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Front Cover; Modeling, Characterization and Production of Nanomaterials: Electronics, Photonics and Energy Applications; Copyright; Contents; List of contributors; Woodhead Publishing Series in Electronic and Optical Materials; Part One: Modeling techniques for nanomaterials; Chapter 1: Multiscale modeling of nanomaterials: recent developments and future prospects; 1.1. Introduction; 1.2. Methods; 1.2.1. Quantum mechanics; 1.2.1.1. Introduction; 1.2.1.2. Hartree-Fock theory; 1.2.1.3. Electron-correlated methods; 1.2.1.4. Density functional theory; 1.2.1.5. Other methods
1.2.2. Classical mechanics
1.2.2.1. Molecular mechanics; 1.2.2.2. Molecular dynamics; 1.2.2.3. Monte Carlo; 1.2.2.4. Forcefields; 1.2.2.5. Applications of classical tools to nanomaterials; 1.2.3. Mesoscale; 1.2.3.1. Models; 1.2.3.2. Forcefields; 1.2.3.3. Potentials; 1.2.3.4. Dynamics; 1.2.3.5. Parameterization; 1.2.4. Multiscale modeling; 1.2.4.1. Hierarchical methods; 1.2.4.2. Hybrid methods; 1.2.4.3. QM/MM; 1.3. Nanomaterials; 1.3.1. Polymer nanocomposites; 1.3.2. Inorganic nanostructures; 1.3.2.1. Zeolites; 1.3.2.2. Metal-organic frameworks (MOFs); 1.3.2.3. Catalysts; 1.3.3. Soft matter
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