

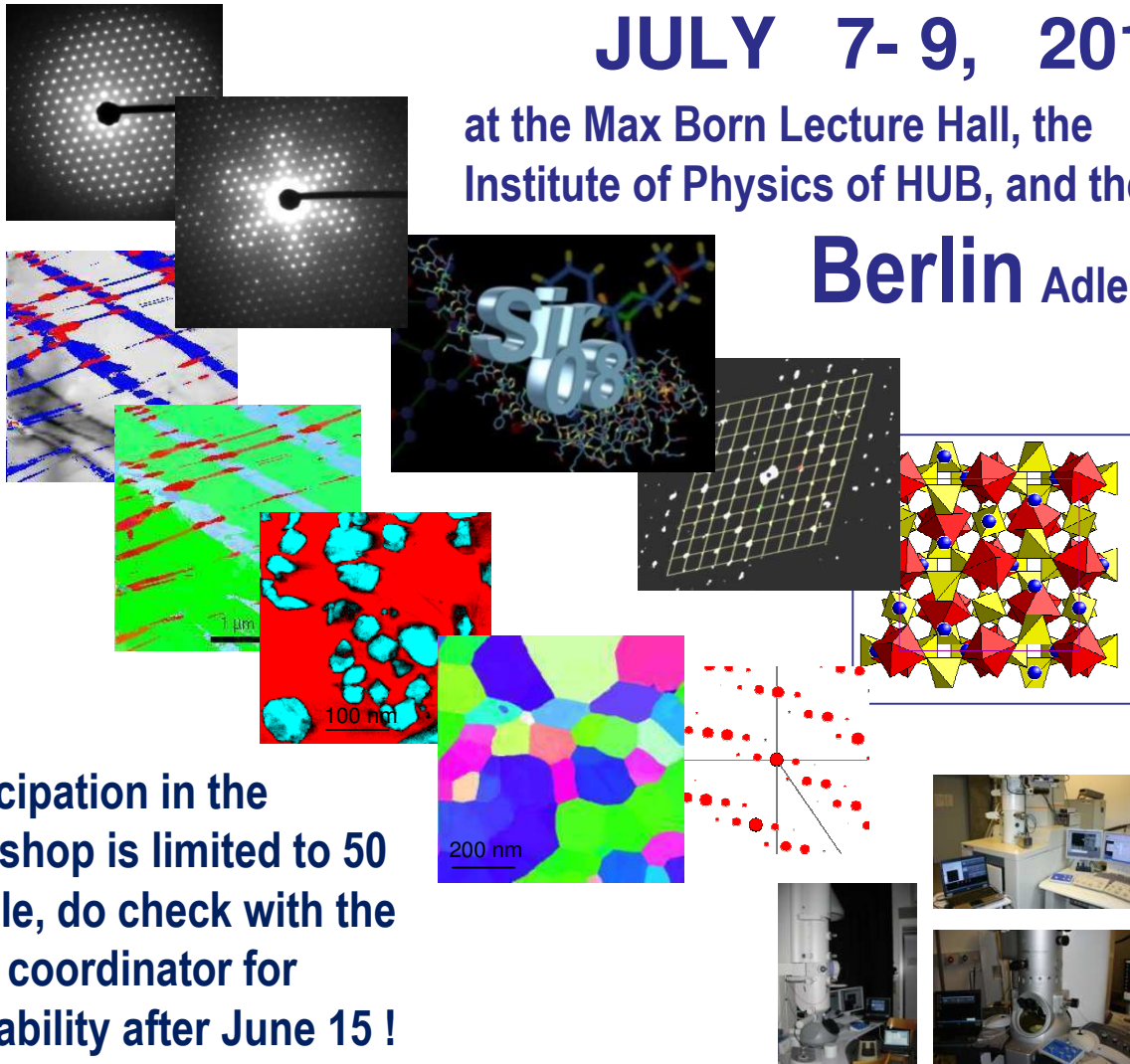
Facets of Electron Crystallography

A three day workshop, organized by the *Joint Laboratory for Electron Microscopy Adlershof* of the Humboldt University Berlin (HUB) and the Leibniz Institute for Crystal Growth (IKZ) in conjunction with the **Electron Microscopy Section of the German Society for Crystallography**

JULY 7-9, 2010

at the Max Born Lecture Hall, the
Institute of Physics of HUB, and the IKZ

Berlin Adlershof



Participation in the workshop is limited to 50 people, do check with the local coordinator for availability after June 15 !

Speakers and hands-on Demonstrators:

Jan Pieter Abrahams (Leiden), Martin Albrecht (IKZ Berlin), Gerd Benner (Oberkochen), Daniel Bultreys (Brussels), Carmelo Giacovazzo (Bari), Meiken Falke (Berlin), Sven Hovmöller (Stockholm), Ute Kolb (Mainz), Holm Kirmse (HUB Berlin), Stephan Kujawa (Eindhoven), Peter Moeck (Portland, USA), Jean-Paul Morniroli (Villeneuve d'Ascq), Wolfgang Neumann (HUB Berlin), Stavros Nicolopoulos (Brussels), Peter Oleynikov (Stockholm), Lukas Palatinus (Prague), Edgar Rauch (Grenoble), Ronald Ries (Muenchen), Matthias Rodewald (Eching), Muriel Véron (Grenoble), Stefan Zaefferer (Duesseldorf)

Mandatory pre-registration and all other inquiries per email pmoeck@pdx.edu to the local coordinator, Prof. Peter Moeck, Tel.: +049 30 2093 8044.

