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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
3.1.6 Transport in Semicrystalline Polymers; 3.2 Computational Methods; 3.2.1 Solubility; 3.2.2 Diffusivity; 3.2.3 Free Volume; 3.2.4 d-Spacing; 3.2.5 Pair Correlation Functions; 3.2.6 Molecular Mobility; 3.2.7 Guidelines for Molecular Simulations; 3.3 Polymer Studies; 3.3.1 Polyetherimide; 3.3.2 Polysulfones; 3.3.3 Polycarbonates; 3.3.4 Poly(2,6-dimethyl-1,4-phenylene oxide); 3.3.5 Polyimides; 3.3.6 Polyphosphazenes; 3.3.7 Main-chain Silicon-containing Polymers; 3.3.8 Poly[1-(trimethylsilyl)-1-propyne]; 3.3.9 Amorphous Teflon; 3.4 Conclusions
Appendices: Primary Force Fields Used in the Simulation of Transport in Polymeric Systems

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
