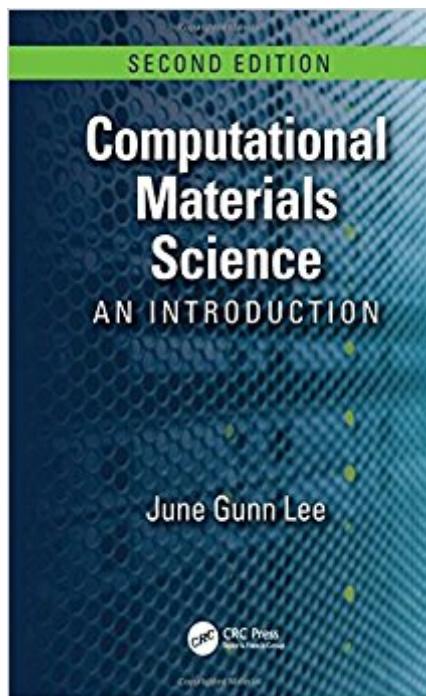


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Computational Materials Science: An Introduction, Second Edition



Synopsis

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.

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June Gunn Lee is an emeritus research fellow in the Computational Science Center at the Korea Institute of Science and Technology, where he has worked for 28 years. Currently, he is also lecturing at the University of Seoul. He has published about 70 papers on engineering ceramics and computational materials science. He received his M.S. and Ph.D. in Materials Science and

Engineering from the University of Utah, U.S.A.

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