FIRST Newsletter
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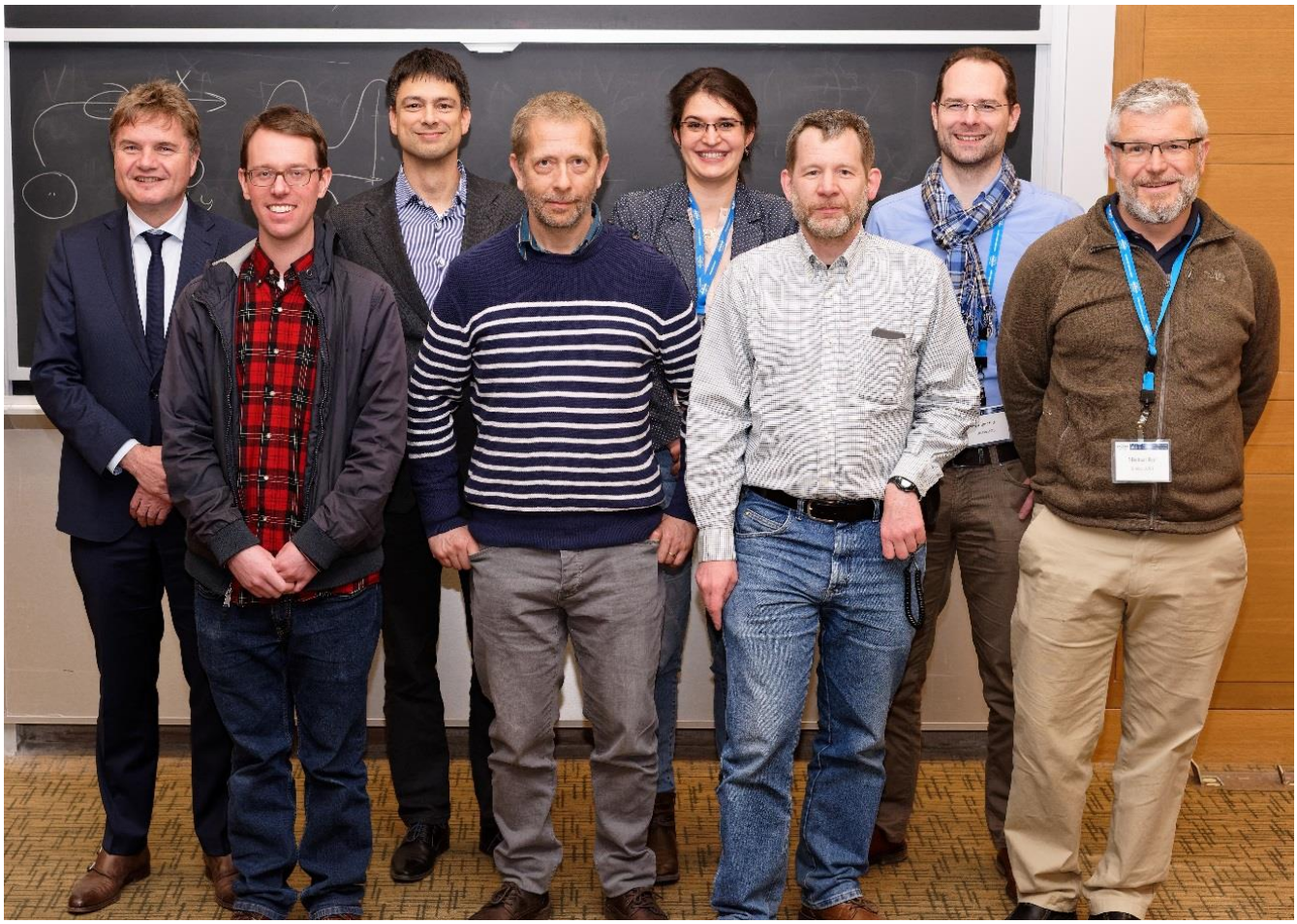
Bruker/MIT Symposium 2019

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 22nd to Sunday, February 24th at the Massachusetts Institute of Technology in Cambridge, MA, was under the motto "**Quantum Crystallography**". With almost 100 registered participants from eight countries (Germany, Switzerland, Spain, Tunisia, France, Oman, Canada and the USA) and 14 US states, this year's Symposium had the flair of an international conference, and the feedback from many participants was enthusiastically positive. As every year, the meeting was hosted by the MIT Department of Chemistry, organized by Peter Müller, Director of the department's X-Ray Diffraction Facility, and sponsored by Bruker AXS.

