



Electronic Structure of Materials (Oxford Science Publications)

Adrian P. Sutton

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In recent years, researchers have increasingly recognized the dominant role of the local atomic environment in controlling the electronic structure and properties of materials. This recognition has spawned the "real-space" approach that provides a coherent framework for the study of perfect and defective crystals and non-crystalline materials. In addition to presenting these ideas, this text details the reciprocal-space approach--exemplified in band theory--and draws powerful links between the two approaches. The book includes illustrations and examples of many up-to-date calculations based on density functional theory that are used today as predictive tools in materials science. Throughout the book, the mathematical complexity is kept to a minimum, while comprehensive problem sets allow readers to master the fundamental concepts. The text provides for students in materials science, physics, and chemistry a unique introduction to predictive modelling of the electronic structure and properties in today's materials.

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