

HERCULES

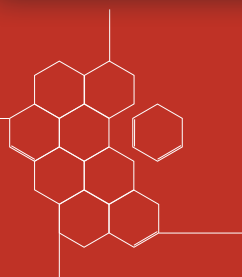
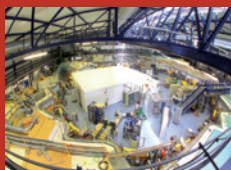
European School

Neutrons and synchrotron radiation
for science

2020

**March 2nd
to April 3rd**

**Grenoble
FRANCE**



HERCULES

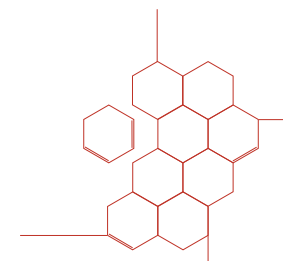
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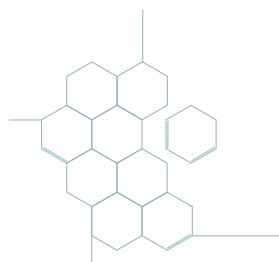
ORGANISATION

ORGANISED BY:

- › Université Grenoble Alpes (UGA)
- › Grenoble INP

SCIENTIFIC ADVISORY COMMITTEE

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SUPPORTED BY:

- › European Commission project CALIPSOplus
- › DECTRIS
- › European Synchrotron Radiation Facility (ESRF)
- › Institut Laue Langevin (ILL)
- › Institut de Biologie Structurale (IBS)
- › Deutsches Elektronen-Synchrotron (DESY)
- › European XFEL
- › Elettra Sincrotrone Trieste:
 - Elettra
 - FERMI
- › Centre National de la Recherche Scientifique (CNRS):
 - Institut National de Physique
 - Laboratoires du Polygone Louis Néel, Grenoble
- › Commissariat à l'énergie atomique (CEA):
 - Direction de la Recherche Fondamentale (DRF)
- › Synchrotron SOLEIL
- › Swiss Light Source (SLS) - Paul Scherrer Institute (PSI)
- › Grenoble Innovation for Advanced New Technologies (GIANT)
- › KIT
- › ALBA
- › FOSTERING SCIENCE
- › Grenoble Alpes Métropole (La Métro)
- › Ministère de l'enseignement supérieur, de la recherche et de l'innovation (MESRI), programme ACCES 2020

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GENERAL INFORMATION

HERCULES is a course designed for training students and scientists from European universities and laboratories in the field of neutron and synchrotron radiation. It includes a common part during a week and a half, followed thereafter by two parallel sessions which are:

Session A:

Physics and chemistry of condensed matter (40 full time and 5 part time participants).

Session B:

Biomolecular structure and dynamics (20 full time participants).

It mainly takes place in Grenoble, at the "Maison des Magistères" on the Polygone Scientifique Louis Néel, where the Institut Laue Langevin (ILL) and the European Synchrotron Radiation Facility (ESRF) are also located.

The HERCULES course includes lectures, tutorials, practicals and visits of laboratories.

It also includes two weeks of practicals and lectures at two different locations (16th to 20th March then 23rd to 27th March) outside Grenoble:

Barcelona-Paris Group:

- at the Spanish synchrotron source, **ALBA**, near Barcelona,
- then on the Paris-Saclay campus, near Paris, at the French synchrotron source **SOLEIL**, with a wide programme on synchrotron science,

Trieste-Hamburg Group:

- in Italy (near Trieste) at **Elettra and FERMI**,
- then in Germany (Hamburg) at **DESY and European XFEL**.

In both places, the programme includes synchrotron and FEL science.

Karlsruhe-Villigen Group:

- in Germany (Karlsruhe) at **KIT Light Source**, with a vast programme of synchrotron science,
- then in Switzerland (Villigen) at **Swiss Light Source (SLS)**, with a programme including synchrotron techniques, as well as lectures and visits about neutrons, muons, and FEL science.

The language of the course is **English**.

LOCATION AND TIMES OF LECTURES, PRACTICALS AND TUTORIALS



Timetable and locations will be provided to you at the beginning of the school.

LECTURES

When:

(see timetable enclosed in the brochure)

- in the morning from **8:45 to 12:25** with a coffee break at 10:25 (except on the first day when it starts at 8:30).
- in the afternoon from **14:00 to 17:40** with a break at 15:40.

Where:

- in the Maison des Magistères amphitheatre located on the CNRS site (see map on page 15).

PRACTICALS AND TUTORIALS

See enclosed the complete list of practicals and tutorials allocated to different groups. The nominative list of groups, together with the practicals and tutorials programme assigned to each of them, will be provided in a separate "daily information" booklet, distributed at the beginning of the school.

VISITS OF LARGE SCALE FACILITIES

- ILL:** B. GRENIER – L. MANGIN-THRO
- ESRF:** G. BEUTIER – M. KRISCH
- ALBA:** B. CALISTO – M. KREUZER – D. PIERUCCI
- Synchrotron SOLEIL:** A. COATI – L. NATAF
- Elettra and FERMI:** N. DEMITRI – L. FOGLIA – E. PEDERSOLI – B. ROSSI
- PSI:** J. G.-H. DREISER – P. HEMBERGER
- DESY and European XFEL:** R. GEHRKE – O. SEECK – S. PASCARELLI – T. TSCHENTSCHER
- KIT:** T. BAUMBACH – M. HAGELSTEIN – A. PLECH



PRACTICAL INFORMATION

TRAVEL INFORMATION

Participants are expected to arrive in Grenoble on **Sunday 1st March 2020**.



TRAINS:

From Paris, Geneva, Milano, Barcelona, etc... arrive at Grenoble train station (Gare SNCF)

Paris-Grenoble by TGV train (high speed train):

www.oui.sncf



INTERNATIONAL FLIGHTS:

Arrival at Lyon Saint-Exupéry (LYS) airport (about 90 kms from Grenoble).

There is a shuttle bus connection from the airport to Grenoble bus/train station and a few trains:

<https://fr.ouibus.com/trajets/lyon-grenoble>

Arrival also possible at Geneva (CH) airport (about 160 kms from Grenoble).

There is a shuttle bus connection from the Geneva airport to Grenoble bus station:

<https://fr.ouibus.com/trajets/geneve-aeroport-grenoble>



DOMESTIC FLIGHTS FROM PARIS (and a few international flights):

Arrival at Grenoble Isère (GNB) airport (about 40 kms from Grenoble).

Regular shuttle bus connection to Grenoble bus/train station:

<https://www.actibus.com/havette-aeroport-grenoble>

WELCOME



When you arrive in Grenoble, whether it is by train, plane or car, **please report to the HERCULES desk in the Hotel "Hipark by Adagio Grenoble", situated just behind the train station, between 5:30 PM and 9:00 PM on Sunday 1st March 2020**. A 'buffet' for dinner will be served from 7:00 to 9:00 PM.

ACCOMMODATION



Participants who have asked for accommodation will be staying in the following hotel:

HIPARK BY ADAGIO

6 rue Auguste Genin - 38000 GRENOBLE

Tel : +33 (0)4 76 39 20 00

Fax : +33 (0)4 76 84 16 83

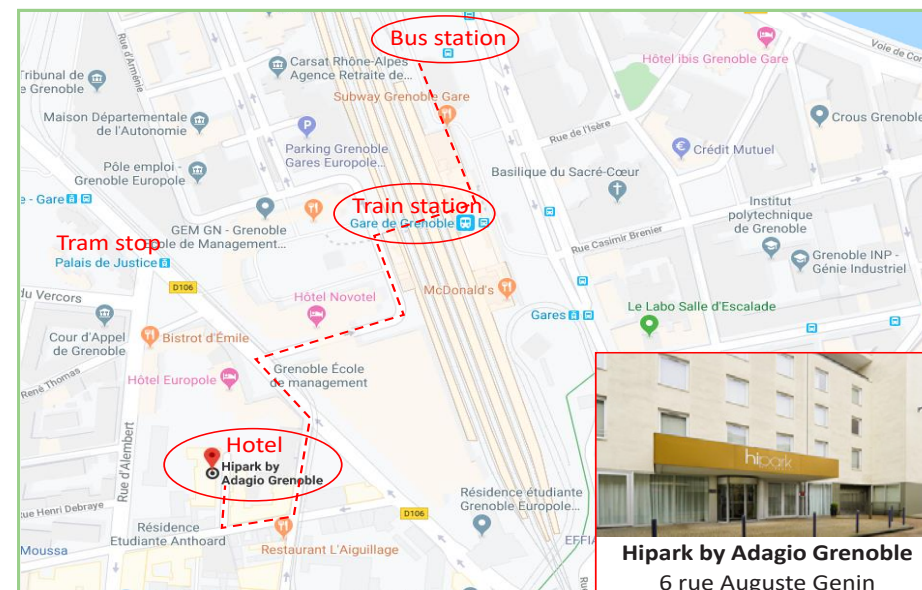
hb2r8@adagio-city.com

Small studio flats are booked from **Sunday 1st March evening to Friday 3rd April morning** in Grenoble and accommodation is organised for the nights in Barcelona, Paris-Saclay, Trieste, Hamburg, Karlsruhe, and Villigen.

A room will be specially booked in Grenoble to store your luggage during the travel outside Grenoble.

The hotel is close to bus and tram stops.

How to go to the hotel from the train/bus station?



MEALS



› Breakfast:

Continental breakfast is available in the hotel from 7:00 AM during the week and from 7:30 AM on the weekends. It is included with the room in the fees.

