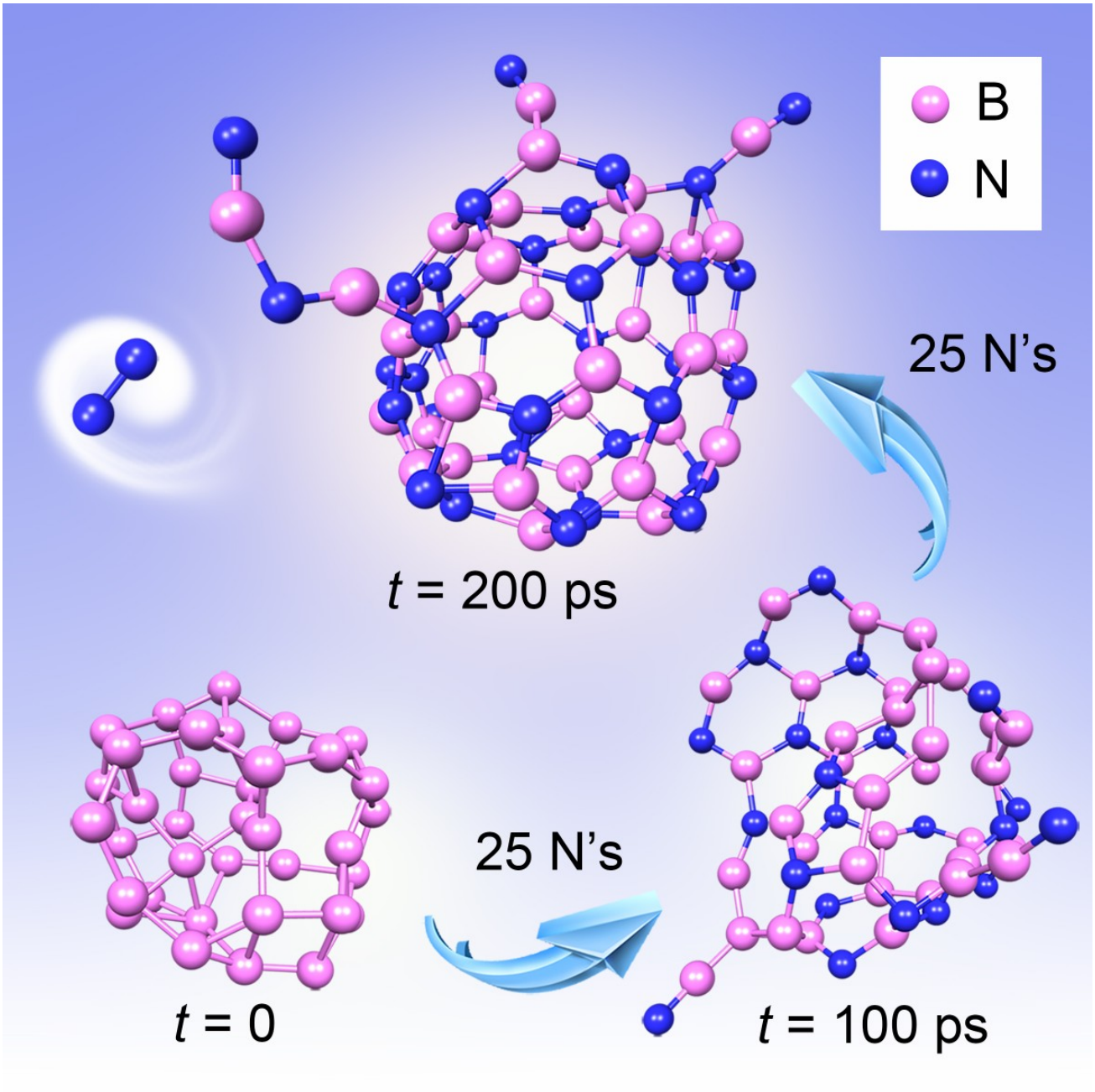
Computational physical chemistry: Quantum dynamics of molecular systems

Yasuhito OHTA [Chemistry Course]



Quantum chemical molecular dynamics simulation of boron nitride fullerene formation from an amorphous boron cluster.

The research in the Ohta laboratory involves theoretical and computational studies of the low dimensional nano material systems such as fullerene, graphene, and nanotube. One of our goals is to elucidate the self-organization process and related reaction processes of the low dimensional nano systems. We mainly use a computational approach based on the quantum chemical molecular dynamics method in order to pursuit the time-evolution of reaction dynamics of the nano systems in atomistic level. Recent computational studies include the rapid formation of the boron nitride fullerene from an amorphous-like boron cluster and defect migration dynamics occurring in a graphene sheet.

Keywords : boron-nitride fullerene, graphene, quantum chemical molecular dynamics, density-functional tight-binding method