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Autore	Lee June Gunn
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Nota di contenuto	chapter 1. Introduction -- chapter 2. Molecular dynamics -- chapter 3. MD exercises with XMD and LAMMPS -- chapter 4. First-principles methods -- chapter 5. Density functional theory -- chapter 6. Treating solids -- chapter 7. DFT exercises with quantum espresso -- chapter 8. DFT exercises with VASP -- chapter 9. DFT exercises with MedeA-VASP.
Sommario/riassunto	This book covers the essentials of Computational Science and gives tools and techniques to solve materials science problems using molecular dynamics (MD) and first-principles methods. The new edition expands upon the density functional theory (DFT) and how the original DFT has advanced to a more accurate level by GGA+U and hybrid-functional methods. It offers 14 new worked examples in the LAMMPS, Quantum Espresso, VASP and MedeA-VASP programs, including computation of stress-strain behavior of Si-CNT composite, mean-squared displacement (MSD) of ZrO2-Y2O3, band structure and phonon spectra of silicon, and Mo-S battery system. It discusses methods once considered too expensive but that are now cost-effective. New examples also include various post-processed results using VESTA, VMD, VTST, and MedeA.