



Getting the Best Structure from your Diffraction Data

Crystal Structure Refinement Workshop



Chemistry

After two successful single-crystal x-ray diffraction workshops in 2019 and 2021, we are excited to announce that we will host this workshop again, this time at the University of Texas at Dallas in 2024.

When? August 5th to 9th, 2024 (5-day workshop with daily instruction from 8:30 am – 5:30 pm). August 4th and 9th (afternoon) are suggested travel days.

Where? Department of Chemistry and Biochemistry, University of Texas at Dallas, Richardson, TX. UT Dallas is centrally located in the north-east of the Dallas-Fort-Worth Metropolitan area.

Travel suggestions. We are easy to reach by car from the greater areas of Texas (e.g., 4 h NW of Houston; 3.5 h NE of Austin). The nearest airport is the Dallas Fort Worth International Airport (DFW), only about 30 minutes driving (Taxi/Huber) to campus.

About the organizers. Drs. [Mario Wriedt](#) of UT Dallas 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: Peter (left) and Mario (right).

Who should attend? Students, post-docs, faculty and industrial partners 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. \$350 for students and postdocs; faculty and staff \$600; and industrial \$900. Instructional materials, computers and snacks/drinks will be provided. Meals are on a self-pay basis from the Student Union Food Court or close-by restaurants.

Housing. We have negotiated a room deal with the DoubleTree by Hilton Hotel in Richardson for \$99.00 per night (plus fees and taxes, no breakfast included) or \$119.00 per night (plus fees and taxes, hot breakfast buffet included). Parking, WiFi, and a shuttle to UT Dallas campus (and back) are complementary. We have a total of 20 rooms with two Queen beds and 20 rooms with one King bed available. To book from this room block, please use the following links: [UTD Workshop with Breakfast](#) and [UTD Workshop No Breakfast](#). The cutoff date is July 13th, 2024, to book at this negotiated rate.

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 multiple travel awards in 2019 and 2021. Fundraising is not completed yet, but we anticipate being in a similar position for 2024. 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 (mario.wriedt@utdallas.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, 2024. The workshop is limited to 40 participants.

Impressions from previous workshops.



2021



2019