› Lunch:

Lunch will be taken in the **ILL / ESRF restaurant** during the stay in Grenoble (excluding the weekend). This restaurant is close to the lectures place. We will provide you with a canteen card, which will be credited by ESRF for week-day lunches.

For your information, each dish is indicated by a number of points. Coffee is also available in the cafeteria next to the restaurant.

› Dinner:

Dinners and weekend meals are not supported by HERCULES. There are many reasonably priced restaurants near the hotel or it will be possible to cook in your studio flat.

ENTERTAINMENT



There is a good choice of restaurants, cinemas, concerts, theatres ... in Grenoble city centre. Several ski resorts are less than one hour drive from Grenoble (direct bus lines available).

For social events organised by HERCULES see the daily information document (snow-shoes outing, dinner party...)

PUBLIC TRANSPORTATION



How to go to the lectures place (CNRS site) from the hotel?

The course takes place at the **Maison des Magistères amphitheatre** on the CNRS site located on the Polygone Scientifique Louis Néel, just outside the city. You can either use **public transportation** (see hereafter) or walk to get there (30 min).

› **Tramway line B** connects directly the hotel to the Polygone Scientifique terminus "Oxford" (get on the tram at "Palais de justice" or "Saint-Bruno" tram stop, shown on the map page 13).

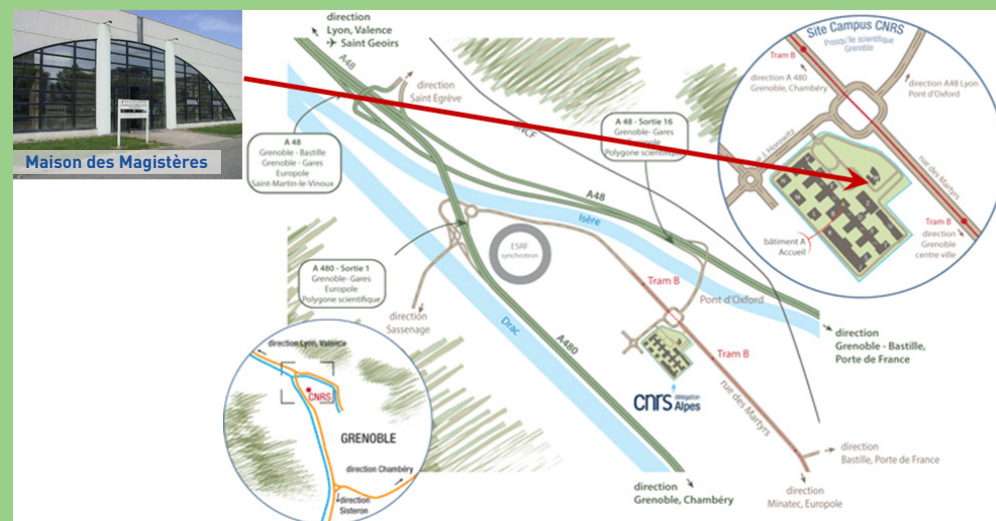
You can buy tickets for public transportation from "TAG" desks on the tram platforms and from tobacco shops (current price: 14.50 € for 10 tickets, or 1.60€ for one ticket (2.10 € on board of the bus)). Tickets are valid for all lines (tram and buses). A ticket is valid for one hour including connections. You have to punch it every time you get on a bus (inside) or tram (before entering it).



› You can also **hire a bike** at the Métrovélo agency located in front of the train station.



› For those who come **by car**, be aware that parking the car downtown or near the station is expensive. You can park at the Maison des Magistères. In this case, please give the information to the HERCULES staff, at the Maison des Magistères.



You should have received your CNRS clearance by email. This clearance, accompanied by a valid ID, must be submitted when entering the site as well as when leaving it, so that presence can be logged.

The security officer needs time to check one by one your identity document (ID or passport). Please arrive in advance at the CNRS entrance gate in order not to be late for the lectures.

MAIL

You can buy stamps at tobacco shops and post-offices. The closest post office to the hotel is located "16 Place Saint-Bruno".

ELECTRONIC MAIL

You will be able to use computer facilities as well as a **wireless network** in the "Maison des Magistères", ground floor.

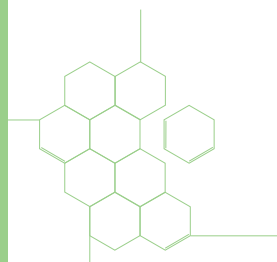
BANKS

You will, of course, find banks downtown.
The nearest ones are "Société Générale" and "Banque Populaire Auvergne Rhône Alpes" located 10 and 10Bis rue Abbé Grégoire.

POSTER SESSION

A **poster session** will be organised on Friday 6th March afternoon. The poster session is an opportunity given to you to present your recent research activities to other HERCULES participants as well as to Grenoble scientists.

It is an important aspect of the HERCULES school. This enables one to initiate an interface between the participants and the local scientific community.
Please prepare your poster in advance and bring it with you to Grenoble.
For your information, the maximum size of the poster should be about:
0.85 m wide x 1.15 m high.

**STAY IN BARCELONA, PARIS-SACLAY, TRIESTE, HAMBURG, KARLSRUHE, AND VILLIGEN****Travel is organised and supported by HERCULES.**

Always carry your identity card/passport with you, as it can be asked when crossing the country borders and it is mandatory for entering on the various sites.

Barcelona – Paris Group:

- ▶ Grenoble to Barcelona on **Sunday 15th March**
- ▶ Barcelona to Paris-Saclay on **Sunday 22nd March**
- ▶ Paris-Saclay to Grenoble on **Sunday 29th March**

Trieste – Hamburg Group:

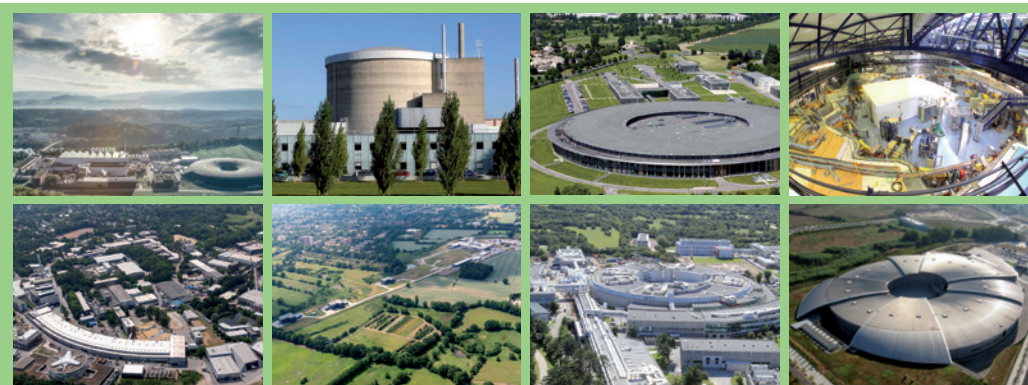
- ▶ Grenoble to Trieste on **Sunday 15th March**
- ▶ Trieste to Venice on **Saturday 21st March**
- ▶ Venice to Hamburg on **Sunday 22nd March**
- ▶ Hamburg to Grenoble on **Sunday 29th March**

Karlsruhe – Villigen Group:

- ▶ Grenoble to Karlsruhe on **Sunday 15th March**
- ▶ Karlsruhe to Villigen on **Sunday 22nd March**
- ▶ Villigen to Grenoble on **Friday 27th March**



You will be accommodated in guest house or in double room in hotel.



PROGRAMME IN GRENOBLE

COMMON LECTURES



EMBL



BASIC METHODS AND INSTRUMENTS

- ▶ Diffraction, refraction and absorption of X-rays and neutrons *V. Favre-Nicolin*
- ▶ Introduction to synchrotron radiation *D. Attwood*
- ▶ Soft X-rays and VUV: specific optics and applications *D. Attwood*
- ▶ Neutrons: scattering and instrumentation *A. Wildes*
- ▶ Neutron and X-ray diffraction by crystals: kinematical approximation and experimental diffraction methods *TBD*
- ▶ Hard X-ray optics for synchrotron radiation beamlines *R. Barrett*
- ▶ Introduction to small angle scattering *M. Blankenburg*
- ▶ Introduction to imaging techniques *F. Marone*
- ▶ X-ray Detectors *H. Graafsma*
- ▶ Introduction to neutron and X-ray inelastic scattering *C. Alba-Simionesco*
- ▶ Full-field coherent imaging *P. Cloetens*
- ▶ Introduction to X-ray Spectroscopies and Fundamentals of X-ray Absorption Fine Structure *S. Pascarelli*
- ▶ Free Electron Lasers and ultra fast applications *S. Pascarelli*
- ▶ Science at neutron spallation sources: exploiting accelerator based facilities *S. Langridge*

REFRESHER LECTURES

- ▶ Crystallography *C. Colin*
- ▶ Introduction to magnetism *L. Paolasini*
- ▶ Fourier Transform: basic concepts (online lecture slides) *C. Boote*
- ▶ Quantum Mechanics (online lecture slides) *E. Belorizky*

SESSION A: PHYSICS AND CHEMISTRY OF CONDENSED MATTER

LECTURES

I- Interaction of radiation with matter: scattering

- Disorder and its effects on neutron and X-ray diffraction *M. de Boissieu*
- Dynamical diffraction theory *T. Baumbach*
- Magnetic neutron scattering *B. Grenier*
- Neutron and X-ray reflectometry *O. Seeck*
- Polarized neutrons: theoretical and experimental techniques *S. Langridge*
- Polarized X-rays *U. Staub*
- Powder diffraction *R. Cerny*
- Resonant diffraction (MAD, DAFS) *V. Favre-Nicolin*
- Single crystal structure analysis *E. Espinosa*

