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Titolo	Electronic Structure and Physical Properties of Solids [[electronic resource] ] : The Uses of the LMTO Method // edited by Hugues Dreyse
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Collana	Lecture Notes in Physics, , 0075-8450 ; ; 535
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Nota di bibliografia	Includes bibliographical references at the end of each chapters.
Nota di contenuto	Ground and Excited-State Formalisms -- Developing the MTO Formalism -- From ASA Towards the Full Potential -- A Full-Potential LMTO Method Based on Smooth Hankel Functions -- Full-Potential LMTO Total Energy and Force Calculations -- Excited States Calculated by Means of the Linear Mu.n-Tin Orbital Method -- Magnetic Properties -- Fully Relativistic Band Structure Calculations for Magnetic Solids - Formalism and Application -- First Principles Theory of Magneto—Crystalline Anisotropy -- On the Implementation of the Self-Interaction Corrected Local Spin Density Approximation for d- and f-Electron Systems -- Ab Initio Theory of the Interlayer Exchange Coupling -- Disordered Alloys -- Disordered Alloys and Their Surfaces: The Coherent Potential Approximation -- Locally Self-Consistent Green's Function Method and Its Application in the Theory of Random Alloys -- Large-Scale Real-Space Calculations -- Sparse Direct Methods: An Introduction -- Real-Space Tight-Binding LMTO Approach to Magnetic Anisotropy: Application to Nickel Films on Copper -- Combining Real Space and Tight Binding Methods for Studying Large Metallic Systems.
Sommario/riassunto	This book displays the latest developments in the determination of the electronic structure of solids and the physical properties which can be described from the electronic structure. Special emphasis is placed on the Linear Muffin Tin Orbital method for ground state and excited state

calculation. The state-of-the-art of the formalisms is presented, from the venerable Atomic Sphere Approximation to the Full Potential schemes. The efficiency of this method is shown in various situations: magnetic properties, interlayer exchange coupling, metallic alloys, d- and f-electron systems. The latter part of the book is devoted to large-scale real-space calculations, including an introduction to sparse direct methods. With the aim of maximizing tutorial value, experts in each domain present over ten years of work, which has been published only in specialised papers before and now becomes available for researchers as well as students and teachers in solid state physics or materials science.

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