This book describes modern thinking about the electronic structure and properties of crystalline and non-crystalline materials in a form that is readily accessible to undergraduates in materials science, physics, and chemistry. In recent years the dominant role of the local atomic environment in controlling electronic structure and properties of materials has been recognized. The 'real-space' approach to electronic structure that this recognition has spawned runs through the book, and provides a coherent framework in which to study perfect and defective crystals and non-crystalline materials. This is the approach that those who have been worried by the conventional preoccupation with perfect crystals and band theory have been waiting for. The reciprocal space approach, exemplified in band theory, is also developed and powerful links between the two approaches are shown. Modern, first principles calculations, based on density functional theory, are now predictive tools in materials science and they are introduced and illustrated with relevant examples. Throughout this book the mathematical complexity is kept to a bare minimum. This book provides a unique introduction to current understanding and predictive modelling of electronic structure and properties in today's materials.

Adrian Sutton is a University Lecturer in Materials Science at Oxford University and a Fellow of Linacre College.

The cover shows a snapshot of the electronic charge density of a chlorine molecule dissociating on a silicon (111) surface as computed self-consistently in density functional theory by A. De Vita, M. J. Gillan, D. King-Smith, M. C. Payne, and I. Stich.

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