Dynamics of Nucleoside and Nucleotide Hydrates by MD Simulation

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Humidity-governed phase transitions of nucleoside and nucleotide hydrates are triggered by adsorption or desorption of crystal water molecules.[1] Lowering temperature, the phase transitions coupled with ordering of crystal water molecules in the hydrates were also observed. To know the dynamics of the phase transitions, we have started molecular dynamics simulation of hydrates of guanosine[2] and disodium inosine 5'-phosphate.

The simulation was performed with the AMBER 6 program in the periodic boundary conditions. The calculation cell was constructed to be about 60 × 60 × 60 Å by replicating the crystallographic unit in the directions of the *a*-, *b*-, and *c*- axes, respectively. The AMBER ff99 energy parameters and the TIP3P water parameters were used. Electrostatic interactions were calculated by the particle-mesh Ewald method.

Averaged structures, atomic displacement parameters, time profile of hydrogen bonding probability, formation of large translocation clusters etc. were analyzed based on the simulation trajectory. The origins of the phonons observed in Raman spectra[3] were also suggested.

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