

4.00 p.m. (Minatec Conference Hall)

Charge density analysis via powder diffraction

Bo B. Iversen

Aarhus University, Denmark

E-mail: bo@chem.au.dk

The electron density of a molecular-scale system is the most information-rich observable available in natural science. It can be obtained either from quantum mechanical calculations or estimated experimentally from accurate X-ray diffraction data. For the past three decades electron densities have been determined in numerous crystals based on modeling of accurate structure factors measured by single crystal X-ray diffraction. The X-ray electron density method is today well established and it has provided important insight into the nature of chemical bonding and physical properties of systems spanning from small organic molecules to inorganic crystals and even proteins. In many ways inorganic materials represent the ultimate challenge for experimental electron density determination. In these systems the scattering from the valence electrons is very weak compared with the core electron scattering and inorganic crystals often suffer from strong absorption effects. In addition the excellent crystal quality makes extinction in the low order reflections highly problematic. Normally single crystal X-ray data are considered to be more accurate than powder diffraction due factors such as peak overlap. However, for simple inorganic structures peak overlap is limited and furthermore in powder diffraction all data are measured on the same scale. In this talk our efforts in determining experimental electron densities from synchrotron powder X-ray diffraction will be discussed.

Keywords: charge density, multipole modeling, synchrotron powder diffraction