II- Interaction of radiation with matter: spectroscopy

- Inelastic X-ray scattering *M. Krisch*
- Neutron time-of-flight, spin echo and back-scattering spectroscopies *T. Perring*
- Neutron triple axis spectroscopy *B. Lake*
- Photoelectron spectroscopy from UV to soft X-rays *H. Dil*
- X-ray absorption spectroscopy: theoretical basis *G. Radtke*
- X-ray photon correlation spectroscopy *G. Grübel*
- X-ray photoemission electron microscopy *C.M. Schneider*

III- Interaction of radiation with matter: imaging

- Coherent diffraction imaging and ptychography *M. Guizar-Sicairos*

IV- Special topics and selected examples of applications

- Ancient materials research with synchrotron and neutron techniques *S. Schoeder*
- Coherent and transient states studied with X-rays FELS *C. Callegari*
- Liquid and amorphous materials *A. Barnes*
- Soft condensed matter *A. Rennie*
- Solving surface problems using SR techniques *G. Renaud*
- Magnetic X-ray and neutron reflectivity *H. Zabel*
- Nanostructures in the light of synchrotron radiation *G. Renaud*

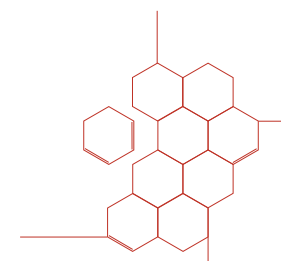
HERCULES 2020: PROGRAMME OF LECTURES

(subject to modification)

Updated : 20/02/2020

- Common lectures
- Session A lectures
- Other

Week 1	Monday 2/03	Tuesday 3/03	Wednesday 4/03	Thursday 5/03	Friday 6/03
8:30 - 8:45 8:45 - 9:30 10' break 9:40 - 10:25	Welcome	Diffraction, refraction and absorption of X-rays and neutrons (1/2) V. Favre-Nicolin	Diffraction, refraction and absorption of X-rays and neutrons (2/2) V. Favre-Nicolin	Introduction to imaging techniques Federica Marone	X-ray detectors Heinz Graafsma
10:45 - 11:30 10' break 11:40 - 12:25	ESRF / ILL badges distribution	Crystallography (1/2) Claire Colin	Neutrons: scattering and instrumentation (1/2) Andrew Wildes	Neutrons: scattering and instrumentation (2/2) Andrew Wildes	Crystallography (2/2) Claire Colin
14:00 - 14:45 10' break 14:55 - 15:40	ESRF / ILL visits	Introduction to synchrotron radiation David Attwood	Neutron and X-ray diffraction by crystals: kinematical approximation and experimental methods TBD	Introduction to small angle scattering Malte Blankenburg	POSTER SESSION
16:00 - 16:45 10' break 16:55 - 17:40	16:00 - 17:30 ESRF / ILL presentations Michael Krish / Helmut Schober 17:30 - 17:45 UGA presentation	ESRF / ILL visits	Hard X-ray optics for SR beamlines Ray Barrett	Full-field coherent Imaging Peter Cloetens	
	18:00 Welcome cocktail at ILL				17:00: NFFA.eu Ennio Capria 17:15 Poster awards
					19:30 Gala dinner



Week 2	Monday 9/03	Tuesday 10/03	Wednesday 11/03	Thursday 12/03	Friday 13/03
8:45 - 9:30 10' break 9:40 - 10:25	Introduction to neutron and X-Ray inelastic scattering Christiane Alba Simionescu	Magnetic neutron scattering Béatrice Grenier	Polarized X-rays Urs Staub	Disorder and its effects on neutron and X-ray diffraction Marc de Boissieu	Soft condensed matter Adrian Rennie OR Solving surface problems using SR techniques Gilles Renaud
10:45 - 11:30 10' break 11:40 - 12:25	Introduction to magnetism Luigi Paolasini	Dynamical diffraction theory Tilo Baumbach	Polarized neutrons: theoretical and experimental techniques Sean Langridge	Neutron and X-ray reflectometry Oliver Seeck	Coherent diffraction imaging and ptychography Manuel Guizar-Sicairos
14:00 - 14:45 10' break 14:55 - 15:40	Introduction to X-ray Spectroscopies and Fundamentals of X-ray Absorption Sakura Pascarelli	FELs & ultrafast applications Sakura Pascarelli	TUTORIALS / LABS	Liquid and amorphous materials Adrian Barnes	Powder diffraction Radovan Cerny
16:00 - 16:45 10' break 16:55 - 17:40	Fine Structure Sakura Pascarelli	Science at neutron spallation sources Sean Langridge		Single crystal structure analysis Enrique Espinosa	Resonant diffraction (MAD, DAFS) Vincent Favre-Nicolin
18:00 - 19:00	Ancient materials research with synchrotron and neutron techniques Sebastian Schoeder	17:45 - 18:00 Fostering Science presentation Thibaud David David Argenti		17:45 - 18:05 DECTRIS presentation Dubravka Sisak Jung	

Week 3 (16th – 20th March), and **week 4** (23th – 27th March): Outside Grenoble

Week 5	Monday 30/03	Tuesday 31/03	Wednesday 1/04	Thursday 2/04	Friday 3/04
8:45 - 9:30 10' break 9:40 - 10:25	ILL PRACTICALS / TUTORIALS	X-ray absorption spectroscopy: theoretical basis Guillaume Radtke	Photoelectron spectroscopy from UV to soft X-rays (1/2) Hugo Dil	Inelastic X ray scattering Michael Krisch	Nanostructures in the light of synchrotron radiation Gilles Renaud
10:45 - 11:30 10' break 11:40 - 12:25		Coherent and transient states studied with X-rays FELS Carlo Callegari	Photoelectron spectroscopy from UV to soft X-rays (2/2) Hugo Dil	Neutron triple axis spectroscopy Bella Lake	Hercules Mythology Chris Buckley 12:00 Farewell wine and cheese lunch
14:00 - 14:45 10' break 14:55 - 15:40	ILL PRACTICALS / TUTORIALS	X ray photon correlation spectroscopy Gerhard Grübel	X-ray photo-emission electron microscopy Claus M. Schneider	TUTORIALS / LABS	
16:00 - 16:45 10' break 16:55 - 17:40		Magnetic X-ray and neutron reflectivity Hartmut Zabel	Neutron time of flight, spin echo and back-scattering spectroscopies Tobias Perring		
18:00 - 19:00			EVALUATION MEETING		

PRACTICALS AND TUTORIALS Session A



COORDINATORS:

- **Grenoble:** G. BEUTIER, A. FERNANDEZ-MARTINEZ, B. GRENIER, L. MANGIN-THRO
- **Barcelona:** B. CALISTO, M. KREUZER, D. PIERUCCI, M. J. SIMANCAS
- **Paris-Saclay:** A. COATI, L. NATAF
- **Trieste:** N. DEMITRI, L. FOGLIA, E. PEDERSOLI, B. ROSSI
- **Hamburg:** R. GEHRKE, S. PASCARELLI, O. SEECK, T. TSCHENTSCHER
- **Karlsruhe:** T. BAUMBACH, M. HAGELSTEIN, L. JOCHIM, A. PLECH
- **Villigen:** J. DREISER, M. FÜGLISTER, P. HEMBERGER

Due to the long shutdown of the European Synchrotron Radiation Facility, there will be no ESRF practicals this year, but all full time participants will go outside Grenoble for 2 weeks on 2 different locations, with practicals on each site. Furthermore, the European Institut Laue Langevin (ILL) high flux reactor will restart after the end of the school, but hands-on simulated neutron practicals are nevertheless maintained at ILL.

In Grenoble, all participants (including part-time participants) will carry out a practical at ILL, as well as a tutorial at ESRF, ILL, and/or CNRS (full-time participants will follow one additional practical or tutorial). Some laboratories at CEA – INAC, Institut Néel, LNCMI, and ILL will also welcome some practicals (LABS) allowing the participants to discover techniques they are not used to (each participant will follow one of them).

Additional practicals will be organized for each full-time participant on 2 different sites among our 6 partner facilities, with three groups:

- the Spanish synchrotron source ALBA near Barcelona, then the French synchrotron radiation facility SOLEIL near Paris (Barcelona-Paris Group)
- the Italian synchrotron light source Elettra and Free Electron laser Radiation for Multidisciplinary Investigations (FERMI) in Trieste, then the German synchrotron radiation facility Deutsches Elektronen-Synchrotron (DESY) and the European XFEL in Hamburg (Trieste-Hamburg Group)
- the KIT Light Source in Karlsruhe, then the Swiss synchrotron radiation facility Swiss Light Source (SLS) at the Paul Scherrer Institute (PSI) in Villigen (Karlsruhe - Villigen Group).

Full time participants have been assigned to one of these travel groups. For the purpose of practicals, groups of four participants have been arranged in agreement with their main research interests and wishes expressed, also taking into account organisational constraints. Each group of 4 will perform selected practicals and tutorials (about 14 half-days during the whole school).



All participants are required to attend the entire practical and tutorial programme assigned to them.

