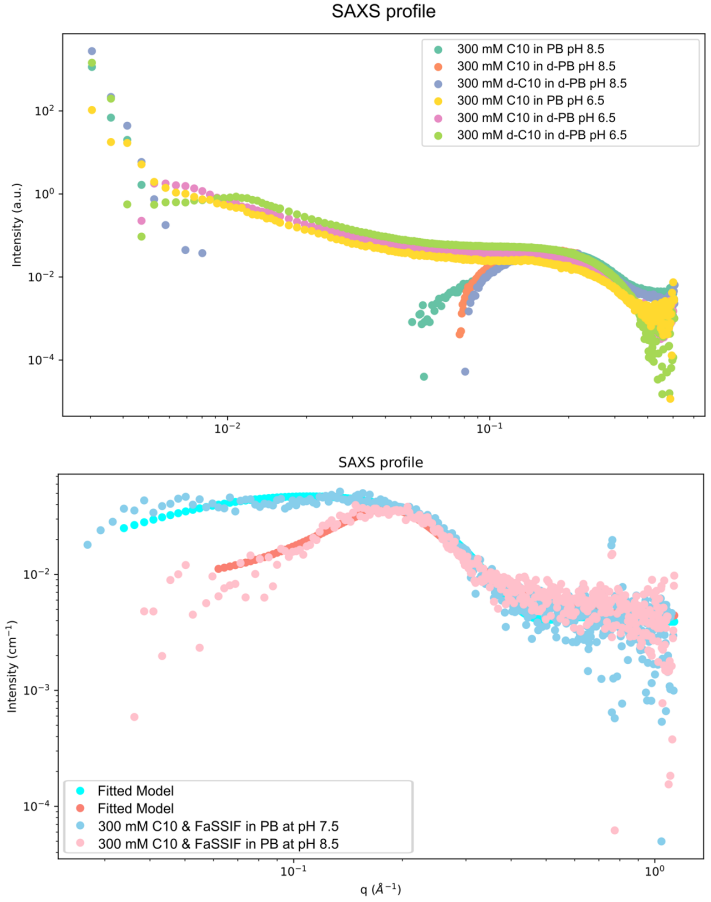
Investigation of the aggregation behavior of Sodium Caprate by Coarse-Grained simulation and Small-angle Scattering

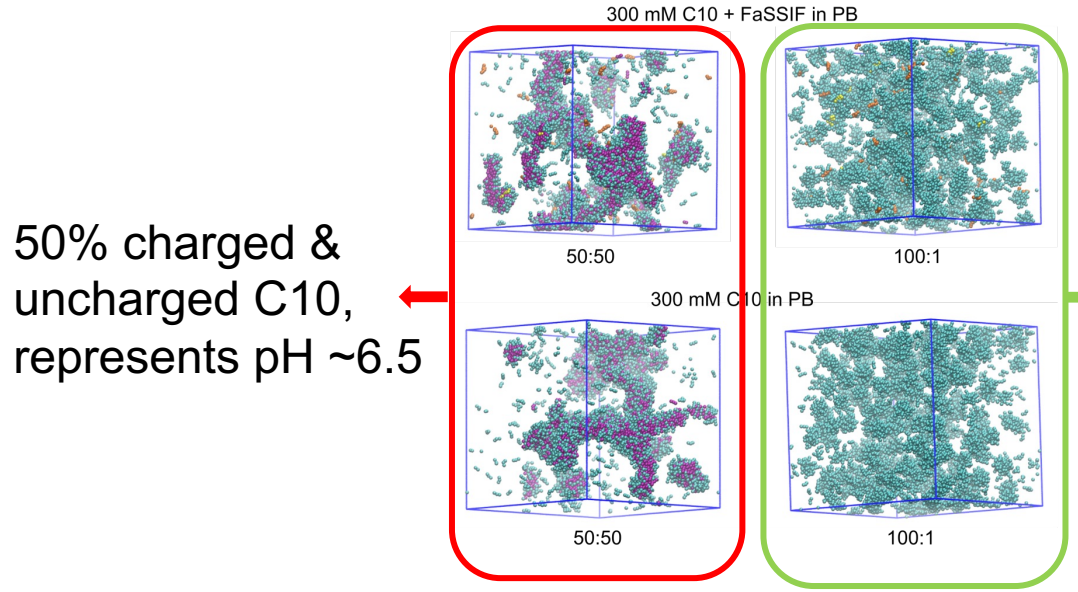
Objective

1. Characterization of aggregation behavior by using Small Angle Scattering (SAS)
2. To develop computational simulation protocols to observe the aggregation behavior



- Figured out the primary structure from SAXS data.
- Need to have low Q SAS data, hence, applied for Beamtime in ILL.

Results and current status



50% charged & uncharged C10, represents pH ~6.5

100% ionized C10, represents pH ~8.5

- Formed larger aggregates in low pH and smaller aggregates in higher pH.
- Determining theoretical SAS spectra from the simulation data by back mapping into All-atom simulation and using PEPSI-SAXS/SANS

Shahina Akter, PhD student, UU