Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Thursday, September 21st 2017 – 2:00 pm
CFEL Seminar room I-II, (Bldg. 99)

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" Supercooled water: Fluctuation, glass transition, and vibrational entropy"

Water is the most common liquid. Its properties are not, however, common. Since the anomalies of water become pronounced at low temperatures, especially below its melting temperature, it has been proposed that the anomalous properties are attributed to the presence of two liquid states corresponding to the two amorphous ices. Experimental studies of supercooled water are however very difficult. This is due to the fact that bulk water is easily transferred to a crystalline phase in the “no man’s land”, which is a temperature range bounded by the crystallization of supercooled water at ~235K and by that of highly viscous liquid water at ~150K. Therefore, various theoretical and computational studies have been conducted for understanding the properties in the no man’s land. We have performed extensive molecular dynamics simulations from normal liquid to deeply supercooled states to reveal the structural and dynamical instabilities in the no man’s land. The spatiotemporal fluctuations, dynamic transition, glass transition, and vibrational contribution to Kauzmann temperature of supercooled water will be discussed.

Host: Dwayne Miller

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