Neutron Practical at ILL, Grenoble		
Local coordinators: Béatrice GRENIER and Lucile MANGIN-THRO		
Name	Instructor(s)	Title
D1B (a)	Françoise DAMAY	Powder diffraction: crystal structure refinement using Fullprof
D1B (b)	Claire COLIN	Powder diffraction: crystal and magnetic structure refinement using Fullprof
CYCLOPS	Laura CANADILLAS DELGADO, Oscar FABELLO ROSA	Neutron Laue diffraction on antiferromagnetic MnO: indexation of nuclear and magnetic Bragg reflections in a Laue pattern
D23	Ketty BEAUVOIS	Single crystal diffraction: crystallographic and magnetic structure refinement using Fullprof
D17	Thomas SAERBECK	Exploring thin-film structure and magnetism with neutron reflectometry
D33	Nina-Juliane STEINKE	Small angle scattering using polarized neutrons
D50	Lukas HELFEN, Alessandro TENGATTINI	Acquisition and analysis of X-ray and neutron tomography
IN3	Ursula HANSEN	Phonons in the high temperature superconductor LSCO studied with triple axis spectroscopy
IN6	Sylvain PETIT	Analysis of time of flight inelastic neutron scattering data
IN16B	Markus APPEL, Tilo SEYDEL	Cold neutron backscattering spectroscopy

Practicals in laboratories (Labs) at CEA, CNRS, and ILL, Grenoble			
Local coordinator: Béatrice GRENIER			
Name	Site	Instructor	Title
LAB1	ILL	Pierre COURTOIS	Characterization of mosaic crystals using hard X-Ray diffraction; Application for the manufacturing of neutron monochromators
LAB2	CEA	Arnaud DE GEYER	Small angle X-ray scattering
LAB3	CEA	Jacques PECAUT	Small molecule structure resolution using single-crystal X-ray diffraction
LAB4	CNRS	Olivier LEYNAUD	X-ray powder diffraction
LAB5	CNRS	Eric MOSSANG	Reflectometry and GIXRD
LAB6	CNRS	Marc-Henri JULIEN	Nuclear Magnetic Resonance in an antiferromagnet

Tutorials at ILL, Maison des Magistères (MM), CNRS, and ESRF, Grenoble			
Local coordinator: Béatrice GRENIER			
Name	Site	Instructor(s)	Title
T1	ILL	Alberto RODRIGUEZ VELAMAZAN	Crystal and magnetic structure determination using single crystal neutron diffraction and the Fullprof suite
T2	ILL	Henry FISCHER	From Q-space to R-space: PDF-analysis
T3	ILL	Arnaud MORIN	Small Angle Scattering in Proton Exchange Membrane Fuel Cell
T4	CNRS	Yves JOLY	Simulation of X-ray absorption spectroscopies
T5(a)	CNRS	Jean-Sébastien MICHA	White Beam Microdiffraction
T5(b)	ESRF		
T6	ESRF	Marius RETEGAN	X-ray spectroscopy simulations using semi-empirical multiplet approaches
T7	ESRF	Juan REYES HERERRA	Modeling a SR beamline
T8(a)	ESRF	Francesco D'ACAPITO	Introduction to EXAFS data analysis
T8(b)		Alessandro PURI	
T9	ESRF	Olivier PROUX	Basic Principles of EXAFS analysis
T10	ESRF	Vincent FAVRE-NICOLIN	Ab initio structure determination from powder diffraction (FOX software)

SESSION B: BIOMOLECULAR STRUCTURE AND DYNAMICS

LECTURES

I- Introduction

- Basics of protein crystallography, data collection, data reduction, phasing *M. Roe*
- Introduction to current trends and challenges of molecular and structural biology *C. Sauter*
- Neutron crystallography *M. Blakeley*

II- Protein dynamics

- Dynamics of macromolecules *G. Zaccai*
- Protein dynamics by neutron scattering *G. Zaccai*

III- Diffusion and diffraction on larger scale biological systems

- Biological small angle X-ray scattering *J. Perez*
- Crystallography of viruses and very large macromolecules *D. Stuart*
- Fibre diffraction *C. Boote*
- Small angle neutron scattering *F. Gabel*

IV- Spectroscopy

- Local order by X-ray absorption spectroscopy *W. Meyer-Klaucke*
- Time-resolved fluorescence and circular dichroism studies with SR *D. Clarke*

V- Imaging

- Coherent diffraction imaging and ptychography *C. Jacobsen*
- Medical imaging with synchrotron radiation *G. Tromba*

VI- Special topics

- Analysis and visualization of 3D X-ray data *C. Buckley*
- Ancient materials research with synchrotron and neutron techniques *S. Shoeder*
- Crystal growth and low resolution structures *M. Spano*
- Electron microscopy for structural biology *A. Desfosses*
- Membrane diffraction *D. Barlow*
- Native Mass Spectrometry to study intact protein complexes *E. Boeri-Erba*
- Non-crystallographic ways of obtaining structural and dynamical information at different length and time scales for biological systems *P. Judge*
- Nuclear Magnetic Resonance *M. Blackledge*
- Super-resolution fluorescence microscopy *D. Bourgeois*
- X-ray and neutron reflectivity in biophysics *Y. Gerelli*

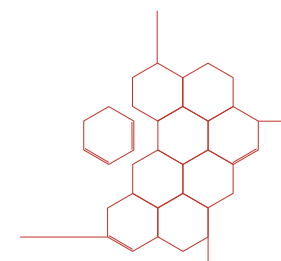
HERCULES 2020: PROGRAMME OF LECTURES

(subject to modification)

Updated : 20/02/2020

- Common lectures
- Session A lectures
- Other

Week 1	Monday 2/03	Tuesday 3/03	Wednesday 4/03	Thursday 5/03	Friday 6/03
8:30 - 8:45 8:45 - 9:30 10' break 9:40 - 10:25	Welcome	Diffraction, refraction and absorption of X-rays and neutrons (1/2) V. Favre-Nicolin	Diffraction, refraction and absorption of X-rays and neutrons (2/2) V. Favre-Nicolin	Introduction to imaging techniques Federica Marone	X-ray detectors Heinz Graafsma
10:45 - 11:30 10' break 11:40 - 12:25	ESRF / ILL badges distribution	Crystallography (1/2) Claire Colin	Neutrons: scattering and instrumentation (1/2) Andrew Wildes	Neutrons: scattering and instrumentation (2/2) Andrew Wildes	Crystallography (2/2) Claire Colin
14:00 - 14:45 10' break 14:55 - 15:40	ESRF / ILL visits	Introduction to synchrotron radiation David Attwood	Neutron and X-ray diffraction by crystals: kinematical approximation and experimental methods TBD	Introduction to small angle scattering Malte Blankenburg	POSTER SESSION
16:00 - 16:45 10' break 16:55 - 17:40	16:00 - 17:30 ESRF / ILL presentations Michael Krish / Helmut Schober 17:30 - 17:45 UGA presentation	ESRF / ILL visits	Hard X-ray optics for SR beamlines Ray Barrett	Full-field coherent Imaging Peter Cloetens	
	18:00 Welcome cocktail at ILL				17:00: NFFA.eu Ennio Capria 17:15 Poster awards
					19:30 Gala dinner



Week 2	Monday 9/03	Tuesday 10/03	Wednesday 11/03	Thursday 12/03	Friday 13/03
8:45 - 9:30 10' break 9:40 - 10:25	Introduction to neutron and X-Ray inelastic scattering Christiane Alba Simionescu	Basics of protein crystallography, data collection, phasing (1/2) and (2/2) Mark Roe	Introduction to current trends and challenges of molecular and structural biology Claude Sauter	Non-crystallographic ways of obtaining structural and dynamical information at different length and time scales for biological systems Peter Judge	IBS+ESRF LABS / TUTORIALS
10:45 - 11:30 10' break 11:40 - 12:25	Introduction to magnetism Luigi Paolasini		Neutron crystallography Matthew Blakekey	Biological Small Angle X-Ray Scattering Javier Perez	
14:00 - 14:45 10' break 14:55 - 15:40	Introduction to X-ray Spectroscopies and Fundamentals of	FELs & ultrafast applications Sakura Pascarelli	Nuclear Magnetic Resonance Martin Blackledge	Electron microscopy for structural biology Ambroise Desfosses	IBS+ESRF LABS / TUTORIALS
16:00 - 16:45 10' break 16:55 - 17:40	X-ray Absorption Fine Structure Sakura Pascarelli	Science at neutron spallation sources Sean Langridge	Super-resolution fluorescence microscopy Dominique Bourgeois	Crystal growth and low resolution structures Monika Spano	
18:00 - 19:00	Ancient materials research with synchrotron and neutron techniques Sebastian Schoeder	17:45 - 18:00 Fostering Science presentation Thibaud David David Argenti		17:45 - 18:05 DECTRIS presentation Dubravka Sisak Jung	

Week 3 (16th – 20th March), and **week 4** (23th – 27th March): Outside Grenoble

Week 5	Monday 30/03	Tuesday 31/03	Wednesday 1/04	Thursday 2/04	Friday 3/04
8:45 - 9:30 10' break 9:40 - 10:25	Native Mass spectrometry to study intact protein complexes Eli. Boeri Erba	ILL PRACTICALS /	Medical imaging with synchrotron radiation Giuliana Tromba	Coherent diffraction imaging and ptychography Chris Jacobsen	Analysis and visualization of 3D X-Ray data Chris Buckley
10:45 - 11:30 10' break 11:40 - 12:25	Local order by X-Ray absorption spectroscopy Wolfram Meyer-Klaucke		Membrane diffraction David Barlow	X-Ray and neutron reflectivity in biophysics Yuri Gerelli	Hercules Mythology Chris Buckley 12:00 Farewell wine and cheese lunch
14:00 - 14:45 10' break 14:55 - 15:40	Crystallography of viruses and very large macromolecules David Stuart	ILL PRACTICALS /	Dynamics of macromolecules Giuseppe Zaccai	Small angle neutron scattering Frank Gabel	
16:00 - 16:45 10' break 16:55 - 17:40	Fibre diffraction James Bell		Protein dynamics by neutron scattering Giuseppe Zaccai	Time resolved fluorescence and circular dichroism studies with SR David Clarke	
18:00 - 19:00			EVALUATION MEETING		

PRACTICALS AND TUTORIALS Session B



COORDINATORS:

- **Grenoble:** B. DEME, B. GRENIER, P. PERNOT, G. SCHIRO
- **Barcelona:** B. CALISTO, M. KREUZER, D. PIERUCCI, M. J. SIMANCAS
- **Paris-Saclay:** A. COATI, L. NATAF
- **Trieste:** N. DEMITRI, L. FOGLIA, E. PEDERSOLI, B. ROSSI
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- **Karlsruhe:** T. BAUMBACH, M. HAGELSTEIN, L. JOCHIM, A. PLECH
- **Villigen:** J. DREISER, M. FÜGLISTER, P. HEMBERGER

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In Grenoble, all participants will carry out two practicals at ILL and two hands-on experiments / data treatment sessions (labs / tutorials), both at Institut de Biologie Structurale (IBS), or one at IBS and the other one at ESRF.

