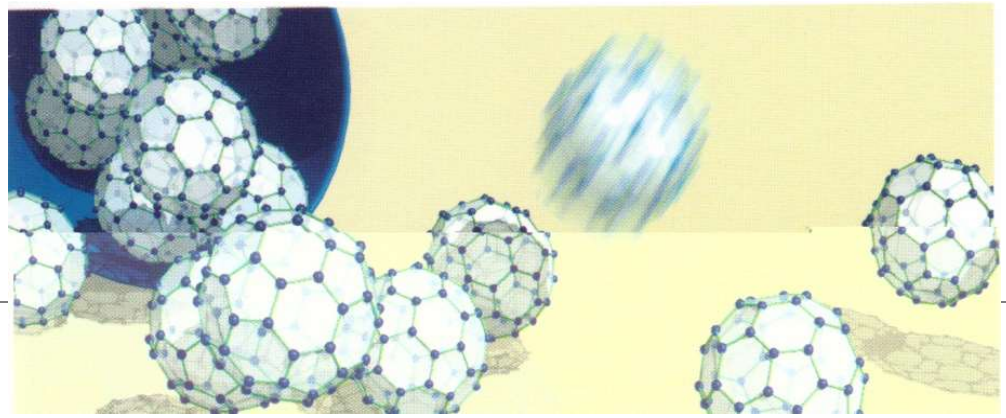
How to apply for time-machine at large scale facilities

