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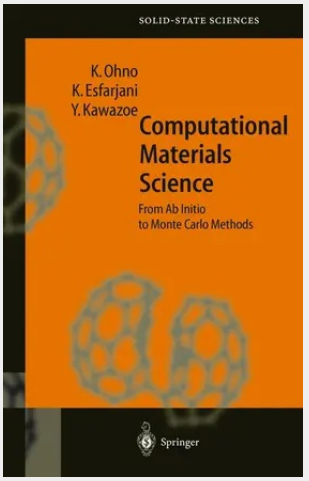
Computational Materials Science

From Ab Initio to Monte Carlo Methods



Powerful computers now enable scientists to model the physical and chemical properties and behavior of complex materials using first principles. This book introduces dramatically new computational techniques in materials research, specifically for understanding molecular dynamics.

There has been much progress in the computational approaches in the field of materials science during the past two decades. In particular, computer simula tion has become a very important tool in this field since it is a bridge between theory, which is often limited by its oversimplified models, and experiment, which is limited by the physical parameters. Computer simulation, on the other hand, can partially fulfill both of these paradigms, since it is based on theories and is in fact performing experiment but under any arbitrary, even unphysical, conditions. This progress is indebted to advances in computational physics and chem istry. Ab initio methods are being used widely and frequently in order to determine the electronic and/or atomic structures of different materials. The ultimate goal is to be able to predict various properties of a material just from its atomic coordinates, and also, in some cases, to even predict the sta ble atomic positions of a given material. However, at present, the applications of ab initio methods are severely limited with respect to the number of par ticles and the time scale of dynamical simulation. This is one extreme of the methodology based on very accurate electronic-level calculations.

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