

Connectivity, dynamics, and structure in a tetrahedral network liquid

We report a detailed computational study by Brownian dynamics simulations of the structure and dynamics of a liquid of patchy particles which forms an amorphous tetrahedral network upon decreasing the temperature. The highly directional particle interactions allow us to investigate the system connectivity by discriminating the total set of particles into different populations according to a penta-modal distribution of bonds per particle. With this methodology we show how the particle bonding process is not randomly independent but it manifests clear bond correlations at low temperatures. We further explore the dynamics of the system in real space and establish a clear relation between particle mobility and particle connectivity. In particular, we provide evidence of anomalous diffusion at low temperatures and reveal how the dynamics is affected by the short-time hopping motion of the weakly bounded particles. Finally we widely investigate the dynamics and structure of the system in Fourier space and identify two quantitatively similar length scales, one dynamic and the other static, which increase upon cooling the system and reach distances of the order of few particle diameters. We summarize our findings in a qualitative picture where the low temperature regime of the viscoelastic liquid is understood in terms of an evolving network of long time metastable cooperative domains of particles.