1. Record Nr. UNINA9910585943503321

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Titolo	Simulation and Modeling of Nanomaterials
Pubbl/distr/stampa	Basel, : MDPI - Multidisciplinary Digital Publishing Institute, 2022
Descrizione fisica	1 online resource (270 p.)
Soggetti	Physics Research & information: general
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Sommario/riassunto	This Special Issue focuses on computational detailed studies (simulation, modeling, and calculations) of the structures, main properties, and peculiarities of the various nanomaterials (nanocrystals, nanoparticles, nanolayers, nanofibers, nanotubes, etc.) based on various elements, including organic and biological components, such as amino acids and peptides. For many practical applications in nanoelectronics., such materials as ferroelectrics and ferromagnetics, having switching parameters (polarization, magnetization), are highly requested, and simulation of dynamics and kinetics of their switching are a very important task. An important task for these studies is computer modeling and computational research of the properties on the various composites of the other nanostructures with polymeric ferroelectrics and with different graphene-like 2-dimensional structures. A wide range of contemporary computational methods and software are used in all these studies.