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MATERIALS MODELLING USING DENSITY FUNCTIONAL THEORY: PROPERTIES AND PREDICTIONS



Oxford University Press. Hardback. Book Condition: new. BRAND NEW, Materials Modelling Using Density Functional Theory: Properties and Predictions, Feliciano Giustino, 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...

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- Authored by Feliciano Giustino
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