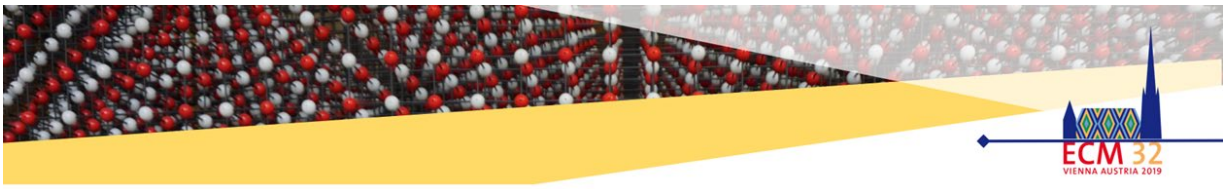

ECM 32
VIENNA AUSTRIA 2019
SATELLITES INFORMATION
13th – 18th August 2019
32nd European Crystallographic Meeting
18th -23rd August 2019
TECHNISCHE UNIVERSITÄT WIEN
universität wien
https://ecm2019.org



Content

Venue Satellite Meetings 32nd ECM

August, 13th – 18th , 2019

Lecture Halls
Electrical Engineering department
Vienna University of Technology
Gußhausstrasse 25-29
A-1040 Vienna
Austria

Welcome Message

Dear participants of the ECM32 satellite meetings, dear Crystallographers and Friends!

On behalf of the entire team of the local organizers it is our pleasure to welcome all participants of the satellite meetings of the 32nd European Crystallographic Meeting (ECM32) in Vienna.

The individual organizers of the satellite meetings set up an attractive programme covering various fields in crystallography and cognate disciplines that attracted about 350 people. The ECM32 with a vibrant five-day scientific programme and numerous social events is subsequent of this satellite's events starting on August 18th. About 1100 attendees will be meeting there to exchange their newest results.

It is important to us to express our gratitude to all sponsors, exhibitors, institutions and foundations for their generous support, to all our volunteers and numerous helping hands for their time and effort, as well as to the organizers of previous ECM's for sharing their valuable experiences. Last but not least, we would like to thank you in particular for coming to Vienna and helping us with your participation to make these satellite meetings a success.

We wish you scientifically fruitful meetings, but also make sure to enjoy the amenities of the city of Vienna and the famous Austrian hospitality during these days.



Klaudia Hradil, Kristina Djinovic-Carugo, Ronald Miletich
Chairs of the ECM32, on behalf of the Local Organization Committee

Gerry Schneider
Congress Management Office of the University of Vienna

Route to the Venue

Address of the Venue

The satellite meetings will take place from August 13th to 18th 2019 at the TU Wien within the buildings of the Electrical Engineering Department:

TU Wien
Department of Electrical Engineering
Gußhausstrasse 25-29
1040 Vienna
GPS coordinates: (48.1983295, 16.3696166,17)

Please find the routes to the venue on pp. 7 - 8.

Travel to Vienna

http://www.tuwien.ac.at/en/contactsearch/visit_us_travelling_information

Main Locations of TU Wien (location maps)

Plane

The Vienna International Airport (VIE) in Schwechat is about 20 km away in the south-eastern direction of Vienna.

On the airport's web site you can find flight information as well as different transfers into the city center:

Train S7 to Landstraße/Wien Mitte

Bus Service Vienna Airport Lines (VIA):

VIA to Wien Schwedenplatz: Travel time 20 minutes
VIA to UNO-City: Travel time 20 minutes
VIA to Wien Südtiroler Platz: Travel time 20 minutes
VIA to Wien Südbahnhof: Travel time 25 minutes
VIA to Wien Westbahnhof: Travel time 35 minutes

City Airport Train (CAT)

A **Taxi** stand is right in front of the Arrival Hall.

Train/bus

If you prefer travelling by train you will find all necessary information at http://www.oebb.at (Austrian Federal Railways) or *via* phone +43 05-1717.

Public transport in Vienna

The building of the electrical engineering department of TU Wien is located in the city centre of Vienna and reachable via the underground lines **U1, U2, U4 (station = Karlsplatz)** and the **tramway 1, 62 or Badeber Bahn (station = Paulanergasse)**. Please not that the U4 is currently under construction, but there is a replacement bus UZ4 between Längenfeldgasse and Karlsplatz. At every station signs as well as personel is positioned to help guiding you to the bus.

Tickets are available at the airport, at the subway stations and in tobacco shops ("Trafik").

city map: www.wienerlinien.at

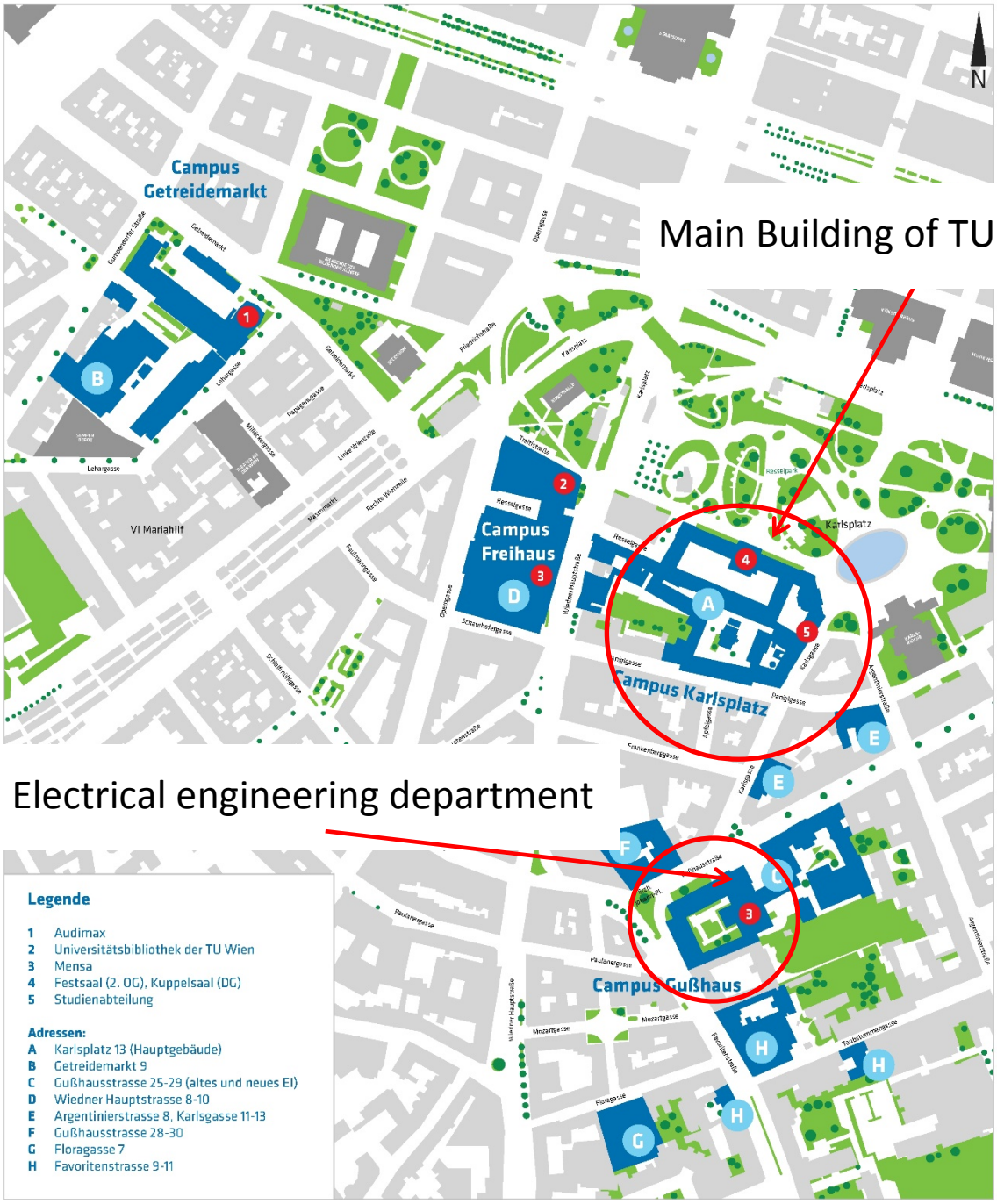
Parking in Vienna

Parking a car is very restricted in Vienna, in particular in the area of the city centre. You have to use pre-paid tickets called "Parkschein" (see picture), which exist in five colours:

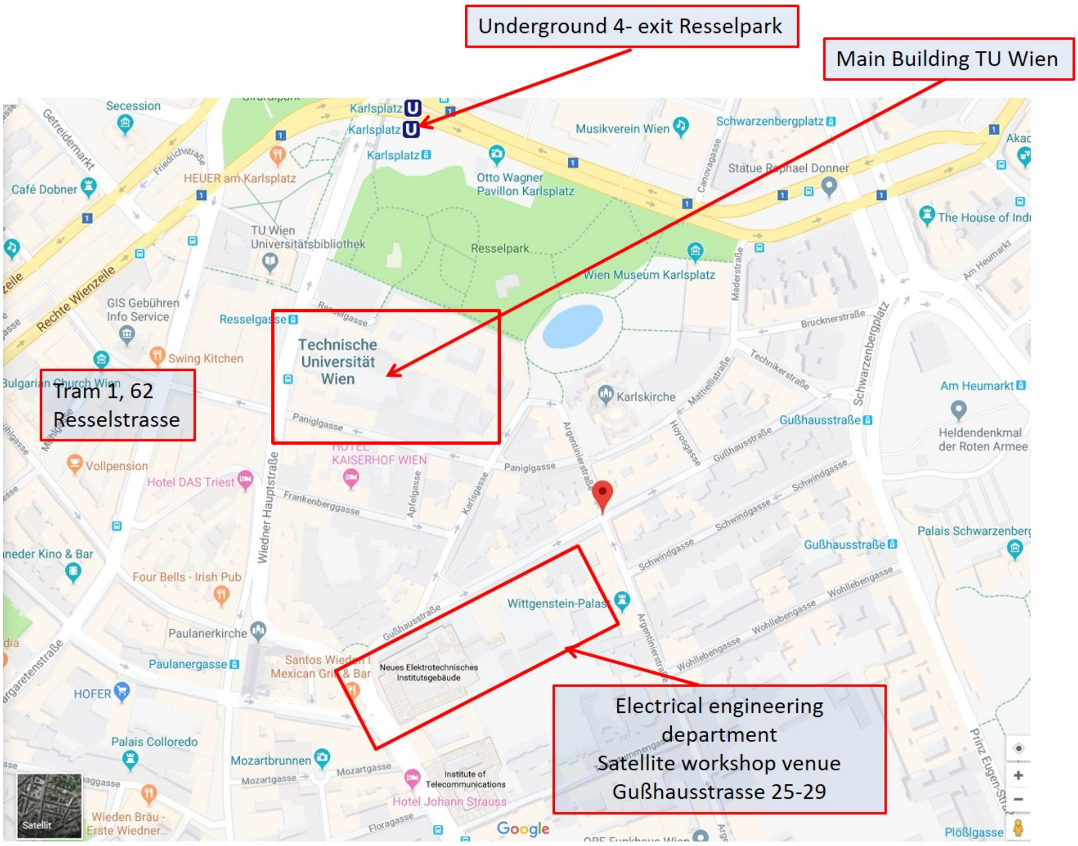
- purple = 15 min., free (only once allowed)
- red = ½ hour, 1.05 €
- blue = 1 h, 2.10 €
- green = 1½ h, 3.15 €
- yellow = 2 h, 4.20 €

