In-vitro Materials Design: Modern Atomistic Simulation Methods for Engineers

Roman Leitsmann, Philipp Plänitz, Michael Schreiber

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An overview of the latest computational materials science methods on an atomic scale.
The authors present the physical and mathematical background in sufficient detail for this highly current and important topic, but without unnecessary complications. They focus on approaches with industrial relevance, covering real-life applications taken from concrete projects that range from tribology modeling to performance optimization of integrated circuits.
Following an introduction to the fundamentals, the book describes the most relevant approaches, covering such classical simulation methods as simple and reactive force field methods, as well as highly accurate quantum-mechanical methods ranging from density-functional theory to Hartree-Fock and beyond. A review of the increasingly important multiscale approaches rounds off this section. The last section demonstrates and illustrates the capabilities of the methods previously described using recent real-life examples of industrial applications. As a result, readers gain a heightened user awareness, since the authors clearly state the conditions of applicability for the respective modeling methods so as to avoid fatal mistakes.

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