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Titolo	Foundations of Molecular Modeling and Simulation : Select Papers from FOMMS 2018 // edited by Edward J. Maginn, Jeffrey Errington
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Descrizione fisica	1 online resource (x, 220 pages) : illustrations
Collana	Molecular Modeling and Simulation, Applications and Perspectives, , 2364-5091
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Soggetti	Molecular dynamics Molecules - Models Chemical engineering Statistical Mechanics Molecular Dynamics Molecular Modelling Chemical Engineering
Lingua di pubblicazione	Inglese
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Nota di bibliografia	Includes bibliographical references.
Nota di contenuto	Strain Controlling Catalytic Efficiency of Water Oxidation for Ni1-xFexOOH alloy -- The Role of Entropy in the Structural Transitions in Zeolitic Imidazolate Frameworks -- Coarse-grained modeling and simulations of thermoresponsive biopolymers and polymer nanocomposites with specific and directional interactions -- Dissipative Particle Dynamics Approaches to Modeling the Self-Assembly and Morphology of Neutral and Ionic Block Copolymers in Solution -- The Statistical Mechanics of Solution-phase Nucleation: CaCO3 Revisited -- Efficient Sampling of High-Dimensional Free Energy Landscapes: A Review of Parallel Bias Metadynamics.
Sommario/riassunto	This highly informative and carefully presented book comprises select proceedings of Foundation for Molecular Modelling and Simulation (FOMMS 2018). The contents are written by invited speakers centered on the theme Innovation for Complex Systems. It showcases new developments and applications of computational quantum chemistry, statistical mechanics, molecular simulation and theory, and continuum

and engineering process simulation. This volume will serve as a useful reference to researchers, academicians and practitioners alike.
