1. Record Nr. UNISA996466704603316

Titolo	Rugged free energy landscapes : common computational approaches in spin glasses, structural glasses, and biological macromolecules / / edited by W. Janke
Pubbl/distr/stampa	Berlin, Germany ; ; New York, New York : , : Springer, , [2008] ©2008
ISBN	3-540-74029-5
Edizione	[1st ed. 2008.]
Descrizione fisica	1 online resource (X, 412 p.)
Collana	Lecture Notes in Physics, , 0075-8450 ; ; 736
Disciplina	530.413
Soggetti	Spin glasses - Mathematical models Condensed matter - Mathematical models Protein folding - Mathematical models
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Bibliographic Level Mode of Issuance: Monograph
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Rugged Free-Energy Landscapes – An Introduction -- Rugged Free-Energy Landscapes – An Introduction -- Spin Glasses -- Some Aspects of Infinite-Range Models of Spin Glasses: Theory and Numerical Simulations -- The Potts Glass Model: A Scenario for the Freezing Transition of Structural Glasses? -- Domain Walls, Droplets and Barriers in Two-Dimensional Ising Spin Glasses -- Local Scale-Invariance in Disordered Systems -- Structural Glasses -- Transport of Mobile Particles in an Immobile Environment: Computer Simulations of Sodium Silicates -- The Gonihedric Ising Model and Glassiness -- Protein Folding -- Thermodynamics of Protein Folding from Coarse-Grained Models' Perspectives -- Exact Energy Landscapes of Proteins Using a Coarse-Grained Model -- Protein Folding, Unfolding and Aggregation Studied Using an All-Atom Model with~a~Simplified Interaction Potential -- All-Atom Simulations of Proteins -- Algorithmic Developments -- Markov Chain Monte Carlo Methods for Simulations of Biomolecules -- A Different Approach to Monte Carlo Simulations in Systems with Complex Free-Energy Landscapes -- Generalized-Ensemble Algorithms for Protein Folding Simulations.
Sommario/riassunto	This collection of lectures and tutorial reviews by renowned experts

focusses on the common computational approaches in use to unravel the static and dynamical behaviour of complex physical systems at the interface of physics, chemistry and biology. Paradigmatic examples of condensed matter physics are spin and structural glasses and protein folding, as well as their aggregation and adsorption to hard and soft surfaces, in physico-chemical biology. Among the most prominent joint key features of the systems considered in this volume are rugged free-energy landscapes. These generate metastability and are often responsible for very slow dynamics allowing for the system to be trapped in one of the many available local minima. The challenge set forth by the authors of this volume is to provide a common basis and technical language for the (computational) technology transfer between the fields and systems considered.