

HERCULES

European School

Neutrons and synchrotron radiation
for science

2019

**18th March
to 19th April**

**Grenoble
FRANCE**



HERCULES

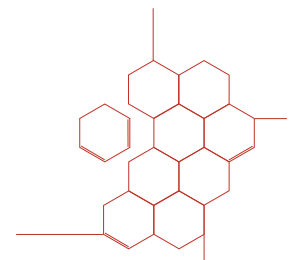
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CONTENT

■ Organisation.....	p6
■ General information.....	p10
■ Practical information.....	p12
■ Programme in Grenoble	
▶ Common lectures.....	p18
▶ Session A:	
Physics and chemistry of condensed matter.....	p20
▶ Session B:	
Biomolecular structure and dynamics.....	p26
■ Programme outside Grenoble.....	p32
▶ Planning in Barcelona (Barcelona - Paris group).....	p34
▶ Planning in Paris-Saclay (Barcelona - Paris group).....	p38
▶ Planning in Trieste (Trieste - Hamburg group).....	p41
▶ Planning in Hamburg (Trieste - Hamburg group).....	p46
▶ Planning in Villigen (Villigen - Karlsruhe group).....	p49
▶ Planning in Karlsruhe (Villigen - Karlsruhe group).....	p54
■ Lecturers.....	p56



ORGANISATION

ORGANISED BY:

- Université Grenoble Alpes (UGA)
- Grenoble INP

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SUPPORTED BY:

- European Commission projects:
 - SINE2020
 - CALIPSOplus
- 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):
 - Formation Permanente (ANF)
 - Délégation Alpes
 - Laboratoires du Polygone Louis Néel, Grenoble
- Commissariat à l'énergie atomique (CEA):
 - Direction de la Recherche Fondamentale (DRF)
 - Institut Nanosciences et Cryogénie (INAC)
- SOLEIL
- Laboratoire Léon Brillouin (LLB)
- Swiss Light Source (SLS) - Paul Scherrer Institute (PSI)
- Grenoble Innovation for Advanced New Technologies (GIANT)
- KIT
- ALBA
- FOSTERING SCIENCE
- Grenoble Alpes Métropole (La Métro)

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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 (1st to 5th April then 8th to 12th April) 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,
 - and **Laboratoire Léon Brillouin (LLB)**, CEA Saclay, with an experimental reinforced neutron programme.

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.

Villigen-Karlsruhe Group:

- 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,
- then in Germany (Karlsruhe) at **KIT Light Source**, with a vast programme of synchrotron 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 FACILITIES

- › **ILL**: B. GRENIER – L. MANGIN-THRO
- › **ESRF**: G. BEUTIER – M. KRISCH
- › **ALBA**: B. CALISTO – D. PIERUCCI
- › **SOLEIL**: A. COATI – L. NATAF
- › **LLB**: F. DAMAY
- › **Elettra and FERMI**: F. BENCIVENGA – A. LOCATELLI
- › **PSI**: J. G.-H. DREISER
- › **DESY and European XFEL**: R. GEHRKE – T. TSCHENTSCHER
- › **KIT**: T. BAUMBACH – M. HAGELSTEIN



PRACTICAL INFORMATION

TRAVEL INFORMATION

Participants are expected to arrive in Grenoble on **Sunday 17th March 2019**.



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:

<http://www.aerocar.fr/>



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/navette-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 "Résidence Hôtelière Séjours et Affaires Marie Curie", situated just behind the train station, between 5:30 PM and 9:00 PM on Sunday 17th March 2019.

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:

Séjours & Affaires Marie-Curie

58 rue Félix Esclangon - 38000 GRENOBLE

Tel : +33 (0)4 76 84 72 22

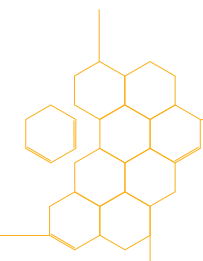
Fax : +33 (0)4 76 84 16 83

Small studio flats are booked from **Sunday 17th March evening to Friday 19th April morning** in Grenoble and accommodation is organised for the nights in Barcelona, Paris-Saclay, Trieste, Hamburg, Villigen, and Karlsruhe.

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 from 7:30 AM in the hotel. 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 (20 min).

› **Tramway line B** connects directly the hotel to the Polygone Scientifique terminus. While registering at the hotel, you will be given maps, timetable and a few tickets for your convenience.

You can buy tickets for public transportation from "TAG" desks and tobacco shops (current price: 42 € for 30 tickets, 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 "Grenoble Gambetta" situated 12 avenue Alsace Lorraine.

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 one to the hotel is located 51 rue Pierre Séward (LCL bank).

POSTER SESSION

A **poster session** will be organised on Friday 22nd 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, VILLIGEN, AND KARLSRUHE

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 31st March**
- ▶ Barcelona to Paris-Saclay on **Sunday 7th April**
- ▶ Paris-Saclay to Grenoble on **Sunday 14th April**

Trieste – Hamburg Group:

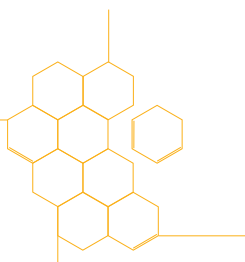
- ▶ Grenoble to Trieste on **Sunday 31st March**
- ▶ Trieste to Venice on **Saturday 6th April**
- ▶ Venice to Hamburg on **Sunday 7th April**
- ▶ Hamburg to Grenoble on **Saturday 13th April**

Villigen – Karlsruhe Group:

- ▶ Grenoble to Villigen on **Sunday 31st March**
- ▶ Villigen to Karlsruhe on **Friday 5th April**
- ▶ Karlsruhe to Grenoble on **Saturday 13th April**



You will be accommodated in guest houses.



PROGRAMME IN GRENOBLE

COMMON LECTURES



EMBL



BASIC METHODS AND INSTRUMENTS

- ▶ Diffraction, refraction and absorption of X-rays and neutrons *W. F. Kuhs*
- ▶ 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 *W. F. Kuhs*
- ▶ Hard X-ray optics for synchrotron radiation beamlines *R. Barrett*
- ▶ Introduction to small angle scattering *M. Müller*
- ▶ Introduction to imaging techniques *F. Marone*
- ▶ X-ray Detectors *H. Graafsma*
- ▶ Introduction to neutron and X-ray inelastic scattering *V. Balédent*
- ▶ Coherent imaging *P. Cloetens*
- ▶ Fundamentals of X-ray Absorption Fine Structure *S. Pascarelli*
- ▶ Free Electron Lasers and ultra fast X-ray science *T. Tschentscher*
- ▶ Science at neutron spallation sources: exploiting accelerator based facilities *S. Langridge*

REFRESHER LECTURES

- ▶ Crystallography *B. Grenier*
- ▶ 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 *N. Qureshi*
- ▶ 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 *T. Weber*
- ▶ Photoelectron spectroscopy from UV to soft X-rays *H. Dil*
- ▶ X-ray absorption spectroscopy: theoretical basis *A. Juhin*
- ▶ 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*

