Insights on Water Structure from the Modeling of Scattering Data

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The structural and dynamic properties of water in bulk and at interfaces are relevant for many physico-chemical processes. Insight can be gained from all-atomistic simulations of interfacial water that nowadays reach the experimentally relevant length and time scales. This is demonstrated with a few examples:

i) For bulk water, simulations reproduce the main features of the experimental SAXS structure factor S(q), including the minimum at small q. Spatial correlations between local density and structural fluctuations are shown to be weak, suggesting that features in density-density correlations (such as measured by the structure factor) are not straightforwardly related to structural spatial correlations in liquid water. [1]

ii) Hydrophobic surfaces in contact with water show a pronounced depletion layer where the water density is highly reduced[2]. The combination of X-ray reflectivity (XR) and atomistic molecular dynamics (MD) simulations provide new insight into simple oil-water interfaces. [3]

iii) The bending rigidity and the structure of the water-vapor interface is obtained from an analysis of the capillary interfacial wave spectra from simulations and grazing-incidence x-ray scattering. A pronounced scale dependence of the bending rigidity points to a crossover at a length scale of about one nanometer: At smaller scales the interface reconstructs and nano-ripples proliferate, at larger scales the interface is governed by tension and bending rigidity. [4]

iv) The combination of x-ray scattering experiments and molecular dynamics simulations yields insight into the structure and the swelling mechanics of hydrated collagen. With a proper choice of simulation force fields the experimental packing distances as well as osmotic pressures for different collagen types are reproduced.

[1] Spatial Correlations of Density and Structural Fluctuations in Liquid Water: A Comparative Simulation Study
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[2] Interfacial Water at Hydrophobic and Hydrophilic Surfaces: Depletion versus Adsorp-

tion, J. Janecek and R.R. Netz, Langmuir 23, 8417 (2007).

[3] Nanoscale Structure of the Oil-Water Interface
M. Fukuto, B. M. Ocko, D. J. Bonthuis, R. R. Netz, H.-G. Steinrück, D. Pontoni, I. Kuzmenko, J. Haddad, and M. Deutsch

PRL 117, 256102 (2016)

[4] Nanoroughness, Intrinsic Density Profile, and Rigidity of the Air-Water Interface
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