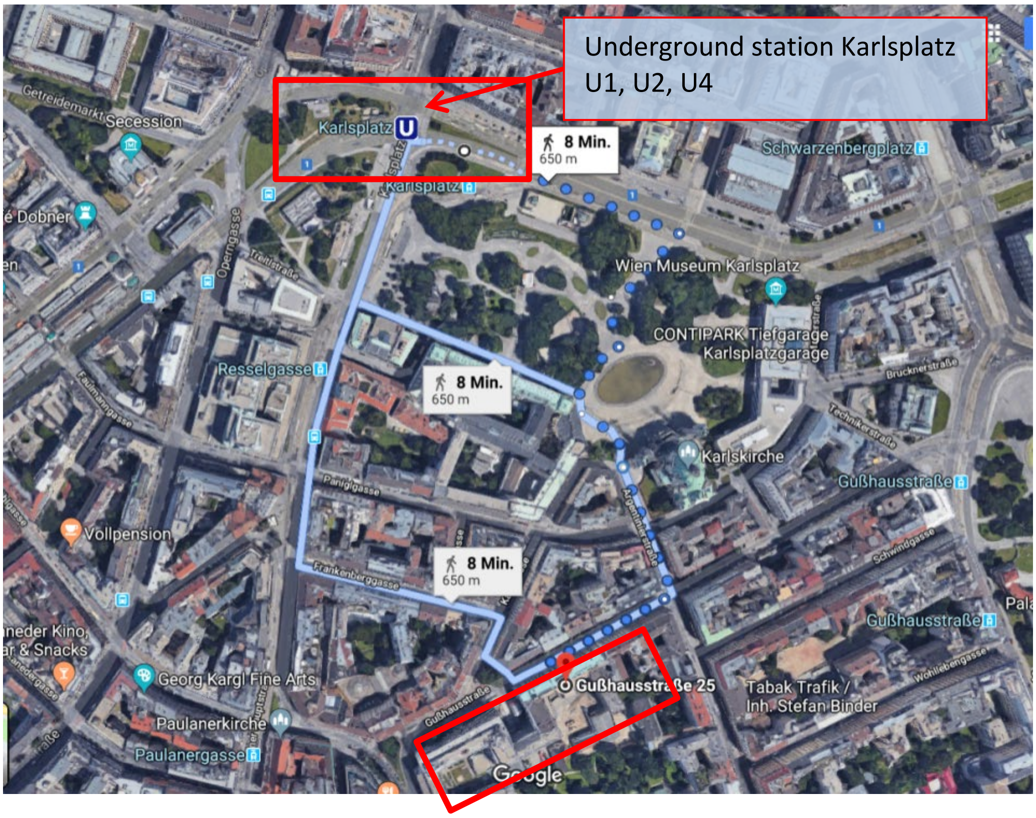
These tickets can be purchased at any tabacco shop ("Trafik"). Parking with these tickets is limited to a maximum of 2 hours. These parking tickets are only available in German.
If you want to park for longer you have to use one of the car parks. The next one is the "WIPARK Operngasse-Garage" in the Operngasse (24 hours open, 4.30 € per hour!). The most **inexpensive** way to park in Vienna would be to use the park & ride stations for 3.60 € per day (you are recommended to be there at 6:00 a.m. to find a parking space). For further details on parking in Vienna follow the link:
https://www.wien.gv.at/english/transportation/parking/

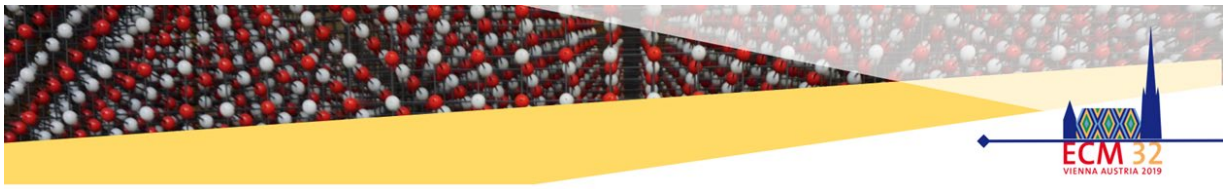
TECHNISCHE UNIVERSITÄT WIEN
Vienna University of Technology



April 2018 | TU GUT, Resselgasse 3, 1040 | www.tuwien.ac.at


Underground 4- exit Resselpark
Main Building TU Wien
Tram 1, 62
Resselstrasse
Technische Universität Wien
Electrical engineering department
Satellite workshop venue
Gußhausstrasse 25-29


Underground station Karlsplatz
U1, U2, U4
8 Min.
650 m
Gußhausstraße 25



General information

Registration/Opening hours

The registration can be found on the ground floor of the building. A floor map is shown on page 14.

Opening hours:	Time
Tuesday, August 13th	8 – 10 a.m. and 3 – 6 p.m.
Wednesday, August 14th	8 – 12 a.m. and 2 – 4 p.m.
Thursday, August 15th	8 – 12 a.m. and 2 – 4 p.m.
Friday, August 16th	8 – 12 a.m. and 2 – 4 p.m.
Saturday, August 17th	8 – 12 a.m. and 2 – 4 p.m.
Sunday, August 18th	8 – 12 a.m. and 2 – 4 p.m.

Contacts

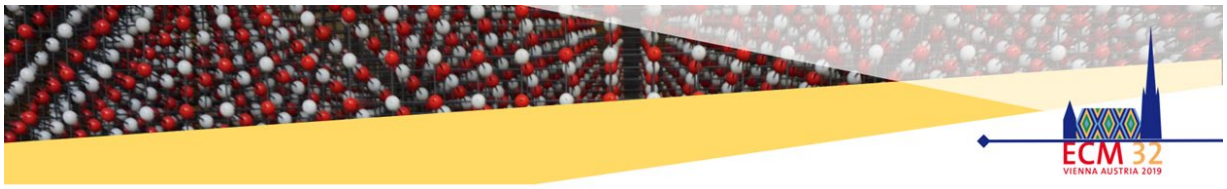
Organisation/Rooms/Registration:

- Klaudia Hradil, Email: klaudia.hradil@tuwien.ac.at; phone: +43 664 88537039
- Herta Effenberger, Email: herta.silvia.effenberger@univie.ac.at; phone: +43 664 49705637

Technique:

- Erik Lübke, Email: erik.luebke@tuwien.ac.at ;phone: +43 660 2502508
- Werner Artner, Email: werner.artner@tuwien.ac.at ; +43 664 60588-7117

Erik Lübke and Werner Artner will guide you the first day of your workshop and show you how to use the presentation technique and microphone functions within the room.



Rooms for the individual workshops

The workshops are taking place in the same building as the registration. They are distributed on the ground, first, third and sixth floor of the building part CA, CB and CD of the electrical engineering department, respectively. The lecture halls and seminar rooms are shown on the floor maps presented on pp 14 and 15. Direction signs to the individual workshops showing the title, logo and organizers' names are also placed within the building to guide you to the individual workshop venue. Additionally, the right screen of the building information system is showing the current running workshops.

You can find a lift directly behind the Porter's room on the left side to reach the other floors. The main stair case #1 is also located there.

Keys for the lecture halls/seminar rooms (only for organizers)

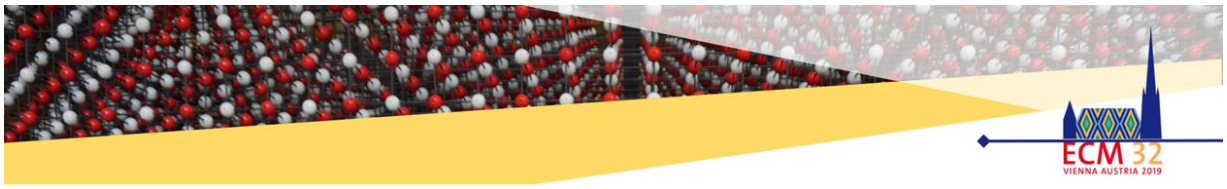
The names of all organizers are deposited with the porter. Please sign in the logbook for the keys. The porter will hand over the keys and you can keep them during the day. Please do not forget to bring them back at the end of the day. Be aware that you are responsible for the borrowed keys during holding it. Make sure to lock the room if you leave it for coffee and/or lunch breaks. The building is open for the public during the entireweek (including Sunday until 6 p.m.).

Poster

Except for the posters for the High Pressure Crystallography workshop (displayed in front of the lecture hall 10), all posters of the individual workshops can be presented throughout the whole week on the ground floor in lunch area. Mounting equipment will be provided at the registration. Please inform them on arriving that you will need mounting material for your poster.

Coffee breaks and lunch

Coffee/tea, soft drinks and small cakes are served on the rooftop terrace located on the 6th floor (see map page 15). Lunch is served in the ground floor caferteria (see map page 14). You can choose between two hot meals (meat/fish or vegan). **Attendees will find vouchers for the catering within their bags for workshops which booked coffee and/or lunch during their breaks.** Lunch is served between 12 a.m. – 2 p.m. on the ground floor (foyer), coffee/tea and soft drinks on the rooftop terrace in the 6th floor. Please follow the direction



signs. All other participants may have drinks and food on their own payment. The mensa of the TU Wien is located within 10 minutes walking distance in the first floor of the Physics Department (Wiedener Hauptstraße 8 – 10). Also there are some restaurants nearby serving lunch menues.

Electricity

The electric current in Austria is 230 V AC (at 50 Hz). You can use your equipment, if the outlet voltage in your country ranges between 220 and 240 V, otherwise you have to use an adapter. You have to use 2-pin type C or type F plugs for Austrian sockets.

Insurance

The ECM 32 satellite organization cannot accept liability for personal injuries, or for loss or damage of personal belongings either during or as a result of the meeting. Please check the validity of your personal insurance.

Smoking

Smoking is not allowed in the entire area of the TU Wien, with the exception of the garden. There is easy access to the garden from the foyer. Thank you for your understanding.