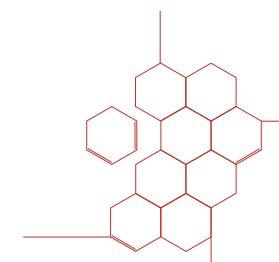
HERCULES 2019: PROGRAMME OF LECTURES

(subject to modification)

Updated : 18/02/2019

- Common lectures
- Session A lectures
- Other

Week 1	Monday 18/03	Tuesday 19/03	Wednesday 20/03	Thursday 21/03	Friday 22/03
8:30 - 8:45	Welcome				
8:45 - 9:30 10' break 9:40 - 10:25	Diffraction, refraction and absorption of X-rays and neutrons (1/2) Werner F. Kuhs	Diffraction, refraction and absorption of X-rays and neutrons (2/2) Werner F. Kuhs	Soft X-rays and VUV: specific optics and applications David Attwood	Fundamentals of X-ray Absorption Fine Structure (1/2) Sakura Pascarelli	X-ray detectors Heinz Graafma
10:45 - 11:30 10' break 11:40 - 12:25	ESRF / ILL badges distribution	Introduction to synchrotron radiation David Attwood	Neutrons: scattering and instrumentation (1/2) Andrew Wildes	Neutrons: scattering and instrumentation (2/2) Andrew Wildes	Crystallography (2/2) Béatrice Grenier
14:00 - 14:45 10' break 14:55 - 15:40	ESRF / ILL visits	Crystallography (1/2) Béatrice Grenier	Neutron and X-ray diffraction by crystals: kinematical approximation and experimental methods Werner F. Kuhs	Fundamentals of X-ray Absorption Fine Structure (2/2) Sakura Pascarelli	POSTER SESSION
16:00 - 16:45 10' break 16:55 - 17:40	16:00 - 17:30 ESRF / ILL presentations Francesco Sette / Mark Johnson 17:30 - 17:45 UGA presentation	ESRF / ILL visits	Free Electron Lasers and ultra fast X-ray science Thomas Tschentscher	Introduction to imaging techniques Federica Marone	16:00: European user facilities: the CERIC-ERIC and wayforlight Matthias Girod 16:45:NFFA.eu Ennio CAPRIA 17:00: Poster awards Gala dinner
	Welcome cocktail at ESRF			DECTRIS presentation	



Week 2	Monday 25/03	Tuesday 26/03	Wednesday 27/03	Thursday 28/03	Friday 29/03
8:45 - 9:30 10' break 9:40 - 10:25	Introduction to neutron and X-Ray inelastic scattering Victor Balédent	Magnetic neutron scattering Navid Qureshi	Disorder and its effects on neutron and X-ray diffraction Marc de Boissieu	Polarized X-rays Urs Staub	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-Sicairo
14:00 - 14:45 10' break 14:55 - 15:40	Full-field coherent imaging Peter Cloetens	Hard X-ray optics for SR beamlines Ray Barrett	TUTORIALS / LABS	Liquid and amorphous materials Adrian Barnes	Powder diffraction Radovan Cerny
16:00 - 16:45 10' break 16:55 - 17:40	Introduction to small angle scattering Martin Müller	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			

Week 3 (1st - 5th April), and week 4 (8th - 12th April) : Outside Grenoble

Week 5	Monday 15/04	Tuesday 16/04	Wednesday 17/04	Thursday 18/04	Friday 19/04
8:45 - 9:30 10' break 9:40 - 10:25	ILL PRACTICALS / TUTORIALS /	X-ray absorption spectroscopy: theoretical basis Amélie Juhin	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	LABS	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 Tobias Weber	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 photoemission electron microscopy Claus M. Schneider	TUTORIALS / LABS	
16:00 - 16:45 10' break 16:55 - 17:40	LABS	Magnetic X-ray and neutron reflectivity Hartmut Zabel	Neutron time of flight, spin echo and back-scattering spectroscopies Tobby Perrin		
18:00 - 19:00			EVALUATION MEETING		

PRACTICALS AND TUTORIALS Session A



Coordinators:

- ▶ G. BEUTIER, B. GRENIER, L. MANGIN-THRO (Grenoble)
- ▶ B. CALISTO, D. PIERUCCI, M. J. SIMANCAS (Barcelona)
- ▶ A. COATI, F. DAMAY, L. NATAF (Paris-Saclay)
- ▶ F. BENCIVENGA, A. LOCATELLI, E. PEDERSOLI, B. ROSSI (Trieste)
- ▶ R. GEHRKE, O. SEECK, T. TSCHENTSCHER (Hamburg)
- ▶ J. DREISER, M. FÜGLISTER (Villigen)
- ▶ T. BAUMBACH, M. HAGELSTEIN, L. JOCHIM (Karlsruhe)

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 will carry out one practical at ILL, as well as two tutorials (one for part-time participants) at ESRF, ILL, and/or CNRS. Some laboratories at CEA – INAC, Institut Néel, LNCMI, and ILL will also welcome some practicals allowing the participants to discover techniques they are not used to.

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** and the French neutron reactor Orphée – **LLB** 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 Swiss synchrotron radiation facility Swiss Light Source (**SLS**) at the Paul Scherrer Institute (**PSI**) in Villigen, then the **KIT Light Source** in Karlsruhe (**Villigen-Karlsruhe 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 16 half-days during the whole school).



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

Practicals in laboratories (Labs) at CEA, CNRS, and ILL, Grenoble

Local coordinator: Béatrice GRENIER

Name	Site	Instructor	Title
LAB1	CEA	Arnaud DE GEYER	Small angle X-ray scattering
LAB2	CNRS	Olivier LEYNAUD	X-ray powder diffraction
LAB3	CNRS	Eric MOSSANG	Reflectometry and GIXRD
LAB4	CNRS	Hadrien MAYAFFRE	Nuclear Magnetic Resonance in an antiferromagnet
LAB5	ILL	Pierre COURTOIS	Characterization of mosaic crystals using hard X-Ray diffraction; Application for the manufacturing of neutron monochromators

Neutron Practical at ILL, Grenoble

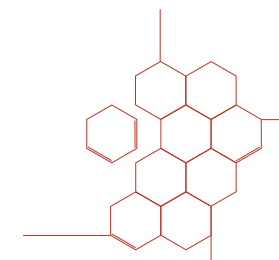
Local coordinators: Béatrice GRENIER and Lucile MANGIN-THRO

Name	Instructor(s)	Title
CYCLOPS	Oscar FABELO ROSA	Neutron Laue diffraction on antiferromagnetic MnO: indexation of nuclear and magnetic Bragg reflections in a Laue pattern
D23	Ketty BEAUVOIS	Single crystal diffraction: nuclear and magnetic structure refinement using Fullprof
D17	Thomas SAERBECK	Exploring thin-film structure and magnetism with neutron reflectometry
D33	Dirk HONECKER	Polarized small angle neutron scattering of magnetic nanoparticle dispersions
IN5	Sylvain PETIT	Time of flight inelastic neutron scattering on powders
IN16B	Markus APPEL / Tilo SEYDEL	Cold neutron backscattering spectroscopy
IN20	Tobias WEBER	Monte-Carlo simulations of neutron triple-axis spectrometers

