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Nota di bibliografia

Includes bibliographical references at the end of each chapters.

Nota di contenuto

1 The Schrödinger equation -- 1.1 The history of quantum mechanics in small bits -- 1.2 Planck versus the ultraviolet catastrophe -- 1.3 An intuitive approach to the Schrödinger equation -- 1.4 The Feynman approach -- 1.5 The Schrödinger equation -- 1.6 Relations between position and momentum wavefunctions -- 1.7 Heisenberg uncertainty principle -- 1.8 Observable and its time evolution -- 1.9 The Hellmann-Feynman theorem -- 1.10 The Pauli exclusion principle -- 1.11 On the numerical solution of the Schrödinger equation -- 2 Ab-initio calculations -- 2.1 The Hartree-Fock description -- 2.2 Density Functional Theory -- 2.3 Concluding remarks on the quantum scale -- 3 Coarse-grained descriptions -- 3.1 Molecular dynamics -- 3.2 Brownian dynamics -- 4 Kinetic theory models. 4.1 Motivation -- 4.2 Kinetic theory description of simple liquids and gases -- 4.3 Complex fluids -- 4.4 The Chemical Master Equation -- References.

Sommario/riassunto

This SpringerBrief covers the main scales of description of matter, starting at its finest level, the quantum scale, moving through ab-initio, molecular dynamics, coarse grained approaches, to finish at the scale of kinetic theory models that allows a nice compromise between the rich but expensive microscopic descriptions and the computationally cheap but sometimes too coarse macroscopic descriptions. The book addresses undergraduate and graduate students, as well as beginners in multi-scale modeling of materials.