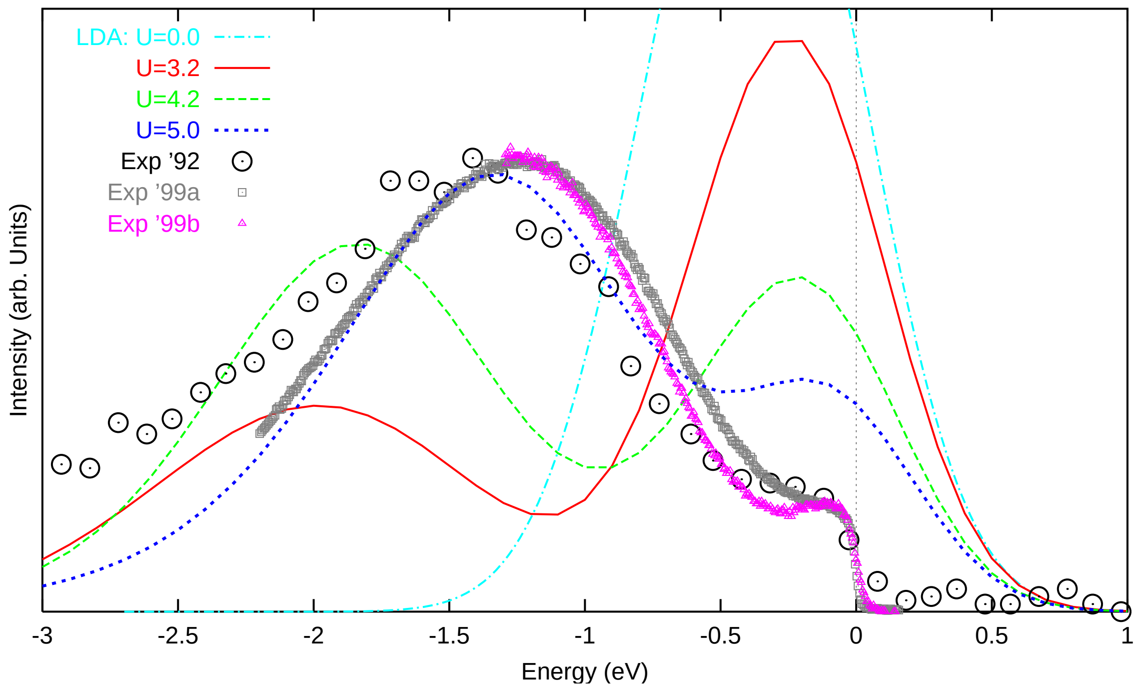


**Figure 5.7:** $La_{1-x}Sr_xTiO_3$ photoemission spectra (x=0.06): LDA+DMFT(QMC) estimates for different $U$ (QMC simulations at $T = 1160$ K, Fermi function for $T \approx 0$ K) in comparison with experiments at $T = 80$ K (Fujimori, Hase, Namatame, Fujishima, Tokura, Eisaki, Uchida, Takegahara and de Groot, 1992), $T = 23$ K (a), and $T = 150$ K (b) (Yoshida et al., 2002). The agreement with experiments improves with increasing $U$ (used in the simulation).

predicted correctly. Although the relative weight originating from the quasiparticle peak is computed to be almost a factor of 5 higher than seen experimentally, the improvement over LDA is impressive. The value of $U \approx 5$ eV which best reproduces the experimental spectra is a bit higher than estimated from LDA, but still within the error range, in particular when the reduction of band width by orthorhombic distortion is considered. The remaining differences may be due to disorder,[19] to a reduced hybridization at the surface, to deficiencies of the theoretical PES treatment, to simplifications inherent in the electronic model, to the too high temperature used in the QMC cimulations, and to numerical errors related to the QMC and MEM treatment of the DMFT problem. This last technical point will be addressed in the following subsections where we also leave the ground of published collaborative work.

We point out that due to the high spectral weight present in $\rho(\epsilon)$ just above the Fermi energy (cf. Fig. 5.5), the spectral weight near the Fermi energy of the resulting PES is very sensitive to the exact position of the Fermi energy. In fact,

[19]Note that, while the experimentally realized form of doping with 3% O should correspond to 6% doping with Sr, the materials are clearly not fully equivalent electronically. In particular, disorder should have much stronger effects for $LaTiO_{3.03\pm0.01}$.