# Quantum Crystallographic Quest for New Polymorphic Forms of Ice and Hydrates

Water is the main constituent of Earth's hydrosphere and the fluids of most living organisms. It is crucial for all known forms of life. It forms18 solid crystalline ices and two amorphous solid forms. It covers the most of the Earth's surface. Water molecules interact with the most important biological substances: proteins, DNA and polysaccharides influencing protein folding, DNA base pairing, and other phenomena crucial to life. Water molecules form hydrogen bonds - one of the most important interactions in modern biology, medicine and pharmacology. Water forms different hydrates and plays a key role in Earth's mantle processes (hydrography, hydrology, hydrogeology, glaciology, oceanography, etc). Water is also present in outer space. It is produced as a by-product of stellar nuclear fusion, was detected in interstellar clouds within the Milky Way, and exists in abundance in other galaxies. **The main goals of this project are: (1) to discover new forms of ice, deuterated ice and hydrates hosting small organic molecules, (2) to improve the known forms of ice by establishing better averaged and local structures and to elucidate the hydrogen atom thermal motion.**

We will accomplish our aims by combining the new approaches of quantum crystallography (QC) with single crystal high pressure studies using wide opening angle diamond anvil cells (DACs) with controlled pressure and temperature and short wavelength synchrotron radiation. QC approaches will include: experimental charge density studies, Hirshfeld atom (HAR) and proposed by us Hirshfeld atom-like refinements (including its periodic version), and X-ray wavefunction refinement (XWR). QC methods are more rigorous (and also more precise and accurate) than routine methods of crystallography. Using HAR we have already refined anisotropic H-atoms in hydrates of very heavy metal derivatives and relativistic and electron correlation effects in a gold complex. Sometimes, we were observing some new structures of ice but they were of very poor quality and we could not have refined them. However, synchrotron X-ray radiation is ca. 10mln times stronger than laboratory X-ray sources and thus we hope to get reliable new ice structures from synchrotron data collections. This is incredible that using our HAR, we have already managed to refine anisotropic hydrogen atoms in ice VI, $D_2O$ ice VI and mixed $H_2O/D_2O$ ice VI for data obtained on our home X-ray silver source. We will generate different forms of ice *in situ* inside the DACs, and produce new forms of ice through changes in temperature and pressure. Decreases in temperature and increases in pressure will reduce the thermal motion of water molecules while increasing temperature and decreasing pressure will increase the dynamic disorder of water molecules. **Using wide angle DACs, QC and synchrotron X-rays, we will simulate ice and hydrate structures and processes inside Earth and other planetary bodies, and characterise and study them at the level of quantitative electron density changes. This is opening new mineralogy far beyond the present state of the art.**

Our project is highly interdisciplinary and combines state-of-the-art methods of quantum crystallography utilising strict ideas of quantum chemistry for the solid state, and high resolution, high pressure and variable temperature mineralogical studies. Additionally, a significant part of our project is focused on development of new software which would allow us to improve quality of results. This includes correction of high resolution single crystal X-ray data to account for absorption of the diamond anvil cell and for diffuse scattering.

We are convinced that with proper DACs allowing for controlling both temperature and pressure we will find some new polymorphic forms of ices and hydrates particularly those carrying important biological molecules in their structures. Water studies have become a hot topic recently. An excellent example of importance of this topic is a series of conferences at DESY(Germany) focused on forming a Centre for Molecular Water Science (CMWS) a joint effort of ca. 85 research groups from all over the world. I am a contributor to Pillar 2 of that application.

**Our research has a fundamental nature and it should allow to get break through in studies of ice (really milions publications in literature) . It will allow for better understanding the role of woter/ice in the mantles of planets, the experimental determination of plastic anisotropy and deformation, ion/holes transition pathways and the better understanding of the dynamics and evolution of Earth and other extraterrestrial planets.**