nanoTBtech webinars

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Water: Decoding the percolation phase transition at 330 K with a nanoparticle ruler.

Abstract:

Liquid water, despite its simple molecular structure, remains one of the most fascinating and complex substances. Most notably, many questions continue to exist regarding phase transitions and anomalous properties of water, which are subtle to observe experimentally.

In a recent work,[1] we report a sharp transition in water at 330 K unveiled through experimental measurements of the instantaneous Brownian velocity of $NaYF_4$:Yb^{3+}/Er^{3+} upconversion nanoparticles in water. Our experimental investigations, corroborated by molecular dynamics simulations, elucidate a geometrical phase transition where a low-density-liquid (LDL) phase becomes percolated below 330 K. Around this critical temperature, we find that the sizes of the LDL clusters to be similar to the nanoparticles, confirming the role of upconversion nanoparticle as a powerful ruler for measuring the extensiveness of the LDL hydrogen-bond network and nanometer-scale spatial changes (20 to 100 nm) in liquids. Additionally, a new order parameter that unequivocally classifies water molecules into two local geometric states is introduced, providing a new tool for understanding and modelling water's many anomalous properties and phase transitions.

In this talk, I will highlight the major findings of our work, in particular, upconversion nanothermometry as a key tool for unveiling the properties of liquid water near its isocompressibility minimum at ambient pressure.

[1] C.D.S. Brites & B. Zhuang *et al.* Phys. Chem. Lett. **2020**, 11, 16, 6704–6711 (https://pubs.acs.org/doi/10.1021/acs.jpclett.0c02147)