

7th December 2022 - 2:00 p.m.
CFEL-bldg. 99, seminar room IV

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Interpretation and modeling of X-ray scattering experiments with molecular dynamics simulations

X-ray scattering in solution, carried out at synchrotrons or FEL facilities, has developed to an increasingly accurate method for obtaining structural information on biomolecules and soft-matter complexes in solution. However, the interpretation of the solution scattering data by computational methods is complicated by (i) the low information content of the data and (ii) by scattering contributions from the hydration layer and excluded solvent, leading to a significant risk of over-interpretation upon fitting structural models against the data.

To overcome such problems, our group develops methods for interpreting and modeling X-ray scattering experiments with all-atom explicit-solvent molecular dynamics (MD) simulations, with a focus on small- and wide-angle scattering data (SWAXS). In this talk I will present an overview of our methods covering (i) predictions of SWAXS curves from MD simulations including an application to time-resolved

WAXS data, (ii) structure and ensemble refinement against SWAXS data, (iii) analysis of the protein hydration layer and validation against a recent worldwide round-robin benchmark, and (iv) modeling of water jet explosion after impact of an X-FEL beam.

