

CHYN MEETS HARBOR

Investigation of water in nanoporous silica (MCM-41) on molecular scale

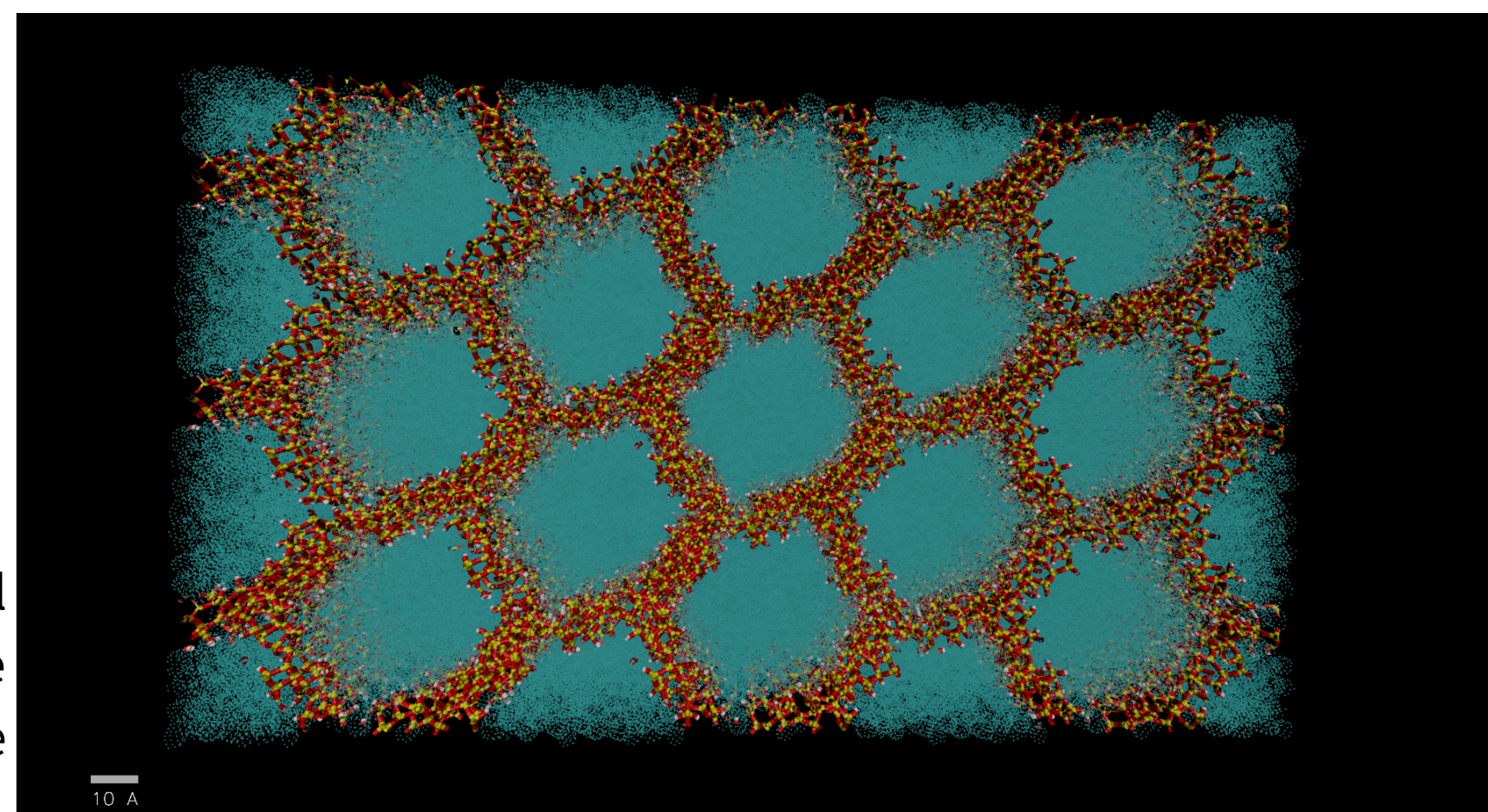
Lars Dammann

Correctness-State Score: an Objective Metric to Guide Background Correction and Data Interpretation of Small Angle X-ray Scattering Data

Yunyun Gao

Abstract Talk 1: The physicochemical properties of water in confined spaces are as yet poorly understood on the molecular scale. One possibility to investigate the structure and the behaviour of confined water are Molecular Dynamics (MD) simulations. In this talk I will give a short introduction on what MD Simulations are and how MD simulations might be used to investigate the molecular properties OF water confined in nanoporous silica (MCM-41) (s. Fig.).

Subsequently, I want to present an approach on how experimental results, e.g. from X-ray scattering measurements, might be combined with MD simulations via the Maximum Entropy principle to improve the validity of MD simulation results.



Abstract Talk 2: Small-angle X-ray scattering (SAXS) experiments provide an estimation of biological macromolecule geometry on the level of domain structure. The reliability of structural inference drawn from SAXS data is dependent on the accurate measurement as well as the proper post-processing procedure. The methods improving raw data quality and gaining more information are widely explored. Among those innovations, size-exclusion chromatography small-angle X-ray solution scattering (SEC-SAXS) has become a standard method for modern bio-SAXS synchrotron light sources. However, the principle of data post-processing for SEC-SAXS remains rather unclear. This includes background correction and averaging of the raw data. Several statistical tools have been developed to assess solution SAXS data quality. These are mostly useful for “rejecting” significantly different data points or data frames, based on the assumption that the rest of the data are close to the “truth”.

But this can lead to a situation where mediocre data, especially data contaminated with radiation damage, are not correctable or simply cannot be evaluated before any interpretation is done. To alleviate this problem, an objective metric, correction-state score (CSS) is proposed. As a metric of “similarity”, CSS was formulated by utilizing several mathematical concepts originating from the Dynamic Time Warping (DTW). CSS can be used to both verify the data quality and identify the optimal data correction procedure for post-processing of SEC-SAXS data. CSS can be represented as a numerical likelihood with a scale of 0 to 1. Using this objective score it is possible to quantitatively assess the “goodness” or appropriateness of a background correction for SEC-SAXS data. Under the guidance of CSS, the metadata recorded during a SEC-SAXS experiment can be used to maximize the fidelity of the post-processing as well as reduce the ambiguity in further data interpretation.

