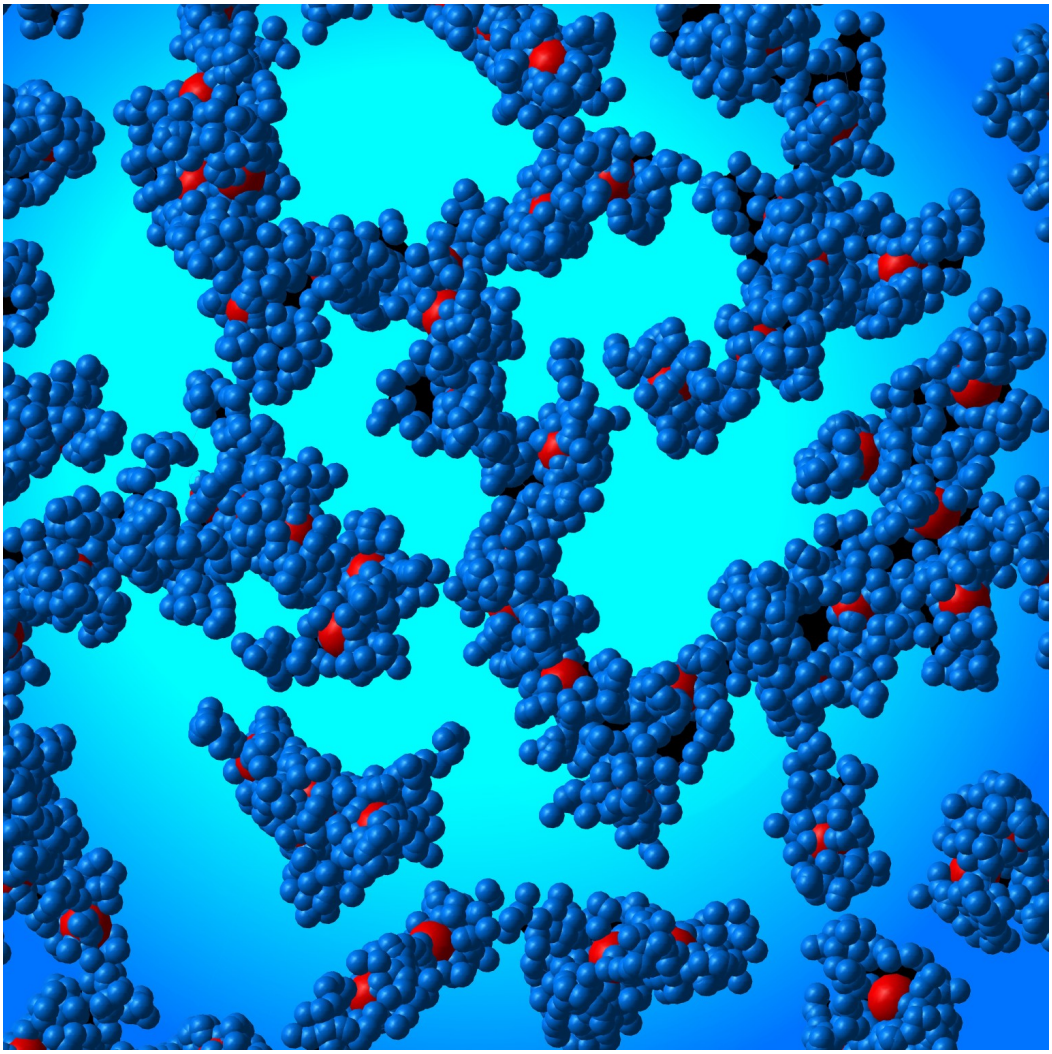
# Quantum molecular dynamics simulations aiming at exploration of dynamics of low-temperature condensed phases of quantum atoms and molecules

Kenichi KINUGAWA [Chemistry Course]



Spatial distribution of hydrogen molecules in liquid para-hydrogen obtained from the path integral centroid molecular dynamics simulation

We aim at exploration of dynamical properties of low-temperature quantum molecular systems containing atoms and molecules with light mass by means of quantum dynamical simulations. Our research targets are liquid and solid hydrogen, liquid helium-4, and ice at low temperature and high pressure. The dynamics of all of these can be approached exclusively by the quantum molecular dynamics simulations. In our researches, not only static properties but also microscopic or collective time-dependent and transport properties of such systems are numerically evaluated to give new insight for the understanding of quantum substances. We seek for a priori revelation of unexplored dynamical properties and phenomena of quantum condensed matter prior to any experimental studies, on the basis of such quantum simulations. We are also attempting to extend theoretically the methodology of quantum dynamics calculation to include the effect of particle permutation in it.

Keywords : quantum dynamics, molecular dynamics simulation, quantum many-body systems, quantum liquids and solids, path-integral quantization