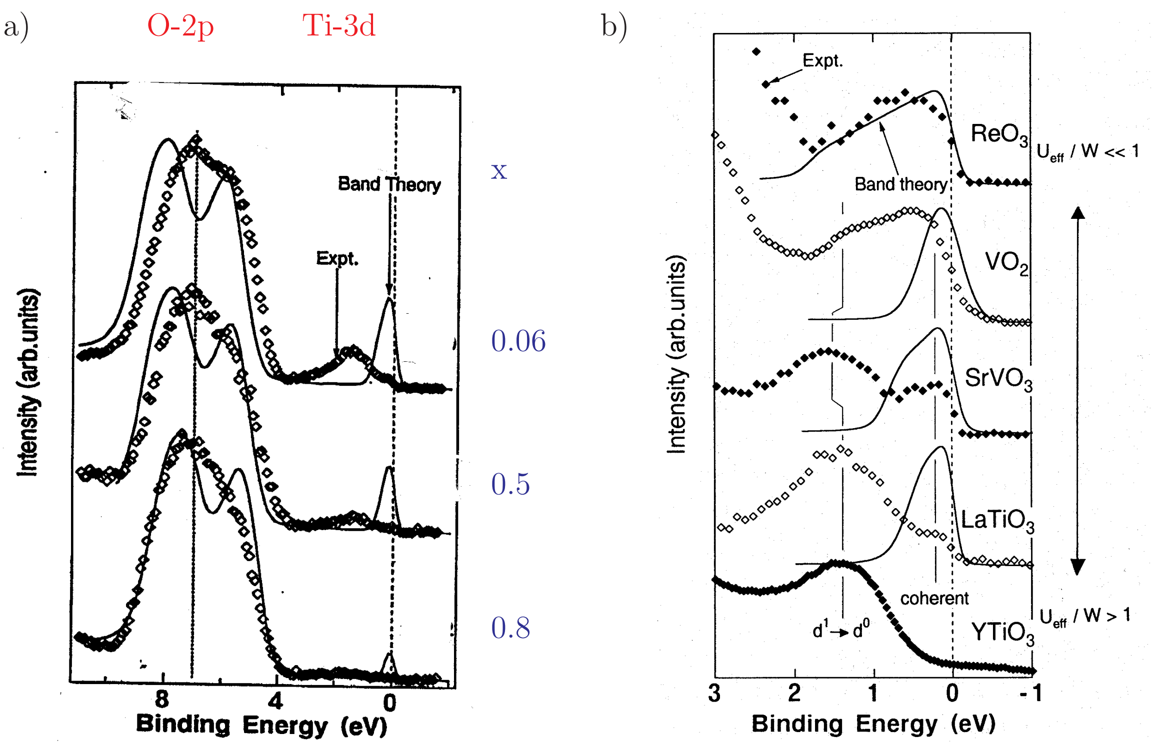

Figure 5.3: a) Photoemission spectra (squares) in comparison with LDA calculations (solid lines) for $La_{1-x}Sr_xTiO_3$ (Fujimori, Hase, Nakamura, Namatame, Fujishima, Tokura, Abbate, de Groot, Czyzyk, Fuggle, Strebel, Lopez, Domke and Kaindl, 1992). **b)** PES over reduced energy range of various transition metal oxides with d^1 configuration with increasing deviations from LDA calculations from top to bottom. The curve "$LaTiO_3$" gives a magnified view of the PES of $La_{1-x}Sr_xTiO_3$ for $x = 0.06$ (Fujimori, Hase, Namatame, Fujishima, Tokura, Eisaki, Uchida, Takegahara and de Groot, 1992).

for interstitial oxygen; instead vacancies form at La and Ti sites in this case (Hays et al., 1999). As seen in Fig. 5.2 a, recent measurements (with 1% relative accuracy of the oxygen content) show a continuous decay of the remanent magnetization with increased Sr doping while the Néel temperature jumps discontinuously with an intermediate plateau. This behavior implies the existence of a two-phase region including AF order for $La_{1-x}Sr_xTiO_3$ with $0.045 \leq x \leq 0.08$ (Hays et al., 1999).

The importance of correlations is directly seen in Fig. 5.3 a, a comparison between measured photoemission spectra (PES) and theoretical estimates based on LDA band structure calculations. Evidently, the oxygen $2p$ bands lying far below the Fermi energy are well reproduced by LDA; in contrast, spectral weight corresponding to t_{2g} bands is predicted by LDA as a peak at the Fermi energy while the experiment shows contributions at around -1.5 eV. The disagreement is strongest for small doping x (i.e., large occupancy $1 - x$ of the Ti t_{2g} band) which is the case we will study in the following. Both a magnified view of the t_{2g} portion of the PES for $La_{1-x}Sr_xTiO_3$ for $x = 0.06$, i.e., just outside the antiferromagnetic phase region, and a comparison to other transition metal oxides with d^1 configuration are shown in Fig. 5.3 b.