Tutorials at ILL, Maison des Magistères (MM), CNRS, and ESRF, Grenoble

Local coordinator: Béatrice GRENIER

Name	Site	Instructor	Title
T1	ILL	Claire COLIN	Magnetic structures formalism
T2	ILL	Alberto RODRIGUEZ VELAMAZAN	Single Crystal Neutron Diffraction Studies for Nuclear and Magnetic Structures: Determination of a Hybrid Compound using FullProf
T3	ILL	Gabriel CUELLO	From Q-space to R-space: PDF-analysis
T4	ILL	Frédéric OTT	Neutron reflectivity
T5	ILL	Sandrine LYONNARD	Quasi-Elastic Neutron Scattering in batteries
T6	ILL	Arnaud MORIN	Small Angle Scattering in Proton Exchange Membrane Fuel Cell
T7	ILL	Peter FOUQUET	Neutron spin-echo spectroscopy: data reduction and fields of application
T8	MM	Jacques PECAUT	Small molecule structure resolution using single-crystal X-ray diffraction
T9	MM	Olivier PEREZ	Aperiodic crystals: from data collection to structure solution
T10	CNRS	Jean-Sébastien MICHA	White Beam Microdiffraction
T11	CNRS	Yves JOLY	Simulation of X-ray absorption spectroscopies
T12	ESRF	Marius RETEGAN	X-ray spectroscopy simulations using semi-empirical multiplet approaches
T13	ESRF	Manuel SANCHEZ DEL RIO	Modeling a SR beamline
T14	ESRF	Francesco D'ACAPITO	Introduction to EXAFS data analysis
T15	ESRF	Olivier PROUX	Basic Principles of EXAFS analysis
T16	ESRF	Vincent FAVRE-NICOLIN	X-ray Coherent Diffraction Imaging and Ptychography
T17	ESRF	Cécile OLIVIER	3D quantitative assessment of human cortical bone by micro-tomography



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 *J. Bell*
- 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*

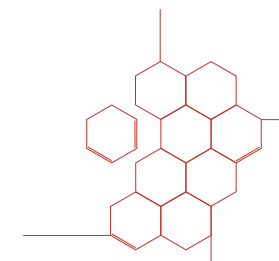
HERCULES 2019: PROGRAMME OF LECTURES

(subject to modification)

Updated : 18/02/2019

- Common lectures
- Session B lectures
- Other

Week 1	Monday 18/03	Tuesday 19/03	Wednesday 20/03	Thursday 21/03	Friday 22/03
8:30 - 8:45	Welcome				
8:45 - 9:30 10' break 9:40 - 10:25	Diffraction, refraction and absorption of X-rays and neutrons (1/2) Werner F. Kuhs	Diffraction, refraction and absorption of X-rays and neutrons (2/2) Werner F. Kuhs	Soft X-rays and VUV: specific optics and applications David Attwood	Fundamentals of X-ray Absorption Fine Structure (1/2) Sakura Pascarelli	X-ray detectors Heinz Graafsma
10:45 - 11:30 10' break 11:40 - 12:25	ESRF / ILL badges distribution	Introduction to synchrotron radiation David Attwood	Neutrons: scattering and instrumentation (1/2) Andrew Wildes	Neutrons: scattering and instrumentation (2/2) Andrew Wildes	Crystallography (2/2) Béatrice Grenier
14:00 - 14:45 10' break 14:55 - 15:40	ESRF / ILL visits	Crystallography (1/2) Béatrice Grenier	Neutron and X-ray diffraction by crystals: kinematical approximation and experimental methods Werner F. Kuhs	Fundamentals of X-ray Absorption Fine Structure (2/2) Sakura Pascarelli	POSTER SESSION
16:00 - 16:45 10' break 16:55 - 17:40	16:00 - 17:30 ESRF / ILL presentations Francesco Sette / Mark Johnson 17:30 - 17:45 UGA presentation	ESRF / ILL visits	Free Electron Lasers and ultra fast X-ray science Thomas Tschentscher	Introduction to imaging techniques Federica Marone	16:00: European user facilities: the CERIC-ERIC and wayforlight Matthias Girod 16:45:NFFA.eu Ennio CAPRIA 17:00: Poster awards Gala dinner
	Welcome cocktail at ESRF			DECTRIS presentation	



Week 2	Monday 25/03	Tuesday 26/03	Wednesday 27/03	Thursday 28/03	Friday 29/03
8:45 - 9:30 10' break 9:40 - 10:25	Introduction to neutron and X-Ray inelastic scattering Victor Balédent	Basics of protein crystallography, data collection, data reduction, 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 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	Full-field coherent Imaging Peter Cloetens	Hard X-ray optics for SR beamlines Ray Barrett	Nuclear Magnetic Resonance Martin Blackledge	Electron microscopy for structural biology Ambroise Desfosses	IBS LABS / TUTORIALS
16:00 - 16:45 10' break 16:55 - 17:40	Introduction to small angle scattering Martin Müller	Science at neutron spallation sources Sean Langridge	Native Mass spectrometry to study intact protein complexes Elisabetta Boeri Erba	Small angle neutron scattering Frank Gabel	
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			

Week 3 (1st – 5th April), and week 4 (8th – 12th April) : Outside Grenoble

Week 5	Monday 15/04	Tuesday 16/04	Wednesday 17/04	Thursday 18/04	Friday 19/04
8:45 - 9:30 10' break 9:40 - 10:25	Crystal growth and low resolution structures Monika Spano	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	TUTORIALS / LABS	Dynamics of macromolecules Giuseppe Zaccai	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 /	Protein dynamics by neutron scattering Giuseppe Zaccai	Super-resolution fluorescence microscopy Dominique Bourgeois	
16:00 - 16:45 10' break 16:55 - 17:40	Fibre diffraction James Bell	TUTORIALS / LABS	Membrane diffraction David Barlow	Time resolved fluorescence and circular dichroism studies with SR David Clarke	
18:00 - 19:00			EVALUATION MEETING		

**PRACTICALS AND TUTORIALS
Session B**

Coordinators:

- ▶ B. DEME, B. GRENIER, P. PERNOT, G.SCHIRO (Grenoble)
- ▶ B. CALISTO, D. PIERUCCI, M. J. SIMANCAS (Barcelona)
- ▶ A. COATI, F. DAMAY, L. NATAF (Paris-Saclay)
- ▶ F. BENCIVENGA, A. LOCATELLI, E. PEDERSOLI, B. ROSSI (Trieste)
- ▶ R. GEHRKE, O. SEECK, T. TSCHENTSCHER (Hamburg)
- ▶ J. DREISER, M. FÜGLISTER (Villigen)
- ▶ T. BAUMBACH, M. HAGELSTEIN, L. JOCHIM (Karlsruhe)

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 will carry out two practicals at ILL or one practical at ILL and a lab on CryoEM at ESRF, as well as hands-on experiments / data treatment at Institut de Biologie Structurale (IBS).

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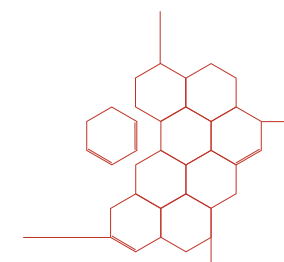


All participants are required to attend the entire practical and tutorial programme assigned to them.

