



Creator Guide

Studio Manual

Material Studio Manual

Sumit Sharma

Material Studio Manual:

Molecular Dynamics Simulation of Nanocomposites using BIOVIA Materials Studio, Lammps and Gromacs

Sumit Sharma,2025-04-10 Molecular Dynamics Simulation of Nanocomposites using BIOVIA Materials Studio Lammps and Gromacs Second Edition introduces the three major software packages essential for the molecular dynamics simulation of nanocomposites providing detailed instructions on utilizing each. This content is accompanied by real world examples that illustrate when each should be applied. Numerous case studies demonstrate how each software package predicts various properties of nanocomposites encompassing metal matrix polymer matrix and ceramic matrix based nanocomposites. Explored properties include mechanical thermal optical and electrical characteristics. This is a valuable resource for students researchers and scientists working in the field of molecular dynamics simulation. All chapters have been fully updated to reflect the latest developments in the field and this new edition has been enriched with additional chapters covering Al composites machine learning polymer coatings and graphene based materials and carbon nanotubes. Provides a detailed explanation on the basic commands and modules of Materials Studio Lammps and Gromacs. Demonstrates how these materials predict the mechanical thermal electrical and optical properties of nanocomposites. Introduces coding in LAMMPS explaining modeling using Materials Studio and LAMMPS. Utilizes case studies to illustrate the appropriate software for solving various nanoscale modeling problems.

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