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Abstract

This book is dedicated to Tight Binding. It explains the principles on which this method is based on and it presents its applications on molecules like the nucleic acid bases and similar ones, as well as on base pairs, which we call monomers. Then we extend it to dimers, trimers, oligomers and polymers as well as to various categories of one-dimensional solids, periodic or aperiodic (quasi-periodic or fractal). It is explained how we arrive to a two-level system as two initially isolated one-level systems approach, and then we extend to multi-level systems. Various one-dimensional systems are solved and principal notions are defined. Conjugated molecules are examined analytically (in simpler cases) as well as numerically. The linear combination of atomic orbitals as well as the linear combination of molecular orbitals is introduced. Then, the electronic structure using all valence orbitals is discussed and it is applied to benzene and 1,3,5-triazine. Afterwards, the electronic structure and the charge transfer in DNA monomers, dimers, trimers, tetramers and polymers is examined either at the base pair level or at the base level. Various well-known models are analyzed like the wire model, the simple and extended ladder model, as well as their combinations with the fishbone model. Then we examine the electronic structure and the charge transfer in atomic carbon wires aka carbynes, either cumulenic or polyynic. Tight binding models are presented in second quantization formulation and various famous aperiodic sequences (quasi-periodic or fractal) are analyzed.