Synchrotron Facilities



MADDALENA PEDIO

CNR – IOM

Istituto Officina dei Materiali

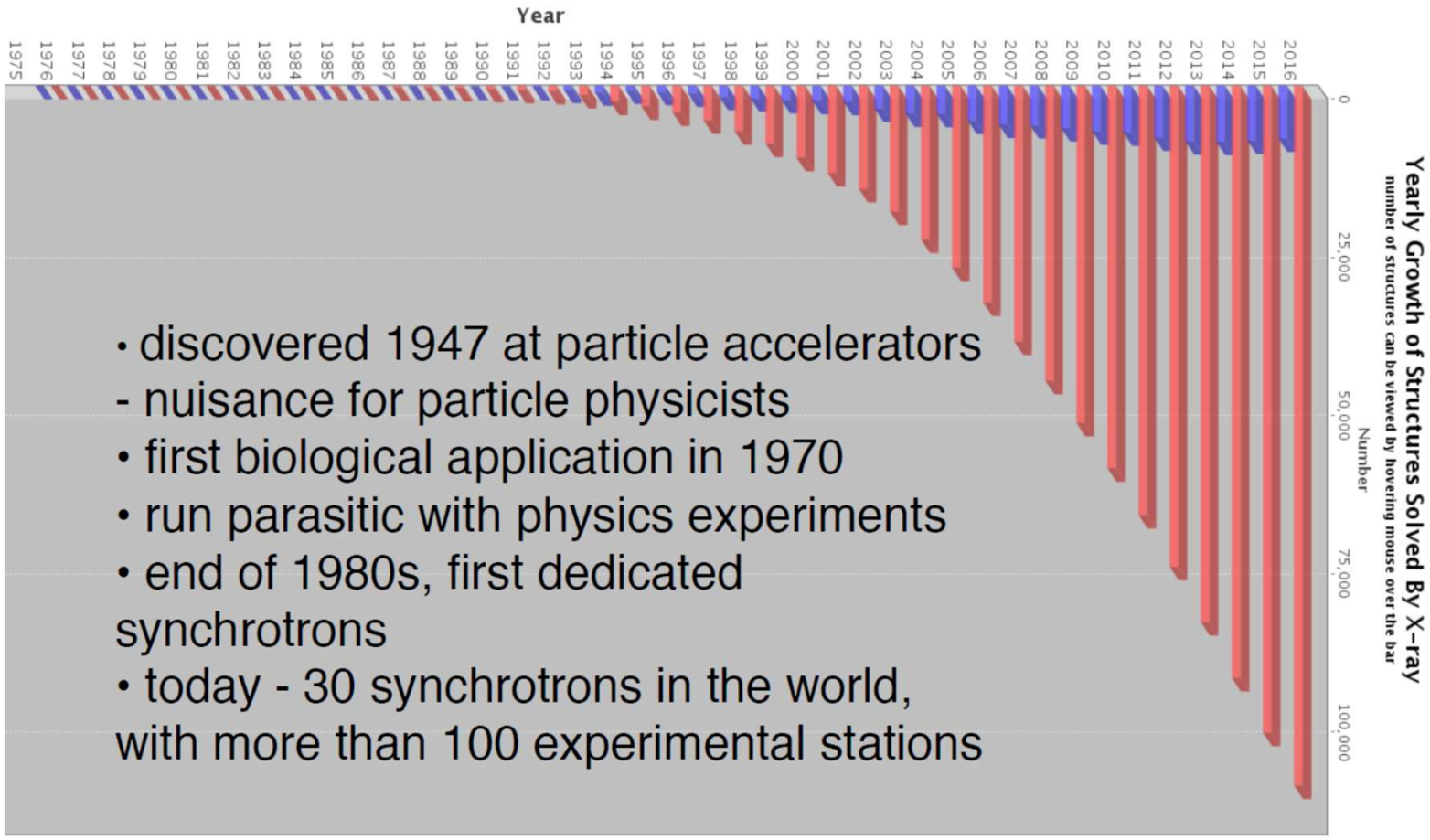
Outline

- Notes on Synchrotron Radiation
- Large-scale facilities
- Planning an experiment
- Example proposals: focus on the main issues for a good proposal

Info on light source in the world

http://www.lightsources.org

Facilities Synchrotron Radiation



A problem in High Energy Physics
A crucial tool in Material Science

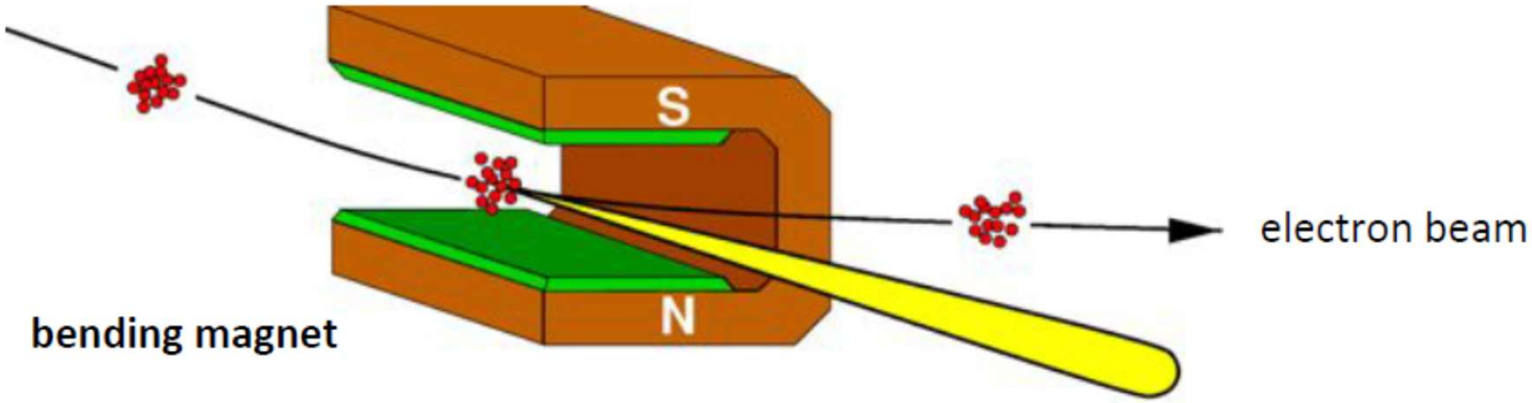
- **What is synchrotron radiation?**
  - It is the electromagnetic radiation radiated by a relativistic accelerated charged particle
  - A relativistic particle is characterized by

$$\beta = \frac{v}{c} = \sqrt{1 - \frac{1}{\gamma^2}},\ v:\ \text{speed of particle},\ c:\ \text{speed of light},\ \beta \cong 1$$

$$E = \gamma m_0 c^2,\ \gamma >> 1,\ m_0:\ \text{particle rest mass}$$

- **How can be produced synchrotron radiation?**
  - the easiest way is by a static magnetic field **B** and the Lorentz force:

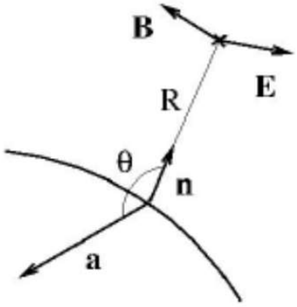
$$\mathbf{F} = e\mathbf{v} \times \mathbf{B},\ e:\ \text{charge of the particle},\ \mathbf{v}:\ \text{velocity}$$



