MAR17-2016-020659

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Water at protein surfaces studied with femtosecond nonlinear spectroscopy[1]

HUIB J. BAKKER, AMOLF, Science Park 104, 1098 XG, Amsterdam

We report on an investigation of the structure and dynamics of water molecules near protein surfaces with femtosecond nonlinear spectroscopic techniques. We measured the reorientation dynamics of water molecules near the surface of several globular protein surfaces, using polarization-resolved femtosecond infrared spectroscopy. [1] We found that water molecules near the protein surface have a much slower reorientation than water molecules in bulk liquid water. The number of slow water molecules scales scales with the size of the hydrophobic surface of the protein. When we denature the proteins by adding an increasing amount of urea to the protein solution, we observe that the water-exposed surface increases by ˜50% before the secondary structure of the proteins changes. This finding indicates that protein unfolding starts with the protein structure becoming less tight, thereby allowing water to enter. With surface vibrational sum frequency generation (VSFG) spectroscopy, we studied the structure of water at the surface of antifreeze protein III.[2] The measured VSFG spectra showed the presence of ice-like water layers at the ice-binding site of the protein in aqueous solution, at temperatures well above the freezing point. This ordered ice-like hydration layers at the protein surface likely plays an important role in the specific recognition and binding of anti-freeze protein III to nascent ice crystallites, and thus in its anti-freeze mechanism. [1] C.C.M. Groot and H.J. Bakker, *Proteins Take up Water Before Unfolding*, J. Phys. Chem. Lett. **7**, 1800–1804 (2016). [2] K. Meister, S. Strazdaite, A.L. DeVries, S. Lotze, L.L.C. Olijve, I.K. Voets, and H.J. Bakker, *Observation of ice-like water layers at an aqueous protein surface*, Proc. Natl. Acad. Sci. USA **111**, 17732-17736 (2014).

[1]This research is supported by the "Nederlandse organisatie voor Wetenschappelijk Onderzoek (NWO)