

Last but not least, the book is a testimonial in itself to the persistence and fruitfulness of a professor (T.M.)–student (E.P.) collaboration—one that has been almost entirely informal and dating back to the early 1990’s.

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## Chapter 1

# Tight-binding modeling of layered perovskites

### 1.1 Introduction

After the discovery of the high- $T_c$  superconductors the layered cuprates became one of the most studied materials in solid state physics. A vast range of compounds were synthesised and their properties comprehensively investigated. The electron band structure is of particular importance for understanding the nature of superconductivity in this type of perovskites [9]. Along this line one can single out the significant success achieved in the attempts to reconcile the photoelectron spectroscopy data [10,11] and the band structure calculations of the Fermi surface (FS) especially for compounds with simple structure such as  $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_{4-\delta}$  [12,13]. A qualitative understanding, at least for the self-consistent electron picture, has been achieved and for the most electron processes in the layered perovskites one can employ adequate lattice models.

At the time when we actually started working on the subject of this book, there was not much analysis of the electronic band structures of the high- $T_c$  materials in the terms of single analytical expressions available. This is something for which there was a clear need, in particular to help in the construction of more realistic many-body Hamiltonians. The aim of this chapter is to analyse the common features in the electron band structure of the layered perovskites within the tight-binding (TB) method (for a nice review see references [14–16]). In the following we shall focus on the metallic (being eventually superconducting) phase only, with the provision that the antiferromagnetic correlations, especially in the dielectric phase, could substantially alter the electron dispersion. It is shown that the linear combination of atomic orbitals (LCAO) approximation can be considered as an adequate tool for analysis of energy