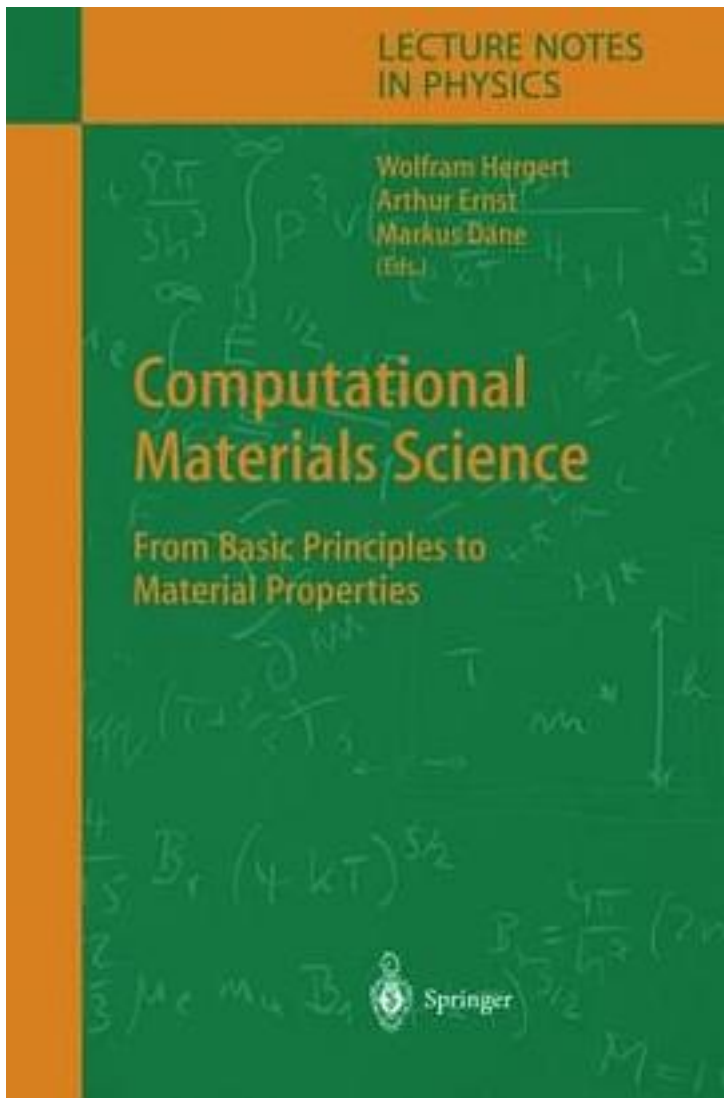


Computational Materials Science



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This book introduces new theoretical techniques in materials research. With the computer power now available, it is possible to use numerical techniques to study various physical and chemical properties of complex materials from first principles. Some typical examples are presented and all the necessary equations and plots are included so that readers can fully understand the details. This book offers the materials scientist access to, and an understanding of the modern development of molecular dynamics and Monte Carlo simulation. It will also be of interest to physicists and chemists engaged in materials research.

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