Practicals in laboratories(Labs) and tutorials at IBS, Grenoble		
Local coordinators: Petra PERNOT and Giorgio SCHIRO		
Name	Instructor(s)	Title
NMR	Adrien FAVIER	Folding characterization, structure and dynamics of proteins by NMR
COOT	David COBESSI	Macromolecular model building and analysis in electron density maps using COOT
Cryst	Monika BUDAYOVA-SPANO	Crystallization of biological macromolecules
Anom	Eric GIRARD	Solving protein structures by crystallography with anomalous-based methods
Mass spec	Elisabetta BOERI-ERBA	Native mass spectrometry to study intact protein complexes
EM	Daphna FENEL, Leandro ESTROZI	Electron microscopy using negative staining

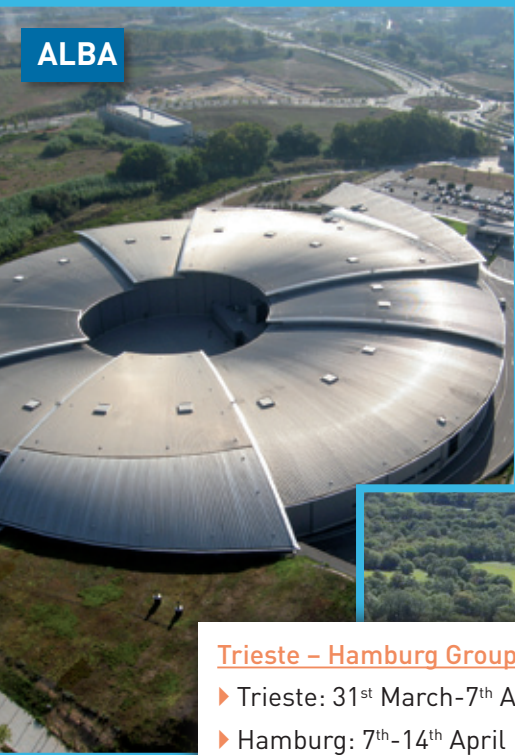
Neutron Practical at ILL, Grenoble		
Local coordinators: Bruno DEME and Petra PERNOT		
Name	Instructor	Title
FIGARO	Armando MAESTRO	Life in two dimensions: From soft to biological matter elucidated by neutron reflectometry
D22	Anne MARTEL	Small-Angle Neutron Scattering for low resolution structure of biological complexes in solution
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
ID30s (Cryobench)	Antoine ROYANT	Overview and practice of crystallo Optical Spectroscopies (Absorption, Fluorescence and Raman)
CryoEM (CM01)	David FERNANDEZ MARTINEZ, Michael HONS	Cryo-EM: vitrification and data collection pipeline

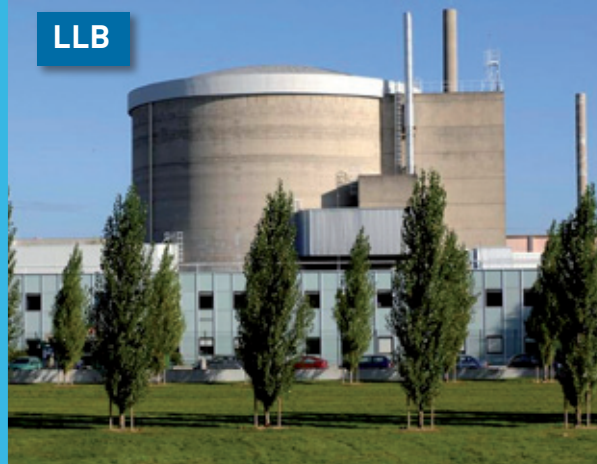


PROGRAMME OUTSIDE GRENOBLE

ALBA



LLB



Elettra-FERMI



Trieste – Hamburg Group:

- ▶ Trieste: 31st March-7th April
- ▶ Hamburg: 7th-14th April

PSI



SOLEIL



Barcelona – Paris Group:

- ▶ Barcelona: 31st March-7th April
- ▶ Paris-Saclay: 7th-14th April

DESY-European XFEL



KIT



Villigen – Karlsruhe Group:

- ▶ Villigen: 31st March-5th April
- ▶ Karlsruhe: 5th-13th April

HERCULES SCHOOL 2019: PLANNING IN BARCELONA

31st March - 7th April 2019 (Sunday-Sunday)

[Session A: Physics and chemistry of condensed matter](#)

[Session B: Biomolecular structure and dynamics](#)



Monday 1st April
in Maxwell Auditorium

Time	Title	Speakers
9:00	Welcome message	Management
9:10	Attendee's background and expectations. Explanation of the program.	
9:30	Soft X-ray absorption and XMCD	Javier HERRERO, Stefano AGRESTINI
10:30	Coffee break	
11:00	Macromolecular Crystallography at ALBA: from data to structure	Xavier CARPENA
12:00	X-ray Photoemission Electron Microscopy (XPEEM): Principles and applications	Michael FOERSTER
13:00	Lunch	
14:30	Soft X-ray Transmission Microscopy	Andrea SORRENTINO
15:30	Near Ambient Pressure Photoemission (NAPP) at ALBA synchrotron: more realistic studies by minimizing the pressure gap	Carlos ESCUDERO
16:30	Coffee break	
17:00	Guided Tour to ALBA	

Tuesday 2nd and Wednesday 3rd April

Time	Title
9:00	Practical at ALBA
13:00	Lunch
14:30-18:00	Practical or Tutorial at ALBA

Thursday 4th April
Session A

Time	Title
9:00	Tutorial: Analysis of data collected at ALBA
11:30	Preparation of an experimental report
13:00	Lunch
14:30	Tutorial: Analysis of data collected at ALBA
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	Instructors	Room
9:00	Macromolecular model building and analysis of electron density maps	Xavier CARPENA Bárbara CALISTO	Ada Lovelace
13:00	Lunch		
14:30	Infrared data handling (chemical imaging and individual spectra) using OPUS and Unscrambler software	Ibraheem YOUSEF	Ada Lovelace
16:30	Coffee break		
17:00	Preparation of an experimental report. One-to one-meetings with ALBA researchers		
20:30	Social dinner		

Friday 5th April

Time	Title	Room
9:00	Preparation of an experimental report: Final touches	Marie Curie Niels Bohr/Bragg
10:00	Presentation of the reports (session A)	Maxwell Audit
11:00	Coffee break	
11:20	Presentation of the reports (session B)	Maxwell Audit
12:00	Wrap-up session	
13:00	Lunch	

Practicals Session A: Physics and chemistry of condensed matter

Synchrotron Radiation Practicals at ALBA, Barcelona Local coordinators: Bárbara CALISTO, Maria José SIMANCAS, and Debora PIERUCCI		
Beamlines	Instructors	Title
GBL22 – CLAESS	Laura SIMONELLI, Carlo MARINI, Giovanni AGOSTINI	X-ray absorption end emission spectroscopy to access the local structural and electronic properties of the matter
BL29 – BOREAS	Stefano AGRESTINI, Javier HERRERO (Part I), Manuel VALVIDARES, Pierluigi GARGIANI (Part II)	XAS and XMCD investigation of bulk and surface science samples
BL11 – NCD-SWEET	Marc MALFOIS, Eduardo SOLANO	SAXS/WAXS study on polymer crystallisation

