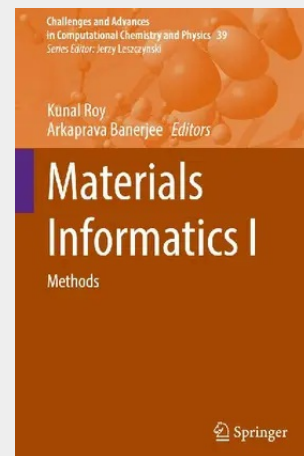


Materials Informatics I

Methods

This contributed volume explores the integration of machine learning and cheminformatics within materials science, focusing on predictive modeling techniques. It begins with foundational concepts in materials informatics and cheminformatics, emphasizing quantitative structure-property relationships (QSPR). The volume then presents various methods and tools, including advanced QSPR models, quantitative read-across structure-property relationship (q-RASPR) models, optimization strategies with minimal data, and in silico studies using different descriptors. Additionally, it explores machine learning algorithms and their applications in materials science, alongside innovative modeling approaches for quantum-theoretic properties. Overall, the book serves as a comprehensive resource for understanding and applying machine learning in the study and development of advanced materials and is a useful tool for students, researchers and professionals working in these areas.

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