

# Real-space investigation of microsolvation: Water structures in the presence of organic molecules or ions

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Solvation science aims at using the solvent to enhance and steer reactivity. However, there is little to no experimental evidence of the exact structure of solvents around molecules and thus very little is known about the solvent-solute interaction on a microscopic level. We use low-temperature scanning tunneling microscopy to reveal structural changes to water ice on the (111) faces of the coin metals in the presence of both organic molecules and cations. By investigating the attachment of individual water molecules to the solute by low-temperature scanning tunnelling microscopy, we gain microscopic insight into the solvent-solute interaction. Moreover, we present an example, how this interaction influences the reactivity of photo-induced reactions. The systems discussed in this talk are benzene and azobenzene [1,2] derivatives as prototypes for polar molecules and lithium and cesium ions as prototypes for cations.

Concerning the formation of a solvation shell, we used differently functionalized azo dyes and follow the attachment of the first water molecule to a fully solvated molecule on the Ag(111) surface. Specific functional groups bind initially one water molecule each, which act as anchor points for additional water molecules.

Concerning the influence of solvation on reactivity, we investigate the photolytic dissociation of halogenated benzene molecules. The molecules are adsorbed on amorphous and crystalline ice islands supported on Cu(111). Energy barrier and dissociation rate are largely altered upon adsorption and moreover depend crucially on the exact water arrangement around the dissociating molecule.

Concerning the solvation of cations, we present the first real space information about the difference in ice structure induced by addition of a chaotrope versus a kosmotrope on the electrochemically important Au(111) surface.

Our STM study gives an unprecedented view of water interacting with polar species on surfaces.

References:

[1] J. Henzl, K. Boom, K. Morgenstern, *J. Am. Chem. Soc.* 136 (2014) 13341

[2] K. Lucht, D. Loose, G. Dyker, K. Morgenstern, *Angew. Chem. Int. Ed.* 57 (2018) 1266-1270