

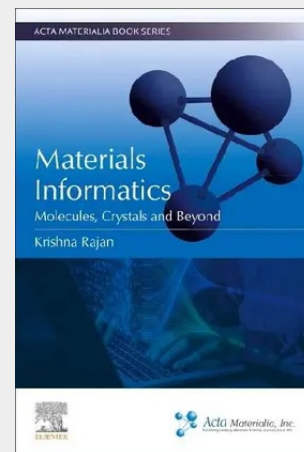
Materials Informatics

Molecules, Crystals, and Beyond

Materials Informatics: Molecules, Crystals and Beyond discusses the role of information science in aiding the discovery and interpretation of multiscale relationships that are critical for materials discovery, design, and optimization. The book covers key challenges in applying information science methods to materials science, including the multidimensional nature of structure-property relationships, data sparsity, and the nature and sources of uncertainty, along with a brief overview of the algorithmic tools used for unsupervised and supervised learning. Building on these topics, chapters then cover the development of physics/chemistry informed data representations of structure and properties, the application of machine learning for structure and property prediction and screening for targeted properties, and the utilization of techniques such as graphics recognition, natural language processing, and statistically driven visualization tools in deciphering processing-structure-property-performance relationships in materials.

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