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Sinopsis

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This book introduces modern techniques based on computer simulation to study materials science. It starts from first principles calculations that enable the physical and chemical properties to be revealed by solving a many-body Schroedinger equation with Coulomb forces. For the exchange-correlation term, the local density approximation is usually applied. After the introduction of the first principles treatment, tight-binding and classical potential methods are briefly introduced to indicate how one can increase the number of atoms in the system. In the second half of the book, Monte Carlo sim.