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Titolo	Foundations of Molecular Modeling and Simulation : Select Papers from FOMMS 2015 / / edited by Randall Q Snurr, Claire S. Adjiman, David A. Kofke
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Descrizione fisica	1 online resource (176 p.)
Collana	Molecular Modeling and Simulation, Applications and Perspectives, , 2364-5083
Disciplina	541.220113
Soggetti	Biochemical engineering Applied mathematics Engineering mathematics Molecular biology Materials science Biochemical Engineering Mathematical and Computational Engineering Molecular Medicine Characterization and Evaluation of Materials
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references at the end of each chapters.
Nota di contenuto	A Discontinuous-Potential Model for Protein-Protein Interactions -- Probing How Defects in Self-Assembled Monolayers Affect Peptide Adsorption with Molecular Simulation -- Development of a Coarse-Grained Water Forcefield Via Multistate Iterative Boltzmann Inversion -- Optimizing Molecular Models through Force Field Parameterization via the Efficient Combination of Modular Program Packages -- A Hierarchical, Component Based Approach to Screening Properties of Soft Matter -- Quantum Virial Coefficients via Path Integral Monte Carlo with Semi-Classical Beads -- Homogeneous Nucleation of [Dmim+][Cl-] from its Supercooled Liquid Phase: A Molecular Simulation Study -- Influence of the Precursor Composition and Reaction Conditions on Raney-Nickel Catalytic System -- Atomistic Modeling and Simulation at Solving Gas-Extraction Problems -- Atomistic Simulations of CO2

	During “Trapdoor” Adsorption Onto Na-Rho Zeolite.
Sommario/riassunto	This book is a collection of select proceedings of the FOMMS 2015 conference. FOMMS 2015 is the sixth triennial FOMMS conference showcasing applications of theory of computational quantum chemistry, molecular science, and engineering simulation. The theme of the 2015 meeting focuses on Molecular Modeling and the Materials Genome.