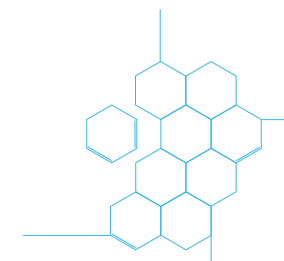
Synchrotron Radiation Tutorials at ALBA, Barcelona Local coordinators: Bárbara CALISTO, Maria José SIMANCAS, and Debora PIERUCCI	
Instructors	Title
Laura SIMONELLI, Carlo MARINI, Giovanni AGOSTINI	Analysis of XAS data collected at CLAESS: XANES linear combination approach (Athena program), XES data treatment: quantification of the local magnetic moment by the IAD method (Origin program)
Stefano AGRESTINI (Part I), Pierluigi GARGIANI (Part II)	Analysis of XAS and XMCD data collected at BOREAS: spectra treatment, sum rules and introduction to multiplet simulations
Marc MALFOIS, Eduardo SOLANO	Analysis of data collected at NCD-SWEET: data reduction using pyFAI and DAWN software. Preliminary data analysis and interpretation

Practicals Session B: Biomolecular structure and dynamics

Synchrotron Radiation Practicals at ALBA, Barcelona Local coordinators: Bárbara CALISTO, Maria José SIMANCAS, and Debora PIERUCCI		
Beamlines	Instructors	Title
BL01 - MIRAS	Immaculada MARTINEZ-ROVIRA, Ibraheem YOUSEF	Using the FTIR microscope and various experimental setups at MIRAS BL
BL09 - MISTRAL	Ana PÉREZ-BERNÁ	Biomedical Applications at the soft X-ray microscope MISTRAL
BL13 - XALOC	Bárbara CALISTO Damià GARRIGA	Protein crystallisation and data collection at XALOC
BL13 - XALOC	Fernando GIL, Roeland BOER	In-situ diffraction and data treatment at XALOC

Synchrotron Radiation Tutorials at ALBA, Barcelona Local coordinators: Bárbara CALISTO, Maria José SIMANCAS, and Debora PIERUCCI	
Instructors	Title
Xavier CARPENA, Bárbara CALISTO	Macromolecular model building and analysis of electron density maps
Ibraheem YOUSEF	Infrared data handling (chemical imaging and individual spectra) using OPUS and Unscrambler software

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



**HERCULES SCHOOL 2019:
PLANNING IN PARIS-SACLAY**
7th-14th April 2019 (Sunday-Sunday)

Session A: Physics and chemistry of condensed matter
Session B: Biomolecular structure and dynamics
Monday 8th April

At SOLEIL all day long

Time	
9:00 - 9:40	Welcome SOLEIL (Jean Daillant) and LLB (Alain Menelle) presentations
9:45-11:00	Claire LAULHE Time-resolved X-ray Scattering <i>Auditorium</i>
11:00-11:15	Coffee break
11:15-12:45	Paul DUMAS Synchrotron infrared emission and spectroscopic applications <i>Auditorium</i>
12:45-14:00	Lunch at SOLEIL
14:00-15:30	Thierry MORENO Calculation of a hard x-rays beamline <i>Phenix (A1.0.59)</i>
15:30-16:00	Coffee break
16:00-17:30	Thierry MORENO Calculation of a hard x-rays beamline <i>Phenix (A1.0.59)</i>
17:30 -18:00	Break
18:00-19:00	Sylvain RAVY How light became a wave? <i>Auditorium</i>

Tuesday 9th and Wednesday 10th April

At SOLEIL all day long

Time	
9:00-17:30	PRACTICALS on SOLEIL beamlines
17:30-19:00	Data Analysis - Talk Preparation

Thursday 11th April

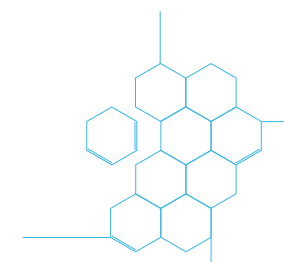
At LLB all day long

Time	
9:00-17:30	PRACTICALS at the LLB

Friday 12th April

At SOLEIL all day long

Time	
9:00-10:30	Frédéric OTT How to build a neutron spectrometer? <i>Auditorium</i>
10:30-11:00	Coffee break
11:00-11:45	François BAUDELET History of Synchrotron <i>Auditorium</i>
11:45-13:00	Lunch at SOLEIL
13:00-15:00	Data Analysis - Talk Preparation
15:00-15:30	Coffee break
15:30-17:30	Students presentation and Evaluation Meeting <i>Auditorium</i>



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
GALAXIES	Jean-Pascal RUEFF	Spin states in Fe-based compounds,
ODE	Lucie NATAF	investigated through XES and XAS
ROCK	Valérie BRIOIS	Memory effect of Layered Double Hydroxide,
CRISTAL	Erik ELKAÏM	by EXAFS and WAXS
AILES	Jean-Blaise BRUBACH	Spin transition in molecular magnets
SAMBA	Emiliano FONDA	studied by IR THz spectroscopy and XAFS

Neutron Practicals at LLB, CEA, Saclay (near Paris) Local coordinator: Françoise DAMAY		
Beamline	Instructors	Title
G4.1	Françoise DAMAY	Neutron powder diffraction: crystal and magnetic structures
IMAGINE	Frédéric OTT	Neutron imaging of water diffusion in porous media
G4.3	Sylvain PETIT	Phonon and magnon excitations in CaF2

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
SWING	Aurélien THUREAU Javier PEREZ	Studies of the TTR protein in complex with ligands by X-ray Crystallography and SAXS.
PROXIMA2	William SHEPARD	

Neutron Practicals at LLB, CEA, Saclay (near Paris) Local coordinator: Françoise DAMAY		
Beamline	Instructors	Title
PACE	Sophie COMBET	Small angle neutron scattering on biological samples
Muses	Stéphane LONGEVILLE	Protein diffusion in crowded solutions

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

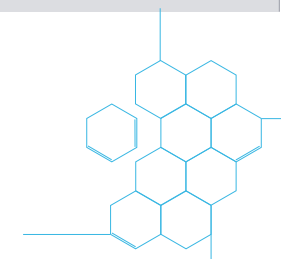
HERCULES SCHOOL 2019:**PLANNING IN TRIESTE**31st March - 7th April 2019 (Sunday-Sunday)

Session A: Physics and chemistry of condensed matter

Session B: Biomolecular structure and dynamics

Monday 1st April

Time	Where	What
	Hotel	Breakfast
9:00-9:10	Training room	Welcome
9:10-9:45	Training room	Claudio MASCIOVECCHIO Frontier science at FERMI
9:45-10:20	Training room	Luca GIANNESI FERMI: the first externally seeded Free Electron Laser in the extreme ultraviolet and soft x-ray spectral regions
10:20-10:50		Coffee break
10:50-11:25	Training room	Luca GREGORATTI Photoelectron spectromicroscopy at Elettra: recent advances and perspectives
11:25-12:00	Training room	Alessandro BARALDI Probing growth and properties of materials using fast and high-resolution x-ray photoelectron spectroscopy
12:00-12:35	Training room	Paolo MORAS Angle-resolved photoelectron spectroscopy studies at synchrotron light sources
12:35-14:10	Canteen	Lunch
14:10-15:30	Elettra/FERMI	Visit to the 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 to the facility Labs
	Hotel	Dinner