Workshop Topics

Fundamentals of electron crystallography

New developments in precession electron diffraction

High resolution crystallite orientation and phase mapping (HRCOPM - very loosely speaking “EBSD like mapping”) in the TEM

Automated Crystallography for the TEM (ACT)

3D Diffraction tomography

Rotation/precession diffraction methods for the collection of 3D data sets

HRTEM image-based electron crystallography

Objective-lens corrected TEM (including aberration-corrected precession diffraction)

Direct methods & charge flipping for electron crystallography

Hands-on activities in small groups

- HRCOPM at an analytical JEOL JEM 2200F
- HRTEM at an objective-lens corrected FEI Titan 80-300
- Software for electron crystallography (SIR 2008 - Superflip – CRISP/ELD, and eMap, eSlice)

The whole workshop will be conducted in English!

All participants are encouraged to present one poster (in English) that gives an introduction to their work. **The best poster, as judged by a committee, will win a prize of 100 Euro.**

The organizers will invite selected participants of our workshop to submit either a research or a review paper for a special issue on “***New developments in electron diffraction***” of the journal ***Crystal Research and Technology*** (<http://www.crystalresearch.com>), guest editors: Peter Moeck and Stavros Nicolopoulos. This special issue is planned to appear in December 2010. The **submission deadline** is, therefore, **October 1, 2010.**

Workshop participation fees (to be paid at the workshop venue on arrival in cash – no credit/debit cards of any kind), after pre-registration with the local coordinator (Peter Moeck, pmoeck@pdx.edu)

Students: 50 Euros (one day), 125 Euros (all three days)

Senior Researches: 100 Euros (one day), 250 Euros (all three days)

Workshop venues: **Max-Born Lecture Hall**, Carl-Scheele-Straße 6; **HUB, Institute of Physics**, Newtonstraße 15; and **IKZ**, Max-Born-Straße 2, all three venues at 12489 Berlin-Adlershof (in 5 minutes walking distance from each other)

Accommodation: Airport Hotel Berlin-Adlershof, prices (per night) range from 62 Euro for a single room, over 73 Euro for two people sharing a double room, to 81 Euro for 3 people sharing a “family room”, and 108 Euro for 4 people sharing such a room, breakfast buffet: 12 Euro (per day), <http://www.airporthotel-berlin-adlershof.de/>; Please download the respective registration forms for this hotel in [English](http://crysta.physik.hu-berlin.de/workshop_FoEC/HUB-electron-crystallography-English.pdf): http://crysta.physik.hu-berlin.de/workshop_FoEC/HUB-electron-crystallography-English.pdf (or [German](http://crysta.physik.hu-berlin.de/workshop_FoEC/HUB-electron-crystallography-German.pdf): http://crysta.physik.hu-berlin.de/workshop_FoEC/HUB-electron-crystallography-German.pdf), fill them out and fax or email them back to the hotel, please do **not** use the websites of this hotel for direct booking. **You completing the form and sending it to them (per fax, or as email attachment to reservierung@airporthotel-berlin-adlershof.de) is the way they want to have this done!** It is also OK with this hotel to arrive on Monday, July 5 and to leave on Saturday, July 10, and to book a room at the special reduced workshop rate. Simply use the form for this and change clearly visible to the requested dates at the top of the form by hand. All prices are inclusive of VAT, wireless internet access is available in this hotel, but not included in the room rate. One public computer is available in the hotel lobby. **There will, however, be access to email for the participants during the workshop in the Physics Department Computer Cluster.** Direct booking at these rates is guaranteed until June 15, keywords **“Electron crystallography”**.

Alternatively, the **Dorit Berlin-Adlershof**, <http://hotel-berlin-adlershof.dorint.com/>, is across the street and offers single rooms starting at 63 Euro and double rooms starting at 73 Euro (including VAT), breakfast buffet: 13 Euro; keywords **“facets of electron crystallography”**. Direct booking at these rates is guaranteed until June 15, as you do not have to fill in a special form **do mention the keywords** in your email or telephone inquiry/booking. Wireless internet access is available in this hotel, but not included in the room rate. There is one public computer in the lobby of this hotel, but you can do your **emailing during the workshop at the computer cluster of the Physics Department**.

Both hotels are located within a short walk of 5 minutes from the workshop venues. There is a stop of **bus 162** in front of these hotels. This bus comes from (and goes to) Schoenefeld Airport directly within less than 20 minutes (three times per hour during the day). Participants arriving at Tegel Airport need to either take a taxi (45 – 90 minutes depending on the time of day) or the **bus TXL** to a(n) S-Bahn/U-Bahn station and from there to Adlershof (about 1 hour). If you want to use public transportation (for 2.10 Euro), the recommendation is: take the bus TXL bus to S-Bahn station Beusselstrasse, walk down the stairs, step into train 41 (it only goes in one direction, the other direction has a different number), change at S-Bahn station Ostkreuz to train S8, step out at S-Bahn station Adlershof, walk some 10 minutes towards the South down the street “Rudower Chaussee”.

Participants arriving at any of the Berlin railway stations should take the S-Bahn to Adlershof.

Public transportation within Berlin can be planned ahead at <http://www.fahrinfo-berlin.de/Fahrinfo/bin/query.bin/en?id=0.1&>

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General Information

The practical sessions “Practice of HRCOPM” is offered on the afternoons of all three days. Up to five sessions (“groups 1 to 5” with a maximum of 10 people) may be held to serve everybody’s interests and needs.

Sessions A are offered three times on the afternoons of the second and third day.

