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X-ray Crystallography, an Important Cog in the Materials Science Machine.

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Materials science is dependent on collaborations around the globe. Research groups often have expertise in one field but not others, yet all are required to see the full picture from synthesis through characterisation and properties to applications.

The Elsegood group's expertise is in structure characterisation through single crystal X-ray diffraction. We collect data in our laboratory in Loughborough, at synchrotron sources in the UK and in the USA, and through the National Crystallography Service in the UK. We also make use of databases like the CSD.

Our structural work supports the research of several synthetic chemistry research groups around the world, including the Redshaw and Allin groups in the UK and China, and the Yamato and Hill/Ariga groups in Japan.

In turn, these groups also require help from groups in Shanghai and Texas to assess the gas adsorption/desorption properties of metal-organic framework (MOF – Fig 1) compounds and lithium-containing calixarenes, and similar compounds. Other collaborators help with molecular modelling and electrochemical experiments.

The talk will discuss the hardware and software we employ in our structural studies and emphasise the importance of 'doing it right'. It will also highlight the links and collaborations in which the Elsegood group is involved with many examples of the sort of compounds studied.

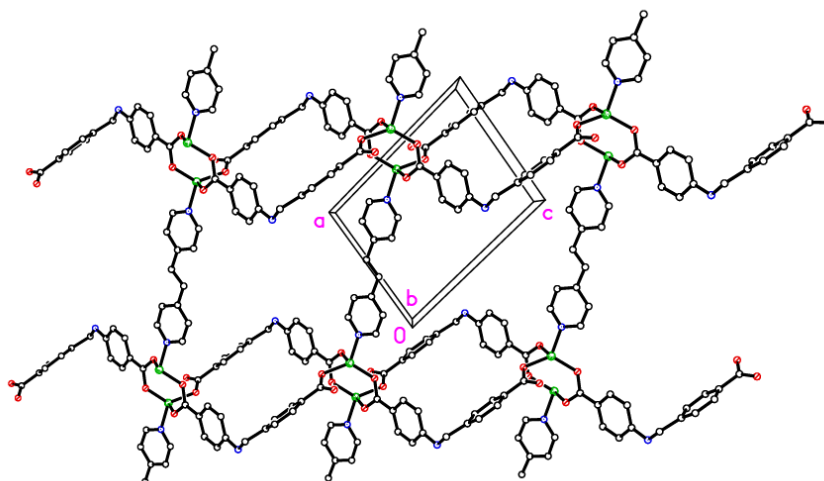


Fig. 1. A MOF from the Elsegood/Redshaw collaboration.