Additional practicals will be organized for each full-time participant on 2 different sites among our 6 partner facilities, with three groups:
 → the Spanish synchrotron source ALBA near Barcelona, then the French synchrotron radiation facility SOLEIL near Paris (Barcelona-Paris Group)
 → the Italian synchrotron light source Elettra and Free Electron laser Radiation for Multidisciplinary Investigations (FERMI) in Trieste, then the German synchrotron radiation facility Deutsches Elektronen-Synchrotron (DESY) and the European XFEL in Hamburg (Trieste-Hamburg Group)
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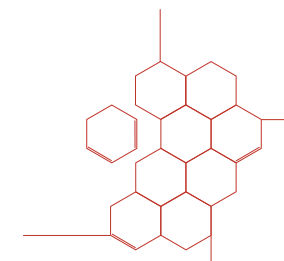


All participants are required to attend the entire practical and tutorial programme assigned to them.

Neutron Practical at ILL, Grenoble Local coordinators: Bruno DEME and Petra PERNOT		
Name	Instructor	Title
FIGARO	Armando MAESTRO	Life in two dimensions: From soft to biological matter elucidated by neutron reflectometry
D11	Sylvain PREVOST	Small-Angle Neutron Scattering
LADI-III	Nicolas COQUELLE	Neutron macromolecular crystallography using the quasi-Laue diffractometer
IN13	Judith PETERS	Molecular dynamics of biological samples probed by incoherent neutron scattering
IN15	Ingo HOFFMANN	Neutron Spin-Echo for diffusion in colloidal systems

Synchrotron Radiation Labs at ESRF, Grenoble Local coordinator: Petra PERNOT		
Name	Instructor(s)	Title
icOS (ID30s)	Antoine ROYANT	Overview and practice of crystallography, Optical Spectroscopies, (Absorption Fluorescence and Raman)
CryoEM (CM01)	David FERNANDEZ MARTINEZ, Eazhisai KANDIAH	Cryo-EM: vitrification and data collection pipeline

Practicals in laboratories(Labs) and tutorials at IBS, Grenoble Local coordinators: Petra PERNOT and Giorgio SCHIRO		
Name	Instructor	Title
NMR	Adrien FAVIER	Folding characterization, structure and dynamics of proteins by NMR
MX-DA	David COBESSI	Macromolecular model building and analysis in electron density maps
Cryst	Monika BUDAYOVA-SPANO	Crystallization of biological macromolecules



PROGRAMME OUTSIDE GRENOBLE

ALBA



Elettra-FERMI



Trieste – Hamburg Group:

- ▶ Trieste: 15th - 22nd March
- ▶ Hamburg: 22nd - 29th March

PSI



Synchrotron SOLEIL



Barcelona – Paris Group:

- ▶ Barcelona: 15th - 22nd March
- ▶ Paris-Saclay: 22nd - 29th March

DESY-European XFEL



KIT



Karlsruhe – Villigen Group:

- ▶ Karlsruhe: 15th - 22nd March
- ▶ Villigen: : 22nd - 27th March

HERCULES SCHOOL 2020:**PLANNING IN BARCELONA****15th - 22nd March 2020 (Sunday-Sunday)**Session A: Physics and chemistry of condensed matterSession B: Biomolecular structure and dynamics

Monday 16th March
in Maxwell Auditorium

Time	Title	Lecturer
9:00	Welcome message and presentation of ALBA synchrotron	Management
9:30	Soft X-ray absorption and XMCD	Javier HERRERO
10:30	Coffee break	
11:00	Macromolecular Crystallography at ALBA: from data to structure	Xavier CARPENA
12:00	Low energy Electron and X-ray Photoemission Electron Microscopy (LEEM & XPEEM): Principles and applications	Michael FOERSTER
13:00	Lunch	
14:30	Full field soft X-ray Transmission Microscopy	Andrea SORRENTINO
15:30	Near Ambient Pressure Photoemission (NAPP) at ALBA synchrotron: more realistic studies by reducing the pressure gap	Carlos ESCUDERO
16:30	Coffee break	
17:00	Guided Tour to ALBA	

Tuesday 17th March
on ALBA beamlines

Time	Title
9:00	Practical 1
13:00	Lunch
14:30-18:00	Practical 1 (continuation) OR Tutorial

Wednesday 18th March
on ALBA beamlines

Time	Title
9:00	Practical 2
13:00	Lunch
14:30-18:00	Practical 2 (continuation) OR Tutorial

Thursday 19th MarchSession A

Time	Title
9:00	Analysis of data collected at ALBA during practical 1 or 2
11:30	Preparation of an experimental report
13:00	Lunch
14:30	Analysis of data collected at ALBA during practical 2 or 1
17:00	Coffee break
17:30	Preparation of an experimental report. One-to one-meetings with ALBA researchers
20:30	Social dinner

Session B

Time	Title
9:00	Tutorial
13:00	Lunch
14:30	Analysis of data collected at ALBA during practical 1 or 2
16:30	Coffee break
17:00	Preparation of an experimental report. One-to one-meetings with ALBA researchers
20:30	Social dinner

Friday 20th March

Time	Title	Room
9:00	Preparation of an experimental report: Final touches	Bragg, Hodgkin, Niels Bohr
10:00	Presentation of the reports by <u>Session A</u> groups: → CLAESS + BOREAS exp. → BOREAS + NCD-SWEET exp. → NCD-SWEET + CLAESS exp.	Maxwell Auditorium
11:00	Coffee break	
11:20	Presentation of the reports by <u>Session A</u> groups: → XALOC + MIRAS exp. → XALOC + MIRAS exp.	Maxwell Auditorium
12:00	Wrap-up session	
13:00	Lunch	

Practicals and Tutorials Session A: Physics and chemistry of condensed matter

Synchrotron Radiation Practicals at ALBA, Barcelona Local coordinators: Bárbara CALISTO, Martin KREUZER, Debora PIERUCCI, and Maria José SIMANCAS		
Beamlines	Instructors	Title
BL11 – NCD-SWEET	Marc MALFOIS, Eduardo SOLANO	SAXS/WAXS study on polymer crystallisation
BL22 – CLAESS	Giulio GORNI, Carlo MARINI, Laura SIMONELLI	X-ray absorption end emission spectroscopy to access the local structural and electronic properties of the matter
BL29 – BOREAS	Pierluigi GARGIANI, Javier HERRERO, Manuel VALVIDARES	XAS and XMCD investigation of bulk and surface science samples

Synchrotron Radiation Tutorials at ALBA, Barcelona Local coordinators: Bárbara CALISTO, Martin KREUZER, Debora PIERUCCI, and Maria José SIMANCAS		
Room	Instructors	Title
Niels Bohr	Marc MALFOIS, Eduardo SOLANO	Analysis of data collected at NCD-SWEET: data reduction using pyFAI and DAWN software. Preliminary data analysis and interpretation.
Tesla	Giulio GORNI, Carlo MARINI, Laura SIMONELLI	Analysis of XAS data collected at CLAESS: XANES linear combination approach, XES data treatment: quantification of the local magnetic moment by the IAD method.
Tesla	Pierluigi GARGIANI, Javier HERRERO	Analysis of XAS and XMCD data collected at BOREAS: spectra treatment, sum rules and introduction to multiplet simulations.

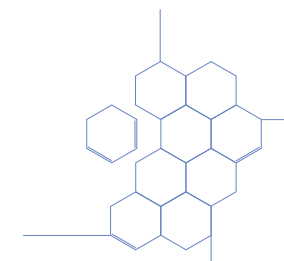
As in Grenoble, each group of 4 full time participants from **session A** will follow practicals selected from the lists above.

Practicals and Tutorials Session B: Biomolecular structure and dynamics

Synchrotron Radiation Practicals at ALBA, Barcelona Local coordinators: Bárbara CALISTO, Martin KREUZER, Debora PIERUCCI, and Maria José SIMANCAS		
Beamlines	Instructors	Title
BL01 - MIRAS	Tanja DUCIC, Martin KREUZER	Using the FTIR microscope and various experimental setups at MIRAS BL
BL13 - XALOC	Bárbara CALISTO, Xavier CARPENA, Iñaki DE DIEGO	Advanced Macromolecular Crystallography Data Collection Protocols

Synchrotron Radiation Tutorials at ALBA, Barcelona Local coordinators: Bárbara CALISTO, Martin KREUZER, Debora PIERUCCI, and Maria José SIMANCAS		
Room	Instructors	Title
Marie Curie	Ana PÉREZ-BERNÁ	Tutorial at BL09 - MISTRAL: Biomedical Applications at the soft X-ray microscope MISTRAL
Ada Lovelace	Roeland BOER, Damià GARRIGA	Macromolecular model building and analysis of electron density maps
Ada Lovelace	Ibraheem YOUSEF	Analysis of data collected at MIRAS: Infrared data handling (chemical imaging and individual spectra) using OPUS and Unscrambler software

Both groups of **session B** complete an identical training.