Wi-Fi

Wi-Fi access is available via eduroam throughout the entire venue. You will find a personal access account to the WLAN network of the TU Wien within your bag.

Social Event: Heurigen Evening@10er Marie

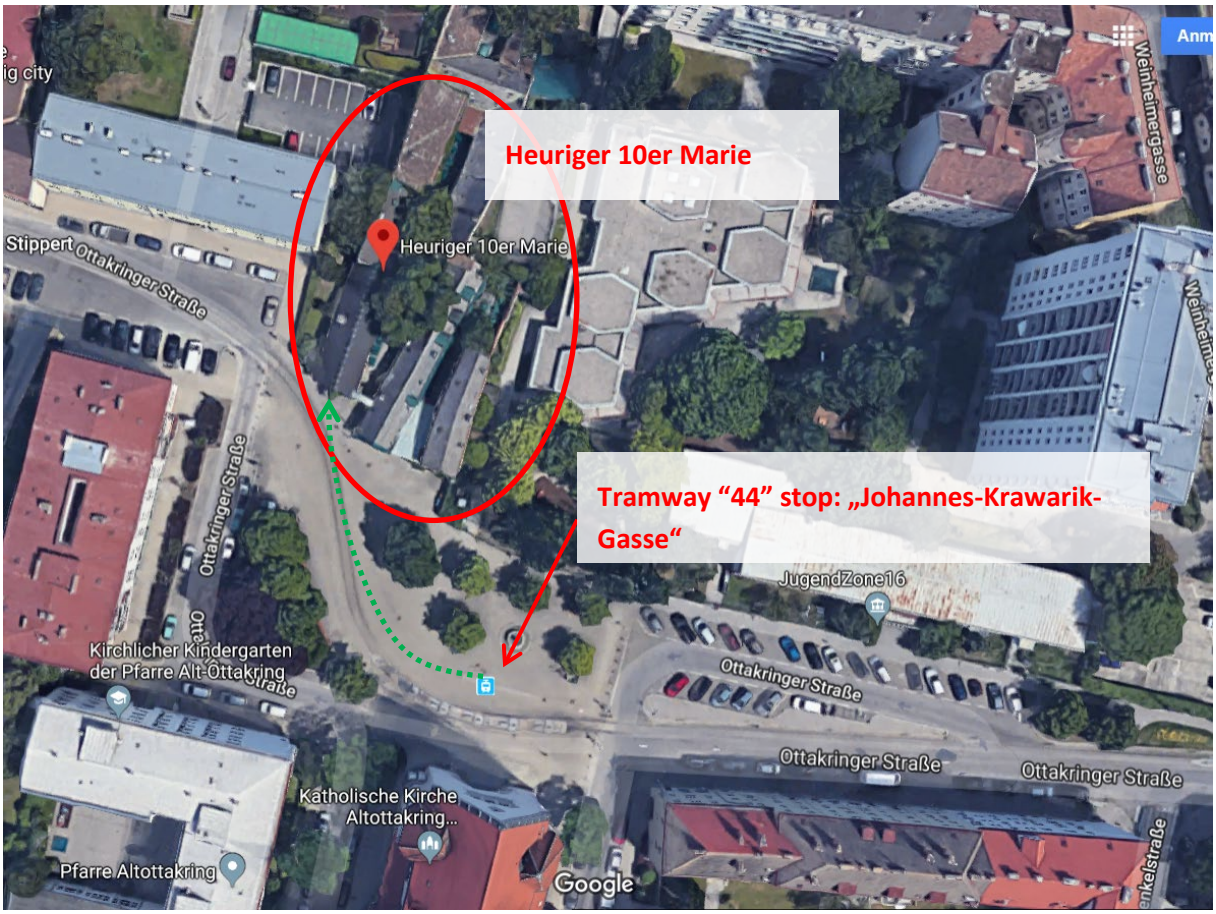
We arranged an evening event for Friday, **August 16th 2019** at a typical Viennese "Heuriger" named *"10-er Marie"* within reach of public transport. The place, first mentioned anno 1740, is the oldest traditional "Heuriger" in the city of Vienna serving local vine and typical Viennese food.

There are still some places left and you can register via our webpage together with the social events of the ECM32:

https://ecm2019.org/programme/social-events/online-registration-social-events/

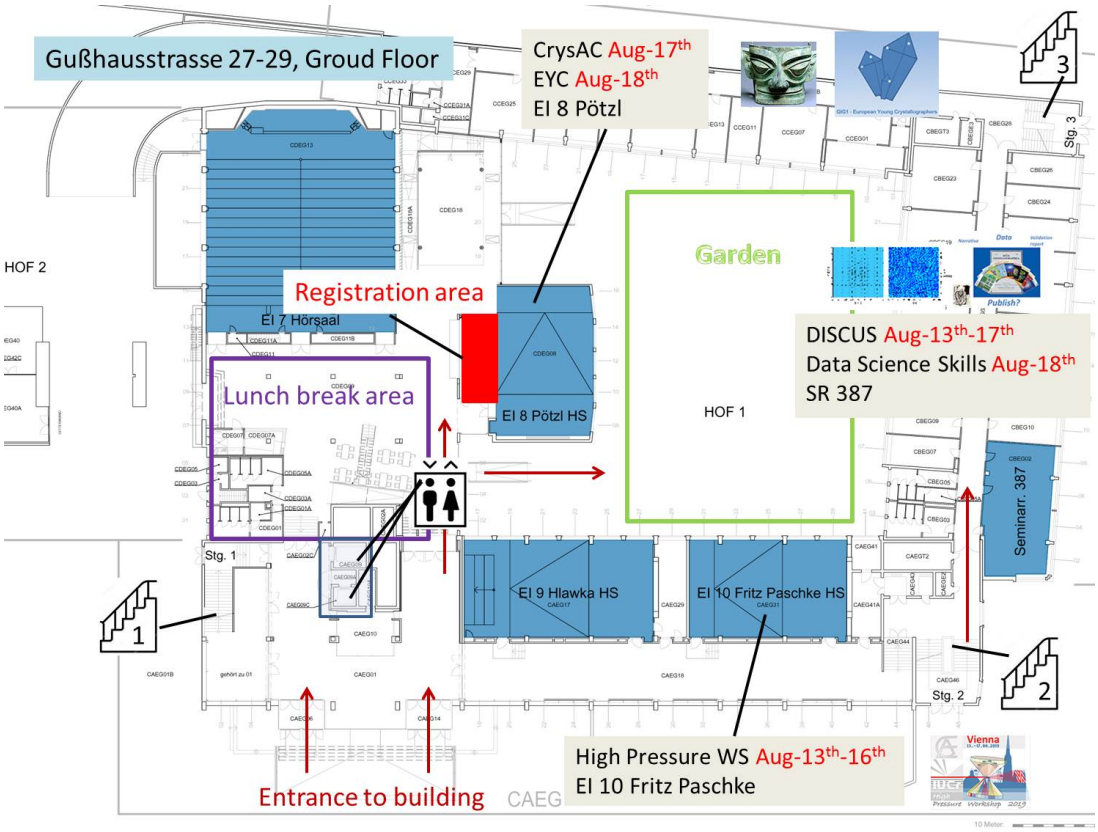
How to reach “10er Marie” by public transport

“10er Marie“, Ottakringer Str. 222-224, 1160 Wien, heuriger@10ermarie.at

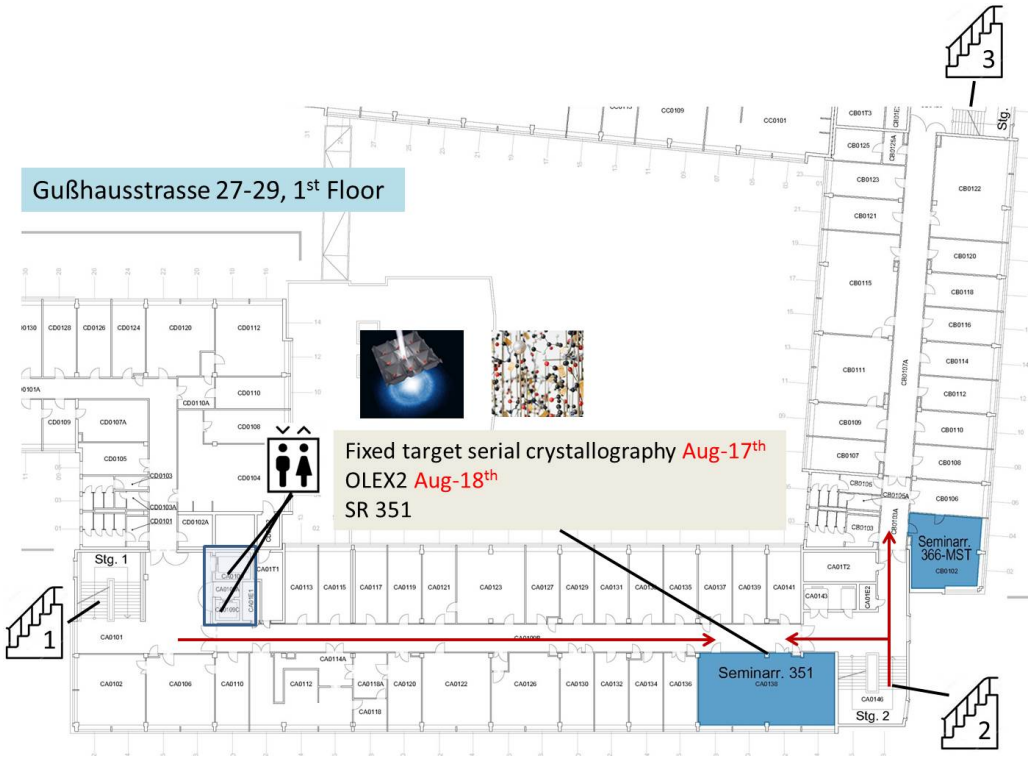


- Walk to the station Karlsplatz/Opera (see page 8)
- Change to "U2" (direction: Seestadt) or tramway lines "1", "D", or "71" (station next to the opera)
- Get out at "Schottentor/Universität" next to the University of Vienna
- Change to tramway "44" (direction Maroltingergasse)
- Exit the tramway at station "Johannes-Krawarik-Gasse" opposite of the “Altotta-kringer Pfarrkirche (17-18 minutes)
- Walk 1 minute to the Zehnermarie.

