

Multiscale and Multiphysics Computational Frameworks for Nano- and Bio-Systems (Springer Theses)



This volume develops multiscale and multiphysics simulation methods to understand nano- and bio-systems by overcoming the limitations of time- and length-scales. Here the key issue is to extend current computational simulation methods to be useful for providing microscopic understanding of complex experimental systems. This thesis discusses the multiscale simulation approaches in nanoscale metal-insulator-metal junction, molecular memory, ionic transport in zeolite systems, dynamics of biomolecules such as lipids, and model lung system. Based on the cases discussed here, the author suggests various systematic strategies to overcome the limitations in time- and length-scales of the traditional monoscale approaches.

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