HERCULES SCHOOL 2020: PLANNING IN PARIS-SACLAY



22nd - 29th March 2020 (Sunday-Sunday)

Session A: Physics and chemistry of condensed matter

Session B: Biomolecular structure and dynamics

Monday 23rd March

Time	Title	Lecturer
9:00	Welcome at Synchrotron SOLEIL	Jean DAILLANT
9:30	Synchrotron infrared emission and spectroscopic applications at Libra	Paul DUMAS
10:30	Coffee break	
11:00	Synchrotron infrared emission and spectroscopic applications at Libra	Paul DUMAS
12:00	Lunch at SOLEIL	
14:00	How light became a wave? at Auditorium	Sylvain RAVY
15:30	Coffee break	
16:00	How to build a neutron spectrometer? at Libra	Frédéric OTT
17:30	Welcome drink	

Tuesday 24th and Wednesday 25th March

Time
9:00-17:30 PRACTICALS on Synchrotron SOLEIL beamlines

Thursday 26th March

Time	Title	Lecturer
9:00	Calculation of a hard x-rays Beam Line at Phenix (A1.0.59)	Thierry MORENO
10:30	Coffee break	
11:00	Calculation of a hard x-rays Beam Line at Phenix (A1.0.59)	Thierry MORENO
12:30	Lunch at SOLEIL	
14:00	Time-resolved X-ray Scattering at Libra	Claire LAULHE
15:30	Coffee break	
16:00-	Data Analysis	
17:30	Talk Preparation	

Friday 27th March

Time	Title
9:00	Data Analysis Talk Preparation
10:30	Coffee break
11:00	Data Analysis Talk Preparation
12:30	Lunch at SOLEIL
14:00-16:00	Students presentation and Evaluation Meeting at Auditorium

Practicals Session A: Physics and chemistry of condensed matter

Synchrotron Radiation Practicals at SOLEIL, Saint-Aubin (near Paris) Local coordinators: Alessandro COATI and Lucie NATAF		
Beamline	Instructors	Title
AILES	Jean-Blaise BRUBACH	Spin transition in molecular magnets
SAMBA	Emiliano FONDA	studied by IR THz spectroscopy and XAFS
GALAXIES	Jean-Pascal RUEFF	Spin states in Fe-based compounds,
SMIS	Ferenc BORONDICS	investigated through XES and XAS
ROCK	Valérie BRIOIS	Memory effect of Layered Double Hydroxide,
CRISTAL	Erik ELKAÏM	by EXAFS and WAXS

Practicals Session B: Biomolecular structure and dynamics

Synchrotron Radiation Practicals at SOLEIL, Saint-Aubin (Paris-Saclay campus) Local coordinators: Alessandro COATI and Lucie NATAF		
Beamline	Instructors	Title
DIFFABS	Solenn RÉGUER	Structural investigations of Membrane Proteins
DISCO	Matthieu RÉFRÉGIERS, Frank WIEN	using SRCD, BioSaxs and X-Ray Crystallography

As in Grenoble, each group of 4 full time participants from **session A** will follow practicals selected from the lists above.

Both groups of **session B** complete an identical training.

HERCULES SCHOOL 2020:

PLANNING IN TRIESTE

15th - 22nd March 2020 (Sunday-Sunday)Session A: Physics and chemistry of condensed matterSession B: Biomolecular structure and dynamicsSunday 15th March

Arrival and dinner at the hotel

Monday 16th March

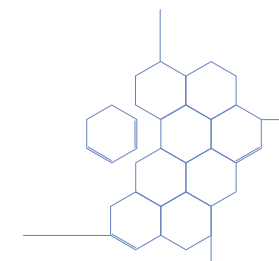
Time	Where	What
	Hotel	Breakfast
9:00-9:10	Training room	Welcome
9:10-9:50	Training room	Andrea LOCATELLI X-ray photoelectron spectroscopy and microscopy at Elettra: advanced methods to unveil the local structure of materials
9:50-10:30	Training room	Claudio MASCIOVECCHIO Frontier Science at FERMI
10:30-11:00		Coffee break
11:00-11:40	Training room	Luca GIANNESI FERMI: the first externally seeded Free Electron Laser in the extreme ultraviolet and soft X-ray spectral regions
11:40-12:10	Training room	Giuliana AQUILANTI Research highlights at the XAFS beamline of Elettra
12:10-12:40	Training room	Nicola DEMITRI Unravelling atomic level details of materials using X-Ray diffraction at Elettra
12:40-14:10	Cafeteria	Lunch
14:10-15:30	Elettra/FERMI	Visit FERMI experimental hall and FERMI/Elettra control room
15:30-16:00	Elettra hall	Coffee break and group photos
16:00-17:30	Elettra/FERMI	Visit Bio/AFM/Cultural Heritage Labs at Elettra
	Hotel	Dinner

Tuesday 17th March

Time	Where	What
	Hotel	Breakfast
9:00-9:30	Training room	Lisa VACCARI Infrared bio-spectroscopy: from Macro to Nano scale on the molecules of life
9:30-10:00	Training room	Sigrid BERNSTORFF Grazing Incidence Small Angle X-ray Scattering: A useful tool in the development of solar energy conversion devices
10:00-10:30	Training room	Lucia MANCINI 3D and 4D X-ray imaging techniques
10:30-11:00		Coffee break
11:00-11:30	Training room	ALESSANDRO BARALDI Physical and chemical properties of solid surfaces probed by means of fast and high-resolution x-ray photoelectron spectroscopy
11:30-12:00	Training room	CARLO CALLEGARI The Low Density Matter beamline at the FERMI Free Electron Laser
12:00-12:30	Training room	FLAVIO CAPOTONDI Magnetization dynamics at FERMI seeded FEL
12:30-14:00	Cafeteria	Lunch
14:00-17:30	Elettra/FERMI	Practicals
	Hotel	Dinner

Wednesday 18th March

Time	Where	What
	Hotel	Breakfast
9:00-12:30	Elettra/FERMI	Practicals
12:30-14:00	Cafeteria	Lunch
14:00-17:30	Elettra/FERMI	Practicals
	Hotel	Dinner



Thursday 19th March

Time	Where	What
	Hotel	Breakfast
9:00-9:40	Training room	Cecilia BLASETTI Hints and tips for a successful beamtime proposal
9:40-10:30	Beamline/lab	One-to-one with researchers
10:30-11:00	Training room	Coffee break
11:00-12:30	Beamline/lab	One-to-one with researchers
12:30-14:00	Cafeteria	Lunch
14:00-17:00		Prepare group presentations and free time
	Hotel	Dinner

Friday 20th March

Time	Where	What
	Hotel	Breakfast
9:00-10:30	Training room	Group presentations
10:30-11:00	Training room	Coffee break
11:00-12:30	Training room	Feedback meeting
12:30-14:00	Cafeteria	Lunch
14:00-19:00		Social program
19:00-22:30		Social Dinner

Saturday 21st March

Breakfast and departure to Venice (until Sunday) from the hotel

Practicals Session A: Physics and chemistry of condensed matter

Synchrotron Radiation Practicals at Elettra, Trieste (Italy) Local coordinators: Nicola DEMITRI and Barbara ROSSI		
Beamline	Instructors	Title
Nanospectroscopy	Andrea LOCATELLI, Tevfik Onur MENTEŞ	Chemical and magnetic imaging by means of synchrotron-based photoemission electron microscopy
ESCAmicroscopy	Matteo AMATI, Luca GREGORATTI	2D materials at the nanometric scale: properties and functionalities
SAXS	Heinz AMENITSCH, Sigrid BERNSTORFF, Barbara SARTORI	Self Assembly of mesoporous materials (MCM-41); in situ experiments of the formation highly ordered hexagonal structures
MCX	Mattia GABOARDI, Lara GIGLI, Jasper PLAISIER	Applications of powder diffraction
XAFS	Giuliana AQUILANTI, Ilaria CARLOMAGNO, Danilo Oliveira DE SOUZA, Luca OLIVI, Simone POLLASTRI	Short-range order in crystalline, amorphous, liquid, and supercooled germanium probed by X-ray absorption spectroscopy
Xpress	Frederico ALABARSE, Boby JOSEPH	Structural determinations at High Pressure, Equation of state, DAC handling, Pressure measurement, Data indexing

Free Electron Laser Practicals at FERMI, Trieste (Italy) Local coordinators: Laura FOGLIA and Emanuele PEDERSOLI		
Beamline	Instructors	Title
MagneDyn	Antonio CARETTA,	Ultrafast optomagnetism in a superconductor/ferromagnetic bilayer
Metrology	Simone GERUSINA, Michele MANFREDDA, Lorenzo RAIMONDI, Alberto SIMONCIG	How to make spots... hot
T-ReX	Federico CILENTO	Time-and-Angle Resolved PhotoElectron Spectroscopy (TR-ARPES) measurements on complex materials

Practicals Session B: Biomolecular structure and dynamics

Synchrotron Radiation Practicals at Elettra, Trieste (Italy) Local coordinators: Nicola DEMITRI and Barbara ROSSI		
Beamline	Instructors	Title
DXRL	Benedetta MARMIROLI, Alessio TURCHET	X-ray lithography to obtain microgears, replica of microstructures using a soft material
IUVS	Francesco D'AMICO, Silvia DI FONZO	UV Resonant Raman spectroscopy applied to bio-macromolecules
SISSI	Giovanni BIRARDA, Lisa VACCARI	Preparation and analysis of thin sections for infrared imaging micro and nano spectroscopy
XRD2	Nicola DEMITRI, Annie HEROUX	Structural characterization of biomolecules using XRD

Free Electron Laser Practicals at FERMI, Trieste (Italy) Local coordinators: Laura FOGLIA and Emanuele PEDERSOLI		
Beamline	Instructors	Title
LDM	Carlo CALLEGARI, Oksana PLEKAN	Molecular dynamics investigated at the sulfur 2p edge
TeraFERMI	Nidhi ADHLAKHA	THz induced birefringence in z-cut quartz

As in Grenoble, each group of 4 full time participants from both **session A** and **session B** will follow practicals selected from the lists above.

