

User Meeting 2020

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Developing High Pressure Single Crystal Crystallography at MX

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Pressure is an important thermodynamic variable, but its effects on chemical systems have been explored to a much smaller extent than that of temperature. High pressure has been shown to induce significant geometrical, configurational and conformation changes within chemical systems.

The development of diamond anvil cells (DACs) in recent years has allowed the study of chemical systems under high pressure by single crystal X-ray crystallography. This has enabled the analysis of the molecular structure of materials at high pressure, which is invaluable for an increased understanding of their properties. Pressure has been shown to be an important tool in the characterisation of structure-property relationships in porous materials, such as metal organic frameworks (MOFs). High pressure has been used as a useful tool for investigating the stability of MOFs, as well as their mechanical properties such as elasticity, stiffness, and hardness.

A diamond anvil cell contains two opposing diamonds which between them create a sample chamber which can reach pressures of up to 10 GPa. The macromolecular crystallography (MX) beamlines at the Synchrotron are a pair of dual-purpose beamlines serving the needs of the Australasian structural biology and chemical crystallography community. The development of small DACs which can be easily mounted on a goniometer has opened the possibility to conduct high pressure crystallography on the MX beamlines, without major changes to the beamline setup. This development of beamline capability will enable users to study chemical systems at high pressure in order to better understand their properties and study the geometric changes which occur at high pressure.

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