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Nota di contenuto	Introduction -- Part I. Structure and Morphology -- Chapter 1. Atomistic and Molecular Modeling of Polymer Nanocomposites -- Chapter 2. Coarse-grained modeling: Particle-based Approaches -- Chapter 3. Coarse-grained modeling: Field-based Approaches -- Chapter 4. Multiscale modeling examples -- Part II. Dynamics and Rheology -- Chapter 5. Diffusion in Polymer Nanocomposites -- Chapter 6. Linear Rheology of Polymer Nanocomposites -- Chapter 7. Nonlinear Rheology and Mechanics of Polymer Nanocomposites -- Part III. Physical Property Prediction -- Chapter 8. Thermal Conductivity -- Chapter 9. Electrical Conductivity -- Chapter 10. Optical Properties -- Chapter 11. Barrier Properties -- Chapter 12. Dielectric Breakdown -- Chapter 13. Flammability -- Summary -- Index.
Sommario/riassunto	This edited volume brings together the state of the art in polymer nanocomposite theory and modeling, creating a roadmap for scientists and engineers seeking to design new advanced materials. The book opens with a review of molecular and mesoscale models predicting equilibrium and non-equilibrium nanoscale structure of hybrid materials as a function of composition and, especially, filler types. Subsequent chapters cover the methods and analyses used for describing the dynamics of nanocomposites and their mechanical and

physical properties. Dedicated chapters present best practices for predicting materials properties of practical interest, including thermal and electrical conductivity, optical properties, barrier properties, and flammability. Each chapter is written by leading academic and industrial scientists working in each respective sub-field. The overview of modeling methodology combined with detailed examples of property predictions for specific systems will make this book useful for academic and industrial practitioners alike.