Sinchrotron radiation

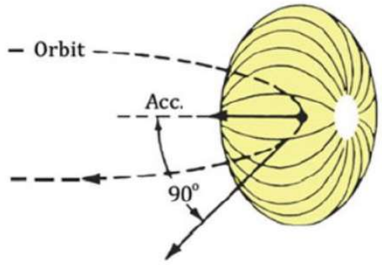
Radiation by a moving charge: $\mathbf{E} = \frac{q}{4\pi\epsilon_0 c^2 R}\mathbf{n} \times \mathbf{n} \times \mathbf{a}$

$$E = \frac{q \sin\theta}{4\pi\epsilon_0 c^2 R}$$



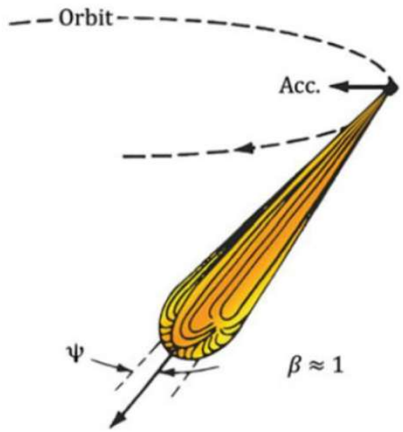
$$\gamma = \frac{1}{\sqrt{1 - v^2/c^2}}$$

Why relativistic electrons? $\left[\beta = \frac{v}{c} \approx 1\right]$



$\beta \ll 1$

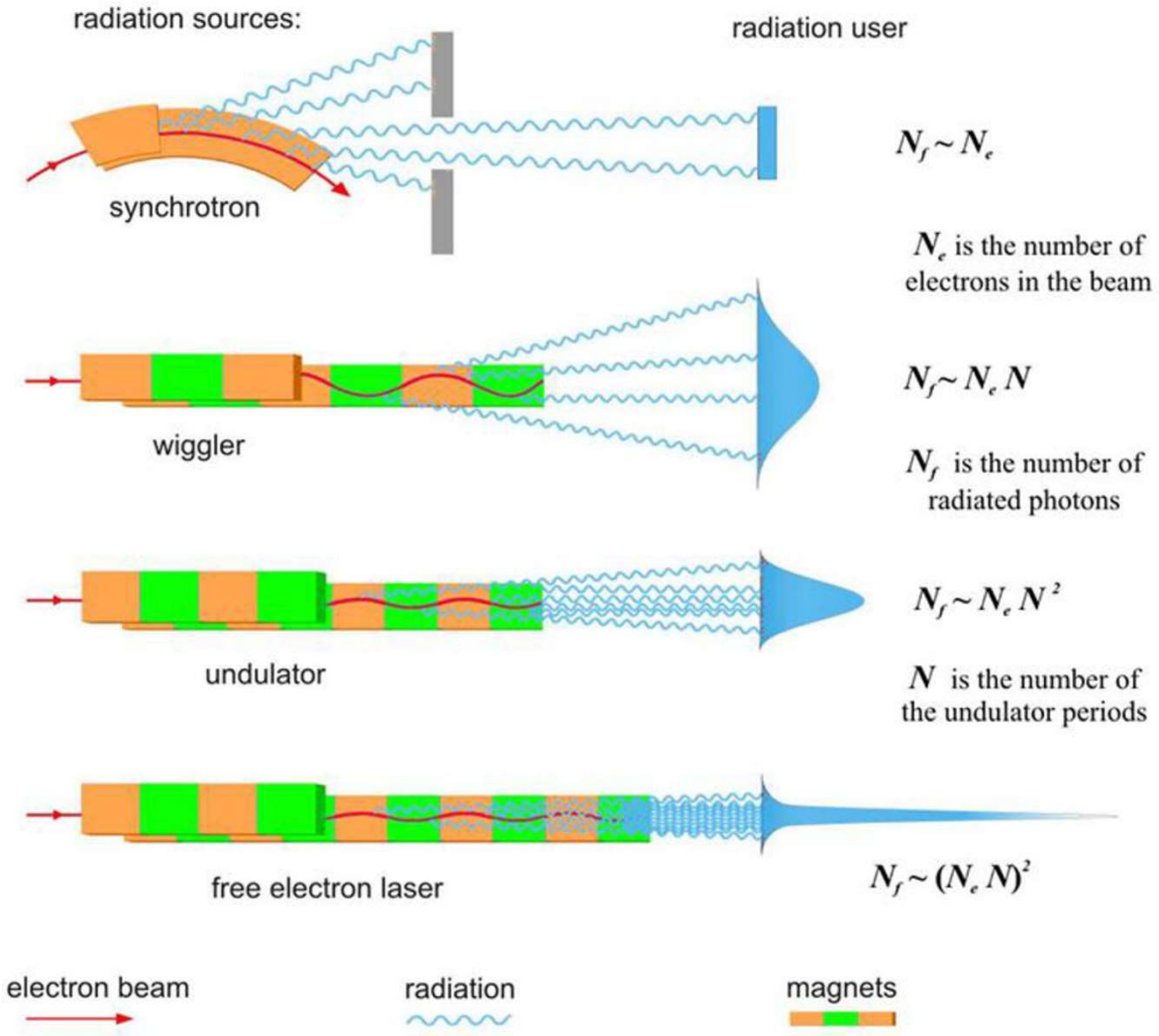
pumpkin-shaped field



highly collimated radiation

- Emission in a cone $\approx 1/\gamma$, with $\gamma = E/m_{e^-}c^2$; $m_0c^2 = 511$ keV; for E = 2.75 GeV, $\gamma = 5382$, $1/\gamma = 0.186$ mrad = 0.01deg
- Polarization

