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Nota di contenuto	Materials Science of Membranes for Gas and Vapor Separation; Contents; Contributors; Preface; 1 Transport of Gases and Vapors in Glassy and Rubbery Polymers; 1.1 Background and Phenomenology; 1.2 Effects of Gas and Polymer Properties on Transport Coefficients; 1.2.1 Effect of Gas Properties on Solubility and Diffusivity; 1.2.2 Effect of Polymer Properties on Transport Parameters; 1.3 Effect of Pressure on Transport Parameters; 1.3.1 Sorption; 1.3.2 Diffusion; 1.3.3 Permeability; 1.3.4 Selectivity; 1.4 Effect of Temperature on Transport Parameters; 1.5 Structure/Property Relations 1.5.1 Connector Groups 1.5.2 CF <sub>3</sub> and Other Fluorinated Moieties as Side-chains; 1.5.3 Polar and Hydrogen Bonding Side-chains; 1.5.4 Para

versus Meta Linkages; 1.5.5 Cis/Trans Configuration; 1.6 Conclusions; References; 2 Principles of Molecular Simulation of Gas Transport in Polymers; 2.1 Introduction; 2.2 Generating Model Configurations for Amorphous Polymers; 2.2.1 Models and Force Fields; 2.2.2 Molecular Mechanics; 2.2.3 Molecular Dynamics; 2.2.4 Monte Carlo; 2.2.5 Coarse-graining Strategies; 2.2.6 Generating Glasses from Melts; 2.3 Validating Model Amorphous Polymer Configurations  
2.3.1 Thermodynamic Properties; 2.3.2 Molecular Packing; 2.3.3 Segmental Dynamics; 2.3.4 Accessible Volume and its Distribution; 2.4 Prediction of Sorption Equilibria; 2.4.1 Sorption Thermodynamics; 2.4.2 Calculations of Low-pressure Sorption Thermodynamics; 2.4.3 Calculations of High-pressure Sorption Thermodynamics; 2.4.4 Ways to Overcome the Insertion Problem; 2.5 Prediction of Diffusivity; 2.5.1 Statistical Mechanics of Diffusion; 2.5.2 Self-diffusivities from Equilibrium Molecular Dynamics; 2.5.3 Diffusivities from Nonequilibrium Molecular Dynamics  
2.5.4 Diffusion in Low-temperature Polymer Matrices as a Sequence of Infrequent Penetrant Jumps; 2.5.5 Gusev-Suter TST Method for Polymer Matrices Undergoing Isotropic 'Elastic' Motion; 2.5.6 Multidimensional TST Approach to Gas Diffusion in Glassy Polymers; 2.5.7 Anomalous Diffusion: Its Origins and Implications; 2.6 Conclusions and Outlook; Acknowledgements; References; 3 Molecular Simulation of Gas and Vapor Transport in Highly Permeable Polymers; 3.1 Fundamentals of Membrane Transport; 3.1.1 Solubility; 3.1.2 Diffusivity; 3.1.3 Permeability; 3.1.4 Free Volume; 3.1.5 d-Spacing  
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Appendices: Primary Force Fields Used in the Simulation of Transport in Polymeric Systems

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## Sommario/riassunto

Materials Science of Membranes for Gas and Vapor Separation is a one-stop reference for the latest advances in membrane-based separation and technology. Put together by an international team of contributors and academia, the book focuses on the advances in both theoretical and experimental materials science and engineering, as well as progress in membrane technology. Special attention is given to comparing polymer and inorganic/organic separation and other emerging applications such as sensors. This book aims to give a balanced treatment of the subject area, allowing the reader an exc

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