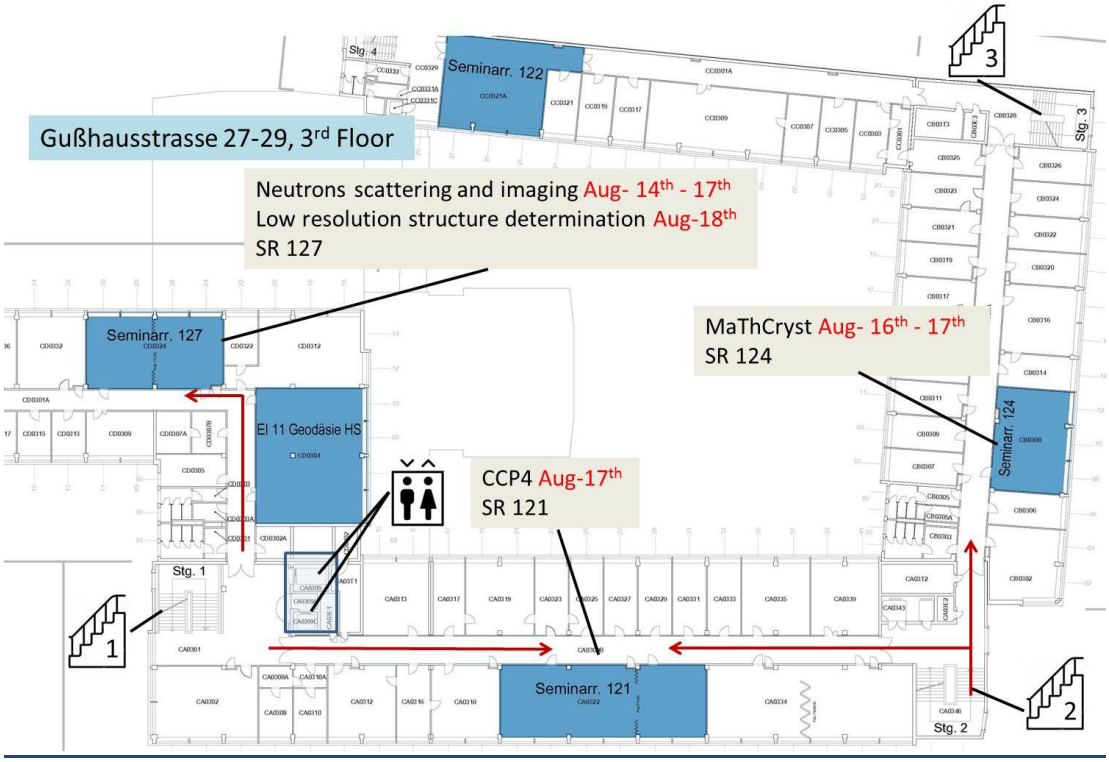
Building Map: Ground Floor



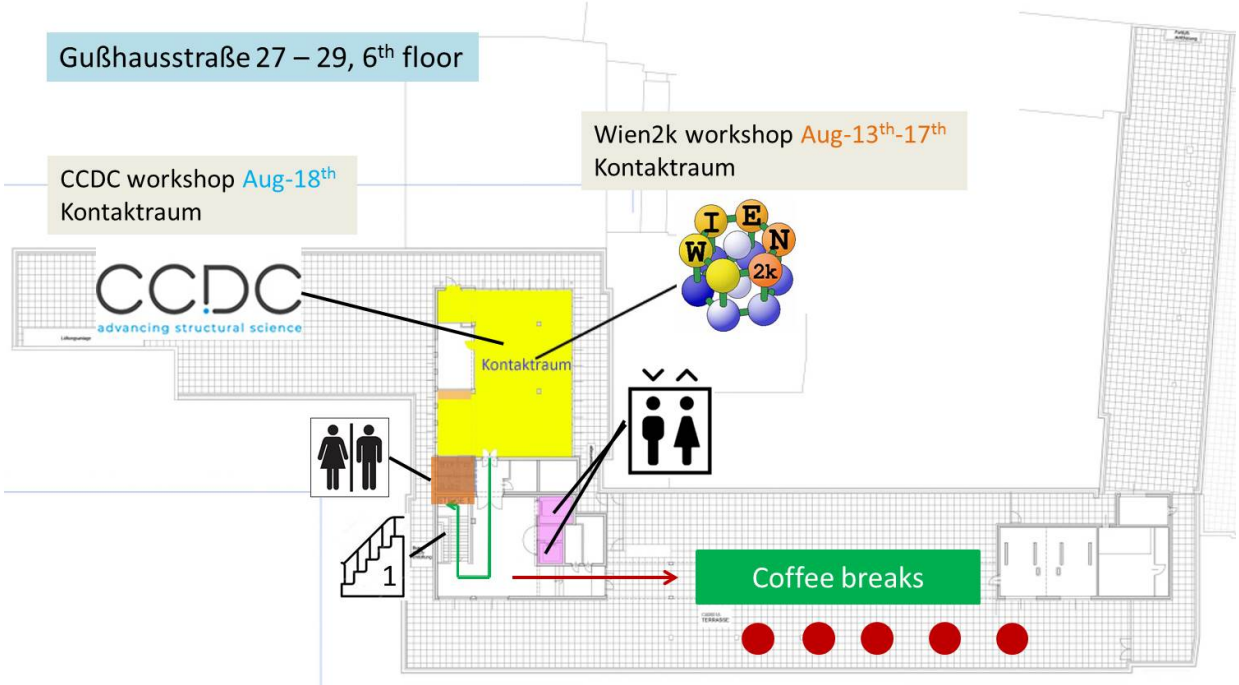
Building Map: First Floor

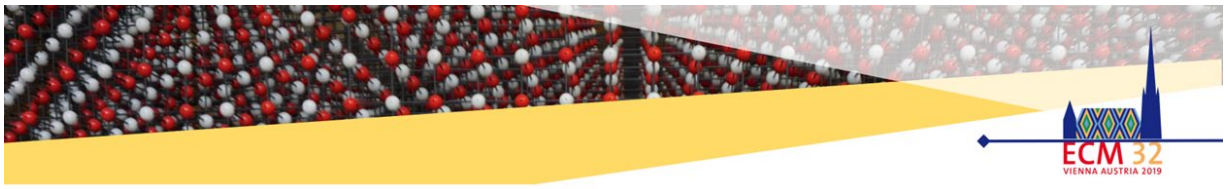


Building Map: Third Floor



Building Map: Sixth Floor





Workshop's Programme

List of satellite workshops

- 26th WIEN2k workshop: DFT based simulations of solids with the WIEN2k code
  Peter Blaha, Karlheinz Schwarz (TU Wien, AT)

- Data Science Skills in Publishing: for authors, editors and referees
  John Helliwell (University of Manchester, UK), Brian McMahon (IUCr, R&D Department, UK)

- CCP4 Structure Solution Workshop
  Eugene Krissinel, Charles Ballard (Collaborative Computational Project No. 4, CCP4, UK)

- MaThCryst satellite meeting: Graph theory and modular structures
  Massimo Nespolo (University Lorraine, F), Bernd Souvignier (Radboud University, NL), Berthold Stöger (TU Wien, AT)

- Neutron Scattering and Imaging for Newcomers
  Jürg Schefer (Paul Scherrer Institute, CH), Martin Meven (RWTH Aachen University and JCNS, FZ Jülich at Heinz Maier-Leibnitz Zentrum (MLZ), D; Arbeitskreissprecher DGK/AK7)

- 5th CrysAC workshop on "Crystallography of ancient metals and metal corrosion"
  IUCr - CrysAC Commission on Crystallography in Art and Cultural Heritage
  Gilberto Artioli (University Padua, I), Manfred Schreiner (Academy of fine Arts, Vienna, AT), Alicja Rafalska-Lasocha (Jagiellonian University, PL), Klaudia Hradil (TU Wien, AT)

- 2019 IUCr & ECA High-Pressure Workshop
  Ronald Miletich (University of Vienna, AT), Haozhe Liu (IUCr HP Commission, CN), Yaroslav Filinchuk (ECA SIG-11, UCL, BE)

- Young Crystallographers Satellite Meeting
  Philipp Hans (TU Wien, Vienna, AT), Filip Topic (McGill University, Montreal, CN)

- Olex2 Workshop
  Horst Puschmann (OlexSys Ltd, Durham University, UK), Michael Bodensteiner (OlexSys UG,D)

- Total scattering analysis with DISCUS
  Reinhard B. Neder (Friedrich-Alexander Universität Erlangen-Nürnberg, D), Thomas E. Proffen (ORNL – Oak Ridge National Laboratory, USA)

- European Crystallographic Computing Forum
  Martin Lutz (University Utrecht, SIG-9, NL), Paul Adams

- Fixed target serial crystallography
  Arwen Pearson, Jennifer Wierman, Pedram Mehrabi, Eike C. Schulz (Universität Hamburg and Hamburg Center for Ultrafast Imaging CUI, D)

- Low resolution structure determination and refinement of Biological Macromolecules by crystallography and cryo-EM
  Paul Adams, Dorothee Liebschner (Lawrence Berkeley National Laboratory, Berkeley, USA)

- Crystal Engineering using the Cambridge Crystallographic Database
  Ioana Sovago (Cambridge Crystallographic Data Centre CCDC, UK)

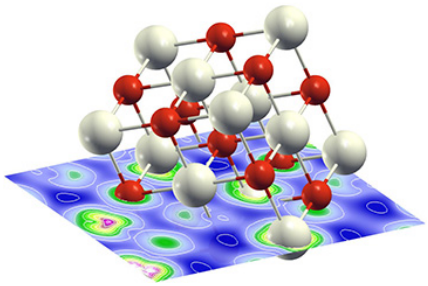
26th WIEN2k workshop: DFT based simulations of solids with the WIEN2k code

Organizers: Peter Blaha (TU Wien, Austria), Karlheinz Schwarz (TU Wien, Austria)

Date: 13th to 17th August 2019 (5 days)

Time: 9 a.m. – 4 p.m.

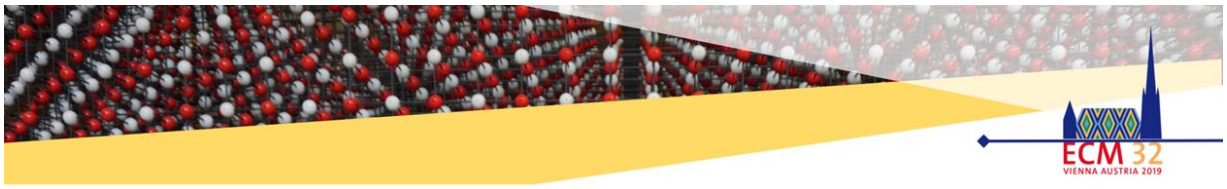
This workshop deals mainly with theoretical simulations of inorganic materials and materials science problems and the structure – property relations. Experimental scientists will learn how to complement their experiments by DFT simulations with WIEN2k; the focus will be on theoretical structure-optimization, analysis of chemical bonding and simulations of various spectroscopies (IR, Raman, UV-Vis, XPS, XAS, EELS, NMR, Mössbauer, STM and AFM).