Sources of radiation at Synchrotrons

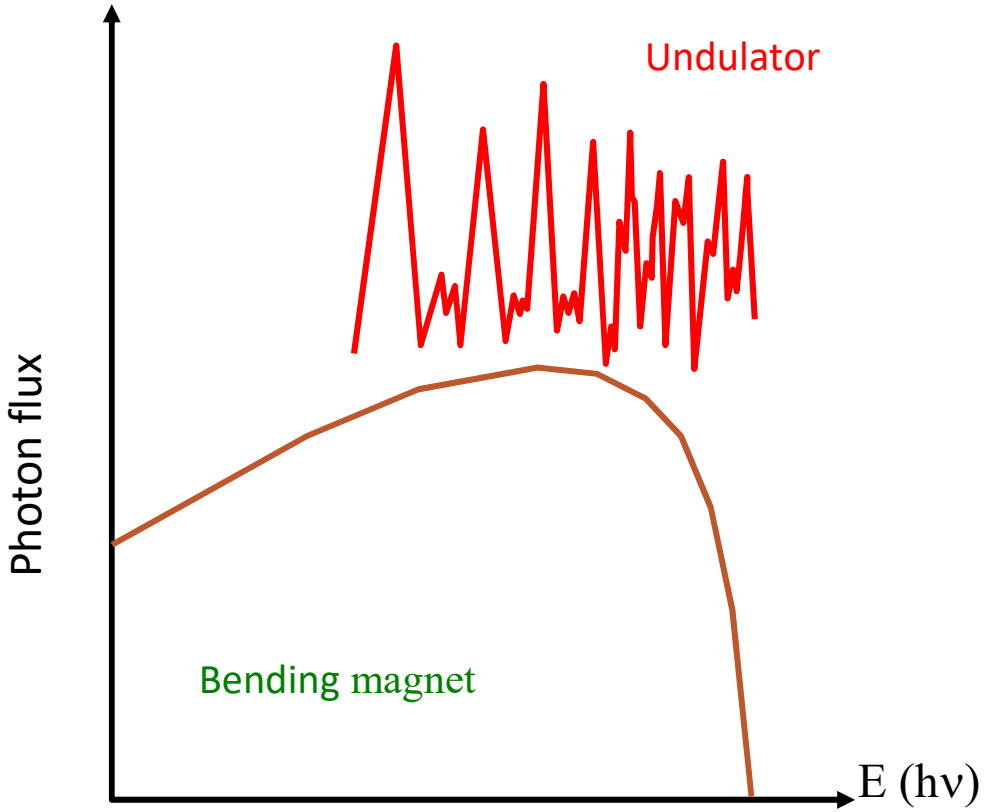


$$K = eB\,\lambda u / 2\pi m_e c$$

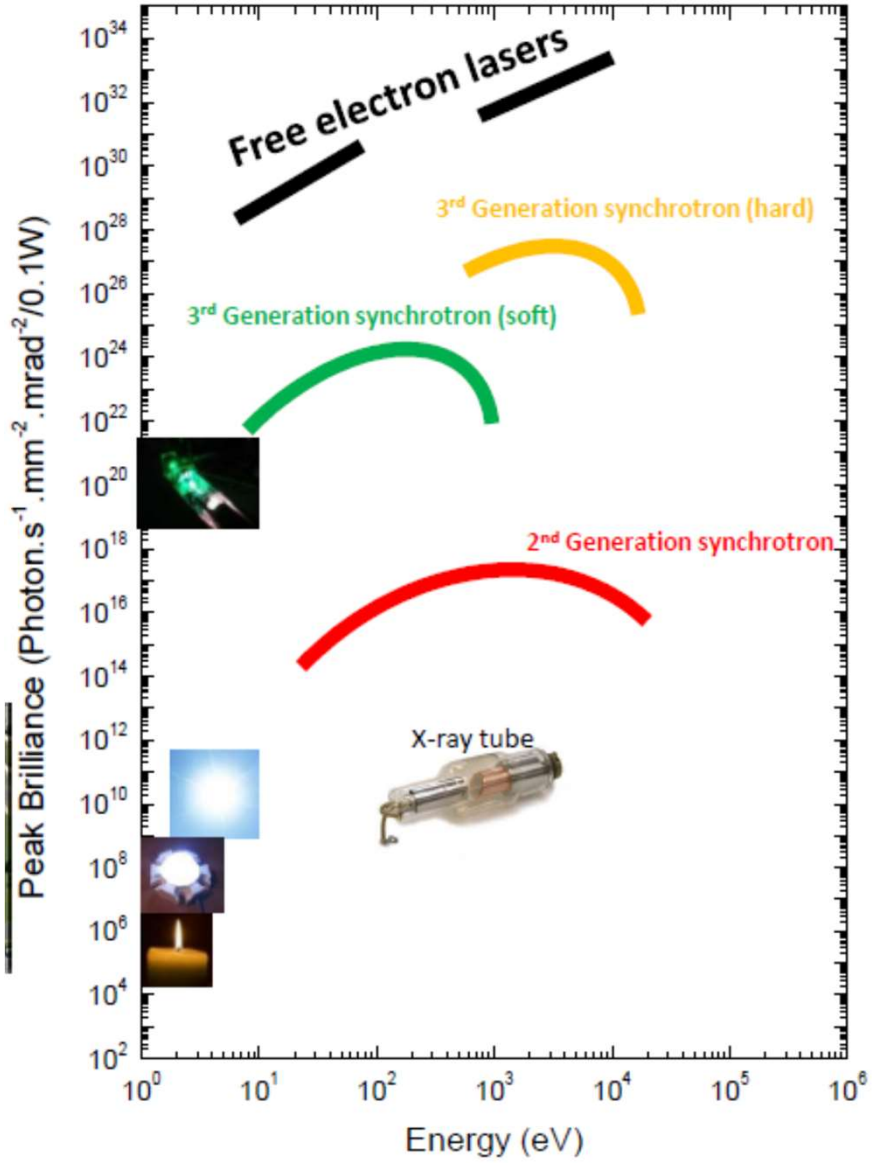
e - electron charge,
B - magnetic field,
λu - spatial period of the undulator magnets
me - electron rest mass
c - speed of light

$K \gg 1$, the oscillation amplitude is big → broad energy spectrum
$K \ll 1$, the oscillation amplitude is small → narrow energy bands

Comparison of SR sources



Comparison of the quality of the photon source



Brilliance

$$\mathcal{B}(\omega) = \frac{Photons/s}{(mm^2) \times (mrad)^2 \times (0.1\%\ bandwidth)}$$

