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Informatics for Materials Science and Engineering: Data-driven Discovery for Accelerated Experimentation and Application

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Materials informatics: a 'hot topic' area in materials science, aims to combine traditionally bio-led informatics with computational methodologies, supporting more efficient research by identifying strategies for time- and cost-effective analysis.

The discovery and maturation of new materials has been outpaced by the thicket of data created by new combinatorial and high throughput analytical techniques. The elaboration of this "quantitative avalanche"—and the resulting complex, multi-factor analyses required to understand it—means that interest, investment, and research are revisiting informatics approaches as a solution.

This work, from Krishna Rajan, the leading expert of the informatics approach to materials, seeks to break down the barriers between data management, quality standards, data mining, exchange, and storage and analysis, as a means of accelerating scientific research in materials science.

This solutions-based reference synthesizes foundational physical, statistical, and mathematical content with emerging experimental and real-world applications, for interdisciplinary researchers and those new to the field.

- Identifies and analyzes interdisciplinary strategies (including combinatorial and high throughput approaches) that accelerate materials development cycle times and reduces associated costs
- Mathematical and computational analysis aids formulation of new structure-property correlations among large, heterogeneous, and distributed data sets
- Practical examples, computational tools, and software analysis benefits rapid identification of critical data and analysis of theoretical needs for future problems



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Editorial Review

Review

"The first half of the volume sets out foundational aspects of data science, and the second half surveys applications in materials science using a case-study approach. The topics include novel approaches to statistical learning in materials science, data dimensionality reduction in materials science,... high-performance computing for accelerated zeolitic materials modeling, and using multivariate analysis to answer questions concerning the conservation of artworks and cultural heritage materials."--Reference & Research Book News, December 2013

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