Sessions B are offered twice on the afternoons of the second and third day.

Sessions C are offered twice but only on the afternoon of the third day.

Section D is only offered once on the afternoon of the third day.

The participants shall select the group by themselves according to their personal preferences, but also ensure that there will be an about even distribution of participants over these sessions.

The 24 computers in rooms 1’428 and 1’429 of the Institute of Physics at Humboldt University Berlin are accessible to all workshop participants from 9:00 to 19:15 each day. The Institute of Physics will be closes each night at 19:30. After these hours in order to leave the closed up building, one needs to call +49 30 2093 2959 for assistance in order to leave the building (There might well be language problems for non-German speakers in accessing this extra service!)

During the parallel sessions, two lectures need to share the above mentioned computers. Participants may also use computers that are not needed for exercises during the parallel sessions for their private emailing, checking on flights, planning their return trips, or other “office work”.

On the last day of the workshop, the lecture sessions will be formally closed just before lunch time. Practical parallel sessions will, however, continue after lunch at the Institute of Physics of Humboldt University until 16:30.

If you are leaving Berlin on the same afternoon, you may leave your luggage in room 2’210 of the Institute of Physics of Humboldt University until about 16:45 (rather than at your hotel).

Information concerning the usage of the computers at the Physics Department Computer Pool, room 1'429

The software demonstrations use part of the Physics Department PC-Pool, running **Debian GNU/Linux** with KDE by default.

For the purpose of this workshop, VirtualBox was added to the installation, with a **virtual Windows XP** as guest system.

The Pool machines are used as compute servers as well, running long jobs in the background. Therefore, even if something goes wrong, **don't press the button, please**.

Login with

username: acomdemo
password: kri-kurs

Click on the **SUN VirtualBox** icon, then **Start** Windows in the virtual machine. (It is configured to run in full-screen mode.)

Keyboard and mouse are shared between host and guest system.

Clicking within Windows **captures** the mouse. (Suppress the confirmation dialog if it bothers you.)

Release the mouse with the **HOST** key, which is bound to **Right_Ctrl**.

HOST+F toggles **full-screen mode**.

HOST+Home brings up the toolbar in full-screen mode.

The ASTAR or ACOM software is found in the **ASTAR** folder on the Windows desktop...

There is also the program enCIFer for the viewing and editing of CIF files.

Accessing a **USB stick** in virtual Windows: insert the stick

- if a KDE window pops up: close it
- open the "Devices" dialog (in full-screen mode: press HOST+Home)
- open "USB Devices" and enable the stick
- an explorer may pop up; if not, access it via ->"Start" ->"My Computer"

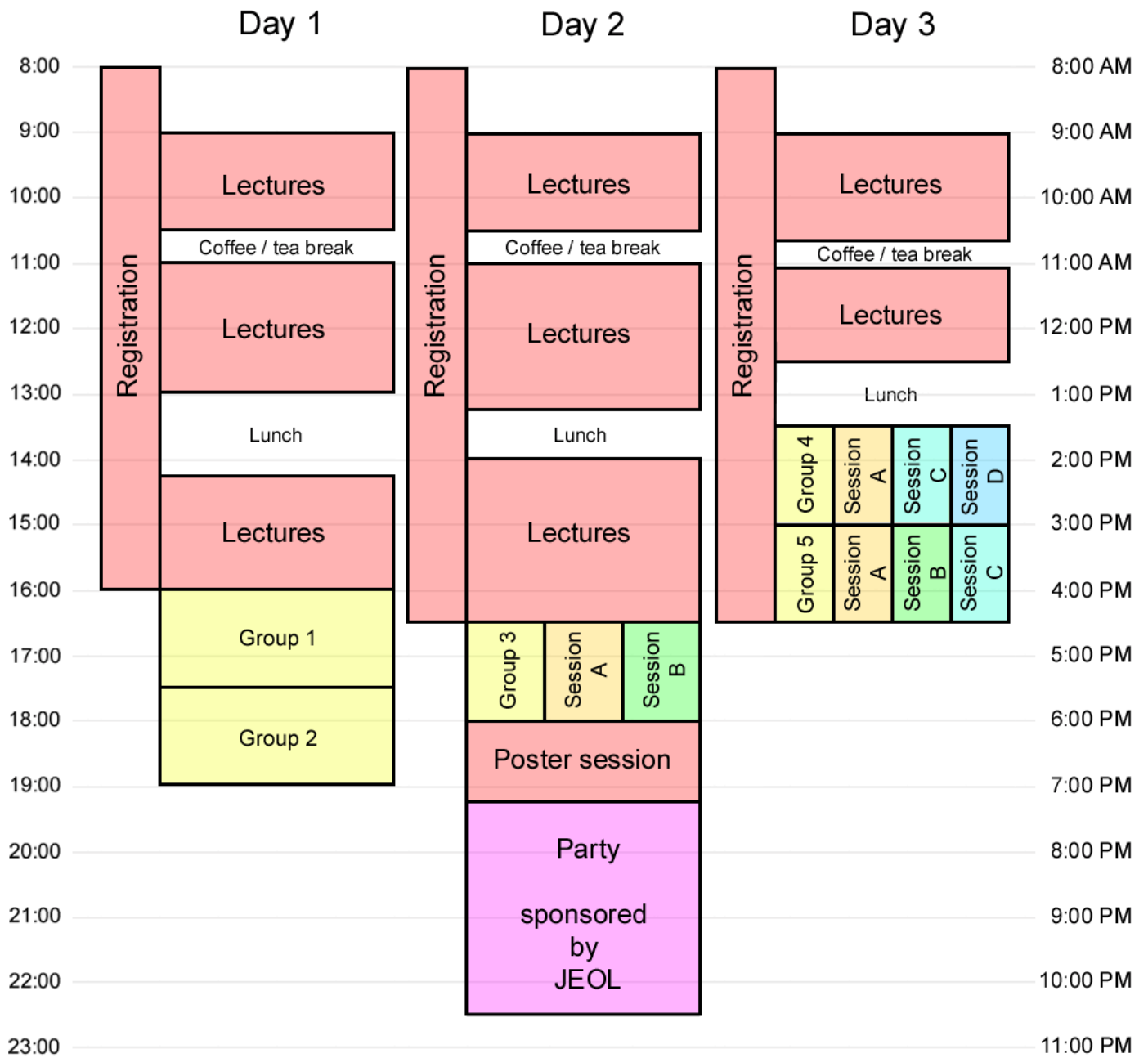
Terminate Windows as usual (**Turn Off** button).

