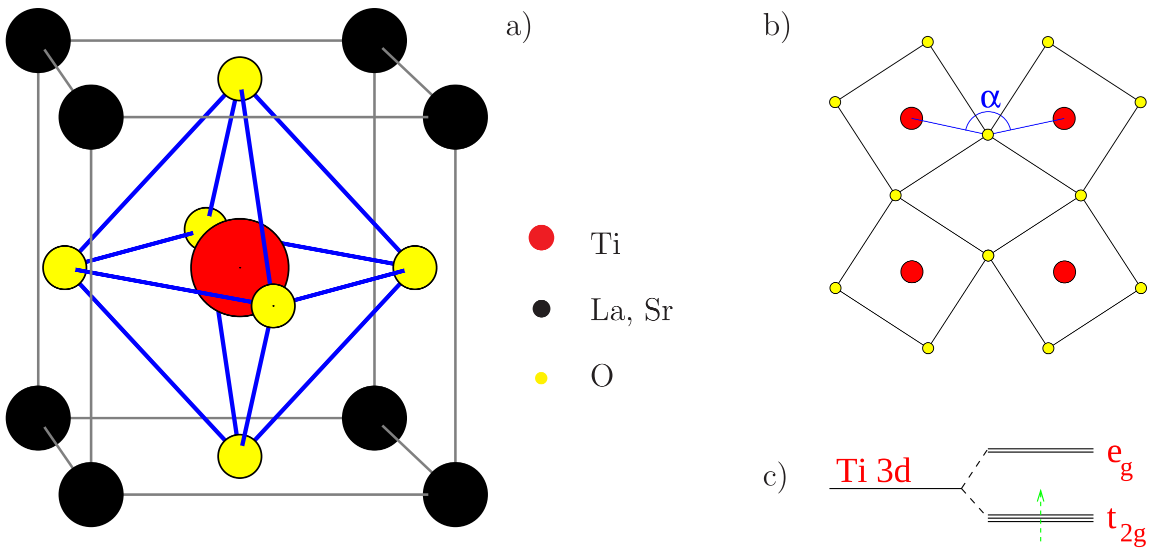

Figure 5.1: Structure of $La_{1\text{-}x}Sr_xTiO_3$: **a)** Idealized (cubic) perovskite structure: Ti ions are octahedrally coordinated by oxygen in a cubic matrix of sites occupied by either La or Sr (presumably disordered). The size of spheres in the figure is not related to ionic radii. **b)** Orthorhombic distortion, i.e., alternating tilting of oxygen octahedra which reduces the angle Ti-O-Ti to $\alpha \approx 155°$. **c)** Scheme of band degeneracy; the t_{2g} band contains one electron per unit cell for $LaTiO_3$ and is empty for $SrTiO_3$.

5.1 $La_{1\text{-}x}Sr_xTiO_3$, a Strongly Correlated Transition Metal Oxide

$La_{1\text{-}x}Sr_xTiO_3$ belongs to a large class of $3d$ transition metal oxides of composition ABO_3, where A is a rare earth or alkalide (or a nonstoichiometric combination thereof) and B a transition metal and which crystallize in the orthorhombically distorted perovskite ($GdFeO_3$-type) structure. The idealized cubic perovskite structure is shown in Fig. 5.1 a. In the distorted perovskite, the almost perfectly rigid oxygen octahedra tilt alternatingly in all space directions so that the angle α (Ti-O-Ti) is reduced from its cubic value of 180° to, e.g., $\alpha \approx 155°$ for $La_{1\text{-}x}Sr_xTiO_3$ (MacLean, Ng, and Greedan, 1979), see Fig. 5.1 b.[1] Formally, pure $SrTiO_3$ is an ionic insulator where all ions reach noble gas configurations.[2] In fact, this material is a band insulator which is seen both in experiment and band structure calculations and makes this material well-suited as substrate or spacer material for high-T_c superconducting films.[3] Both experiment and band-structure calculations imply that La donates 3

[1] The degree of distortion can in general be estimated from ionic radii in terms of the tolerance factor $f = (r_A + r_O)/(\sqrt{2}(r_B + r_O))$, where $f \approx 0.8$ corresponds to $\alpha \approx 140°$ and $f \approx 0.95$ corresponds to $\alpha \approx 157°$, respectively (Imada et al., 1998).

[2] O needs 2 electrons to obtain the [Ne] configuration; the atomic configuration is [Kr] $5s^2$ for Sr, [Ar] $3d^1 4s^2$ for Ti, and [Xe] $5d^1 6s^2$ for La.

[3] The chemically reduced component, $SrTiO_{3-\delta}$, is a superconductor with $T_c \lesssim 0.5$ K (Schooley, Hosler, Ambler, Becker, Cohen, and Koonce, 1965).