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Titolo	Molecular Dynamics Simulations of Disordered Materials : From Network Glasses to Phase-Change Memory Alloys / / edited by Carlo Massobrio, Jincheng Du, Marco Bernasconi, Philip S. Salmon
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Disciplina	519 530.1 530.41 620.11 620.14
Soggetti	Structural materials Physics Mathematical physics Applied mathematics Engineering mathematics Ceramics Glass Composites (Materials) Composite materials Solid state physics Structural Materials Numerical and Computational Physics, Simulation Mathematical Applications in the Physical Sciences Mathematical and Computational Engineering Ceramics, Glass, Composites, Natural Materials Solid State Physics
Lingua di pubblicazione	Inglese
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Livello bibliografico	Monografia
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Nota di bibliografia	Includes bibliographical references and index.

Nota di contenuto	From the Contents: The atomic structure of network forming glass systems -- First-principles molecular dynamics methods applied to glasses -- Computational Modeling of Glasses: A QSPR perspective -- Novel methods for modeling network glasses modeling of silicate liquids -- The numerical challenge of sampling the energy landscape and the long-time dynamics of amorphous networks -- Topology and rigidity in connection to the understanding of the atomic structure of glasses -- Network modeling in variable dimensions.
Sommario/riassunto	This book is a unique reference work in the area of atomic-scale simulation of glasses. For the first time, a highly selected panel of about 20 researchers provides, in a single book, their views, methodologies and applications on the use of molecular dynamics as a tool to describe glassy materials. The book covers a wide range of systems covering "traditional" network glasses, such as chalcogenides and oxides, as well as glasses for applications in the area of phase change materials. The novelty of this work is the interplay between molecular dynamics methods (both at the classical and first-principles level) and the structure of materials for which, quite often, direct experimental structural information is rather scarce or absent. The book features specific examples of how quite subtle features of the structure of glasses can be unraveled by relying on the predictive power of molecular dynamics, used in connection with a realistic description of forces.