Both the Linux **account** and the virtual Windows have the same initial configuration. In fact, they reside on the **local** disk. Adapt it to your needs.

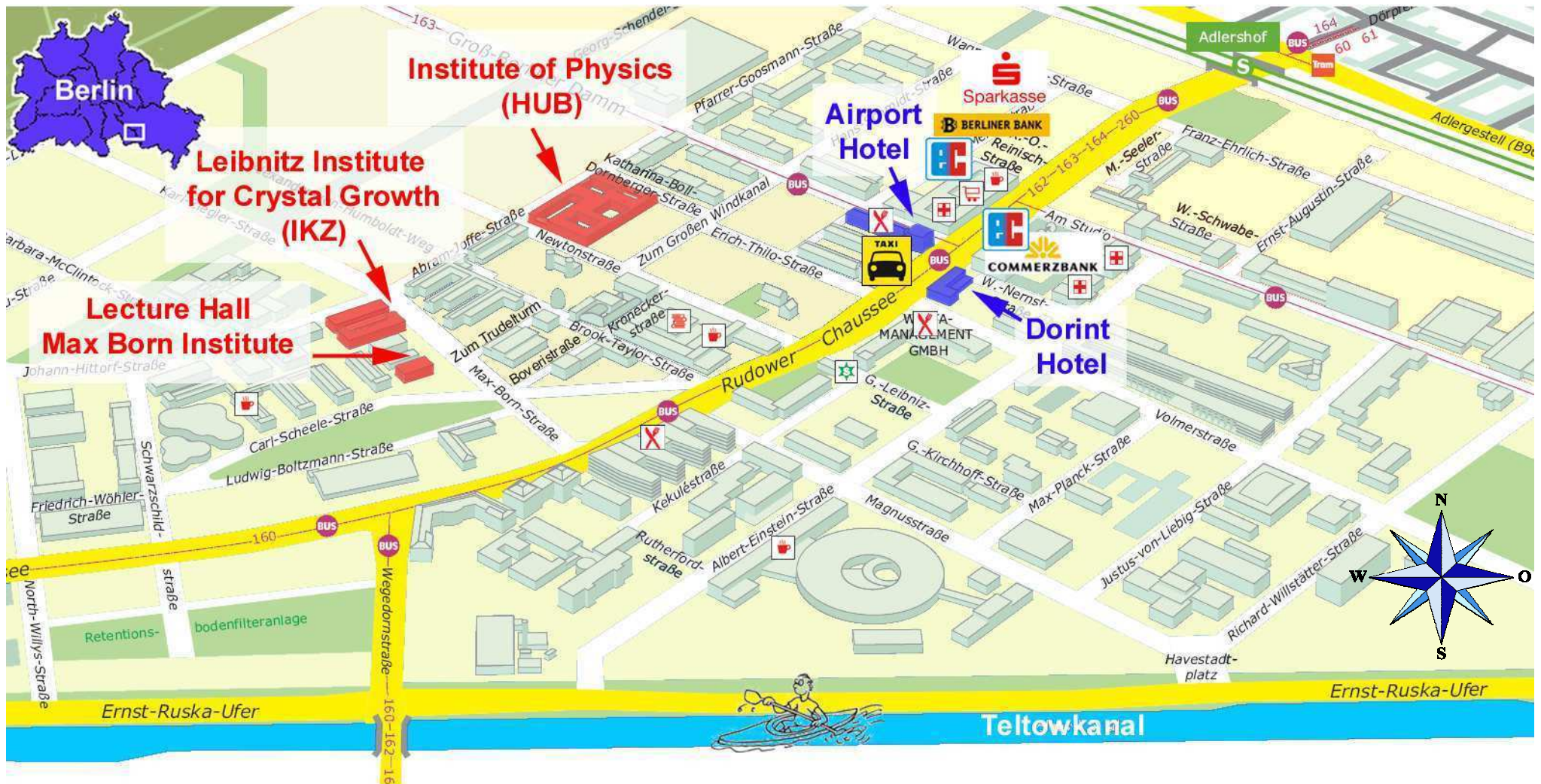
Note that everything will be deleted after the course.

To access your **emails**, login to your home institution or access the mailserv via a webinterface. Direct access with a mailclient is discouraged: outgoing SMTP connections are blocked by Humboldt's firewall.