HERCULES SCHOOL 2020:**PLANNING IN HAMBURG**22nd – 29th March 2020 (Sunday-Sunday)**Session A:** Physics and chemistry of condensed matter**Session B:** Biomolecular structure and dynamics**Monday 23rd March**

DESY Site

Time	What	Who	Where
9:00-9:45	Introduction to DESY	Christian SCHROER	Rm109/Bldg.25B
9:45-10:30	Introduction to EuXFEL	Sakura PASCARELLI	Rm109/Bldg.25B
10:30-13:00	PETRA III and FLASH Tour		
13:00-14:00	Lunch		
14:00-18:00	Session A: DESY Practical Training – Part 1		PETRA/ P07B, P23, or P24
	Session B: P11 Lab Work		PETRA/P11/L407

Tuesday 24th March

European XFEL site

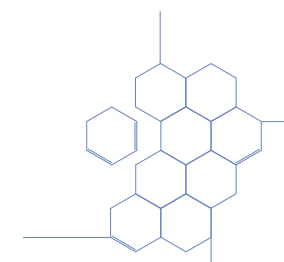
Session A

Time	What	Where
9:00-9:30	Introduction	
9:30-10:30	Experimental Hall and Labs Tour	
10:30-10:45	Coffee Break	
10:45-18:00	European XFEL Practical training	FXE, HED, or SQS

Session B

DESY site

Time	What	Where
9:00-18:00	DESY Practical Training – Part 1	PETRA/P11



Wednesday 25th March

European XFEL Site

Session A

Time	What
9:00-18:00	European XFEL Tutorial training
19:00	Social dinner

Session B

Time	What	Where
9:00-9:30	Introduction	
9:30-13:00	European XFEL Practical training	Biology Lab or XPD
13:00-14:00	Lunch	
14:00-14:30	Experimental Hall Tour	
14:30-18:00	European XFEL Practical training	Biology Lab or XPD
19:00	Social dinner	

Thursday 26th March

DESY site

Session A

Time	What	Where
9:00-13:00	DESY Practical Training – Part 2	PETRA/P07B, P23, or P24
13:00-14:00	Lunch	
14:00-18:00	DESY Practical Training – Part 3	PETRA/P07B, P23, or P24

Session B

DESY site

Time	What	Where
9:00-13:00	DESY Practical Training – Part 2	PETRA/P11
13:00-14:00	Lunch	
14:00-18:00	DESY Practical Training – Part 3	PETRA/P11

Friday 27th March

DESY Site

Time	What	Where
9:00-13:00	Preparation of students presentations	DESY/Rm456/Bldg.25F
13:00-14:00	Lunch	
14:00-17:00	Students presentations	DESY/Rm456/Bldg.25F

Students presentations:

Each groups will report on specific parts of the training with the aim to get all students informed about all parts of the program.

Practicals Session A: Physics and chemistry of condensed matter
Synchrotron Radiation Practicals at DESY – PETRA III, Hamburg (Germany)
 Local coordinators: Rainer GEHRKE and Oliver SEECK

Beamline	Instructors	Title
P07B	Malte BLANKENBURG, Peter STARON	Small-angle X-ray scattering from precipitation hardened aluminium alloys
P23	Dmitri NOVIKOV	Surface Diffraction
P24	Martin TOLKIEHN	Single Crystal Diffraction

Free Electron Laser Practicals at European XFEL, Hamburg (Germany)
 Local coordinator: Sakura PASCARELLI

Beamline	Instructors	Title
FXE	Yi FENG, Katharina KUBICEK	Dispersive X-ray emission spectroscopy of Ni-based samples
HED	Jan Patrick SCHWINKENDORF, Ulf ZASTRAU	Alignment and dispersion determination of von-Hamos spectrometers
SQS	Rebecca BOLL, Tommaso MAZZA, Michael MEYER	Coherent diffraction and electron imaging experiments

Free Electron Laser Tutorials at European XFEL, Hamburg (Germany)
 Local coordinator: Sakura PASCARELLI

Instructor	Title
Ruslan KURTA	Angular X-Ray Cross-Correlation Analysis with an XFEL

All three student groups of **session A** subsequently complete all three practical trainings at the three involved DESY PETRA III beamlines while at European XFEL, each practical training will be exclusive to one group.

Practicals Session B: Biomolecular structure and dynamics

Synchrotron Radiation Practicals at DESY – PETRA III, Hamburg (Germany) Local coordinators: Rainer GEHRKE and Oliver SEECK		
Beamline	Instructors	Title
PETRA/P11	Johanna HAKANPAEAE, Dominik OBERTHUER, Thomas WHITE	Protein Crystallography
P11 Lab work	Johanna HAKANPAEAE Sofiane SAOUANE	Sample Crystallization and Preparation

Free Electron Laser Practicals at European XFEL, Hamburg (Germany) Local coordinator: Sakura PASCARELLI		
Beamline	Instructors	Title
Bio-labs	Huijong HAN, Kristina LORENZEN, Robin SCHUBERT	Nano-crystallization, sample characterization, and jetting test
XPD	Jan GRÜNERT, Naresh KUJALA	Single-shot spectral measurement for Hard X-ray FEL beam

Both groups of **session B** complete an identical training at the two large facilities.

**HERCULES SCHOOL 2020:
PLANNING IN KARLSRUHE**

15th-22nd March 2020 (Sunday – Sunday)



Session A: Physics and chemistry of condensed matter

Session B: Biomolecular structure and dynamics

Monday 16th March

Time	What	Who
9:00-11:00	Welcome, safety instruction	Michael HAGELSTEIN Anton PLECH
	Lecture 1: machine physics	Marcel SCHUH, Anke-Susanne MÜLLER
11:00-11:30	Coffee break	
11:30-12:30	Lecture 2: photon science at KIT	Tilo BAUMBACH Anton PLECH
12:30-14:00	Lunch	
14:00-15:30	Hands-on KARA, FLUTE, UHV Lab, FME Lab	
15:30-16:00	Coffee break	
16:00-18:00	Hands-on KARA, FLUTE, UHV Lab, FME Lab	

Tuesday 17th, Wednesday 18th, Thursday 19th, and Friday 20th March

One day-long practical on a different beamline each day

Time	What
9:00-11:00	Hands-on experiment
11:00-11:30	Coffee break
11:30-12:30	Hands-on experiment
12:30-14:00	Lunch
14:00-15:30	Hands-on experiment
15:30-16:00	Coffee break
16:00-18:00	Hands-on experiment
19:00-21:00	Social dinner on Thursday

Practicals Session A: Physics and chemistry of condensed matter

Synchrotron Radiation Practicals at KIT Light Source, Karlsruhe (Germany) Local coordinators: Michael HAGELSTEIN, Leyla JOCHIM, and Anton PLECH		
Beamline	Instructors	Title
IR1	Alexander BORIS, Yves-Laurent MATHIS	Synchrotron Fourier Transform Infra-red spectroscopy, IR ellipsometry
IR2	Biliana GASHAROVA, David MOSS	Synchrotron Fourier Transform Infra-red spectroscopy
WERA	Michael MERZ, Peter NAGEL, Stefan SCHUPPLER	Soft X-ray spectroscopy of solid state materials
XSPEC	Dirk HAUSCHILD, Lothar WEINHARDT	Photon-in photon out spectroscopy
FLUO	Mateusz CZYZYCKI, Rolf SIMON	Fluorescence spectroscopy of biological materials
INE	Kathy DARDENNE, Jörg ROTHE	X-ray absorption spectroscopy of actinides
LIGA	Martin BÖRNER, Heike FORNASIER, Uwe KÖHLER	X-ray lithography and fabrication of microparts
TOPOTOMO	Elias HAMANN, Thomas VAN DE KAMP, Marcus ZUBER	Tomography and laminography
SCD	Gernot BUTH, Anton PLECH	X-ray reflectivity of thin films and surfaces
UHV Lab	Bärbel KRAUSE, Anette WEISSHARDT	Sample preparation and characterization using laboratory techniques
MFE Lab	Dirk HAUSCHILD	Sample preparation for energy materials
KARA	Marcel SCHUH	Operation of the circular accelerator KARA
FLUTE	Nigel SMALE	Operation of the linear accelerator FLUTE

