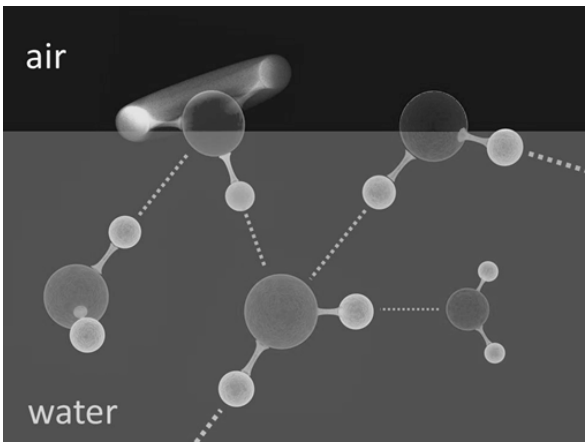
Structure and Dynamics of Interfacial Water

Mischa Bonn
Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany
e-mail: bonn@mpip-mainz.mpg.de

At the surface or interface of water, the water hydrogen-bonded network is abruptly interrupted, conferring properties on interfacial water different from bulk water. Owing to its importance for disciplines such as electrochemistry, atmospheric chemistry and membrane biophysics, the structure of interfacial water has received much attention [1].

We elucidate the structure and structural dynamics of interfacial water using ultrafast surface-specific sum-frequency generation (SFG) vibrational spectroscopy. Specifically, for the water-air interface, we find that the interface is both structurally heterogeneous [2] and highly dynamical [3]. We reveal the nature of the heterogeneity, find surprisingly rapid inter- and intramolecular energy transfer processes and quantify the reorientational dynamics of interfacial water. We quantify the concentration of ions at the surface, compared to the bulk, and find a large surface propensity of halide ions at the water-air surface [4]. At the water-mineral interface, we report a dramatic effect of flow of water along the mineral surface on the organization of water at the interface [5].



At the water-air interface, the hydrogen-bonded network is interrupted, giving rise to undercoordinated water with distinct structure and dynamics at the interface – for instance fast reorientation of 'free' OH groups, as indicated in the cartoon.

References

[1] Bonn, M.; Nagata, Y.; Backus, E.H.G.; *Angew. Chem.-Intern. Ed.* **2015**, (in print).

[2] Hsieh, C.S.; Okuno, M.; Backus, E. H. G.; Hunger, J.; Nagata, Y.; Bonn, M., *Angew. Chem.-Intern. Ed.* **2014**, *31*, 8146 (VIP paper).

[3] Hsieh, C. S.; Campen, R. K.; M. Okuno; E. H. G. Backus; Y. Nagata; and M. Bonn, *Proc. Nat. Acad. Sci. USA* **2013**, *110*, 18780.
[4] Piatkowski, L.; Zhang, Z.; Backus, E. H. G.; Bakker, H.J.; Bonn, M., *Nature Commun.* **2014,** *5*, 4083.
[5] Lis, D.; Backus, E. H. G.; Hunger, J.; Parekh, S. H.; Bonn, M., *Science* **2014**, *344*, 1138.