1. Record Nr. UNINA9911006626103321

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Titolo	Nano-engineering in science and technology : an introduction to the world of nano-design / / Michael Rieth
Pubbl/distr/stampa	Singapore ; ; River Edge, NJ, : World Scientific, c2003
ISBN	9786611871956 9781281871954 1281871958 9789812560032 9812560033
Descrizione fisica	1 online resource (164 p.)
Collana	Series on the foundations of natural science and technology ; ; v. 6
Disciplina	620/.5
Soggetti	Nanotechnology Nanostructures
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 (p. 133-138) and index.
Nota di contenuto	ch. 1. Introduction -- ch. 2. Interatomic potentials. 2.1. Quantum mechanical treatment of the many-particle problem. 2.2. Potential energy surface. 2.3. Pair potential approximation. 2.4. Advantages and limitations of the pair potential approximation. 2.5. Phenomenological potentials. 2.6. Pseudo potentials. 2.7. Many-body potentials -- ch. 3. Molecular dynamics. 3.1. Models for molecular dynamics calculations. 3.2. Visualization techniques. 3.3. Solution of the equations of motion. 3.4. Efficient force field computation. 3.5. Implementation -- ch. 4. Characterization of nano-systems. 4.1. Thermal stability. 4.2. Basic material properties. 4.3. Wear at the nanometer level. 4.4. Mean values and correlation functions -- ch. 5. Nano-engineering - studies and conclusions. 5.1. Functional nanostructures. 5.2. Nano-machines. 5.3. Nano-clusters. 5.4. Stimulated nano-cluster transformations. 5.5. Analogy considerations. 5.6. The bifurcation phenomenon at the nanometer scale. 5.7. Analogies to biology. 5.8. Final considerations.
Sommario/riassunto	This important book provides a vivid introduction to the procedures, techniques, problems and difficulties of computational nano-engineering and design. The reader is given step by step the scientific

background information, for an easy reconstruction of the explanations. The focus is laid on the molecular dynamics method, which is well suited for explaining the topic to the reader with just a basic knowledge of physics. Results and conclusions of detailed nano-engineering studies are presented in an instructive style. In summary, the book puts readers immediately in a position to take their f