PROGRAMME:

Day1: Tuesday, Aug 13th

- 8:30: Registration
- 8:50: Welcome address
- 9:00-10:00: *K.Schwarz:* Density functional theory (DFT) and the concepts of the augmented-plane-wave plus local orbitals (APW+lo) method
- 10:30-12:00: *P.Blaha:* An overview of the WIEN2k package for beginners
- 13:30-14:30: *P.Blaha:* Input files, Volume optimization, AIM,
- Exercises



Day2: Wednesday, Aug 14th

- 9:00-9:30: *P.Blaha*: Forces, structure optimization, supercells, surfaces, phonons
- 9:30-10:00: *K.Schwarz*: Magnetism (FM, FSM, AFM)
- 10:30-11:30: *F.Tran*: Advanced DFT: Hybrid-DFT, vdw-DFT, LDA+U, mBJ
- 11:30-12:00: *J.Tomczak*: DMFT Afternoon
- 13:30-14:30: *R.Laskowski*: Relativistic effects, non-collinear magnetism (NCM)
- Exercises

Day3: Thursday, Aug 15th

- 9:00-10:00: *O.Rubel*: Wannier fuctions + Berry phases + fold2B loch
- 10:30-12:00: *P.Blaha*, *R.Laskowski*: Optical properties, XPS, XAS, EELS, BSE
- Exercises

Day4: Friday, Aug 16th

- 9:00-10:00: *P.Blaha*: Hyperfine interactions
- 10:30-11:30: *R.Laskowski*: NMR shifts
- 11:30-12:00: Poster
- 13:30-14:30: *G.Madsen*: Boltztrap2 (Transport)
- Exercises
- 18:30: Conference Dinner

Day5: Saturday, Aug 17th

- 9:00-10:00: *M.Arrigoni*: Point defects in solids
- 10:30-11:00: *M.Arrigoni*: “Spinney”
- 11:00-12:00*: P.Blaha:* Installation of Wien2k, parallelization
- 12:00-12:30: Round table & closing
- Free Exercises

For further details visit: http://www.wien2k.at/events/ws2019

Organizers: John Helliwell (University of Manchester, UK), Brian McMahon (IUCr, R&D Department, UK)

Date: 18th August 2019 (1 day)

Time: 8:25 a.m. to 5 p.m.

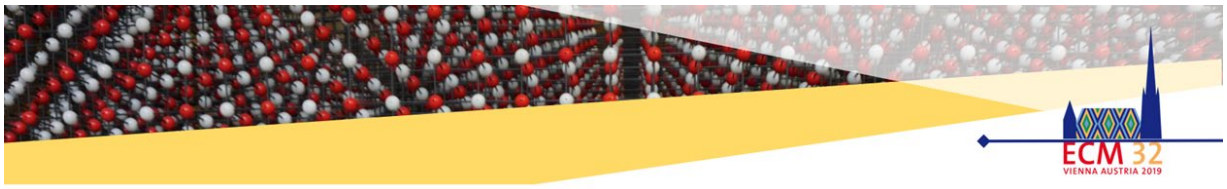
The trend of modern science research data being findable, accessible, interoperable and reusable (i.e., FAIR is something that crystallographers have done for many decades with its excellent crystallographic databases always exploiting the digital hardware archiving available. FAIR is necessary but not sufficient, as physicists would say, since the archived data should also be true facts. So FACT and FAIR are needed for reproducibility. The crystallographic community has developed automatic checking software by pooling its experiences from hundreds of thousands of crystal structure analyses into validation procedures with numerous data file checks on both coordinates and processed diffraction data sets. Alarm alerts can then be scrutinised by journal editors and referees. With such exemplary procedures is there anything to be improved? Crystallographers conclude that there is. Firstly, the IUCr journal Acta Crystallographica Section C for structural chemistry has always required submission of article with validation report with underpinning data files. Thus, the specialist subject expertise of referees can involve their own direct calculations to supplement the automatic checks before article and data set acceptance as versions of record by the editor. This has inspired others to look to improve their own crystallographic disciplines and journals to follow the Acta Crystallographica C standard. Secondly the digital archives have enhanced their capacity in recent years owing to amazing hardware advances so that even the Gigabyte sized raw data sets can also be preserved as versions of record. A reader of a publication can thereby revisit even the earliest calculation decisions of the authors of a publication. As the Royal Society of London puts it: science is about not taking someone's word and so, instead, the science is always in the data. FACT and FAIR, indeed scientific objectivity itself, is possible. This Workshop will address the state of the art in the field and the data science skills hoped for, indeed to be expected, of all those involved in publishing crystallography results, and of results from all the cognate methods such as scattering, microscopy and spectroscopy.

PROGRAMME:

Sunday Aug, 18th

Session 1 Chair: *A.Guerri*

- 08:25-08:30: *J.Helliwell*: "Introduction to the Workshop"
- 08:30-09:00: *T.Linden*: "Data refereeing and editing in chemical crystallography; the Acta Cryst C experience"



- 09:00-09:30: *B.McMahon:* "The vital role of Crystallographic Information Files in chemical and biological crystallography to underpin the databases' validation reports"
  09:30-10:00: *T.Spek*: "Platon and raw diffraction data opportunities for chemical crystallography publishing"
- 10:00-10:30: Coffee Break

Session 2 Chair: *B.McMahon*

- 10:30-11:00: *M.Aranda*: "The role of raw powder diffraction data in peer review; past, present and future"
- 11:00-11:30: *M.Weiss*: "Diffraction data deposition and publication"
- 11:30-12:00: *L.Kroon-Batenburg*: "Raw data opportunities for biological crystallography publishing"
- 12:00-13:00: Lunch

Session 3 Chair: *S.Coles*

- 13:00-13:30: *S.Ward*: "Correcting the public record of chemical crystallography science"
- 13:30-14:00: *M.Jaskolski*: "Correcting the public record of biological crystallography science"
- 14:00-14:30: *P.Bombicz*: "Overview of the role of data reviews and tutorial reviews in improving crystallographic science training"
- 14:30-14:45: Comfort break

Session 4 Chair: B.McMahon

- 14:45-15:15*: S.Billinge*: "Moving towards a more data-centric scientific literature"
- 15:15-15:45: *G.Holmes*: "IUCrData - update on data publication and practices at the IUCr"
- 15:45-16:00*: J.Helliwell*: "Overview of the new opportunities in and a harmonisation of peer review of "data with validation report with article narrative" practices"
- 16:00-16:30: General Discussion
- 16:30-17:00: Tea break
- 18:00: Opening Ceremony of ECM32

For further details visit: www.iucr.org/resources/data/commdat/vienna-workshop

Organizers: Eugene Krissinel, Charles Ballard (Collaborative Computational Project No. 4, CCP4, UK)

Date: 17th August 2019 (1 day)

Time: 9 a.m. – 4 p.m.

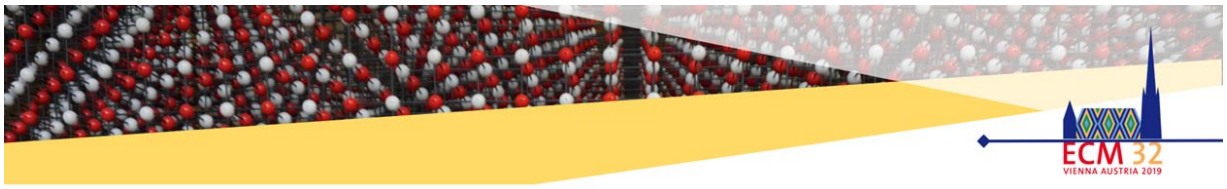
The workshop will demonstrate the use of CCP4 Software Suite for solving macromolecular structures starting from X-ray diffraction images and target sequence. Two main approaches: Molecular replacement and experimental phasing will be presented, for which two corresponding crystallographic projects will be gradually developed by tutors, each one building on the results obtained by the predecessor. The tutors will also make theoretical presentations relevant to their parts of structure solution process.

The workshop will aim at highlighting novel features and components of the CCP4 Software Suite, and both automated and staged approaches to structure solution will be shown. In particular, the newly developed CCP4 Cloud (also presented as an invited talk at MS-11) will be used for developing crystallographic projects.

PROGRAMME:

Saturday, Aug 17th

- 9:00*: E.Krissinel*: CCP4 Cloud Setup and General Introduction
- 9:45: *C.Ballard*: Data Processing and Data Quality
- 10:45: Coffee break
- 11:00: *R.Keegan*: Experimental Phasing and Density Modification
- 12:00: Lunch
- 13:00: *R.Keegan*: Molecular Replacement
- 13:45: *R.Nicholls:* Model Building and Refinement
- 14:45: Coffee break
- 15:00: *S.Kantamneni*: Arp/wArp Software for automated model building
- 15:30: *E.Krissinel:* Validation and Deposition



MaThCryst satellite meeting: Graph theory and modular structures

Organizers: Massimo Nespolo (University Lorraine, France), Bernd Souvignier (Radboud University, Netherlands), Berthold Stöger (TU Wien, Austria)

Date: 16th to 18th August 2019 (3 days)

Time: 9 a.m. – 6 p.m.

This workshop deals with mathematical and theoretical aspects of crystal structure descriptions beyond space group symmetry. The workshop will take place on two-and-a-half days. The first day is devoted to the application of graph theory to crystal structure description. The combinatorial topology of a crystal structure is captured in a natural way by a graph with vertices representing the atoms (or functional groups) and edges representing the bonds between them. Using the periodicity of the crystal structure, this graph can be reduced to a finite labeled quotient graph with elements from the translation subgroup assigned to the edges. By reversing this construction, labeled quotient graphs provide a method to obtain hypothetical crystal structures. The second day will treat the description of modular structures. These structures are built of distinct layers, rods or blocks. They are ubiquitous in all classes of compounds, from minerals to technological materials and pose challenging crystallographic problems, such as twinning, polytypism, disorder and systematic non-space group absences. Standard space group symmetry only considers global symmetry and does not reflect additional local symmetry of these structures. The full symmetry can be described using space groupoids. The order-disorder (OD) theory deals with special, though common, families of modular structures, where all members of a family are locally equivalent. The morning of the third day is reserved for contributions by participants. Poster space will be provided. The workshop will consist of introductory lectures and exercise sessions, where concrete examples will be worked out. Participants are expected to be familiar with the basic concepts of crystallography. No previous knowledge on graph theory or local symmetry is presupposed.

PROGRAMME:

Day1: Friday, Aug 16th

- Fundamentals of graph theory and its application to the description and interpretation of crystal structures.

