

Coarse-graining molecular dynamics for crystalline solids

Xiantao Li

Penn State University

Abstract: I will discuss a coarse-grained model of molecular dynamics in crystalline solids. Such system usually has an underlying lattice structure, and the empirical potentials are of quite simple forms. Thus it provides a nice setting in which coarse-graining (CG) methods can be considered. The goal of the CG method is to reduce the atomic degrees of freedom, and arrive at an effective model in which only a small number of atoms are explicitly involved.