

Summer School 2019

X-ray Crystallography

Summer School 2018 on X-ray Crystallography of the Core Facility BioSupraMol at Freie Universität Berlin, May 23-24 and 27-29, 2019.

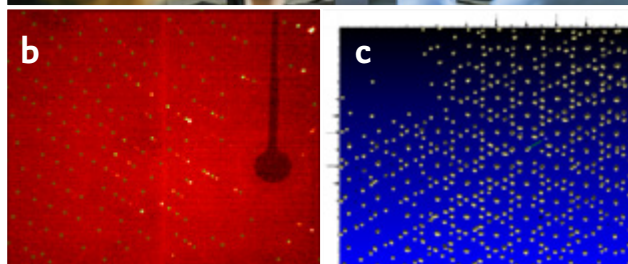
In X-ray crystallography, a beam of X-rays interacts with the crystalline solid, producing a diffraction pattern of regular reflections according to Bragg's law. By measuring the angles and intensities of the spots, the positions of the atoms in the crystal can be determined, from which the molecular structure of the compound in the crystal is derived.

As X-ray diffraction is a technique for determining the electron distribution in solids, the density-based quantum theory of atoms in molecules provides the possibility to interpret crystallographic data in terms of charge densities. Modern crystallography thus allows the correlation between structural features and physical properties of a compound.

The Core Facility BioSupraMol of the Freie Universität Berlin focuses in its crystallography unit on state of the art X-ray crystallography and makes these techniques available to scientists and students.

In this five-day summer school, Dr. Peter Müller from the Massachusetts Institute of Technology (MIT, Cambridge, USA) will present an overview of cutting edge research and recent technical developments in the field of X-ray crystallography. Workshops will give valuable insights and practical training in cutting edge techniques, data analysis and software usage.

Prof. Dr. Christian Müller



a) structure model; b) diffraction pattern of a twin with 3 domains (reflexes of main domain are highlighted by green circles); c) depiction of the twins lattices in reciprocal space (pictures: a: Michael Fahrig; b/c: Steinhauer, FU Berlin)



Dr. Peter Müller

Principal Research Scientist

Massachusetts Institute of Technology (MIT),
Cambridge MA (USA),
Department of Chemistry,
X-Ray Diffraction Facility

<http://web.mit.edu/x-ray/pmueller/pmueller.html>

MIT since 2004 | UCLA 2001 - 2004
Göttingen 1994 - 2001 | Kaiserslautern 1991 - 1993

Program

Thursday, May 23, 2019 | day 1

morning: lecture "Datensammlungsstrategie und Phasenproblem" (Patterson- und direkte Methoden)

afternoon: lecture "Einführung in die SHELX Programme, Übung am Diffraktometer" (sample mounting etc.), software installation if necessary
workshop with one simple structure for beginners to teach how which program is used to do what.

Friday, May 24, 2019 | day 2

morning: lecture "atom type assignment and disorder"

afternoon: workshop "Refinement of Disorder"

Monday, May 27, 2019 | day 3

morning: lecture "non-crystallographic symmetry, twinning and whole-molecule disorder"

afternoon: workshops (a) "twinning by merohedry and pseudo-merohedry", (b) "non-crystallographic symmetry"

Tuesday, May 28, 2019 | day 4

morning: workshop "non-merohedral twinning"

afternoon: workshop "whole-molecule disorder"

Wednesday, May 29, 2019 | day 5

all-day: individuell problem solving, structures of participants



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