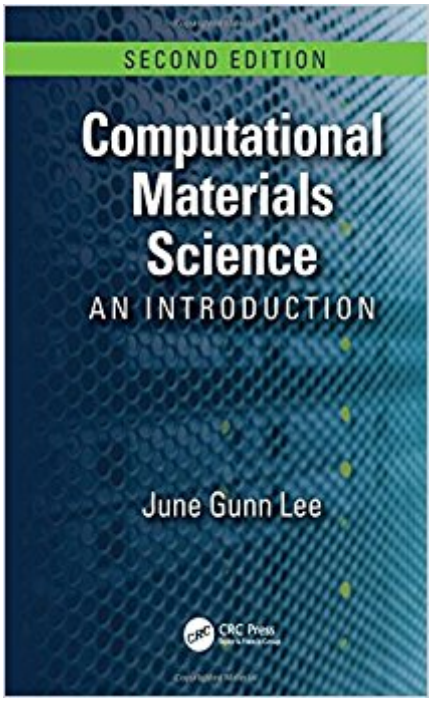
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Computational Materials Science: An Introduction, Second Edition



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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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"The delightful and pragmatic style of this book is irresistible. It intrigues the reader to start using the leading methods in computational materials science, to simulate interesting systems, and to become excited about the remarkable capabilities of todayÃ¢â ¬â„¢s computational methods." Ã¢â ¬â ¢ Erich Wimmer, Materials Design, Inc., Angel Fire, New Mexico, USA "Books such as this allow my students Ã¢â ¬â œ the new generation - to catch up with our fast progressing knowledge and technology. Definitely, this book has help me to teach density functional theory to my students and mentees. I will continually use this book for my class and research. "Ã¢â ¬â ¢ Al Rey Villagracia, De La Salle University, Manila, Philippines "This text takes you on a Ã¢â ¬Ëœworking Ã¢â ¬â„¢

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