Ionic liquids: the prepeak paradox

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Room-temperature ionic liquids are pure salts which are liquid at room temperature. Their chemical structure is a subtle combination of two antagonist counterparts, a polar and an apolar domains which are chemically linked together. This intimate assembly leads to nanoscale segregation, which have:
i) a dynamical signature: cation dynamics present a multi modal scale-dependant behavior, with a localized motion within the IL nanometric domains at shorter time scale and a genuine long-range translational motion for longer times.[1]
ii) a structural signature: a strong scattering called pre-peak is often observed at small scattering vector (below 0.5 $Å^{-1}$) corresponding to correlation lengths larger than the size of the ions (1 – 3 nm).[2]
However, the physical origin of the prepeak is still not explicit: it is related to the segregation between polar and apolar unfriendly domains but only slight change of the molecular structure may wipe off this specific feature.
In this talk, we propose a robust approach to describe S(Q) scattering curves and propose a clearer image of IL nanostructuration: wide-angle neutron scattering (WANS) on selectively deuterated IL samples allows to contrast the different counterparts of these complex liquids. A detailed analysis of these findings will be proposed from a molecular dynamic approach.

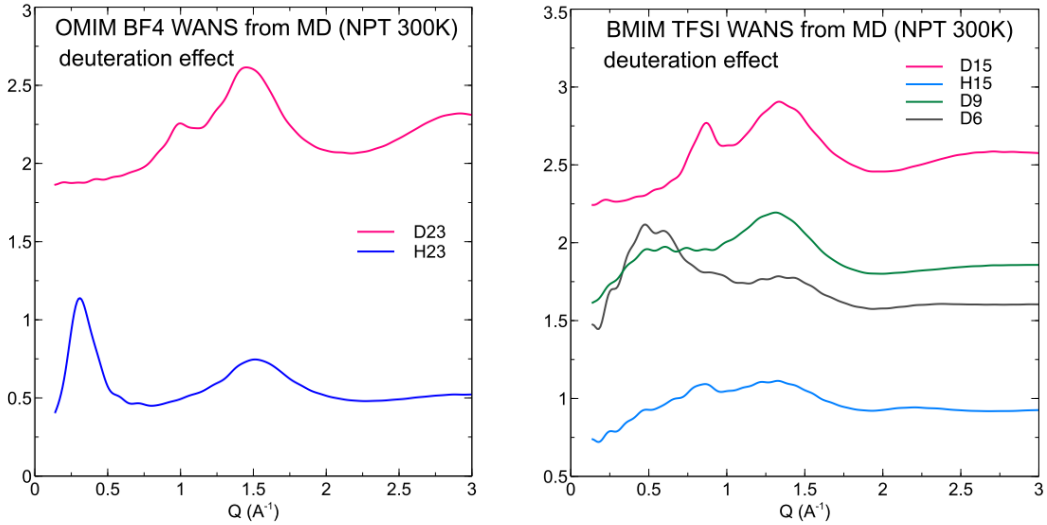

Figure 1: Effects of deuteration sites on neutron structure factor S(Q) profiles as obtained from Molecular Dynamic approach for two different ionic liquids: i) $OMIMBF_4$ (left) ; H23 all hydrogen, D23 all deuterium ; ii) BMIMTFSI (right); H15 all hydrogen, D15 all deuterium, D6 imidazolium deuterated, D9 alkyl chain deuterated.

[1] F. Ferdeghini, Q. Berrod, J.-M. Zanotti, P. Judeinstein, et al., Nanoscale, **9**, 1901 (2017)
[2] A. Martinelli, M. Maréchal, Å. Östlund, J. Cambedouzou, Phys. Chem. Chem. Phys., **15** 5510 (2013)