Source size

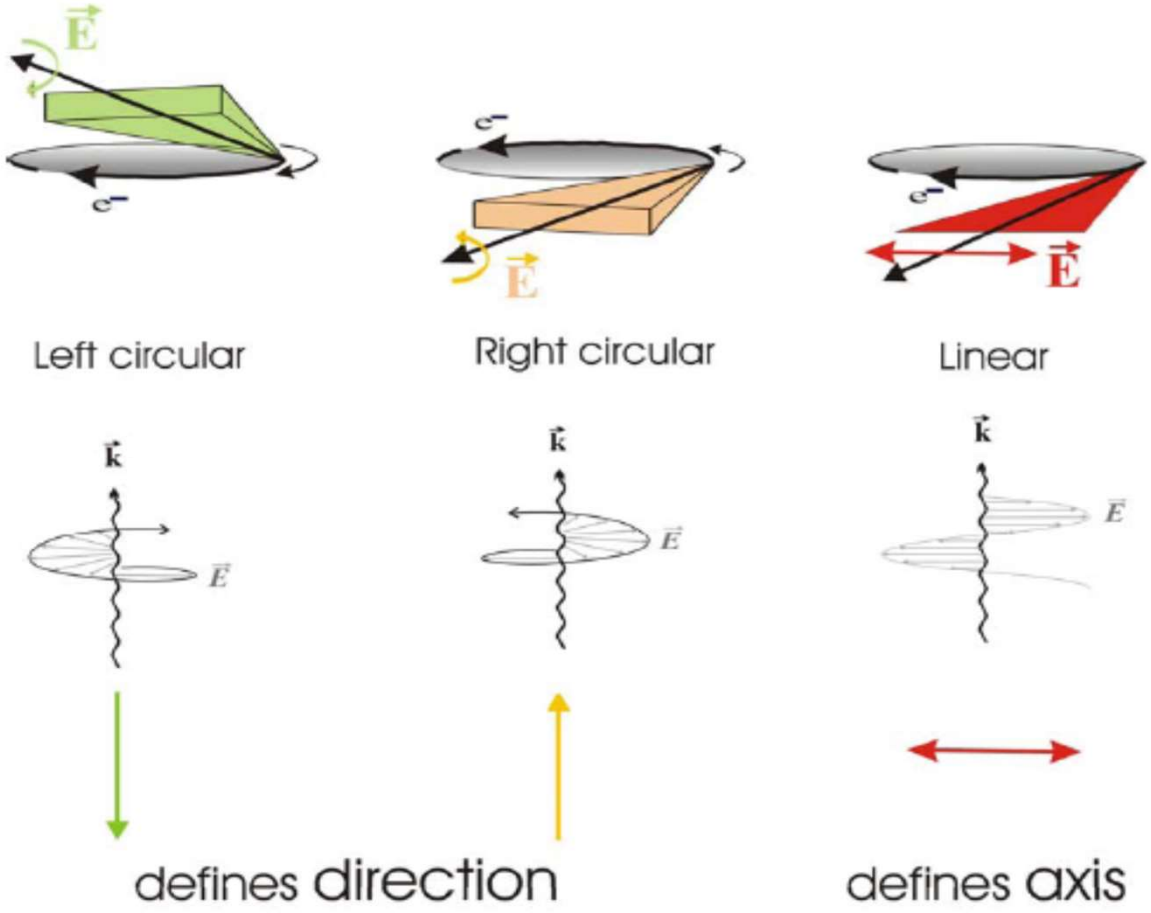
Beam angular divergence

Systems presenting anisotropy

Chemistry - Physics