Tuesday 2nd April

Time	Where	What
	Hotel	Breakfast
9:00-9:35	Training room	Lisa VACCARI Infrared bio-spectroscopy: from macro to nano scale on the molecules of life
9:35-10:10	Training room	Heinz AMENITSCH Small angle x-ray scattering: the answer to dynamics in biological matter?
10:10-10:45	Training room	Lucia MANCINI 3D and 4D x-ray imaging techniques for comprehensive microstructural properties of materials: from medicine to geosciences
10:45-11:10		Coffee break
11:10-11:45	Training room	Simone POLLASTRI Research highlights at the XAFS beamline of Elettra
11:45-12:20	Training room	Carlo CALLEGARI The Low Density Matter beamline at the FERMI Free Electron Laser
12:20-12:55	Training room	Emanuele PEDERSOLI Magnetization dynamics at FERMI seeded FEL
12:55-14:20	Canteen	Lunch
14:20-17:50	Elettra/FERMI	Practicals at the beamlines (including LASER safety at FERMI)
	Hotel	Dinner

Wednesday 3rd April

Time	Where	What
	Hotel	Breakfast
9:00-12:30	Elettra/FERMI	Practicals at the beamlines
12:30-14:00	Canteen	Lunch
14:00-17:30	Elettra/FERMI	Practicals at the beamlines
	Hotel	Dinner

Thursday 4th April

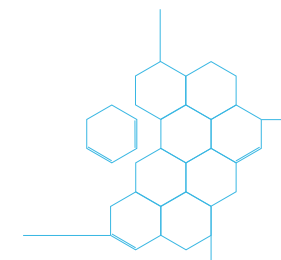
Time	Where	What
	Hotel	Breakfast
9:00-9:35	Training room	Cecilia BLASETTI Hints and tips for writing a successful beamtime proposal
9:35-9:50	Training room	Introduction to one-to-one meetings
9:50-10:20		Coffee break
10:20-12:40	Elettra/FERMI	One-to-one meeting with researchers
12:40-14:10	Canteen	Lunch
14:10-16:00	Elettra/FERMI	Prepare group presentations
		Free evening out

Friday 5th April

Time	Where	What
	Hotel	Breakfast
9:00-10:30	Training room	Group presentations
10:30-11:00		Coffee break
11:00-12:30	Training room	Feedback meeting
12:30-14:00	Canteen	Lunch
15:00-19:00	Trieste	Social tour
19:00-22:30		Social Dinner

Saturday 6th April

Departure to Venice (until Sunday)



Practicals Session A: Physics and chemistry of condensed matter

Synchrotron Radiation Practicals at Elettra, Trieste (Italy) Local coordinators: Andrea LOCATELLI and Barbara ROSSI		
Beamline	Instructors	Title
Nanospectroscopy	Andrea LOCATELLI, Tevfik Onur MENTEŞ, Francesca GENUZIO	Chemical and magnetic imaging of graphene-capped thin films
APE	Ivana VOBORNIK	ARPES and spin-ARPES investigation of systems with strong spin-orbit coupling
ESCA	Matteo AMATI, Luca GREGORATTI, Patrick ZELLER	2D materials at the nanometric scale: properties and functionalities
SuperESCA	Silvano LIZZIT, Paolo LACOVIG, Daniel LIZZIT	Growth and intercalation of graphene on metals studied by fast XPS
ALOISA	Luca FLOREANO, Albano COSSARO, Alberto VERDINI	On-surface modification of organic semiconductors
XAFS	Simone POLLASTRI, Luca OLIVI, Danilo Oliveira DE SOUZA	Unraveling the local and electronic structure in metal oxides

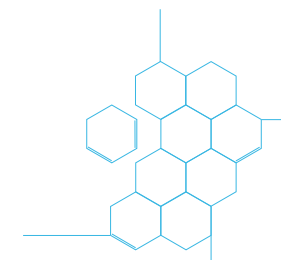
Free Electron Laser Practicals at FERMI, Trieste (Italy) Local coordinators: Filippo BENCIVENGA and Emanuele PEDERSOLI		
Beamline	Instructors	Title
T-ReX	Federico CILENTO, Simone PELI	Time-resolved ARPES experiments on complex materials
MagneDyn	Antonio CARETTA, Marco MALVESTUTO	Ultrafast optomagnetism in a superconductor/ferromagnetic bilayer
LDM	Carlo CALLEGARI, Daniela RUPP	Imaging of resonantly excited helium nanodroplets

Practicals Session B: Biomolecular structure and dynamics

Synchrotron Radiation Practicals at Elettra, Trieste (Italy) Local coordinators: Andrea LOCATELLI and Barbara ROSSI		
Beamline	Instructors	Title
SISSI	Lisa VACCARI, Giovanni BIRARDA	FTIR microscopy and nanoscopy
Twinmic	Alessandra GIANONCELLI	X-ray microscopy and low energy XRF on cells and tissues
SAXS	Heinz AMENITSCH, Sigrid BERNSTORFF	Self assembly of mesoporous materials (MCM-41)
DXRL	Benedetta MARMIROLI, Alessio TURCHET	X-ray lithography to obtain microgears, replica of microstructures using a soft material

Free Electron Laser Practicals at FERMI, Trieste (Italy) Local coordinators: Filippo BENCIVENGA and Emanuele PEDERSOLI		
Beamline	Instructors	Title
EIS	Laura FOGLIA, Riccardo MINCIGRUCCI	Nanoscale thermal transport
TeraFERMI	Nidhi ADHLAKHA	THz induced birefringence in z-cut quartz

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



HERCULES SCHOOL 2019:

PLANNING IN HAMBURG

7th – 14th April 2019 (Sunday-Sunday)Session A: Physics and chemistry of condensed matterSession B: Biomolecular structure and dynamicsMonday 8th April

DESY Seminar Room 109, Building 25B

Time	What
9:00-10:00	Welcome - Christian SCHROER: Introduction to DESY
10:00-11:00	Thomas TSCHENTSCHER: Introduction to European XFEL
11:00-13:00	PETRA III and FLASH Tour
13:00-14:00	Lunch
14:00-18:00	Session A: DESY Practical Training Part 1 Session B: Introduction to the background of the EMBL Practical Trainings

Tuesday 9th April

DESY Site

Time	What
9:00-13:00	Session A: DESY Practical Training Part 2 Session B: EMBL Practical Training Part 1
13:00-14:00	Lunch
14:00-18:00	Session A: DESY Practical Training Part 3 Session B: EMBL Practical Training Part 2

Wednesday 10th April

European XFEL Site

Time	What
9:00-18:00	European XFEL Practicals for Session A and Session B
19:00	Social dinner

Thursday 11th April

European XFEL site

Time	What
9:00-18:00	Continuation of European XFEL Practicals for Session A and Session B

Friday 12th April

DESY Site

Time	What
9:00-13:00	Data Analysis related to the Practical Trainings
12:00-14:00	Lunch
14:00-16:00	Continuation of Data Analysis
16:00-17:00	Course Review

