RESOLV Summer School Solvation Science 2019, advanced hands-on module

Exploring solvation and protonation in the solid state using synchrotron and electron diffraction

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As result of the interaction between particle waves and periodic matter (single crystals), the electron density of a molecular material can be observed in diffraction studies. Single crystal diffraction analyses allow to determine the 3d structure of chemical compounds such as large supramolecular assemblies and can also reveal their protonation state and position of co-crystallized solvent molecules. Compounds featuring large void volumes tend to crystallize with a high solvent content and hence deliver precious data on solvation phenomena in atomic resolution that can be compared to results of solution studies. Besides normal in-house datasets obtained at single crystal X-ray diffractometers, diffraction experiments conducted at highly brilliant synchrotron radiation sources such as DESY in Hamburg allows for extremely small crystal sizes. In addition, the emerging technique of 3D Electron Diffraction (microED) using a special Electron Microscope even allows for structure elucidation at atomic resolution using submicron-sized crystals with a volume of only 1 μm^3.

The practical course will introduce you to modern in-house X-ray facilities and basic crystallographic concepts. Using modern crystallographic software (SHELXL, ShelXle GUI) You will hands-on learn to model chemical structures against synchrotron X-ray and electron diffraction datasets and determine the position of co-crystallized solvent molecules as well as the protonation state of molecules in the solid state. Discussion about possibilities and limits of the technique will be experienced-based on the examples provided. Furthermore, interfacing crystallographic results with modern QM and MD methods will be discussed. We will end the module by discussing potential links with your projects.

Participants are requested to bring their own laptop.