Dangling/distorted bonds-boundary conditions

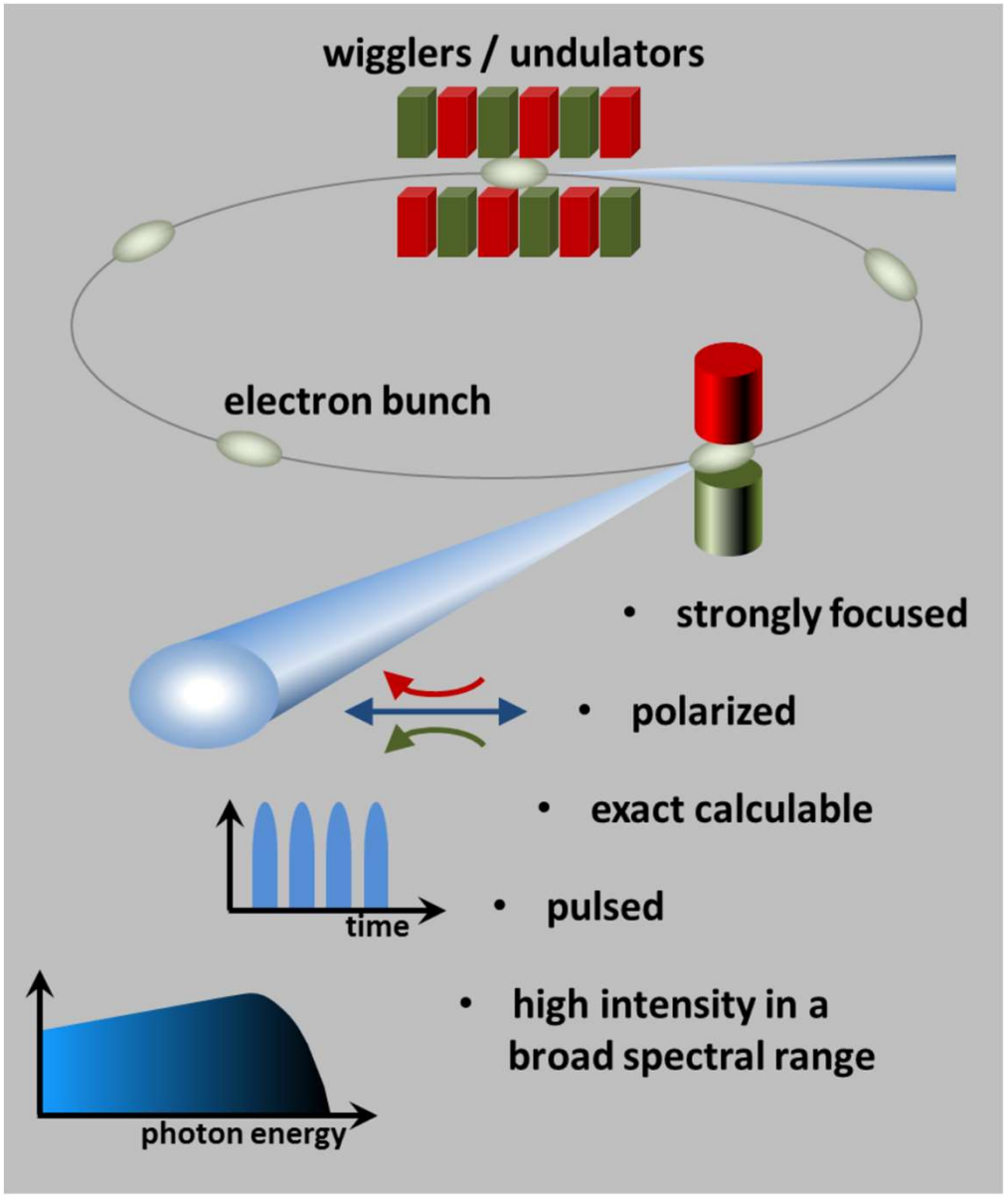
Polarization LdS:
Probing Charge orientations and Spin directions



