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Titolo	Multiscale Paradigms in Integrated Computational Materials Science and Engineering : Materials Theory, Modeling, and Simulation for Predictive Design / / edited by Pierre Deymier, Keith Runge, Krishna Muralidharan
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Disciplina	003.3
Soggetti	Physics Optical materials Electronics - Materials Solid state physics Applied mathematics Engineering mathematics Nanotechnology Numerical and Computational Physics, Simulation Optical and Electronic Materials Solid State Physics Mathematical and Computational Engineering
Lingua di pubblicazione	Inglese
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Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references at the end of each chapters and index.
Nota di contenuto	Orbital-free Density Functional Theory (OFDFT) -- Path Integral Molecular Dynamics (PIMD) -- Interatomic Potentials Including Chemistry -- Consistent Embedding -- Nano- and Meso-Scale Materials Phenomena -- Phase Field Methods -- Multiscale Spatial and Temporal Data Fusion and Fission in Materials -- Multiscaling and Materials Imaging -- Peridynamics -- Conclusions and Industrial Perspectives.
Sommario/riassunto	This book presents cutting-edge concepts, paradigms, and research highlights in the field of computational materials science and engineering, and provides a fresh, up-to-date perspective on solving

present and future materials challenges. The chapters are written by not only pioneers in the fields of computational materials chemistry and materials science, but also experts in multi-scale modeling and simulation as applied to materials engineering. Pedagogical introductions to the different topics and continuity between the chapters are provided to ensure the appeal to a broad audience and to address the applicability of integrated computational materials science and engineering for solving real-world problems.