



Computational Quantum Mechanics for Materials Engineers: The EMTO Method and Applications (Engineering Materials and Processes)

Levente Vitos

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This is the only book to cover the most recent developments in applied quantum theory and their use in modeling materials properties. It describes new approaches to modeling disordered alloys and focuses on those approaches that combine the most efficient quantum-level theories of random alloys with the most sophisticated numerical techniques. In doing so, it establishes a theoretical insight into the electronic structure of complex materials such as stainless steels, Hume-Rothery alloys and silicates.

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