

1. Record Nr.	UNINA9910141285603321
Autore	Karger Jorg
Titolo	Diffusion in nanoporous materials [[electronic resource] /] / Jorg Karger, Douglas M. Ruthven, and Doros N. Theodorou
Pubbl/distr/stampa	Weinheim, Germany, : Wiley-VCH, c2012
ISBN	1-283-59214-2 9786613904591 3-527-65130-6 3-527-65127-6 3-527-65129-2
Descrizione fisica	1 online resource (904 p.)
Altri autori (Persone)	RuthvenDouglas M <1938-> (Douglas Morris) TheodorouDoros Nicolas
Disciplina	541.34 620.1/16 620.116
Soggetti	Porous materials - Diffusion rate Materials science Electronic books.
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 and index.
Nota di contenuto	Diffusion in Nanoporous Materials; Contents; Preface; Acknowledgments; Part I: Introduction; 1 Elementary Principles of Diffusion; 1.1 Fundamental Definitions; 1.1.1 Transfer of Matter by Diffusion; 1.1.2 Random Walk; 1.1.3 Transport Diffusion and Self-Diffusion; 1.1.4 Frames of Reference; 1.1.5 Diffusion in Anisotropic Media; 1.2 Driving Force for Diffusion; 1.2.1 Gradient of Chemical Potential; 1.2.2 Experimental Evidence; 1.2.3 Relationship between Transport and Self-diffusivities; 1.3 Diffusional Resistances in Nanoporous Media; 1.3.1 Internal Diffusional Resistances 1.3.2 Surface Resistance 1.3.3 External Resistance to Mass Transfer; 1.4 Experimental Methods; References; Part II: Theory; 2 Diffusion as a Random Walk; 2.1 Random Walk Model; 2.1.1 Mean Square Displacement; 2.1.2 The Propagator; 2.1.3 Correspondence with Fick's Equations; 2.2 Correlation Effects; 2.2.1 Vacancy Correlations; 2.2.2

Correlated Anisotropy; 2.3 Boundary Conditions; 2.3.1 Absorbing and Reflecting Boundaries; 2.3.2 Partially Reflecting Boundary; 2.3.3 Matching Conditions; 2.3.4 Combined Impact of Diffusion and Permeation; 2.4 Macroscopic and Microscopic Diffusivities  
2.5 Correlating Self-Diffusion and Diffusion with a Simple Jump Model  
2.6 Anomalous Diffusion; 2.6.1 Probability Distribution Functions of Residence Time and Jump Length; 2.6.2 Fractal Geometry; 2.6.3 Diffusion in a Fractal System; 2.6.4 Renormalization; 2.6.5 Deviations from Normal Diffusion in Nanoporous Materials: A Retrospective; References; 3 Diffusion and Non-equilibrium Thermodynamics; 3.1 Generalized Forces and Fluxes; 3.1.1 Mechanical Example; 3.1.2 Thermodynamic Forces and Fluxes; 3.1.3 Rate of Generation of Entropy; 3.1.4 Isothermal Approximation  
3.1.5 Diffusion in a Binary Adsorbed Phase  
3.2 Self-Diffusion and Diffusive Transport; 3.3 Generalized Maxwell-Stefan Equations; 3.3.1 General Formulation; 3.3.2 Diffusion in an Adsorbed Phase; 3.3.3 Relation between Self- and Transport Diffusivities; 3.4 Application of the Maxwell-Stefan Model; 3.4.1 Parameter Estimation; 3.4.2 Membrane Permeation; 3.4.3 Diffusion in Macro- and Mesopores; 3.5 Loading Dependence of Self- and Transport Diffusivities; 3.5.1 Self-Diffusivities; 3.5.2 Transport Diffusivities; 3.5.3 Molecular Simulation; 3.5.4 Effect of Structural Defects  
3.6 Diffusion at High Loadings and in Liquid-Filled Pores  
References; 4 Diffusion Mechanisms; 4.1 Diffusion Regimes; 4.1.1 Size-Selective Molecular Sieving; 4.2 Diffusion in Macro- and Mesopores; 4.2.1 Diffusion in a Straight Cylindrical Pore; 4.2.1.1 Knudsen Mechanism; 4.2.1.2 Viscous Flow; 4.2.1.3 Molecular Diffusion; 4.2.1.4 Transition Region; 4.2.1.5 Self-Diffusion/Tracer Diffusion; 4.2.1.6 Relative Importance of Different Mechanisms; 4.2.1.7 Surface Diffusion; 4.2.1.8 Combination of Diffusional Resistances; 4.2.2 Diffusion in a Pore Network; 4.2.2.1 Dusty Gas Model  
4.2.2.2 Effective Medium Approximation

---

## Sommario/riassunto

Atoms and molecules in all states of matter are subject to continuous irregular movement. This process, referred to as diffusion, is among the most general and basic phenomena in nature and determines the performance of many technological processes. This book provides an introduction to the fascinating world of diffusion in microporous solids. Jointly written by three well-known researchers in this field, it presents a coherent treatise, rather than a compilation of separate review articles, covering the theoretical fundamentals, molecular modeling, experimental observation and techni

---