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Autore	Maezono Ryo
Titolo	Ab initio Calculation Tutorial : For Materials Analysis, Informatics and Design / / by Ryo Maezono
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ISBN	9789819909193
Edizione	[1st ed. 2023.]
Descrizione fisica	1 online resource (285 pages)
Disciplina	780
Soggetti	Density functionals Materials science - Data processing Electronic structure Quantum chemistry - Computer programs Materials Chemistry Computer simulation Density Functional Theory Electronic Structure Calculations Computational Materials Science Computational Design Of Materials
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Introduction -- Preparing tutorial environments -- Sequence of computational procedure -- Determining computational conditions -- Points to understand in background theories. .
Sommario/riassunto	This textbook covers the framework of first-principles analysis applied to materials using density functional theory (DFT). It provides a set of hands-on tutorials using the Quantum ESPRESSO package, an open-source software for DFT. The tutorials are well chosen, designed for maximum effectiveness while requiring a minimum of the reader’s time, and the book describes how the essential components are combined to create the practical applications based on the idea of modeling practical problems of materials. The book carefully explains how to prepare the platform to run the tutorials assisted by free

software. This textbook is useful for students in experimental laboratories, for industrial researchers, and for those not majoring in theoretical studies but learning individually.