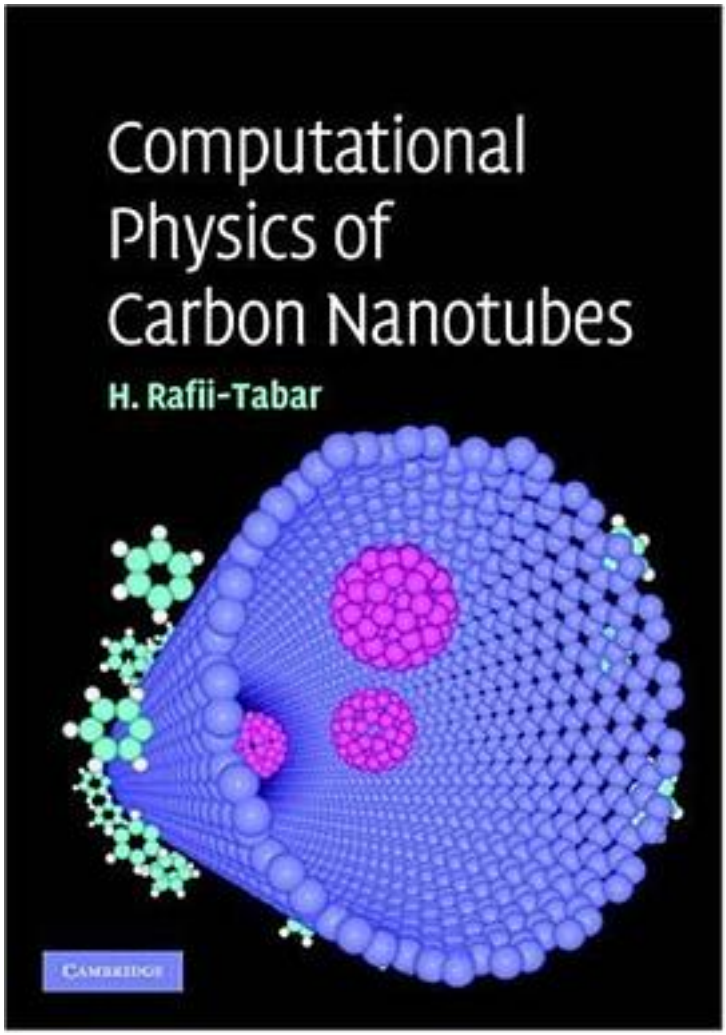
Computational Physics of Carbon Nanotubes



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Carbon nanotubes are the fabric of nanotechnology. Investigation into their properties

has become one of the most active fields of modern research. This book presents the key computational modelling and numerical simulation tools to investigate carbon nanotube characteristics. In particular, methods applied to geometry and bonding, mechanical, thermal, transport and storage properties are addressed. The first half describes classic statistical and quantum mechanical simulation techniques, (including molecular dynamics, Monte Carlo simulations and ab initio molecular dynamics), atomistic theory and continuum based methods. The second half discusses the application of these numerical simulation tools to emerging fields such as nanofluidics and nanomechanics. With selected experimental results to help clarify theoretical concepts, this is a self-contained book that will be of interest to researchers in a broad range of disciplines, including nanotechnology, engineering, materials science and physics.

作者介绍:

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