xTiO_3$ as a function of doping (Hays et al., 1999). **b)** Phase diagram for $LaTiO_{3+x}$ (Lichtenberg et al., 1991).

electrons, i.e., formally reaches noble gas configuration in $La_{1-x}Sr_xTiO_3$ as well, so that Ti obtains the configuration $3d^1$ in pure $LaTiO_3$. As discussed in App. A.1, cubic symmetry splits the $3d$ band into a twofold degenerate e_g and a threefold degenerate t_{2g} band as depicted in Fig. 5.1c. While in principle the reduced symmetry due to distortion should further split up the t_{2g} band, this effect is negligible in practice since the local ligand field of the Ti ion is dominated by the local octahedral oxygen coordination which retains cubic symmetry. The single electron per unit cell therefore occupies predominantly the threefold degenerate t_{2g} bands hybridizing via oxygen $2p$ states. The effective overlap between Ti states of neighboring unit cells and, consequently, the effective band width (in a single-particle picture) is reduced by orthorhombic distortion compared to the idealized cubic structure for $La_{1-x}Sr_xTiO_3$ (and even more for $YTiO_3$ where $\alpha \approx 142°$).

Experimentally, pure $LaTiO_3$ is an antiferromagnetic insulator with a Néel temperature estimated between $T_N \approx 125$K (Eitel and Greedan, 1986) and $T_N \approx 145$ K (Hays, Zhou, Markert, and Goodenough, 1999); see Fig. 5.2. The Ti magnetic moment saturates at 0.45 μ_B and the energy gap is about 0.2 eV (Goral, Greedan, and MacLean, 1982; Crandles, Timusk, Garrett, and Greedan, 1994). At doping $x \approx 0.05$, $La_{1-x}Sr_xTiO_3$ undergoes an insulator-to-metal transition and becomes a correlated paramagnetic metal with a strongly enhanced susceptibility and electronic specific heat coefficient (Pickett, Erwin, and Ethridge, 1998). Apparently, the fabrication of samples of controlled stoichiometry and even the a posteriori analysis of their composition are still nontrivial tasks for experimentalists. Often, only the formal deviation $\delta = x + y/2$ from integer t_{2g} filling of a composition $La_{1-x}Sr_xTiO_{3+y}$ is stated in results (Lichtenberg et al., 1991) as seen in Fig. 5.2b. For $y > 0$ such a formula does no longer correspond to a unit cell since there is no place in the structure