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Nota di contenuto	1. Descriptors for Machine Learning of Materials Data -- 2. Potential Energy Surface Mapping of Charge Carriers in Ionic Conductors Based on a Gaussian Process Model -- 3. Machine learning predictions of factors affecting the activity of heterogeneous metal catalysts -- 4. Machine Learning-based Experimental Design in Materials Science -- 5. Persistent homology and materials informatics -- 6. Polyhedron and Polychoron codes for describing Atomic Arrangements -- 7. Topological Data Analysis for the Characterization of Atomic Scale Morphology from Atom Probe Tomography Images -- 8. Atomic-scale nanostructures by advanced electron microscopy and informatics -- 9.

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Sommario/riassunto

This open access book brings out the state of the art on how informatics-based tools are used and expected to be used in nanomaterials research. There has been great progress in the area in which "big-data" generated by experiments or computations are fully utilized to accelerate discovery of new materials, key factors, and design rules. Data-intensive approaches play indispensable roles in advanced materials characterization. "Materials informatics" is the central paradigm in the new trend. "Nanoinformatics" is its essential subset, which focuses on nanostructures of materials such as surfaces, interfaces, dopants, and point defects, playing a critical role in determining materials properties. There have been significant advances in experimental and computational techniques to characterize individual atoms in nanostructures and to gain quantitative information. The collaboration of researchers in materials science and information science is growing actively and is creating a new trend in materials science and engineering. This book is open access under a CC BY license.