Chapter 5

Realistic Modeling of Strongly Correlated Materials

Well-controlled studies of abstract models like the one-band Hubbard model as presented in the preceding chapters shed light on important physical phenomena, even when the models themselves are neither fully realistic nor complete (full frustration, single-band assumption, etc.). Still, one ultimate goal of condensed matter theory is a controlled description of materials which is as realistic as possible and allows for a material-specific calculation of a wide range of properties. One step into this direction, although not fully controlled, is the recently developed LDA+DMFT method which we will apply in this chapter for modeling the doped transition metal oxide $La_{1\text{-}x}Sr_xTiO_3$. We will introduce the material under investigation and demonstrate the failure of LDA to reproduce its photoemission spectrum in Sec. 5.1, then discuss conventional density functional theory in Sec. 5.2 and introduce the LDA+DMFT method in Sec. 5.3. Numerical results will be presented and compared with experiments in Sec. 5.4.

The work presented in this chapter was started in a collaboration with the Optics of Metals Laboratory at the Institute of Metal Physics of the Ural Division of the Russian Academy of Sciences in Yekaterinburg lead by Prof. V. I. Anisimov. In particular, all LDA calculations were performed by Igor Nekrasov from Anisimov's group. The initial QMC and MEM results presented in subsection 5.4.1 were mainly calculated by Nekrasov and Held using Held's multi-band version of the QMC code while the photoemission spectra were obtained using an analysis program written as part of this thesis. The QMC computations at higher accuracy and the study of the impact of different MEM procedures on the resulting spectra presented in subsection 5.4.2 as well as the calculation of transport properties in subsection 5.4.3 were also performed by the author of this thesis.