Synchrotron Radiation

Electrons are accelerated to high energy, and pass through magnetic fields. They emit light (radiation), which is very **intense and brilliant**
$\Delta E/E\ 10^4$

- Broad Spectrum
- Selectable Energy
- High Flux
- High Brilliance
- High Stability
- Selectable Polarization
- Clean Light Source
- ***Pulsed Time Structure***



Synchrotron Facilities in Europe

https://lightsources.org/

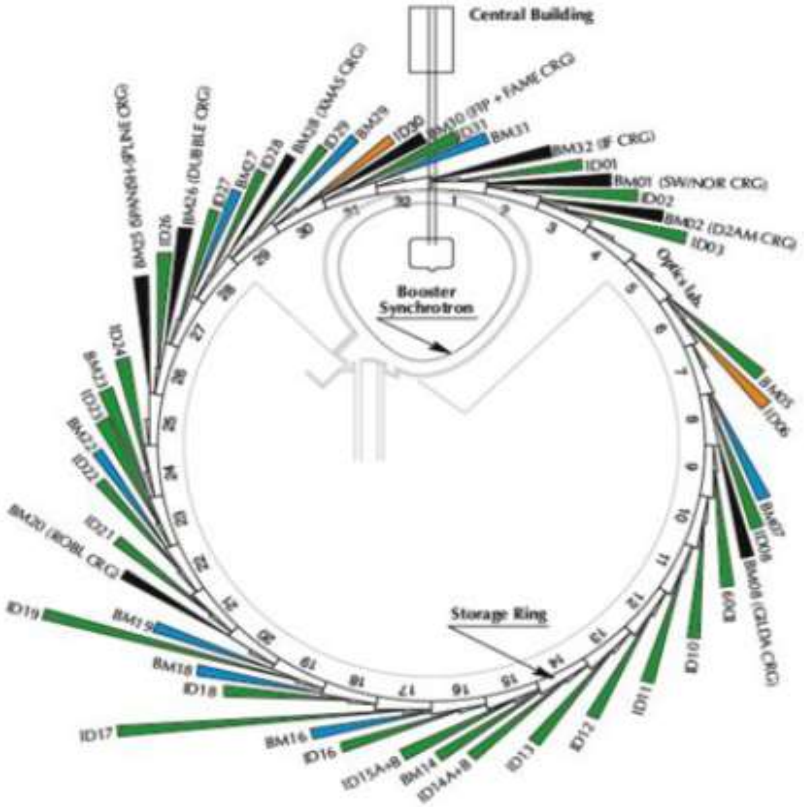


Name	Where	Website	Proposal Deadlines
European Synchrotron Radiation Facility	Grenoble, France	http://www.esrf.eu	1st March - 10th Sept
SOLEIL	Paris, France	http://www.synchrotron-soleil.fr/	March - September
BESSY II - Helmholtz-Zentrum	Berlin, Germany	http://www.helmholtz-berlin.de/	March - September
PETRA III at DESY	Germany	http://photon-science.desy.de	1st March - 1st Sept
Elettra Synchrotron Light Laboratory	Italy	http://www.elettra.eu	15th March - 15th Sept
ALBA	Spain	http://www.cells.es/	March - September
MAX IV Laboratory	Sweden	https://www.maxiv.se	Not official yet
Swiss Light Source	Switzerland	http://www.psi.ch/sls/	April - October
Diamond Light Source	United Kingdom	http://www.diamond.ac.uk/	1st April- 1st Oct