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
P01	Hlynur GRETARSSON, Martin SUNDERMANN	Imaging of orbitals with Inelastic X-Ray Scattering
P07B	Malte BLANKENBURG, Peter STARON	Small-angle X-ray scattering from precipitation hardened aluminium alloys
P08	Florian BERTRAM	Scattering on thin films and surfaces

The experiments at P07B are supervised by Helmholtz Zentrum Geesthacht HZG

Synchrotron Radiation Tutorials at DESY – PETRA III, Hamburg (Germany)

Local coordinators: Rainer GEHRKE and Oliver SEECK

Instructors	Title
Hlynur GRETARSSON, Martin SUNDERMANN, Malte BLANKENBURG, Peter STARON, Florian BERTRAM	Evaluation of data from DESY practicals

Free Electron Laser Practicals at European XFEL, Hamburg (Germany)

Local coordinator: Thomas TSCHENTSCHER

Beamline	Instructors	Title
SA1	Jan GRÜNERT, Naresh KUJALA	FEL spectra and conversion to time domain
FXE	Andreas GALLER, Mykola BIEDNOV	Laser pump X-ray probe fs time resolved X-ray spectroscopy techniques
SQS	Michael MEYER, Tommaso MAZZA	Ion Spectroscopy at Highly Ionized Atoms

*All three student groups of **session A** at the DESY PETRA III beamlines subsequently complete all three Practical Trainings. 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	Instructor	Title
P12	Melissa Ann GRAEWERT, Cy JEFFRIES	Small angle X-Ray scattering on biological samples in solution
P13	Guillaume POMPIDOR	Macromolecular crystallography

The experiments at P12 and P13 are supervised by the European Molecular Biology Laboratory EMBL

Free Electron Laser Practicals at European XFEL, Hamburg (Germany)
 Local coordinator: Thomas TSCHENTSCHER

Beamline	Instructor	Title
Bio-labs	Huijong HAN, Robin SCHUBERT	Crystallization and nano-crystal injection
SPB/SFX	Klaus GIEWEKEMEYER, Henry KIRKWOOD, Ruslan KURTA, Adam ROUND	Small-angle scattering using coherent beams

**Free Electron Laser Tutorials at DESY – PETRA III
or European XFEL (TBD), Hamburg (Germany)**
 Local coordinator: Thomas TSCHENTSCHER

Instructors	Title
Ruslan KURTA	Evaluation of data from European XFEL practicals

Both at the DESY PETRA III beamlines and at European XFEL the two student groups of **session B** subsequently complete two times two Practical Trainings.

HERCULES SCHOOL 2019:**PLANNING IN VILLIGEN**
31st March – 5th April 2019 (Sunday-Friday)
[Session A: Physics and chemistry of condensed matter](#)
[Session B: Biomolecular structure and dynamics](#)
**Sunday 31st March**

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

Monday 1st April

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 2nd April

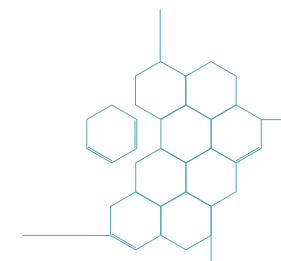
Time	Where	What
8:00 – 9:00	TIMEOUT PSI west	Breakfast
9:00 – 12:30	@ SLS beamlines	Experiments / work in groups
12:30 – 13:30	TIMEOUT PSI west	Lunch
13:30 – 17:00	@ SLS beamlines	Experiments / work in groups
17:00 – 18:00		Free time
18:00	OASE PSI east	Dinner
19:00	Outside PSI guesthouse West	Departure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

Wednesday 3rd April

Time	Where	What
8:00 - 9:00	TIMEOUT PSI west	Breakfast
9:00 - 9:30	WBGB/019	Dubravka SISAK JUNG: Detectors - a view from the application side
9:30 - 10:00	WBGB/019	Cinthia PIAMONTEZE Soft X-ray magnetic circular dichroism
10:00 - 10:30	WBGB/019	Nicholas PLUMB Angle-resolved photoelectron emission spectroscopy
10:30 - 10:45		Break
10:45 - 11:50		Andreas LÜDEKE et al. Tour SLS tunnel
11:50 - 12:30	WBGB/019	Christopher MILNE Intro to SwissFEL
12:30 - 13:30	TIMEOUT PSI west	Lunch
13:30 - 14:45		Christopher MILNE Tour SwissFEL
14:45 - 18:00	WBGB/019 +020, WSLA/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 4th April

Time	Where	What
8:00 - 9:00	TIMEOUT PSI west	Breakfast
9:00 - 9:35	WBGB/019	Michel KENZELMANN Intro to SINQ
9:35 - 10:10	WBGB/019	Zaher SALMAN Muon spin spectroscopy in condensed matter and chemistry - Introduction and examples
10:10 - 10:40	WBGB/019	Henrik Till LEMKE First experiments at SwissFEL
10:40 - 11:00	WBGB/019 + 021 WSLA/105 TIMEOUT	Break / presentation final touches
11:00 - 11:30	WBGB/019	Student presentations part 1
11:30		‣ADRESS-SXARPES
11:45		‣PHOENIX
12:00		‣SIM
12:30 - 13:30	TIMEOUT PSI West	Lunch
13:30 - 14:00	WBGB/019	Oksana ZAHARKO Neutron diffraction: Examples
14:00 - 15:30		TBD + Zaher Salman Tour SINQ + SmuS
15:30 - 15:45		Break
15:45 - 16:25	WBGB/019	Francis GAGNON-MOISAN Introduction to Proton Therapy
16:25 - 17:05		Francis GAGNON-MOISAN Tour Center for Proton Therapy
17:05 - 18:30		Free time
18:30 - 18:50	Bus stop PSI West	Departures of minibus shuttle to restaurant
18:40 - 22:00	“Zur Tenne” Rüfenach	Aperitif and farewell dinner
21:50 - 22:10	Outside “Zur Tenne”	Departures of minibus shuttle to guesthouse



Friday 5th April

Time	Where	What
8:30 - 9:30	PSI guesthouse West PSI reception West TIMEOUT PSI west	Checkout of rooms & store luggage Return room key Breakfast
9:30 - 9:40		Setup for presentations
9:40 - 10:40	WBGB/019	Student presentations part 2 ‣TOMCAT+POLLUX ‣cSAXS ‣MS+MX ‣superXAS
10:40 - 11:00		Break
11:00 - 11:30	WBGB/019	Jochen STAHN Polarized neutron reflectometry
11:30 - 12:00	WBGB/019	Simone FINIZIO Scanning transmission X-ray microscopy and applications
12:00 - 12:30	WBGB/019	Carlos VAZ X-ray photoelectron emission microscopy and applications
12:30 - 13:30	TIMEOUT PSI West	Lunch
13:30 - 13:45	PSI guesthouse West	Load luggage, return badge and board coach
13:45	PSI guesthouse West	Departure to Karlsruhe

