

Handbook of Materials Modeling (Vol 1&2)



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The first reference of its kind in the rapidly emerging field of computational approachs to materials research, this is a compendium of perspective-providing and topical articles written to inform students and non-specialists of the current status and capabilities of modelling and simulation. From the standpoint of methodology, the development follows a multiscale approach with emphasis on electronic-structure, atomistic, and mesoscale methods, as well as mathematical analysis and rate processes. Basic models are treated across traditional disciplines, not only in the discussion of methods but also in chapters on crystal defects, microstructure, fluids, polymers and soft matter. Written by authors who are actively participating in the current development, this collection of 150 articles has the breadth and depth to be a major contributor toward defining the field of computational materials. In addition, there are 40 commentaries by highly respected researchers, presenting various views that should interest the future generations of the community.

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