Two-Dimensional Terahertz-InfraRed-Visible Spectroscopy Reveals Inhomogeneity of Water Hydrating Ions

Mischa Bonn[1*]; Laura Vietze[1], Maksim Grechko[1]

[1]Department of Molecular Spectroscopy, Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany

**bonn@mpip-mainz.mpg.de*

In aqueous solutions, many chemical and biological substances, from simple salts to proteins and DNA, are charged. The solvation of ions in water is accompanied by the formation of a hydration shell – a layer of water molecules, which interacts strongly with the ions. Intermolecular thermal fluctuations of a hydration shell are important for, e.g., thermal reactions, where they provide the energy needed to surmount the reaction barrier. Due to the altered intermolecular forces, the spectrum of thermal fluctuations of a hydration shell is significantly different from that of the bulk water, as revealed by the far-infrared absorption spectroscopy. However, many questions remain regarding these intermolecular vibrations. Here, we use Two-Dimensional Terahertz-InfraRed-Visible (2D TIRV) spectroscopy [1] to investigate the inhomogeneity of the intermolecular terahertz vibrations in the hydration shells of simple inorganic ions.

Our results reveal a direct correlation between the strength of the hydrogen bonds and the frequency of the solvating water molecules' terahertz fluctuations, highlighting the difference between water-water and water-ion hydrogen bonds, and demonstrating the increased heterogeneity of the latter.

References

[1] M. Grechko et al., (2018) Nat. Commun., 9:885.