

1. Record Nr.	UNINA9910829138403321
Titolo	Metal-organic frameworks : materials modeling towards engineering applications / / edited by Jianwen Jiang
Pubbl/distr/stampa	[Singapore] : , : Pan Stanford, , 2014
ISBN	0-429-07632-0 981-4613-46-0
Descrizione fisica	1 online resource (572 p.)
Disciplina	661.895
Soggetti	Organometallic compounds - Industrial applications Porous materials - Industrial applications Organometallic compounds - Mathematical models Porous materials - Mathematical models Supramolecular organometallic chemistry
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	""Cover""; ""Contents""; ""Foreword""; ""Preface""; ""Chapter 1: Computational Approaches to the Design, Crystal Structure Prediction, and Structurea€?Property Relationships of Metala€?Organic Frameworks""; ""Chapter 2: On the Application of Classical Molecular Simulations of Adsorption in Metala€?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 Metala€?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 Metala€?Organic Frameworks""; ""Chapter 7: Molecular Modeling of Gas Separation in Metala€?Organic Frameworks""; ""Chapter 8: Molecular Modeling of Metala€?Organic Frameworks for Carbon Dioxide Separation Applications""; ""Chapter 9: Modeling of Zeolitic-Like Hybrid Materials for Gas Separation""

""Chapter 10: Modeling Adsorptive Separations Using Metal-Organic Frameworks""; ""Chapter 11: Computer Simulations of Ionic Metal-Organic Frameworks""; ""Chapter 12: Computational Modeling of Catalysis in Metal-Organic Frameworks""; ""Chapter 13: Modeled Catalytic Properties of MOF-Based Compounds""; ""Back Cover""

---