Practicals Session B: Biomolecular structure and dynamics

Synchrotron Radiation Practicals at KIT Light Source, Karlsruhe (Germany) Local coordinators: Michael HAGELSTEIN, Leyla JOCHIM, and Anton PLECH		
Beamline	Instructors	Title
IR2	Biliana GASHAROVA, David MOSS	Synchrotron Fourier Transform Infra-red spectroscopy
FLUO	Mateusz CZYZYCKI, Rolf SIMON	Fluorescence spectroscopy of biological materials
INE	Kathy DARDENNE, Jörg ROTHE	X-ray absorption spectroscopy of actinides
TOPOTOMO	Elias HAMANN, Thomas VAN DE KAMP, Marcus ZUBER	Tomography and laminography
KARA	Marcel SCHUH	Operation of the circular accelerator KARA

*As in Grenoble, each group of 4 full time participants from **session A** will follow practicals selected from the first list above, while the single group from **session B** will follow all practicals listed in the second table.*

HERCULES SCHOOL 2020:

PLANNING IN VILLIGEN

22nd – 27th March 2020 (Sunday-Friday)Session A: Physics and chemistry of condensed matterSession B: Biomolecular structure and dynamics

PAUL SCHERRER INSTITUT

Sunday 22nd March

Time	Where	What
Late Afternoon	Guesthouse PSI West	Arrival
18:50	Meeting point: Outside guesthouse entrance	Walk to OASE restaurant
19:00 – 20:00	OASE PSI east	Dinner

Monday 23rd March

Time	Where	What
8:00 – 9:00	TIMEOUT PSI west	Breakfast
9:00 – 9:15	WBGB/019	Welcome (Frithjof NOLTING)
9:15 – 12:30	@ SLS beamlines	Experiments / work in groups
12:30 – 13:30	TIMEOUT PSI west	Lunch
13:30 – 17:00	@ SLS beamlines	Experiments / work in groups
17:00 – 19:00		Free time
19:00 – 20:00	OASE PSI east	Dinner

Tuesday 24th March

Time	Where	What
8:00 – 9:00	TIMEOUT PSI west	Breakfast
9:00 – 12:30	@ SLS beamlines	Experiments / work in groups
12:30 – 13:30	TIMEOUT PSI west	Lunch
13:30 – 17:00	@ SLS beamlines	Experiments / work in groups
17:00 – 18:00		Free time
18:00	OASE PSI east	Dinner
19:00	Departure of bus to Bad Zurzach	Excursion to thermal bath Bad Zurzach
21:45	Bad Zurzach	Departure of bus to PSI

Wednesday 25th March

Time	Where	What	Who
8:00 – 9:00	TIMEOUT PSI west	Breakfast	
9:00 – 9:45	WSLA/008	Chemical spectroscopy	Olga SAFONOVA, Patrick HEMBERGER
9:45 – 10:30	WSLA/008	Intro to SwissFEL	Christoph BOSTEDT
10:30 – 10:45		Break	
10:45 – 11:45		Tour SLS tunnel	Andreas LÜDEKE et al.
11:45 – 12:30	WSLA/008	Specialized talk SwissFEL	Kirsten SCHNORR
12:30 – 13:30	TIMEOUT PSI west	Lunch	
13:30 – 14:45		Walk to SwissFEL, Tour SwissFEL	Henrik LEMKE
14:45 – 18:00	WSLA/008 + 108 +105, TIMEOUT	Walk back to PSI West, then prepare presentations	
18:00 – 19:00		Free time	
19:00 – 20:00	OASE PSI east	Dinner	

Thursday 26th March

Time	Where	What	Who
8:00 – 9:00	TIMEOUT PSI West	Breakfast	
9:00 – 9:45	WSLA/008	Intro to SmuS	Hubertus LUETKENS
9:45 – 10:30	WSLA/008	Specialized talk SmuS	Zaher SALMAN
10:30 – 11:00	WSLA/008 + 108 +105, TIMEOUT	Break / presentation final touches	
11:00 – 11:45	WSLA/008	Intro to SINQ	Christof NIEDERMAYER
11:45 – 12:30	WSLA/008	Student presentations part 1: ▶TOMCAT ▶PHOENIX ▶SIM	
12:30 – 13:30	TIMEOUT PSI West	Lunch	
13:30 – 14:15	WSLA/008	Examples from neutron spectroscopy	Fanni JURANYI
14:15 – 15:30		Tour SINQ + SmuS	Christof NIEDERMAYER Zaher SALMAN
15:30 – 16:00		Break	
16:00 – 16:45	WSLA/008	Introduction to Proton Therapy	David MEER Serena PSOROULAS
16:45 – 17:30		Tour Center for Proton Therapy	David MEER Serena PSOROULAS
17:30 – 18:30		Free time	
18:30		Bus stop PSI West Departure to farewell dinner	

Friday 27th March

Time	Where	What	Who
8:30 - 9:30	PSI reception West	Checkout of rooms, store luggage in TV room (will be locked as of 09:40) Return room key to reception	
9:30 - 9:40	TIMEOUT PSI west	Breakfast Setup for student presentations	
9:40 - 11:30	WSLA/008	Student presentations part 2 •PEARL •cSAXS •X-Treme •superXAS •Pollux •microXAS •XIL	
11:30 - 11:45		Break	
11:45 - 12:30	WSLA/008	X-ray microscopy	Jörg RAABE
12:30 - 13:30	TIMEOUT PSI West	Lunch	
13:30 - 14:15	WSLA/008	ARPES	Nick PLUMB
14:15 - 15:00	WSLA/008	Detectors - a view from the application side	Dubravka SISAK JUNG
15:00 - 15:30	Guesthouse	Return badge Load luggage and board bus	
15:30	Guesthouse	Departure to Grenoble	

Practicals Session A: Physics and chemistry of condensed matter

Synchrotron Radiation Practicals at SLS, Villigen (Switzerland)		
Local coordinator: Jan DREISER		
Beamline	Instructors	Title
cSAXS / X12SA	Johannes IHLI, Dmitry KARPOV	Ptychographic Nanotomography of an Integrated Circuit
microXAS	Dario FERREIRA SANCHEZ	Identifying degradation mechanisms on Solid Oxide Cells through X-ray μ -XRD and μ -XRF synchrotron studies
PEARL	Matthias MUNTWILER	Elemental composition and electronic band structure of a two-dimensional boron nitride layer
PHOENIX	Camelia BORCA, Thomas HUTHWELKER	Iron spatial distribution and its oxide forms in fluid catalytic cracking particles
SIM	Armin KLEIBERT, Carlos A. F. VAZ	Imaging Magnetic Nanostructures using Soft X-ray Photoemission Electron Microscopy (PEEM)
SuperXAS	Adam CLARK, Olga SAFONOVA	Evolution of silica supported Cu-Zn catalyst for CO ₂ hydrogenation under reducing conditions
XIL-II	Iacopo MOCHI, Michaela VOCKENHUBER	Nano patterning of grating structures
X-Treme	Jan DREISER	X-ray magnetic circular dichroism of Fe(II) spin crossover molecules

Practicals Session B: Biomolecular structure and dynamics

Synchrotron Radiation Practicals at SLS, Villigen (Switzerland)		
Local coordinator: Jan DREISER		
Beamline	Instructors	Title
TOMCAT	Federica MARONE, Christian SCHLEPÜTZ	Absorption and phase contrast X-ray tomographic microscopy
Pollux	Benjamin WATTS	Composition mapping of a thin-film polymer blend

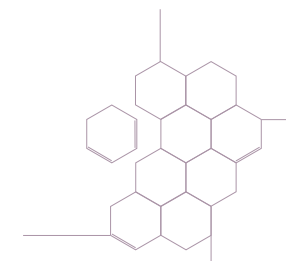
As in Grenoble, each group of 4 full time participants from **session A** will follow practicals selected from the first list above, while the single group from **session B** will follow the two practicals listed in the second table.

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IN CASE OF EMERGENCY

Appel d'urgence européen
(European emergency call)

☎ 112

SAMU

(Emergency services)

☎ 15

POLICE

☎ 17

POMPIERS

(Fire brigade)

☎ 18

Centre Anti-Poison
(Poisons unit)

☎ 04 76 42 42 42

CHEMIST

Pharmacie Saint Bruno

82 cours Berriat

☎ 04 76 96 06 61

DOCTORS

(near the hotel)

ROUX Jean-François

3 rue Arago

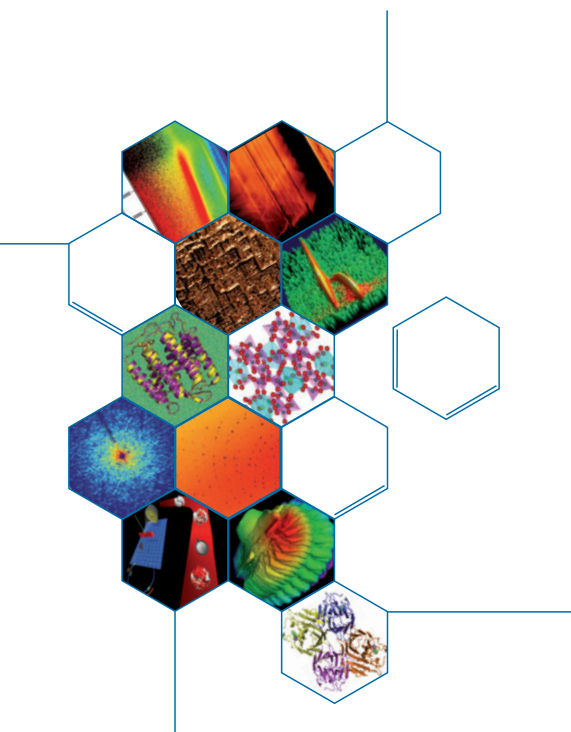
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