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Universal behavior of mesoscopic dynamics in molecular liquids: spectroscopy with polarized neutrons and MD-simulations

In spite of its fundamental interest, the dynamics –collective and self–of molecular liquids and glass-forming systems at the mesoscale is still poorly understood. Quasielastic neutron scattering (QENS) is the ideal technique to carry on this kind investigations in a wide Q-range (Q: momentum transfer) due to the high energy resolution available. The problem is that the measured intensity always contains a combination of coherent and incoherent contributions, which can be very relevant at the mesoscale. The development of spectroscopy methods by using polarized neutrons –that allow separating both neutron components– has fueled a new revival of this topic of utmost importance in the general field of liquids. By means of the recently implemented neutron polarization analysis on a wide time-of-flight spectrometer (LET @ ISIS) and also by using the wide-angle neutron spin echo spectrometer WASP at the ILL, we have been able to separate coherent and incoherent neutron scattering in different liquids with different molecular interaction [A. Arbe et al., Phys. Rev. Research 2, 022015(R) (2020); A. Arbe et al., Phys. Rev. Lett. 134, 098001 (2025)]. Our results show that, independently of the intermolecular interactions, all liquids follow some kind of universal behavior at the mesoscale: (i) density-density fluctuations decay –apart from hydrodynamic-like modes–through a non-diffusive exponential process; (ii) the fingerprint of the local molecular motions involved in this process can be observed in the short time regime of the incoherent intermediate scattering function. These results were interpreted with the help of massive MD-simulations carried on in different systems. In this talk I will give an overview of the current status of these investigations.

Session

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