Day2: Saturday, Aug 17th

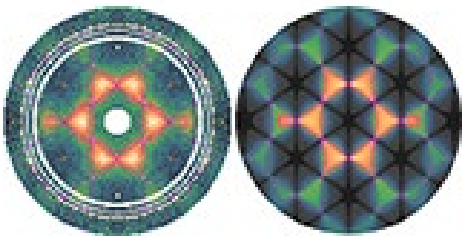
- Modular structures, partial operations and space groupoids

Day3: Sunday, Aug 18th

- Contributed talks from the participants

For further details visit: www.crystallography.fr/mathcryst/wien2019.php

Neutron Scattering and Imaging for Newcomers



Organizers: Jürg Schefer (Paul Scherrer Institute, Switzerland), Martin Meven (RWTH Aachen University and JCNS, FZ Jülich at Heinz Maier-Leibnitz Zentrum (MLZ), Germany, Arbeitskreissprecher DGK/AK7)

Date: 14th to 17th August 2019 (4 days)

Time: 9 a.m. – 5 p.m.

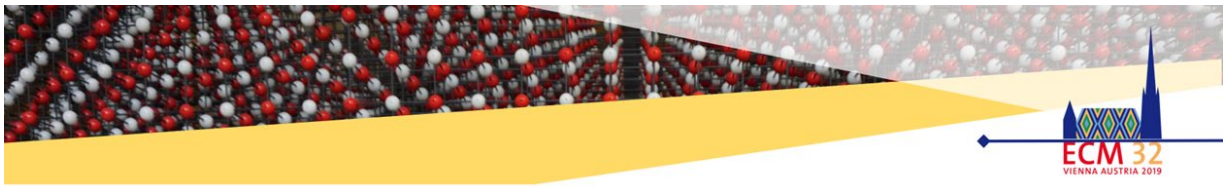
Neutron scattering is a very powerful method to investigate novel materials. Especially when focusing on magnetic properties or light atoms, neutron scattering is often the first-choice method. As neutron wavelength and neutron energy are simultaneously in the range of interatomic distances and nuclear or magnetic excitations, neutron scattering has proven to be a key technology in materials science.

This workshop is organized jointly by the German Crystallographic Society (DGK), AK7 and the Swiss Society for Crystallography (SGK) with kind support from the ECM organizing committee (Dr. K. Hradil) and TU Wien, RWTH Aachen, Paul Scherrer Institute, MLZ and SINE2020.

We intend in this workshop to teach the basic techniques to the participants. This is essential to allow them to make the best use of these expensive large-scale facilities during their future career. Workshops in this field are more and more important as small- and medium flux facilities are closing and are lowering or ending their teaching duties. Going to ECM32 is an ideal location as related scientists are gathering at this conference, especially PhD and postdoc students. Teaching the use of state-of-the-art data evaluation programs will round up this workshop.

Funding and Support

This workshop is organized jointly by the German Crystallographic Society (DGK, AK7) and the Swiss Society for Crystallography (SGK) with kind support from the ECM32 organizing committee (Dr. K. Hradil), RWTH Aachen, Paul Scherrer Institute and SINE2020.



PROGRAMME:

Day1: Wednesday, Aug 14th

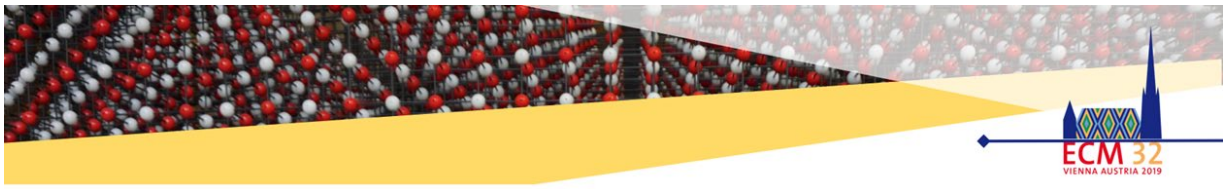
- 9:00-10:30: Introduction
- 10:30-12:00: *J.Schefer*: Neutron Sources
- 12:00-14:00: Lunch
- 14:00-15:30: *M.Meven*: Nuclear Diffraction
- 15:30-16:00: Break
- 16:00-17:30: *Y.Filinchuk*: Fullprof
- 17:30-19:00: Tutorials

Day2: Thursday, Aug 15th

- 9:00-10:30: *V.Pomjakushin*: Magnetic Diffraction
- Break
- 10:30-12:00: *M.Janoschek:* Polarimetrie
- 12:00-14:00: Lunch
- 14:00-15:30: *R.Neder:* Diffuse Scattering
- 15:30-16:00: Break
- 16:00-17:30: *M.Henriques*: JANA 2000, Focus Magnetic
- 17:30-19:00: Tutorials

Day3: Friday, Aug 16th

- 9:00-10:30: *A.Schneidewind*: Inelastic Neutron Scattering
- Break
- 10:30-12:00: *S.Allenspach*: IN Simulations/Tutorials
- 12:00-14:00: Lunch
- 14:00-15:30: *S.Mühlbauer*: SANS/Magnetic Matter
- 15:30-16:00: Break
- 16:00-17:30: *T.Schrader*: Biocrystallography
- 17:30-19:00: Tutorials



Day4: Saturday, Aug 17th

- 9:00-10:30: *M.Strobl*: Neuron Imaging
- 10:30-12:00: *A.Kaestner*: Image information and Processing
- 12:00-14:00: Lunch
- 14:00-17:30: Excursion Atominstitut
- Heuriger - Vienna Wine Event (Satellites Coming Together)

5th CrysAC workshop: "Crystallography of ancient metals and metal corrosion"

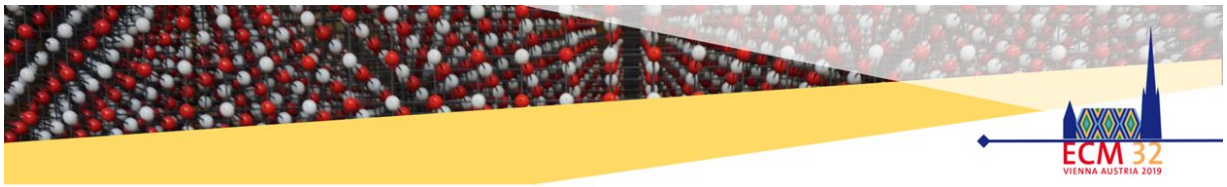
Organizers: IUCr - CrysAC Commission on Crystallography in Art and Cultural Heritage
Gilberto Artioli (University Padua, I), Manfred Schreiner (Academy of fine Arts, Vienna, AT), Alicja Rafalska-Lasocha (Jagiellonian University, PL), Klaudia Hradil (TU Wien, AT)

Date: 17th August 2019 (1 day)

Time: 9 a.m. – 5 p.m.

In keeping with the terms of reference of the Commission, the CrysAC workshop on "The crystallography of ancient metals and metal corrosion" is within the series of one-day workshops organized by the IUCr Commission on Crystallography in Art and Cultural Heritage, aimed to stimulate knowledge exchange between Crystallographers and researchers interested in Cultural Heritage investigations. Different communities are invited to present reviews of established research, recent results and envisaged trends in key areas of Archaemetry and Conservation Science.

The present workshop will invite scientists from research institutions, museums, and conservation bodies, in order to illustrate state-of-the-art applications of materials science in the field of archaeometallurgy, diagnostics and conservation of metals, authentication, corrosion processes, and other themes related to ancient metals and metallurgy. Although only invited contributions are planned, all interested people are invited to exchange ideas and discuss the presented topics.



PROGRAMME:

Saturday, Aug 17th

- 9:00: *K.Hradil; G.Artioli*: Opening
- 9:10-9:50: *A.Brandt*: Unveiling the secrets of ancient metal artifacts
- 9:50-10:30: *E.Tereschenko*: New data of metal artifacts from old museum collections – experiences of NRC Kurchatov Institute
- 10:30-11:00: Break
- 11:00-11:40: *P.Craddock*: What the miners left behind they didn't want: So which minerals did they smelt in the Bronze Age
- 11:40-12:20: *M.Scheiner; R.Wiesinger*: Corrosion of silver coins
- 12:20-13:00: *S.Rabitsch; A.Malissa:* Corrosion of silver links
- 13:00-14:30: Lunch
- 14:30-15:10: *M.Thoury*: High spatial dynamics-photoluminescence imaging
- 15:10-15:50: *F. Grazzi*: The ancient steel sword technology receasled through neutron imaging and Bragg edge neutron transmission
- 15:50-16:10: Break
- 16:10-16:50: *Q.Wang*: Unusual pale blue copper corrosion products on metal objects in museum collections
- 16:50-17:30: *T.Blanton*: Laboratory microXRD Methods for Analysis of Metals, Alloys, and Corrosion Materials
- 17:30-17:45: Discussion and closing

2019 IUCr & ECA High-Pressure Workshop

Organizer: Ronald Miletich (University of Vienna, Austria), Haozhe Liu (IUCr HP Commission, CN), Yaroslav Filinchuk (ECA SIG-11, UCL, BE)

Date: 13th to 16th August 2019 (4 days)

Time: 8:30 a.m. – 6 p.m.

Crystallography under extreme conditions has become a multidisciplinary field dealing with unique states of matter and their changes, and simulating processes in materials at extraordinary conditions. Modern high-pressure science provides among others insights to inaccessible environments such as of planetary interiours, it allows the synthesis of novel materials and access to new material states, and it promotes extraordinary physical properties of solids.

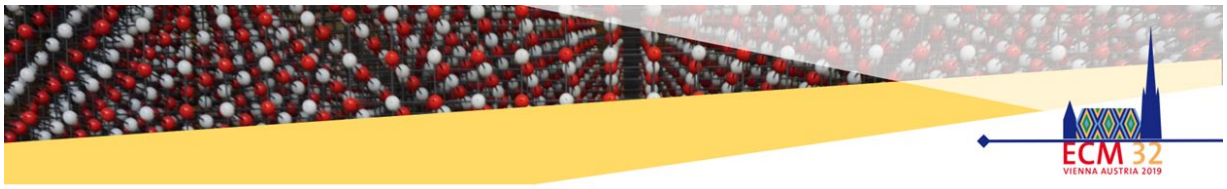
The last decade has seen milestones reached in innovative instrumentations and improvements in experimental methodology and software, as well as ab initio techniques. Structure determination at pressures up to a megabar has become routine. Methods have been developed that enable the analysis of multi-grain data collected on samples composed of hundreds of individual crystallites. Advances in X-ray detector technology and pressure-controlling devices facilitate the collection of crystallographic data with unprecedented speed, at controlled stress and strain rates, and enabling time-resolved experiments.

The purpose of the 2019 High-Pressure Workshop, this year jointly organized by the International Union of Crystallography (IUCr) Commission on High Pressure and the European Crystallographic Association (ECA) Special Interest Group SIG-11 is to bring together researchers, who apply these tools of extreme-condition crystallography to different disciplines of science and to stimulate exciting research directions for the future.

