

Materials Modelling using Density Functional Theory: Properties and Predictions

By Feliciano Giustino

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This book is an introduction to the quantum theory of materials and first-principles computational materials modelling. It explains how to use density functional theory as a practical tool for calculating the properties of materials without using any empirical parameters. The structural, mechanical, optical, electrical, and magnetic properties of materials are described within a single unified conceptual framework, rooted in the Schrodinger equation of quantum mechanics, and powered by density functional theory.

This book is intended for senior undergraduate and first-year graduate students in materials science, physics, chemistry, and engineering who are approaching for the first time the study of materials at the atomic scale. The inspiring principle of the book is borrowed from one of the slogans of the Perl programming language, 'Easy things should be easy and hard things should be possible'. Following this philosophy, emphasis is placed on the unifying concepts, and on the frequent use of simple heuristic arguments to build on one's own intuition. The presentation style is somewhat cross disciplinary; an attempt is made to seamlessly combine materials science, quantum mechanics, electrodynamics, and numerical analysis, without using a compartmentalized approach. Each chapter is accompanied by an extensive set of references to the original scientific literature and by exercises where all key steps and final results are indicated in order to facilitate learning. This book can be used either as a complement to the quantum theory of materials, or as a primer in modern techniques of computational materials modelling using density functional theory.

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Editorial Review

Review
At last an undergraduate/graduate textbook that demonstrates the power of density functional theory not only to help interpret experimental data but also to predict the properties of new materials. Each chapter is lucidly presented with heuristic, intuitive arguments leading to the main ideas before numerous examples illustrate the often remarkable accuracy of density functional theory over a wide range of electronic, structural, mechanical, optical and magnetic properties. A book that should be on the shelves of every library in Materials Science and Engineering, Physics and Chemistry departments. David Pettifor, University of Oxford The density functional theory has finally brought quantum mechanics into materials science. Its proven ability to produce correct predictions of properties of real materials means that it has taken over as the premier method in solid state materials, ultimately because of its suitability as a numerical method. While traditional books still build from analytically tractable models, this book reflects more accurately current practice. The book will be ideal for a graduate-level student with a grounding in quantum mechanics, and could be tackled in an undergraduate course. Graeme Ackland, University of Edinburgh

About the Author

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Feliciano Giustino is a University Lecturer in the Department of Materials at the University of Oxford, the co-Director of the Materials Modelling Laboratory, and Associate Editor of the European Physical Journal B. He holds an MSc in Nuclear Engineering from the Politecnico di Torino, a PhD in Physics from the Ecole Polytechnique Federale de Lausanne, and before joining the Department of Materials at Oxford he was a researcher in the Department of Physics at the University of California at Berkeley. His research team specializes in the computational modelling of nanomaterials and the development of methods for electronic structure calculations. He has been recipient of the European Research Council Starting Grant and of the Leverhulme Research Leadership Award. Besides his research work, he teaches two undergraduate courses on the quantum theory of materials at the University of Oxford.

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