Burkhard Bunk, bunk@physik.hu-berlin.de, Physics Institute, Humboldt University
fax: ++49-30 2093 7628 Newtonstr. 15
phone: ++49-30 2093 7980 12489 Berlin, Germany



- at Max Born Institute Lecture Hall
- Group at Institute of Physics (HUB) Room 0'503
- Session A at Institute of Physics (HUB) Room 0'504
- Session B Session C Session D at Institute of Physics (HUB) Room 1'428 & 1'429
- Party at Leibniz Institute for Crystal Growth (IKZ)



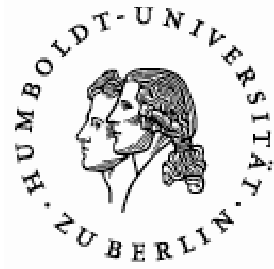
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Participants arriving at any of the Berlin railway stations should take the S-Bahn to Adlershof.

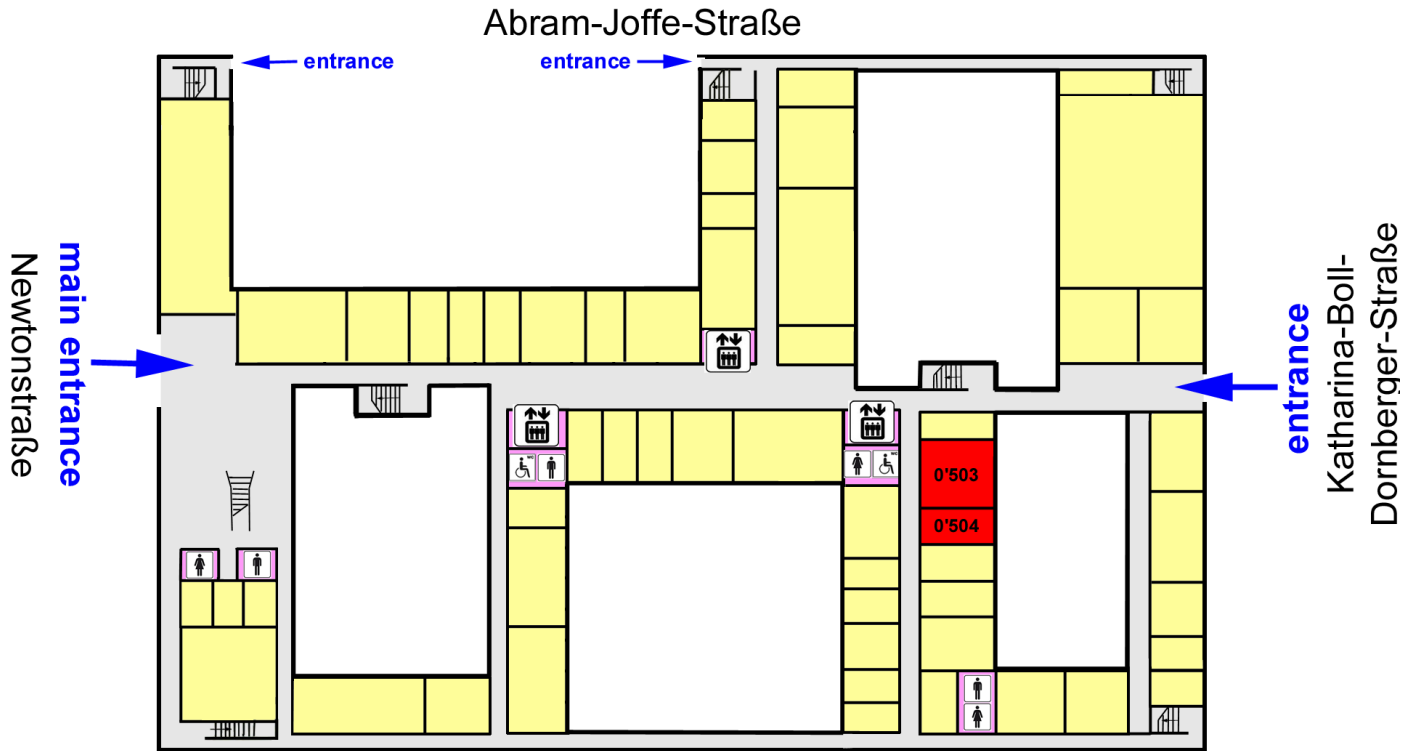
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Humboldt University of Berlin
Institute of Physics