PROGRAMME:

Day1: Tuesday, Aug 13th

- 16:30-18:30: Registration
- 18:30-19:00: Opening Remarks
- 19:00-21:00: Icebreaker Party

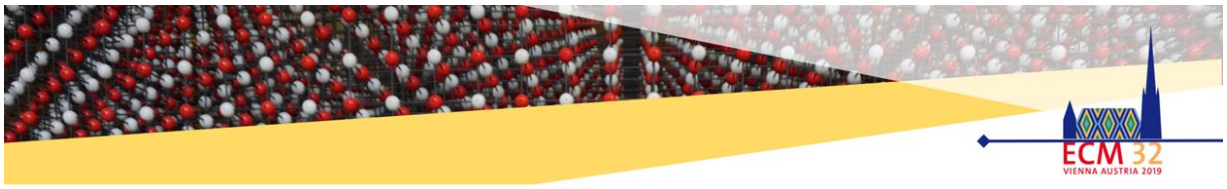


Day2: Wednesday, Aug 14th

- 9:00-10:00: *E.Zurek*: Plenary lecture: Theoretical Predictions of Superconducting and Superhard Materials
- 10:00-10:30: Coffee break
- 10:30-10:50: *L.Caron*: Minimizing hysteresis in phase transforming magnetocaloric Heusler alloys
- 10:50-11:10: *I.Lyubutin*: High-pressure transformation of $GdFe_3(BO_3)_4$ into the multiferroic phase and crystal structure determination based on the Raman and Mössbauer spectroscopy data
- 11:10-11:30: *C.Weber*: Rewriting the structural and magnetic systematics of the lanthanide elements
- 11:30-11:50: *Z.Wu:* Constraining the water content at the top of the mantle transition zone with the elasticity of wadsleyite and olivine
- 11:50-12:10: *J.M.Recio*: The anions in metallic matrices model in the light of the chemical pressure formalism
- 12:10-13:30: Lunch
- 13:30-13:50: *N.Garg*: High pressure phase transitions in transition metal doped topological insulators
- 13:50-14:10*: M.Hasegawa*: Synthesis, crystal chemistry and electronic states of novel transition metal nitrides under high pressures
- 14:10-14:30: *S.I.Kawaguchi*: Structure determination of liquid Fe-Ni-S alloy
- 14:30-14:50*: B.Lavina*: Crystal structure, bonding and stability a new high-pressure polymorph of GaP
- 14:50-15:10: *P.Toulemonde*: Structural and magnetic properties of superconductuing $Fe(Se_{1-x}S_x)$ under pressure probed by neutron and x-ray diffraction, x-ray emission and absorption spectroscopies
- 15:10-16:00: Coffee break
- 16:00-17:30: Lightening talks

Day3: Thursday, Aug 15th

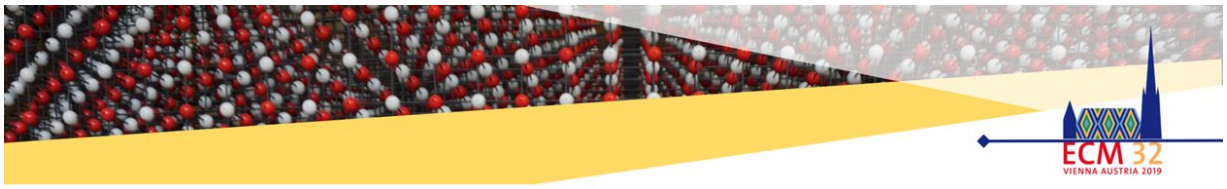
- 9:00-10:00: Plenary lecture: *S.McWilliams*: Static High Pressure Experiments at Free Electron Lasers: Results and Prospects
- 10:00-10:30: Coffee break
- 10:30-10:50: *K.Scheidl*: Elastic behaviour of α-quarz over its entire stability range and its use as a pressure standard



- 10:50-11:10: *F.Zhang*: The lattice dynamics calculation and Infrared spectra of hydrous ringwoodite under the Earth mantle transition zone conditions
- 11:10-11:30: *B.Lavina*: Crystalline forsterite to 160 GPa
- 11:30-11:50: *V.Dimitriev*: Complex structures of simple metals: Strain induced incommensurate structures in vicinity of reconstructive phase transitions
- 11:50-12:10: *M.Ende*: Hidden structural phase transitions in the Cs-stuffed rhombohedral beryl-type framework $Cs[Be_2LiAl_2(Si_6O_{18})]$
- 12:10-12:30: *K.Friese*: The $GeSe_xTe_{x-1}$ phase diagram from experiment and theory
- 12:30-13:30: Lunch
- 13:30-13:50: *L.Dresselhaus-Cooper*: Experimental techniques and data analysis for high-resolution X-ray imaging
- 13:50-14:10: *L.Benedetti*: Time-resolves X-ray diffraction during laser compression experiments: Challenges and progress toward measuring kinetics of structural changes
- 14:10-14:30: *J.Boby*: Xpress: latest results from the dedicated high pressure diffraction beamline at Elettra-Sincrotrone Trieste
- 14:30-14:50: *Y.Meng*: Exploring properties of matter at extreme conditions with advances synchrotron techniques at HPCAT beamline 16-IDB of the Advanced Photon Source
- 14.50-15:10: *W.Yang*: Pressure induced enhancement of physical properties an in-situ characterizations
- 15:10-16:00: Coffee break
- 16:00-16:30: *J.Graf*: Getting the most data out of your high-pressure experiment
- 16:30-17:30: Poster session
- 19:30: Conference Dinner

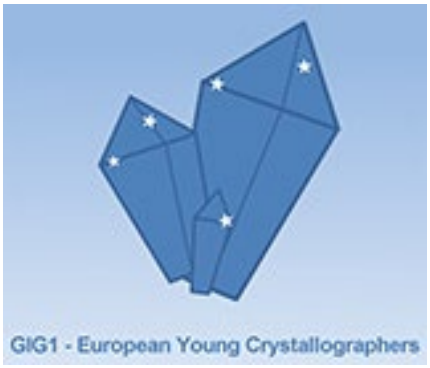
Day4: Friday, Aug 16th

- 9:00-10:00: Plenary lecture: *T.Hattori*: What can we do with High-Pressure Neutrons?
- 10:00-10:30: Coffee break
- 10:30-10:50: *V.Solozhenko*: Chemical interaction and phase relations in the B-X (X=S, Se, Te) systems at high pressure and high temperature
- 10:50-11:10: *D.Scelta*: High pressure and high temperature chemical reactivity of black phosphorus and nitrogen
- 11:10-11:30: *B. Zakharouv*: Selecting hardware and experimental strategy for high-pressure singe-crystal X-ray diffraction studies
- 11:30-11:50: *F.Safari:* Pressure-dependent crystallization preference of resorcinol polymorphs
- 11:50-12:10: *J.Lee*: High pressure structure and magnetism of 1-D molecular magnetic material



- 12:10-12:30: *R.Vilaplana*: Structural and vibrational study of β-As_2Te_3 under hydrostatic pressure
- 12:30-13:30: Lunch
- 13:30-13:50: *Y.Kim*: Shock growth of water ice IV single crystal near equilibrium melting pressure with dynamic diamond anvil cell
- 13:50:14:10: *B.Li*: Single crystal x-ray diffraction of diamond above 2 Mbar
- 14:10-14:30: *R.Husband*: X-ray diffraction of tera-pascal per second fast compression using the dynamic-DAC
- 14:30-14:50: *A.Lazicki*: Extending X-ray diffraction measurements above 2 TPa
- 14:50-15:10: *M.Hanfland*: The surprising stability of certain molecular crystals to very high compressions
- 15:10-16:00: Coffee break
- 16:00-16:30: *T.Donath*: CdTe-based hybrid photon counting detectors PILATUS3 and EIGER2 for high-energy X-ray diffraction under extreme conditions
- 16:30-16:50: *A.Grzechnik*: Single-crystal diffraction in diamond-anvil cells with hot neutrons at the Heinz Maier-Leibnitz Zentrum (MLZ)
- 16:50-17:10: *K.Dziubek*: Clustering of spatially subnanoconfined oxygen compressed in unidimensional channels
- 17:10-17:30: *C.Park*: In-situ observation of polycrystalline texture and microstructure evolution with P using scanning XRD microscopy technique
- 17:30-17:50: *A.Liu:* Pressure induced phase transitions in MO_2 and the potential hard materials
- 17:50-18:15: Closing remarks
- 19:30-22:00: Heuriger (Zehnermarie)

For further details visit: https://www.univie.ac.at/Mineralogie/HPWS/index.html



Organizers: Philipp Hans (TU Wien, Vienna, Austria), Filip Topic (McGill University, Montreal, Canada)

Date: 18th August 2019 (1 day)

At this event, early career researchers will have the opportunity to present their work and socialize with their peers in an informal and friendly environment.

Oral and poster presentations from all aspects of crystallography will ensure that there is something for everyone's interests!

Please send your abstract to philipp.hans@tuwien.ac.at and indicate, which type of contribution you prefer. Depending on time slots and contributions the organizers will make a schedule and will try to respect all wishes. The time per talk will be announced on 28/07/2019 latest. Poster submissions will be possible until the final ECM32 deadline.

For inquiries and details contact Filip Topic or Philipp Hans:

philipp.hans@tuwien.ac.at

filip.topic@mcgill.ca

Olex2 Workshop


Michael Bodensteiner


Lena Rummel


Oleg Dolomanov


Horst Puschmann

Organizers: Horst Puschmann (OlexSys Ltd, Durham University, UK), Michael Bodensteiner (OlexSys UG, Germany)

Date: 18th August 2019 (1 day)

Time: 9 a.m. – 4:30 p.m.

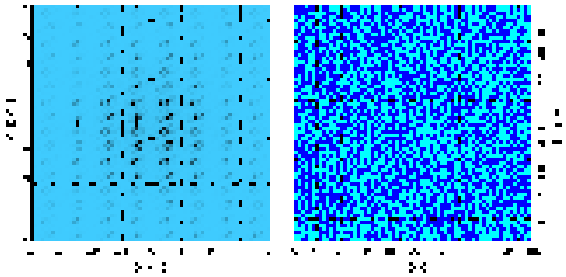
Welcome to the ECM32 and to the official Olex2 workshop, which will be held on the first day of the conference from 9 a.m. until about 4.30 p.m. (in time to make it to the opening ceremony!)

We will be around throughout the conference and please don't hesitate and talk to us about any questions you may have.

