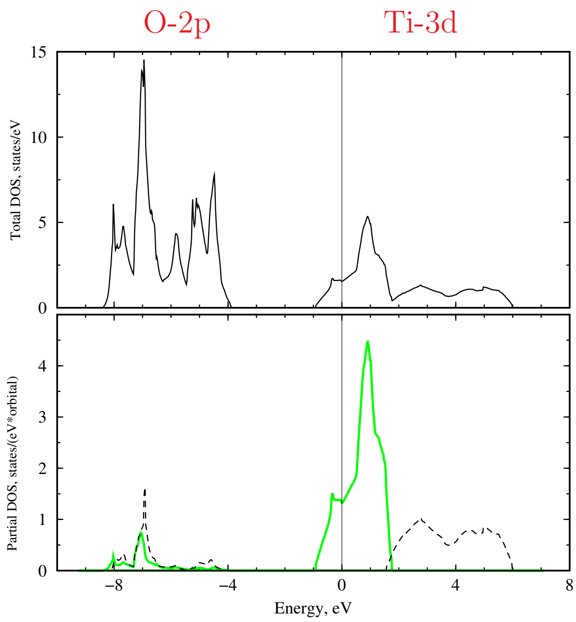

Figure 5.4: Upper part: LDA DOS $\rho(\epsilon)$ for $|\epsilon| < 10$ eV. The band is clearly split into contributions with O-2p and Ti-3d character, respectively. Lower part: partial Ti-3d LDA DOS. The t_{2g} contribution (solid line) forms the peak at the Fermi level, the e_g contribution (dashed lines) is primarily located above.

the Stuttgart TB-LMTO-ASA program in version 4.7 (Jepsen and Andersen, 2000) within the basis set Ti($4s, 4p, 3d$) La($6s, 6p, 5d$) O($2s, 2p$) at a Wigner Seitz radius of 2.37 atomic units for Ti. The average on-site interaction for t_{2g} orbitals was calculated as $U \approx 4.2$ eV which contrasts with an estimate of $U \approx 3.2$ eV previously obtained within LMTO-ASA in orthogonal representation (Solovyev, Hamada, and Terakura, 1996). Since LDA is a ground state method, its numerical results apply to temperature $T = 0$.

The low-energy part (measured from the chemical potential) of the resulting full LDA DOS is shown in the upper part of Fig. 5.4. In comparing to the lower part of Fig. 5.4, which displays only the Ti 3d contribution (note the different scales), split up into t_{2g} and e_g parts, we find a situation typical of early[15] transition metal oxides: The band at about -8 to -4 eV corresponds to the completely filled O 2p bands, while the Ti 3d band is located near the Fermi level. Very importantly, the t_{2g} orbitals account for nearly all the weight of the peak at the Fermi energy and have very small overlap with other bands. Therefore, we can disregard all t_{2g} contributions to the DOS below about -1 eV. Then the t_{2g} band has a total width (edge to edge) of about 2.8 eV with a root-mean-square spread in the energy distribution of 0.65 eV. Double counting corrections not yet included in the plot should move the bottom of the t_{2g} band down compared to the rest by at most 2 eV. We note that the O 2p bands also lead to some contribution near the Fermi energy which will also be neglected in the

[15]Here, "early" refers to the position of the transition metal in the periodic table of elements, i.e., denotes a small number of valence d electrons per atom.