

1. Record Nr.	UNINA9910788150303321
Titolo	Modeling, characterization and production of nanomaterials : electronics, photonics and energy applications // edited by Vinod K. Tewary and Yong Zhang
Pubbl/distr/stampa	Amsterdam, [Netherlands] : , : Woodhead Publishing, , 2015 ©2015
ISBN	1-78242-235-8
Descrizione fisica	1 online resource (555 p.)
Collana	Woodhead Publishing Series in Electronic and Optical Materials ; ; Number 73
Disciplina	620.5
Soggetti	Nanostructured materials
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 at the end of each chapters and index.
Nota di contenuto	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 1.3.3.1. Lipids 1.3.3.2. Surfactants and polymers; 1.3.3.3. Peptide assemblies; 1.4. Application examples; 1.4.1. Polymer nanodielectrics;

1.4.2. Lithium-ion batteries; 1.4.3. Reinforced resins for aerospace; 1.5. Conclusion; References; Chapter 2: Multiscale Green's functions for modeling of nanomaterials ; 2.1. Introduction; 2.1.1. Need for bridging length scales; 2.1.2. Bridging the time scales; 2.1.3. Application; 2.2. Green's function method: the basics; 2.3. Discrete lattice model of a solid; 2.4. Lattice statics Greens function; 2.5. Multiscale Green's function  
2.6. Causal Green's function for temporal modeling  
2.7. Application to 2D graphene; 2.8. Conclusions and future work; Acknowledgments; References; Chapter 3: Numerical simulation of nanoscale systems and materials; 3.1. Introduction; 3.2. Molecular statics and dynamics: an overview; 3.3. Static calculations of strain due to interface; 3.4. Dynamic calculations of kinetic frictional properties; 3.5. Fundamental properties of dynamic ripples in graphene; 3.6. Conclusions and general remarks; Disclaimer; Acknowledgments; References; Part Two: Characterization techniques for nanomaterials  
Chapter 4: TEM studies of nanostructures  
4.1. Introduction; 4.2. Polarity determination and stacking faults of 1D ZnO nanostructures; 4.2.1. Polarity determination in 1D ZnO nanostructures; 4.2.2. Stacking-fault-induced growth of ultrathin ZnO nanobelts; 4.3. Structure analysis of superlattice nanowire by TEM: a case of SnO<sub>2</sub> (ZnO:Sn)<sub>n</sub> nanowire; 4.4. TEM analysis of 1D nanoheterostructure; 4.4.1. Axially heterostructured nanowires; 4.4.2. Coaxial core-shell nanowires; 4.4.2.1. Highly lattice-mismatched ZnO/ZnSe and ZnO/ZnS core-shell nanowires  
4.4.2.2. Nearly lattice-matched CdSe/ZnTe core-shell nanowires

---