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Titolo	Forcefields for Atomistic-Scale Simulations: Materials and Applications / / edited by Akarsh Verma, Sanjay Mavinkere Rangappa, Shigenobu Ogata, Suchart Siengchin
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Descrizione fisica	1 online resource (395 pages)
Collana	Lecture Notes in Applied and Computational Mechanics, , 1860-0816 ; ; 99
Disciplina	531.6
Soggetti	Materials science - Data processing Molecular dynamics Nanotechnology Atomic structure Molecular structure Microclusters Atomistic Models Molecular Dynamics Atomic and Molecular Structure and Properties Atomic and Molecular Clusters
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Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	1. Introduction to Forcefields -- 2. Forcefields for characterization of metals/metal alloys -- 3. Forcefields for characterization of nuclear materials -- 4. Forcefields and Atomistic insights to study high entropy alloys -- 5. Coarse-grained forcefields for anisotropically interacting particles -- 6. Forcefields for 2D nanomaterials (Graphene and h-BN) and the universal solvent “water” -- 7. Reactive forcefield (ReaxFF) for the combustion application -- 8. Reactive forcefield (ReaxFF) for the 2D nanomaterials synthesis -- 9. Forcefields and Modelling of Polymer Coatings and nanocomposites -- 10. Accelerated reactive forcefields for studying nanomaterials and polymers.
Sommario/riassunto	This book describes the forcefields/interatomic potentials that are used in the atomistic-scale and molecular dynamics simulations. It covers

mechanisms, salient features, formulations, important aspects and case studies of various forcefields utilized for characterizing various materials (such as nuclear materials and nanomaterials) and applications. This book gives many help to students and researchers who are studying the forcefield potentials and introduces various applications of atomistic-scale simulations to professors who are researching molecular dynamics.