

The Challenge of Modeling Multiple Scales: From DNA to Dislocations

Rob Phillips

Professor of Mechanical Engineering and Applied Physics
California Institute of Technology

Abstract

The aim of this talk is to examine progress that has been made in recent years in merging atomistic and continuum perspectives for problems ranging from macromolecules of biological significance to defects in crystalline solids. On the positive side of the ledger, I will describe the use of kinematic constraints in conjunction with atomistic force fields for modeling the properties of defects in materials. By way of contrast, I will also highlight the difficulties faced in describing macromolecular assemblies such as packaged DNA in viruses and cells as well as in thinking about critical cellular processes such as gene regulation.