P1-003

Introduction to Molecular Dynamic Simulation Employing a Reactive Force Field (ReaxFF) for Simulating Chemical Reactions of SiHx Radicals on Si Surfaces

한상수

한국표준과학연구원

In this talk, I will introduce a reactive force field (ReaxFF) molecular dynamics (MD) simulation. In contrast to common MD simulations with empirical FFs, we can predict chemical reactions (bond breaking and formation) in large scale systems with the ReaxFF simulation where all of the ReaxFF parameters are from quantum mechanical calculations such as density functional theory to provide high accuracy. Accordingly, the ReaxFF simulation provides both accuracy of quantum mechanical calculations and description of large scale systems of atomistic simulations at the same time. Here, I will first discuss a theory in the ReaxFF including the differences from other empirical FFs, and then show several applications for studying chemical reactions of SiHx radicals on Si surfaces, which is an important issue in Si process.