

1. Record Nr.	UNINA9910299869303321
Autore	Chinesta Francisco
Titolo	A Journey Around the Different Scales Involved in the Description of Matter and Complex Systems : A Brief Overview with Special Emphasis on Kinetic Theory Approaches // by Francisco Chinesta, Emmanuelle Abisset-Chavanne
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2018
ISBN	3-319-70001-4
Edizione	[1st ed. 2018.]
Descrizione fisica	1 online resource (X, 125 p. 16 illus.)
Collana	SpringerBriefs in Applied Sciences and Technology, , 2191-530X
Disciplina	530.136
Soggetti	Mechanics Mechanics, Applied Quantum theory Materials science Theoretical and Applied Mechanics Quantum Physics Characterization and Evaluation of Materials
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
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.

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.