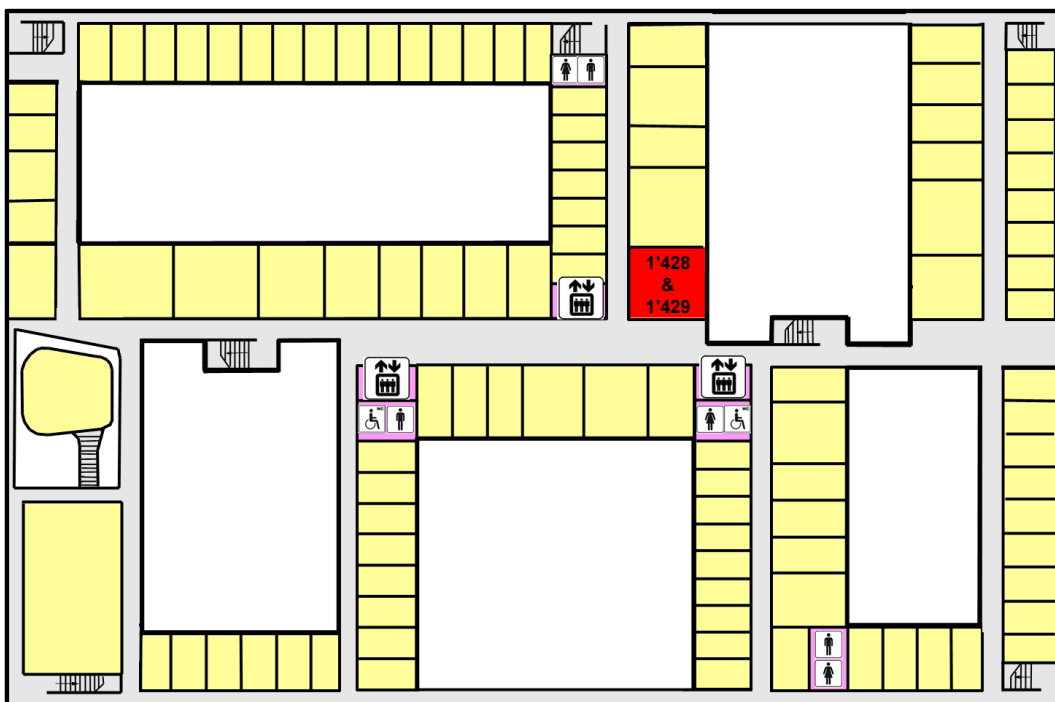
Newtonstr. 15
12489 Berlin



Ground floor

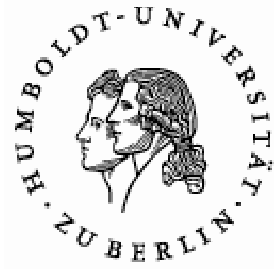


1st floor

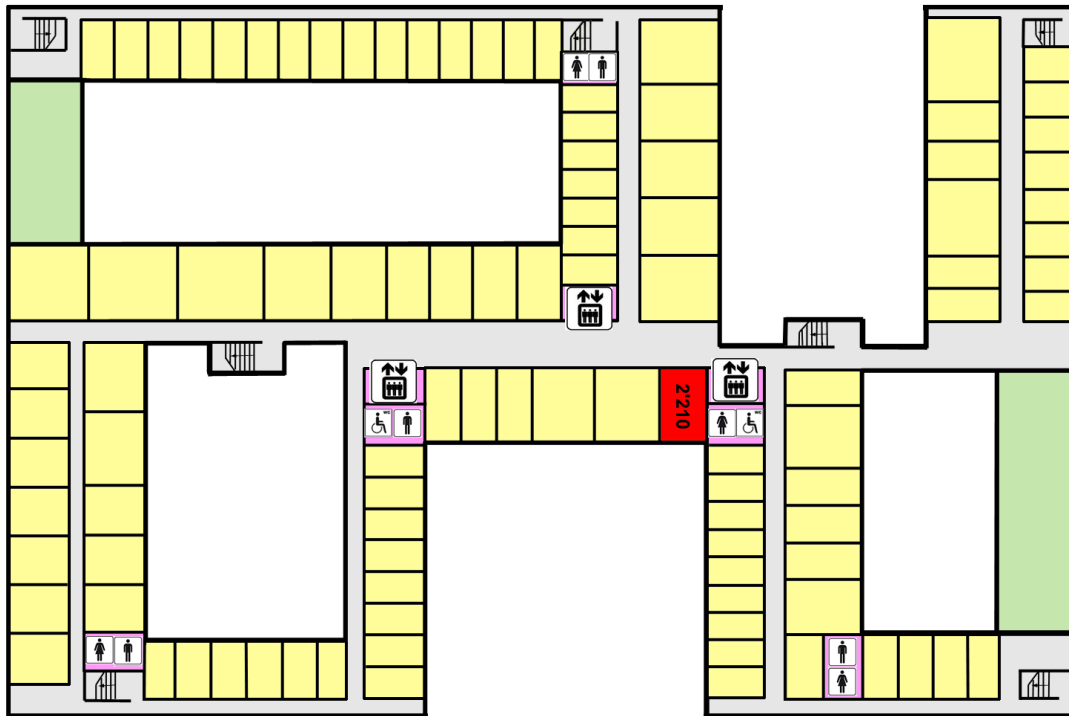


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Institute of Physics

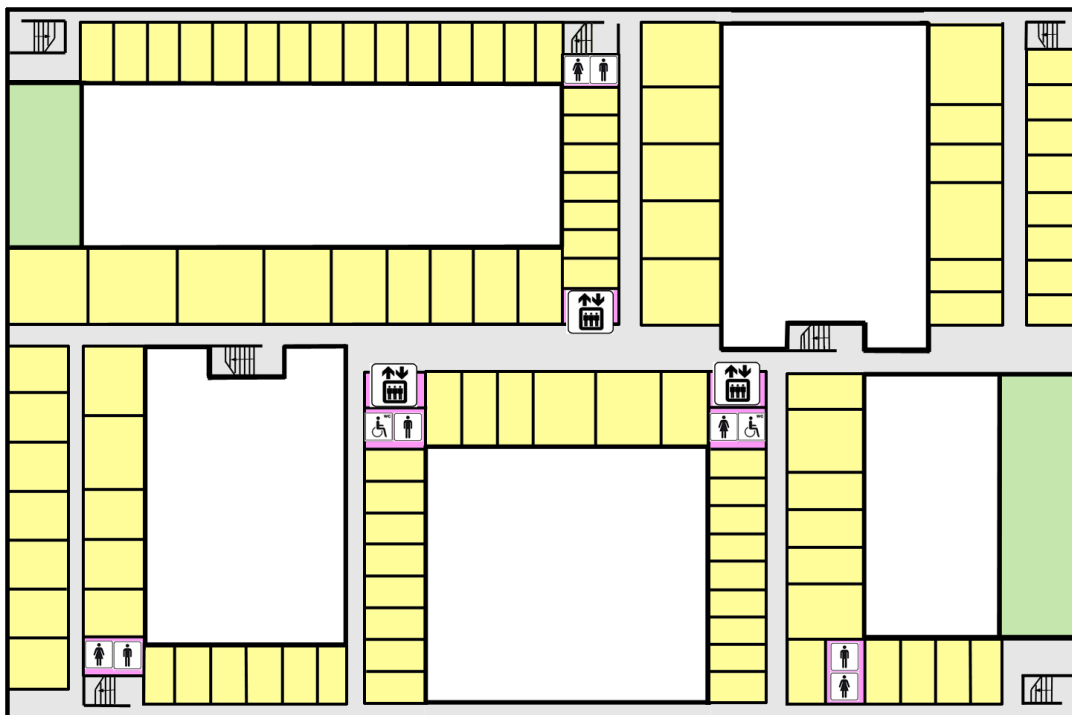
Newtonstr. 15
12489 Berlin



2nd floor



3rd floor



Facets of Electron Crystallography

JULY 7-9, 2010

Berlin Adlershof

PROGRAM

Topics of the day:

Day 1:

High resolution crystallite orientation and phase mapping (HRCOPM) in the TEM

Day 2:

Electron Crystallography (theory and practice), automated techniques and instrumentation

Day 3:

Direct methods, charge flipping, and symmetry determination for electron crystallography

DAY 1: Wednesday, July 7th 2010

Registration 8:00 – 16:00 Foyer at Max Born Lecture Hall

Poster set up, can be continued over the breaks, and group practice sessions

Opening of workshop 9:00 – 9:15 Max Born Lecture Hall
Wolfgang Neumann
(HUB, Germany)

Topic of the day:

High resolution crystallite orientation and phase mapping (HRCOPM) in the TEM

Lectures 9:15 – 15:55 Max Born Lecture Hall

9:15 Wolfgang Neumann (Humboldt University of Berlin, Germany)

Microstructure diagnostics of modern materials by transmission electron microscopy - need for advanced diffraction techniques

9:50 Stavros Nicolopoulos (NanoMEGAS, Belgium)

New techniques for TEM nano-analysis: precession diffraction for structure determination and ("EBSD-TEM like") high resolution crystallite phase/orientation maps

10:35 Coffee break

10:55 Edgar F. Rauch (Grenoble, France)

Coupling template matching and precession electron diffraction for reliable identification of crystallite orientations and phases in TEM

11:45 Muriel Véron (Grenoble, France)

Advanced applications of HRCOPM in materials science

12:35 Peter Moeck (Portland State University, USA)

Structural Fingerprinting in the TEM and open access crystallographic databases

13:05 Lunch

14:15 Stefan Kujawa (FEI Company, The Netherlands)

Imaging and analysis with electrons - where are we today and what are the possibilities for tomorrow?