PROGRAMME:

- 8:30-9:00 Set-up Session: Bring your own Laptop with Olex2 and any other crystallographic software (ShelXL, PLATON). Chance to sort out any last-minute problems you might have experienced.
- 9:00-10:00 Introduction to Olex2: Introducing the key concepts or workings with Olex2 and work through one or two very simple example structures.
- 10:00-12:00: It's your turn now! Work for yourself, or pair up in teams -- and try for yourself what we have covered in the previous section. If it's all familiar to you, work on your own samples (don't forget to bring some!). We will be here to help!
- 12:00-13:30: Working Lunch: We won't provide lunch, instead here's our chance to find some food in the nearby cafes, get to know each other and gossip about crystallography and Olex2.
- 13:30-14:30 Advanced topics in Olex2: Another lecture-style session: disorder modelling, solvent masking, HAR – anything that you might want to find out about. We will cover this here.
- 14:30-16:30: Working out Advanced Techniques: With our help, you are now free to try anything you may want to tackle. This could be simple cases, complicated sample disorder or your own structures -- the choice is yours!
- 4.30: Closing

Total scattering analysis with DISCUS



Organizers: Reinhard B. Neder (Friedrich-Alexander Universität Erlangen-Nürnberg, Germany), Thomas E. Proffen (ORNL – Oak Ridge National Laboratory, USA)

Date: 13th to 17th August 2019 (5 days)

Time: 9 a.m. – 6 p.m.

The workshop will give you an overview of total scattering techniques and data analysis procedures. We will describe single crystal diffuse scattering as well as powder scattering respectively the Pair Distribution Function (PDF) technique.

The data analysis will be described using the DISCUS suite. This program suite allows to simulate structure models of perfect crystals, disordered crystals as well as nanocrystals. The program suite encompasses a wide set of tools to modify a perfect crystal structure in order to introduce defects like stacking faults, chemical short-range order, strain fields, clusters or domains etc. A particular strength is the simulation of finite nanoparticles that can be decorated on the surface by stabilizing molecules. Based on such structural models the program can calculate and refine the structural models against single crystal and powder diffraction pattern or the PDF.

European Crystallographic Computing Forum

Organizers: SIG 9 - Martin Lutz (University Utrecht SIG 9)

Date: 14th - 17th August 2019 (4 days)

Venue: Melk, Lower Austria

Time: t.b.a.

The European Crystallographic Computing Forum will be a participant driven event that welcomes both beginners and experienced software developers in crystallography. Mornings will be filled with plenary discussions and lectures on topics of general interest to computing in all disciplines of crystallography, afternoons and evenings will be run code-camp style: groups of participants will work together on small software projects, being helped by the invited speakers, and at the end present their results. We encourage informal tutorials between participants.

The European Crystallographic Computing Forum will be held from the 14th to 17th of August 2019 in the town of Melk (lower Austria), immediately preceding the European Crystallographic Meeting ECM32 in Vienna, the capital of Austria. We especially welcome registrations from families and parents with children, and offer family rooms as well as babysitting during the morning sessions.

PROGRAMME:

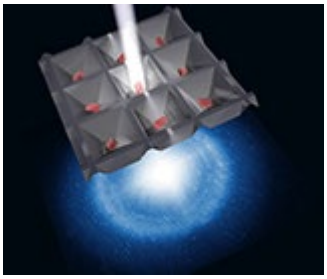
Day1: Wednesday, Aug 14th

- 18:00: Beginning of the forum

Day2: Thursday, Aug 15th, Day3: Friday, Aug 16th & Day4: Saturday, Aug 17th

- Mornings will be filled with plenary discussions and lectures on topics of general interest to computing in all disciplines of crystallography, afternoons and evenings will be run code-camp style, intersparsed with tutorials as needed.

For further details visit: http://www.cryst.chem.uu.nl/lutz/ecacomsig/melk.html



Fixed target serial crystallography

Organizers: Arwen Pearson, Jennifer Wierman, Pedram Mehrabi, Eike C. Schulz (Universität Hamburg and Hamburg Center for Ultrafast Imaging CUI, Germany)

Date: 17th August 2019 (1 day)

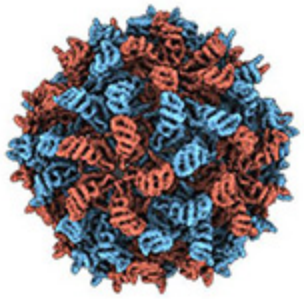
Time: 10 a.m. – 6 p.m.

Serial approaches in crystallography are becoming increasingly prevalent as the improvement in data collection techniques are reducing the constraints for systems amenable to these approaches. Fixed-target approaches have a number of advantages, such as low sample consumption and enabling new methods for time-resolved experiments. This provides novel approaches for structure solution and observing protein dynamics with systems that are otherwise not approachable to classical or other serial approaches.

Workshop goals: The primary goal of the workshop is to discuss and define a set of standard parameters within which individual groups and beamlines can develop the tools and software to make fixed-target methods, including time-resolved approaches, a reliable and routine method for user operation. The participants will learn about the different fixed-target approaches that are currently available, as well as important considerations to make about the workflow to make best use of your fixed-target experiments.

PROGRAMME:

The following areas will be covered primarily in talks and informal round table discussion:
Introduction to fixed targets
Making fixed-target methods reliable for routine user operation
Implementation at different facilities
SSX applications beyond TRX?
Fixed target parameters / dimensions / materials
Translation stage systems and integration of control software into beamline software
Fixed-target mounting solutions (e.g. magnetic mounts, robots, etc.)
Fixed-target storage and shipment options
Auto Processing / Workflows and Pipelines

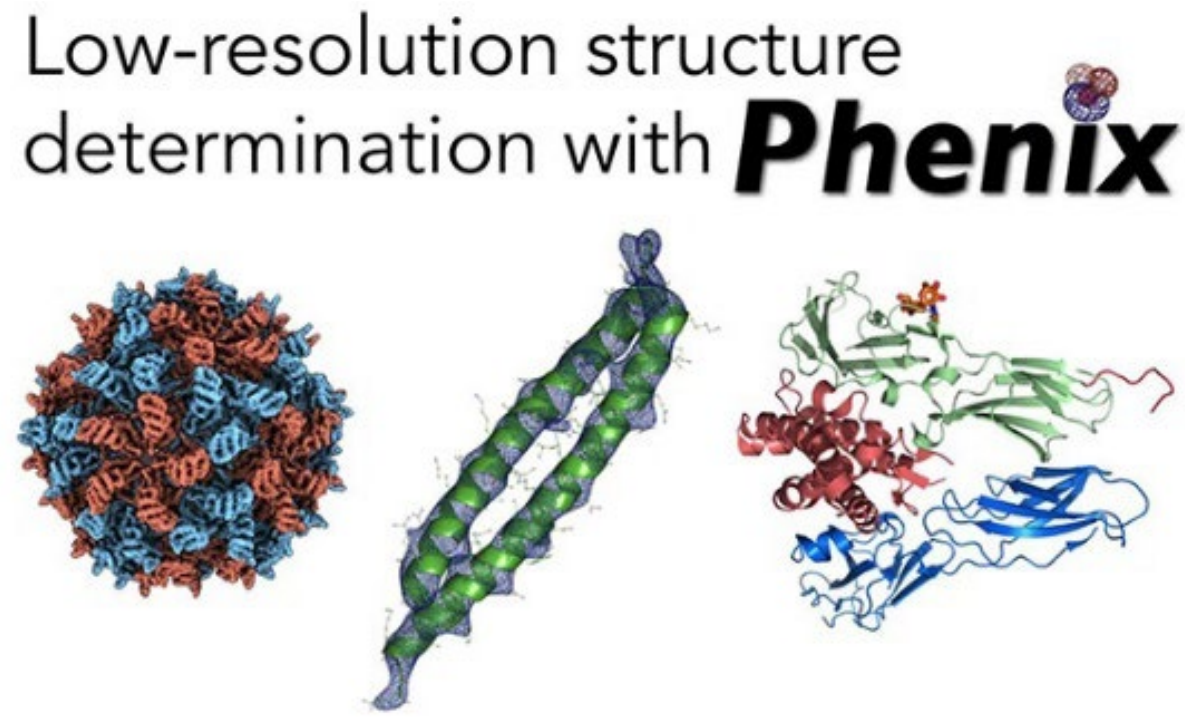


Organizers: Paul Adams, Dorothee Liebschner (Lawrence Berkeley National Laboratory, Berkeley, USA)

Date: 18th August 2019 (1 day)

Time: 9 a.m. – 5 p.m.

This workshop is on low-resolution structure determination of biological macromolecules with the software package Phenix. The lectures and tutorials will cover experimental phasing, automated model building and (real-space) refinement. The focus is on Phenix tools and methods that are designed for handling the challenges of low-resolution data from X-ray crystallography and cryo-electron microscopy.



Crystal Engineering using the Cambridge Structural Database

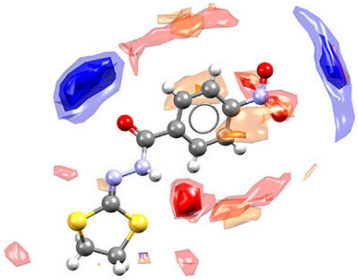
CCDC
advancing structural science

Organizer: Ioana Sovago (Cambridge Crystallographic Data Centre CCDC, UK)

Date: 18th August 2019

Time: 9 a.m. – 4 p.m.

This workshop will involve training on Crystal Engineering applications of the CSD, and associated software, with real case studies including the following: Polymorph assessment using Hydrogen Bond Propensity, Structural analysis using Full Interaction Maps, Geometry Check Analysis, Knowledge-based Co-Crystal Design, Hydrate and Solvate crystal structure analysis.



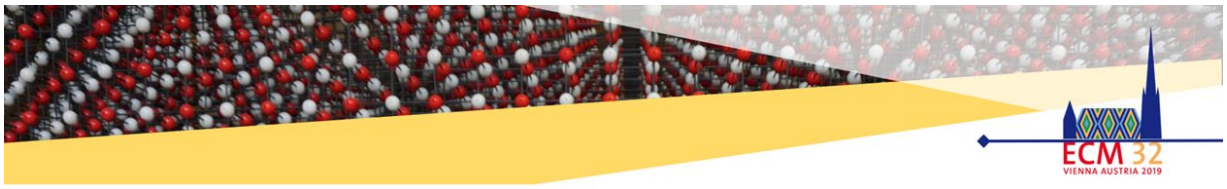
PROGRAMME:

Sunday, Aug 18th

- 09:00-10:45: Polymorph assessment using Hydrogen Bond Propensity, Structural analysis using Full Interaction Maps, Conformational analysis using Mogul Geometry Check
- 10:45-11:00: Coffee break
- 11:00-12:00: Hydrate Structure Analysis
- 12:00-13:00: Lunch break
- 13:00-14:30: Knowledge-based Co-Crystal Design
- 14:30-14:45: Coffee break
- 14:45-15:45: Solvate Structure Analysis
- 15:45:16:00: Q&A Session

For further details visit:

- https://www.ccdc.cam.ac.uk/Community/educationalresources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