



## FIRST Newsletter

Apr 2020, Issue 52

### Bruker/MIT Symposium 2020

*By Dr. Peter Müller, Director of X-Ray Diffraction Facility, MIT Department of Chemistry, Cambridge, MA, USA*

This year's Bruker/MIT Symposium, held from Friday February 21<sup>st</sup> to Saturday February 22<sup>nd</sup> at the Massachusetts Institute of Technology in Cambridge, MA, was under the motto **Porous Materials**. With close to 100 registered participants from six countries (Canada, Germany, Korea, Oman, South Africa and 13 US States), the Symposium once again had the flair of an international conference and we received enthusiastically positive feedback from many participants. As every year, the meeting was hosted by the MIT Department of Chemistry, organized by Peter Müller, Director of the Departmental X-Ray Diffraction Facility, and sponsored by Bruker AXS.

Several of this year's participants had also been present at the Bruker/MIT Symposia about **Metal Organic Frameworks** in 2012 with presentations by Wenbin Lin, Jeff Long, Omar Yaghi, George Whitesides and Mirecea Dinca; however this year's topic, **Porous Materials** explicitly included other types of porous materials. In some cases, the contents of the pores matter most and the framework around them merely provides structure and separation. In other cases, the extended supramolecular framework itself generates the interesting electronic or optical properties. In spite of this variety, this type of chemistry relies heavily on diffraction methods for structure elucidation and the 2020 Bruker/MIT Symposium assembled some

of the most interesting heads of the world of porous materials.

The first talk of the Symposium by **Michael Ruf** (Bruker AXS) introduced what is "New and Exciting at Bruker", giving an update on some of the improvements to Bruker software and hardware since the last Symposium. **K. Travis Holman** (Georgetown College) gave a breathtaking presentation about "Shape Persistent Macrocycles as 'OD' Porous Molecular Solids and Templates for Polymorphic Metal-Organic Frameworks", illustrating his group's work on gas- and solvent-capturing compounds with surprising thermodynamic and kinetic behavior. One of the specialties of the Barbour lab at Stellenbosch University in South Africa is the study of crystals under non-ambient conditions. **Leigh Loots** from Stellenbosch showed and described environmental gas cells developed in her group which allow pressurizing a crystal inside a glass capillary with a relevant gas and subsequently collecting complete diffraction data from the sample under pressure. The last talk before lunch was given by **Xiaoyue Qi**, a postdoc in Robert Langer's lab at MIT who introduced the audience to "Functional Metal-Organic Frameworks (MOFs)-Based Devices for Cell Recognition and Drug Delivery". This impressive work included MOFs with cavities engineered to accommodate small protein molecules and release them in a controlled fashion inside animal tissue samples.

The lunch break was combined with a poster exhibition to which seven participants had brought posters reflecting their most recent research. As every year, an independent jury awarded the best

poster with a \$500 prize. The poster jury was headed by Allen Oliver from the University of Notre Dame and selected the poster “A crystallographer's nightmare or a fascinating case of disorder?” by **Matthew Crawley** (University at Buffalo) for the **2020 Bruker/MIT Poster Prize**.

The first talk after the lunch break was given by MIT's own **Mircea Dinca** who described “Conductive MOFs: Challenging Structures with Unusual Electronic Properties” which find applications as high-performance capacitors to be used, for example, in electric sports cars. Under the title “New 'flavors' of photon-counting detectors: serial versus integrating and direct versus indirect”, **Roger Durst** (Bruker AXS) gave a fascinating overview of the current state-of-the-art of detector technologies across platforms and manufacturers, pointing out advantages and disadvantages of the various detector types. The final talk was presented by **Len Barbour** from Stellenbosch University. In his presentation with the title “Structural flexibility in the solid state – implications for porosity”, he introduced several systems with pores that change shape and properties depending on, for example, pressure or humidity. The crystallographic work in

this context is made possible by the gas pressure cell described by Leigh Loots as well as some other nifty devices developed and built by Len Barbour.

Coupled to the symposium was a workshop about structure refinement using the X-Seed interface. X-Seed is a Windows program for X-ray crystallographers written by Len Barbour. It serves as a front-end to the SHELX 2013-2018 program suite and facilitates exploration, analysis and manipulation of crystal structures, especially of extended structures such as MOFs. In addition, X-Seed produces high-quality molecular graphics images from crystal structure data. The workshop was taught by **Len Barbour** and **Leigh Loots** and was attended by over 30 participants who learned the ropes of X-Seed based on provided datasets while being guided by Len, Leigh and excellent handouts.

Next year's Bruker/MIT Symposium will take place on February 19<sup>th</sup> and 20<sup>th</sup> 2021 and the motto will be **Phosphorous Chemistry**. The program is already coming together and there will be exciting presentations by, among others, **Christopher Cummins** (MIT) and **Christian Müller** (FU Berlin) as well as a hands-on structure refinement workshop.



*Bruker/MIT Symposium 2020 presenters, from left to right: Leigh Loots, Roger Durst, Len Barbour, Travis Holman, Matthew Crawley, Peter Müller, Michael Ruf.*