Getting the Best Structure from your Diffraction Data

Crystal Structure Refinement Workshop

Chemistry

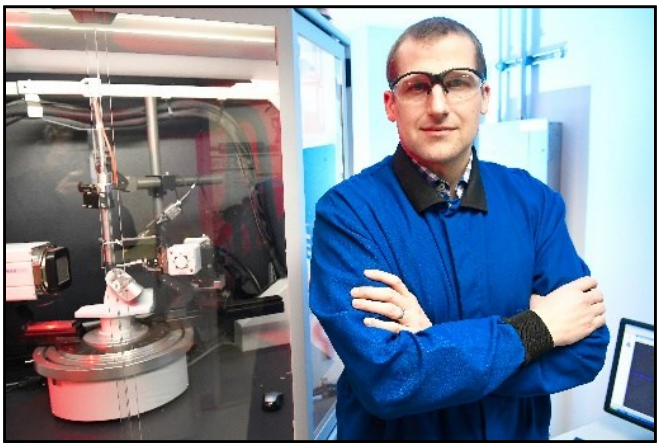
After a successful single-crystal x-ray diffraction workshop in 2019, we are excited to announce that we will host this workshop again at Clarkson University in 2021. Please read here about our success story from 2019.

When? August 16th to 20th 2021 with on-site registration in the late afternoon of August 15th.

Where? Department of Chemistry & Biomolecular Science, Clarkson University, Potsdam, NY. Clarkson is located in upstate NY at the foothills of the beautiful Adirondack Mountains.

Travel suggestions. We are easy to reach by car from the greater areas of New York, Vermont, Quebec and Ontario (e.g., 2 h SW of Montreal, QC; 2 h SE of Ottawa, ON; 2.5 h NE of Syracuse, NY; 3 h W of Burlington, VT). Nearest airports in the order of distance from Clarkson: Ogdensburg, NY (OGS), Massena, NY (MSS), Ottawa, ON (YOW), Montreal, QC (YUL), and Syracuse, NY (SYR).

About the organizers. Drs. Mario Wriedt of Clarkson University and Peter Mueller of the Massachusetts Institute of Technology are the instructors. We both share a passion for crystallography with strong backgrounds in related educational and research areas. Peter has offered this workshop all over the world for many years.



The two workshop instructors: Mario (left) and Peter (right) with their favorite toys.

Who should attend? Students, post-docs and faculty who have already gained at least some practical experience with structure determinations are invited to participate. Some basic knowledge on crystal symmetry and space groups would be welcome.

Registration fee. $300 for students and postdocs. Faculty are charged $600. This covers lodging and all instructional materials. Computers and snacks/drinks will be provided. Lodging is in newly renovated and air-conditioned dorms in single occupancy to meet social distancing requirements. Meals are on a self-pay basis in student cafeteria or close-by restaurants.

Travel awards. We will have limited funds available to help students and postdocs to attend our workshop. Thanks to the support of our generous sponsors, we were able to issue five travel awards in 2019. Fundraising is not completed yet, but we anticipate being in a similar range for 2021. Please send a cover letter, your CV, and a letter of support from your research advisor along with your registration if you want to be considered. Awards will be distributed at the workshop.

Details and background about the content. Single-crystal X-ray diffraction is one of the most widely used methods of structure elucidation. The relatively small experimental effort for a routine X-ray structure determination as well as the revolution in data processing has led to an enormous spread of this method in recent years, which means that even inexperienced users can perform their own structure determinations. Unfortunately, however, sometimes problems arise that impede data collection or structure refinement, and may lead to unusual or simply incorrect structural models. Even if a structure seems to be successfully determined, errors might have occurred which are difficult to detect. All of these problems will be addressed at this workshop. The workshop is divided into five topics: (day 1) sample preparation, data collection strategies, structure solution and refinement; (day 2) refinement of disorder; (day 3) twinning and pseudo symmetry; (day 4) non-merohedral twinning and working with CIF files, structure validation etc.; (day 5) individual problem structures. Each topic will be introduced with a lecture followed by hands-on problem sets using common crystallographic software as described in the workshop manual. Finally, the solutions for all problems will be discussed with the whole group.

How to register? Please email Mario Wriedt (mwriedt@clarkson.edu) and include your name, affiliation, address, email, and a brief justification on why you are a good fit to attend the workshop. If accepted, you will be provided a link with instructions to process the payment of the registration fee. Registration closes on May 31, 2021. The workshop is limited to 30 participants.

COVID-19 addendum. Clarkson's COVID-19 taskforce team approved the plan for this workshop. Considering the current national decrease in positive cases coupled with the increased availability of vaccines for broader communities, we are optimistic that we will be able to offer this workshop in person. In any case, we must meet NY state guidelines, and we are well prepared to implement all associated social distancing requirements for our lecture room and computer lab. We may request a negative test prior to your arrival. However, state and local guidelines may be less strict in August and we will adapt accordingly. In the (hopefully unlikely) case that we will not be allowed to host this workshop in person, we would refund you the full registration fee. We would make this decision not later than July 1st. An alternative online workshop is not planned, we would re-advertise for summer 2022.