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| Descrizione fisica | 1 online resource (x, 220 pages) : illustrations |
| Collana | Molecular Modeling and Simulation, Applications and Perspectives, , 2364-5091 |
| Disciplina | 541.220113 |
| Soggetti | Molecular dynamics Molecules - Models Chemical engineering Statistical Mechanics Molecular Dynamics Molecular Modelling Chemical Engineering |
| Lingua di pubblicazione | Inglese |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
| 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: CaCO ₃ 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.