The last time a Bruker/MIT Symposium dealt with quantum crystallography was 2007 and time has not stood still. In 2007, the Symposium was coupled with a workshop based on the program XD. Since then, another program has emerged: Christian Jelsch's MoPro is well on its way to becoming the software standard for experimental charge density. Another change that has occurred since 2007 is the name of the field itself. What was known as "experimental charge density" is now called "quantum crystallography". What has not changed, however, are the challenges with respect to data quality, and this year's Symposium assembled some of the world's most renowned experts in the field of instrumentation, data collection and charge-density structure refinement: Michael Ruf and Holger Ott (both Bruker AXS), Dietmar Stalke (Göttingen University), Birger Dittrich (Novartis), Alexander Radosevic (MIT), and Christian Jelsch (Université de Lorraine) gave insightful presentations about the current state of the art in quantum crystallography.

The first talk of the Symposium by **Michael Ruf** (Bruker AXS) introduced what is "New and Exciting at Bruker", focusing mostly on hardware, namely the latest generation of CPAD detectors and the new diamond class of *IμS* Microfocus sources. Like few people, **Dietmar Stalke** (Göttingen University), who is a highly accomplished chemist, well-known crystallographer, and engaging teacher, can relate to broad audiences how experimental charge density can make the world a better place. Under the title "Basic Chemical Concepts Challenged by Experimental Charge Density", he illustrated how lone pair regions are as important to study as the bonding region (demonstrated especially in low-valent silicon and phosphorus chemistry), how hypervalency can be ruled out for the sulfate dianion, and that lithium amide bonds are on par with lithium amine bonds. **Birger Dittrich** (Novartis) is a pioneer in method development for advanced crystallographic applications and his invarioms are the basis for the IDEAL approach in Bruker's APEX3 refinement plugin. At this year's Symposium, he talked about his program BAERLAUCH that, through repeated optimizations of the high layer and re-generation of the cluster environment using space group symmetry, leads to a better understanding of co-crystal formation and disorder.



Bruker/MIT Symposium 2019 presenters, from left to right: Dietmar Stalke, Alexander Radosevich, Birger Dittrich, Christian Jelsch, Sabine Becker, Peter Müller, Holger Ott, and Michael Ruf.

The lunch break was combined with a poster exhibition to which seven participants had brought posters reflecting their most recent research. An independent jury awarded the best poster with a $500 prize. The poster jury was headed by Mike Takase (Caltech) and selected the poster "A crystallographer's nightmare or a fascinating case of disorder?" by **Sabine Becker** (TU Kaiserslautern) for the **2019 Bruker/MIT Poster Prize**.

The first talk after the lunch break was given by MIT's own **Alexander Radosevich** who introduced his tri-coordinate phosphorus compounds, which have remarkable structural and electronic features. A collaboration between the labs of Dietmar Stalke and Alexander Radosevich to analyze those compounds with quantum crystallographic methods is underway. Under the title "Accurate Experimental Charge Density Data: Tips & Tricks for Data Collection & Processing", **Holger Ott** (Bruker AXS) gave recommendations for successful charge density research, including suggestions to optimize the instrument performance and his approach to "Good Crystallography Practice". The final talk was presented by **Christian Jelsch** (Université de Lorraine). Christian is one of the world's leading charge-density experts and author of the charge density refinement program MoPro. In his presentation about "Advanced Electron Density Refinement & Transferability: Application to Bio-Macromolecules and Molecular Recognition", he introduced various methods implemented in MoPro, including multipole modeling and Hirshfeld surfaces.

Coupled with the symposium was a two-day workshop about refinement of experimental charge density with the program MoPro taught by **Christian Jelsch** and **Birger Dittrich**. The workshop was attended by over 30 participants who were able apply charge density methods to several structures based on provided datasets while being guided by Christian, Birger and an excellent handout.

Next year's Bruker/MIT Symposium will take place on February 21st and 22nd 2020 and the motto will be **Porous Materials**. The program is already coming together and there will be exciting presentations and a hands-on workshop based on the program X-Seed.

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