

## Interactions Between Water and a *cis*-1,4-Polyisoprene

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Hydrophobic polymers such as *cis*-1,4-polyisoprene (PI) are main components of rubbers for tires. For safe driving of vehicles, high braking performance of tire rubber on wet roads is essential. To improve the performance, it is important to understand the structure and properties of water in contact with the hydrophobic polymers and their effects on properties of the hydrophobic polymers. In this study, MD calculations and Raman spectroscopic measurements were performed to investigate the effects of the interactions between PI and water on their structures and dynamics.

MD calculations were performed using the Amber 16 program. Fundamental cells consisting of PI (39 C<sub>5</sub>H<sub>8</sub>) with 0–5010 H<sub>2</sub>O with three-dimensional periodic boundary conditions were used. The structures and diffusive properties were analyzed in the temperature range of 158–378 K. Raman spectra were measured at room temperature using a JASCO NRS-3100 spectrometer.

The results indicate that the radius of gyration  $R_g$  of PI in water depends on temperature, whereas  $R_g$  of PI without water is almost constant. This indicates that the PI in water undergoes a coil-globule transition owing to temperature dependences of density and diffusivity of water. The volume expansion of the supercooled liquid induces the coil structure of PI, while the increase in the diffusivity of water around PI can be a cause of the globule structure. PI has effects to decrease the strength of hydrogen bonds of water. Furthermore, the thin layer of the intermediate water around PI is a possible cause of the higher diffusion coefficients of free water.