14:50 Gerd Benner (Carl Zeiss NTS, Germany)

Energy filtered Nano Beam Diffraction (NBD) - the prerequisite for highly resolved crystallography

15:25 Matthias Rodewald (JEOL, Germany)

Atomic scale structural and elemental analysis using the new JEOL JEM-ARM200F

Practical courses 16:00 – 19:00 Institute of Physics, HUB
Room 0'503

16:00 – 17:30 **Group 1 Practice HRCOPM ("EBSD like" - TEM)**

Institute of Physics, HUB Room 0'503	<i>Daniel Bultreys</i>	(NanoMEGAS, Belgium)
	<i>Edgar F. Rauch</i>	(Grenoble, France)
	<i>Muriel Véron</i>	(Grenoble, France)
	<i>Holm Kirmse</i>	(HUB, Germany)

17:30 – 19:00 **Group 2 Practice HRCOPM ("EBSD like" - TEM)**

Institute of Physics, HUB Room 0'503	<i>Daniel Bultreys</i>	(NanoMEGAS, Belgium)
	<i>Edgar F. Rauch</i>	(Grenoble, France)
	<i>Muriel Véron</i>	(Grenoble, France)
	<i>Holm Kirmse</i>	(HUB, Germany)

DAY 2: Thursday, July 8th 2010

Registration 8:00 – 16:30 Foyer at Max Born Lecture Hall

Poster set up, can be continued over the breaks, and group practice sessions

Topic of the day:

Electron Crystallography (theory and practice), automated techniques and instrumentation

Lectures 9:00 – 16:30 Max Born Lecture Hall

9:00 *Sven Hovmoeller* (Stockholm University, Sweden)

Electron crystallography - an introduction

9:35 *Jean-Paul Morniroli* (Université Lille I, France)

Introduction to precession electron diffraction

10:25 Coffee break

10:45 *Ute Kolb* (Johannes Gutenberg-University Germany)

Ab-initio structure solutions of nanocrystalline materials by Automated electron Diffraction Tomography (ADT)

11:35 *Sven Hovmoeller* (Stockholm University, Sweden)

Rotation diffraction method for the collection of 3D data sets

12:25 *Jan Pieter Abrahams* (Leiden Institute of Chemistry, The Netherlands)

Electron Crystallography of Three-Dimensional Protein Crystals

13:10 Lunch

14:00 *Stefan Zaefferer* (Max Planck Institute for Iron Research, Germany)

A critical review of orientation microscopy techniques in SEM and TEM

14:45 *Roland Ries* (Gatan GmbH, Germany)

