



# Computational Materials Science: An Introduction, Second Edition

*June Gunn Lee*

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# Computational Materials Science: An Introduction, Second Edition

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## **Computational Materials Science: An Introduction, Second Edition** June Gunn Lee

The book covers the essentials of computational science and gives tools and techniques to solve materials science problems using molecular dynamics 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 methods. It offers 14 new worked examples in the VASP and GUI-VASP programs, including computation of stress-strain behavior of Si-CNT composite, band structure of silicon, and Li<sub>2</sub>MnO<sub>3</sub> 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, and VTST.

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