Practicals Session A: Physics and chemistry of condensed matter

Synchrotron Radiation Practicals at SLS, Villigen (Switzerland)		
Local coordinator: Jan DREISER		
Beamline	Instructors	Title
Phoenix	Camelia BORCA	Iron spatial distribution and its oxide forms in fluid catalytic cracking particles
Adress/ARPES	Vladimir STROCOV	What is the Fermi Surface of your Smartphone? Explore electronic structure of semiconductor heterostructures by soft-X-ray ARPES
SuperXAS	Olga SAFONOVA	Palladium state in advanced heterogeneous catalyst for automotive pollution control
SIM	Carlos VAZ	Imaging Magnetic Nanostructures using Soft X-ray Photoemission Electron Microscopy (PEEM)
cSAXS	Ana DIAZ	X-ray nanotomography with quantitative contrast

Practicals Session B: Biomolecular structure and dynamics

Synchrotron Radiation Practicals at SLS, Villigen (Switzerland)		
Local coordinator: Jan DREISER		
Beamline	Instructors	Title
TOMCAT	Federica MARONE	Absorption and phase contrast X-ray tomographic microscopy
PX III	Vincent OLIERIC	Macromolecular crystallography data collection
Materials science	Nicola CASATI	Quantification of two components powder via Rietveld refinement
Pollux	Ben WATTS	Composition mapping of a thin-film polymer blend

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

HERCULES SCHOOL 2019:

PLANNING IN KARLSRUHE

5th-13th April 2019 (Friday-Saturday)

[Session A: Physics and chemistry of condensed matter](#)

[Session B: Biomolecular structure and dynamics](#)

Monday 8th April

Time	
9:00-10:00	Michael HAGELSTEIN Welcome, introduction, safety instruction
10:00-11:00	Marcel SCHUH, Anke-Susanne MÜLLER Lecture Machine: Accelerator physics at KIT
11:00-11:30	Coffee break
11:30-12:30	Tilo BAUMBACH Lecture Beamlines: Experiments and beamlines at KIT
12:30-14:00	Lunch
14:00-15:30	Thomas SCHALLER Tutorial: Introduction to the Karlsruhe Nano Micro Facility or Marcel SCHUH, Anke-Susanne MÜLLER Practical: Injection to the storage ring KARA or Robert RUPRECHT, Nigel SMALE, Michael NASSE, Thimo SCHMELZER Practical: FLUTE linear accelerator for the generation of THz radiation
then	
16:00-18:00	
	Coffee break in between

Tuesday 9th, Wednesday 10th, Thursday 11th, and Friday 12th April

One day-long practical on a different beamline each day

Time	
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: Tilo BAUMBACH, Michael HAGELSTEIN, Anton PLECH, and Leyla JOCHIM

Beamline	Instructors	Title
INE	Jörg ROTHE, Kathy DARDENNE	X-ray Absorption Spectroscopy of radioactive materials
IR1	Alexander BORIS, Yves-Laurent MATHIS	Synchrotron Fourier Transform Infra-red ellipsometry
IR2	David MOSS, Biliana GASHAROVA	Synchrotron Fourier Transform Infra-red spectroscopy
TOPOTOMO	Daniel HÄNSCHKE, Marcus ZUBER, Thomas VAN DE KAMP	Tomography, laminography
NANO	Sondes BAUER	X-ray full field microscopy
WERA	Stefan SCHUPPLER, Peter NAGEL, Michael MERZ	Soft X-ray spectroscopy and microscopy, X-ray Magnetic Circular Dichroism
LIGA	Uwe KÖHLER, Martin BÖRNER	X-ray lithography
SCD	Gernot BUTH, Anton PLECH	X-ray reflectivity
Storage ring	Marcel SCHUH, Anke-Susanne MÜLLER	Injection to the storage ring
FLUTE	Robert RUPRECHT, Nigel SMALE, Michael NASSE, Thimo SCHMELZER	FLUTE linear accelerator for the generation of THz radiation
KNMF	Thomas SCHALLER	Introduction to the Karlsruhe Nano Micro Facility

Practicals Session B: Biomolecular structure and dynamics

Synchrotron Radiation Practicals at KIT Light Source, Karlsruhe (Germany)

Local coordinators: Tilo BAUMBACH, Michael HAGELSTEIN, Anton PLECH, and Leyla JOCHIM

Beamline	Instructors	Title
KNMF	Thomas SCHALLER	Introduction to the Karlsruhe Nano Micro Facility
IR2	David MOSS, Biliana GASHAROVA, Yves-Laurent MATHIS	Synchrotron Fourier Transform Infra-red spectroscopy
TOPOTOMO	Daniel HÄNSCHKE, Marcus ZUBER, Thomas VAN DE KAMP	Tomography, laminography
NANO	Sondes BAUER	X-ray full field microscopy
INE	Jörg ROTHE	X-ray absorption spectroscopy

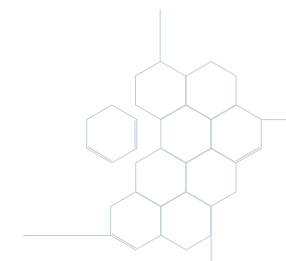
As in Grenoble, each group of 4 full time participants will follow practicals selected from the lists above.

LECTURERS

Surname	Name	Institut
AGRESTINI	Stefano	ALBA
AMENITSCH	Heinz	Elettra Sincrotrone Trieste
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BARRETT	Ray	ESRF
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BAUMBACH	Tilo	KIT
BELL	James	Cardiff University
BLAKELEY	Matthew	EMBL
BLAKLEDGE	Martin	IBS
BLASETTI	Cecilia	Elettra Sincrotrone Trieste
BOERI ERBA	Elisabetta	IBS / EMBL / UVHCI
BOURGOIS	Dominique	IBS
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CLOETENS	Peter	ESRF
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DE BOISSIEU	Marc	Grenoble INP
DESFOSSÉS	Ambroise	IBS
DIL	Hugo	EPFL
DUMAS	Paul	Synchrotron SOLEIL

Surname	Name	Institut
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JUDGE	Peter	Biochemistry, University of Oxford
JUHN GOUEL	Amélie	Univ. Pierre et Marie Curie
KENZELMANN	Michel	PSI
KRISCH	Michael	ESRF
KUHS	Werner F.	University of Göttingen
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MARONE WELFORD	Federica	PSI
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OTT	Frédéric	CEA-LLB
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PASCARELLI	Sakura	ESRF

Surname	Name	Institut
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PIAMONTEZE	Cinthia	PSI
PLECH	Anton	KIT
PLUMB	Nicholas	PSI
POLLASTRI	Simone	Elettra Sincrotrone Trieste
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SCHALLER	Thomas	KIT
SCHNEIDER	Claus	Forschungszentrum Jülich
SCHOEDER	Sebastian	Synchrotron SOLEIL
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SORRENTINO	Andrea	ALBA
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STAUB	Urs	PSI
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TROMBA	Giuliana	Elettra Sincrotrone Trieste
TSCHECHTSCHER	Thomas	European XFEL
VACCARI	Lisa	Elettra Sincrotrone Trieste
VAZ	Carlos	PSI
WEBER	Tobias	ILL
WILDES	Andrew	ILL
YOUSEF	Ibraheem	ALBA
ZABEL	Hartmut	Ruhr Universität Bochum
ZACCAI	JOSEPH	ILL
ZAHARKO	Oksana	PSI



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 du Caducée
68 avenue des Martyrs

☎ 04 76 46 04 40

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