Development of a fast CCD Camera for Electron Diffraction Imaging in Conventional TEM

15:05 Meiken Falke (Bruker Nano GmbH Berlin, Germany)

Liquid nitrogen free EDS for Scanning Transmission Electron Microscopy

15:25 Peter Oleynikov (AnaliteX, Sweden)

New software developments for electron crystallography: eMap and eSlice

15:45 Sven Hovmoeller (Stockholm University, Sweden)

HRTEM image-based electron crystallography

Practical courses 16:35 – 18:00 Institute of Physics, HUB

Parallel sessions

16:35 – 18:00 **Group 3** **Practice HRCOPM ("EBSD like" - TEM)**

Institute of Physics, HUB Room 0'503	<i>Daniel Bultreys</i> (NanoMEGAS, Belgium) <i>Edgar F. Rauch</i> (Grenoble, France) <i>Muriel Véron</i> (Grenoble, France) <i>Holm Kirmse</i> (HUB, Germany)
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16:35 – 18:00 **Session A** **Objective lens aberration corrected TEM, practice**

Institute of Physics, HUB Room 0'504	<i>Martin Albrecht</i> (Leibniz Institute for Crystal Growth, Germany) <i>N.N.</i> (FEI Company, The Netherlands)
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16:35 – 18:00 **Session B** **ELD -CRISP, possibly also eMap and eSlice**

Institute of Physics, HUB Room 1'428 & 1'429	<i>Sven Hovmoeller</i> (Stockholm University, Sweden)
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Poster session 18:05 – 19:15 Foyer and Max Born Lecture Hall

Party 19:30 – 22:30 at Leibniz Institute for
 sponsored by JEOL Crystal Growth (IKZ)

Introduction to the IKZ, visit of labs, food, beer, announcement of best poster winner

DAY 3: Friday, July 9th 2010

Registration 8:00 – 16:30 Foyer at Max Born Lecture Hall

Topic of the day:

Direct methods, charge flipping, and symmetry determination for electron crystallography

Lectures 9:00 – 12:20 Max Born Lecture Hall

9:00 Jean-Paul Morniroli (Université Lille I, France)

Space group identification from electron diffraction

9:50 Carmelo Giacovazzo (Istituto di Cristallografia, Italy)

Direct methods and electron diffraction data

&

The BEA algorithm: an additional tool for crystal structure solutions from PED data, theory

10:40 Coffee break

11:00 Lukas Palatinus (Academy of Sciences of the Czech Republic, *Czech Republic*)

Solving structures from PED data by charge flipping, theory

11:30 Carmelo Giacovazzo (Istituto di Cristallografia, Italy)

Solve structures with PED by direct methods and the BEA algorithm, theory and exercises

Closing of lecture sessions 12:20 – 12:25 Max Born Lecture Hall

Wolfgang Neumann
(HUB, Germany)

12:25 Lunch

Practical courses 13:25 – 14:55 Institute of Physics, HUB

Parallel sessions

13:25 – 14:55 **Group 4** **Practice HRCOPM ("EBSD like" - TEM)**

Institute of Physics, HUB Room 0'503	<i>Daniel Bultreys</i> <i>Edgar F. Rauch</i> <i>Muriel Véron</i> <i>Holm Kirmse</i>	(NanoMEGAS, Belgium) (Grenoble, France) (Grenoble, France) (HUB, Germany)
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13:25 – 14:55 **Session A** **Objective lens aberration corrected TEM, practice**

Institute of Physics, HUB Room 0'504	<i>Martin Albrecht</i> <i>N.N.</i>	(Leibniz Institute for Crystal Growth, Germany) (FEI Company, The Netherlands)
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13:25 – 14:55 **Session C** **Solving structures from PED data by charge flipping, practice**

Institute of Physics, HUB Room 1'428 & 1'429	<i>Lukas Palatinus</i>	(Academy of Sciences of the Czech Republic, <i>Czech Republic</i>)
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13:25 – 14:55 **Session D** **Solve structures with PED by direct methods and the BEA algorithm, more exercises**

Institute of Physics, HUB Room 1'428 & 1'429	<i>Carmelo Giacovazzo</i>	(Istituto di Cristallografia, Italy)
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Practical courses 15:00 – 16:30 Institute of Physics, HUB

Parallel sessions

15:00 – 16:30 **Group 5** **Practice HRCOPM ("EBSD like" - TEM)**

Institute of Physics, HUB	<i>Daniel Bultreys</i>	(NanoMEGAS, Belgium)
Room 0'503	<i>Edgar F. Rauch</i>	(Grenoble, France)
	<i>Muriel Véron</i>	(Grenoble, France)
	<i>Holm Kirmse</i>	(HUB, Germany)

15:00 – 16:30 **Session A** **Objective lens aberration corrected TEM, practice**

Institute of Physics, HUB	<i>Martin Albrecht</i>	(Leibniz Institute for Crystal Growth, Germany)
Room 0'504	<i>N.N.</i>	(FEI Company, The Netherlands)

15:00 – 16:30 **Session B** **ELD -CRISP, possibly also eMap and eSlice**

Institute of Physics, HUB	<i>Sven Hovmoeller</i>	(Stockholm University, Sweden)
Room 1'428 & 1'429		

15:00 – 16:30 **Session C** **Solving structures from PED data by charge flipping, practice**

Institute of Physics, HUB	<i>Lukas Palatinus</i>	(Academy of Sciences of the Czech Republic, <i>Czech Republic</i>)
Room 1'428 & 1'429		