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Nota di contenuto	""Cover""; ""Contents""; ""Foreword""; ""Preface""; ""Chapter 1: Computational Approaches to the Design, Crystal Structure Prediction, and Structure-Property Relationships of Metal-Organic Frameworks""; ""Chapter 2: On the Application of Classical Molecular Simulations of Adsorption in Metal-Organic Frameworks""; ""Chapter 3: Modeling the Adsorption of Small Molecules at Coordinatively Unsaturated Metal Sites: Density Functional Theory and Molecular Mechanics Approaches"" ""Chapter 4: Accurate ab initio Description of Adsorption on Coordinatively Unsaturated Sites in Metal-Organic Frameworks"" Chapter 5: Modeling Sorbate Equilibria and Transport in Porous Coordination Polymers""; ""Chapter 6: Modeling Quantum Effects on Adsorption and Diffusion of Hydrogen in Metal-Organic Frameworks""; ""Chapter 7: Molecular Modeling of Gas Separation in Metal-Organic Frameworks""; ""Chapter 8: Molecular Modeling of Metal-Organic Frameworks for Carbon Dioxide Separation Applications""; ""Chapter 9: Modeling of Zeolitic-Like Hybrid Materials for Gas Separation""

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