



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

By Robert A. Evarestov

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Editorial Review

From the Back Cover

Quantum Chemistry of Solids 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 wavefunction-based (Hartree-Fock), density-based (DFT) and hybrid hamiltonians. The translation and site symmetry consideration is included to establish connection between k-space solid-state physics and real-space quantum chemistry methods in the framework of cyclic model of an infinite crystal. The inclusion of electron correlation effects for periodic systems is considered on the basis of localized crystalline orbitals. The possibilities of LCAO methods for chemical bonding analysis in periodic systems are discussed. The second part deals with the applications of LCAO methods for calculations of bulk crystal properties, including magnetic ordering and crystal structure optimization. The discussion of the results of some supercell calculations of point defects in non-metallic solids and of the crystalline surfaces electronic structure illustrates the efficiency of LCAO method for solids.

About the Author

Born 1937 in St.Petersburg (Russia). A study of Theoretical Physics at St.Petersburg State University (SPBU). 1964 PhD. From 1964 to 1968 assistant at SPBU, mathematical physics department. From 1968- quantum chemistry department at SPBU-associate Professor (1968). Professor (1979),since 1995 Head of Quantum Chemistry Department , SPBU. Full Member of Russian Academy of Natural Sciences (1992),Humboldt Foundation award winner (1998), foreign member of Latvian Academy of Science (2003), Author of 200 scientific publications on theory of symmetry and electronic structure of crystals and 6 books, including Site Symmetry in Crystals.Theory and applications, published in Springer Series in Solid State sciences in two editions (1993,1997)

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