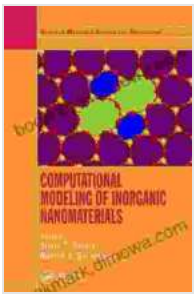
Computational Modeling of Inorganic Nanomaterials: A Comprehensive Guide for Researchers

Inorganic nanomaterials have attracted considerable attention in recent years due to their unique properties and promising applications in various fields, including electronics, optics, catalysis, and biomedicine. Computational modeling provides a powerful tool for understanding the behavior of these materials and predicting their properties.



Computational Modeling of Inorganic Nanomaterials (Series in Materials Science and Engineering Book 18)

by Harold Bloom

★★★★★ 5 out of 5

Language	: English
File size	: 43072 KB
Screen Reader	: Supported
Print length	: 437 pages

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This book provides a comprehensive overview of computational modeling techniques for inorganic nanomaterials, including their synthesis, characterization, and applications. It is written by a team of leading scientists in the field and provides a unique resource for researchers working on inorganic nanomaterials.

Overview of Computational Modeling Techniques

The book begins with an overview of the different computational modeling techniques that can be used to study inorganic nanomaterials. These techniques include:

* Density functional theory (DFT) * Molecular dynamics (MD) * Monte Carlo (MC) * Phase-field modeling * Machine learning

Each of these techniques is described in detail, and its strengths and weaknesses are discussed. The book also provides guidance on how to choose the appropriate technique for a given application.

Synthesis and Characterization of Inorganic Nanomaterials

The next section of the book focuses on the synthesis and characterization of inorganic nanomaterials. Computational modeling can be used to predict the growth mechanisms of nanomaterials and to identify the factors that affect their properties. It can also be used to characterize the structure and properties of nanomaterials, including their size, shape, and surface chemistry.

This section of the book provides a comprehensive overview of the different computational methods that can be used to study the synthesis and characterization of inorganic nanomaterials. It also includes a number of case studies that demonstrate how these methods can be used to solve real-world problems.

Applications of Inorganic Nanomaterials

The final section of the book focuses on the applications of inorganic nanomaterials. Computational modeling can be used to predict the performance of nanomaterials in a variety of applications, including:

* Electronics * Optics * Catalysis * Biomedicine

This section of the book provides a comprehensive overview of the different computational methods that can be used to study the applications of inorganic nanomaterials. It also includes a number of case studies that demonstrate how these methods can be used to design and optimize nanomaterials for specific applications.

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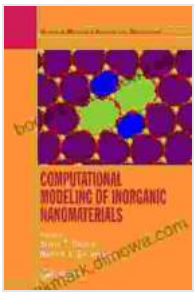

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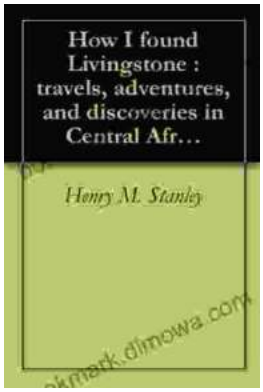

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