



Quantum Chemistry of Solids: The LCAO First Principles Treatment of Crystals (Springer Series in Solid-State Sciences)

Robert Evarestov

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This book delivers a comprehensive account of the main features and possibilities of LCAO methods for the first principles calculations of electronic structure of periodic systems. The first part describes the basic theory underlying the LCAO methods applied to periodic systems and the use of wave-function-based, density-based (DFT) and hybrid hamiltonians. The second part deals with the applications of LCAO methods for calculations of bulk crystal properties.

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