ESFR

ELETTRA

List of beamlines for Surface Science at ESRF



ID01 Coherent Diffraction
ID03 Surface diffraction
ID10 Troïka / Multipurpose-liquid surfaces
ID21 X-ray microscopy (soft X ray)
ID31 High energy diffraction
ID32 Spectroscopy by polarised soft X-rays photoemission, Resonant Inelastic X ray Scattering
BM02 D2AM (France) Materials science
BM08 LISA (Italy) Absorption and diffraction
BM25 SPLINE (Spain) Absorption and diffraction
BM32 IF (France) Surfaces and interfaces

http://www.esrf.eu/home/UsersAndScience/find-a-beamline.html

SOURCE POSITION	NUMBER OF INDEPENDENT END-STATIONS	BEAMLINE NAME	STATUS
ID01	1	Anomalous scattering	Operational since 07/97
ID02	1	High brilliance	Operational since 09/94
ID03	1	Surface diffraction	Operational since 09/94
ID08	1	Dragon	Operational since 02/00
ID09	1	White beam	Operational since 09/94
ID10	2	Soft interfaces and coherent scattering	Operational from 06/12
ID11	1	Materials science	Operational since 09/94
ID12	1	Circular polarisation	Operational since 01/95
ID13	1	Microfocus	Operational since 09/94
ID14A	2	Protein crystallography DH 1	Operational since 07/99
		Protein crystallography DH 2	Operational since 12/97
ID14B	2	Protein solution small-angle scattering DH 3	Operational since 12/98
		Protein crystallography DH 4	Operational since 07/99
ID15A	1	High energy diffraction	Operational since 09/94
ID15B	1	High energy inelastic scattering	Operational since 09/94
ID16	1	Inelastic scattering I	Operational since 09/95
ID17	1	Medical	Operational since 05/97
ID18	1	Nuclear scattering	Operational since 01/96
ID19	1	Topography and tomography	Operational since 06/96
ID21	1	X-ray microscopy	Operational since 12/97
ID22	1	Microfluorescence	Operational since 12/97
ID23	2	Macromolecular crystallography MAD	Operational since 06/04
		Macromolecular crystallography microfocus	Operational since 09/05
ID24	1	Dispersive EXAFS	Operational since 02/96
ID26	1	X-ray absorption and emission	Operational since 11/97
ID27	1	High pressure	Operational since 02/05
ID28	1	Inelastic scattering II	Operational since 12/98
ID29	1	Multiwavelength anomalous diffraction	Operational since 01/00
ID31	1	Powder diffraction	Operational since 05/96
BM14	1	Macromolecular crystallography (MAD)	Operational since 01/10
BM23	1	X-ray absorption spectroscopy	Operational since 03/11

Elettra - Sincrotrone Trieste, Italy





Ligthsources in Italy:

Elettra: 3rd generation ring in operation since 1993 / operates at 2.0 and 2.4 GeV

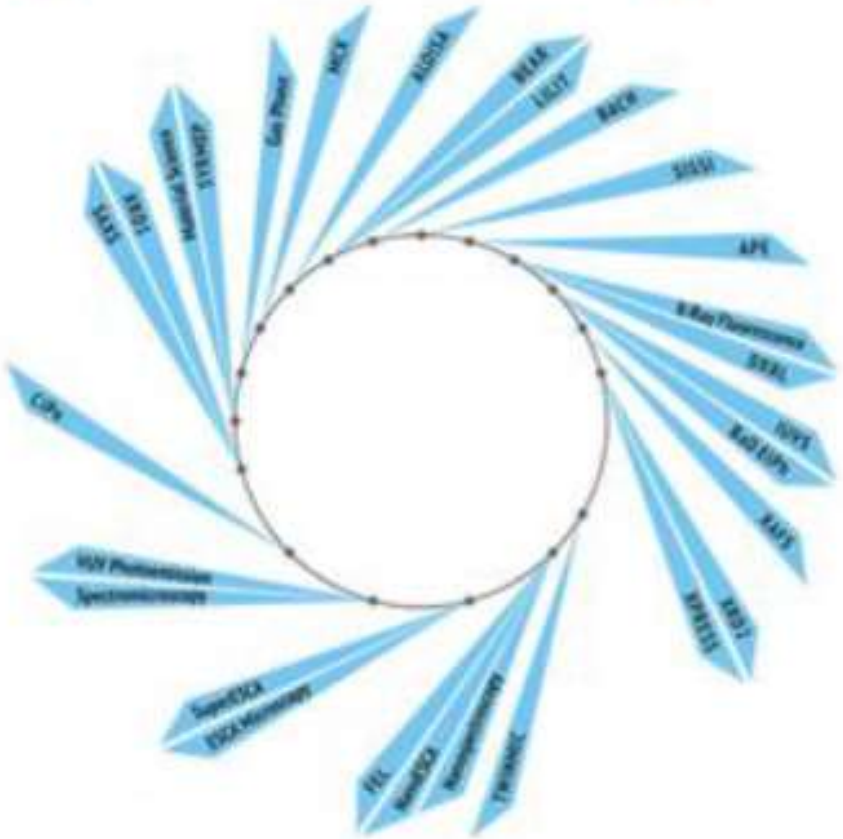
FERMI: the new seeded free electron laser open since 2012

ELETTRA (Trieste)

Elettra's Beamlines

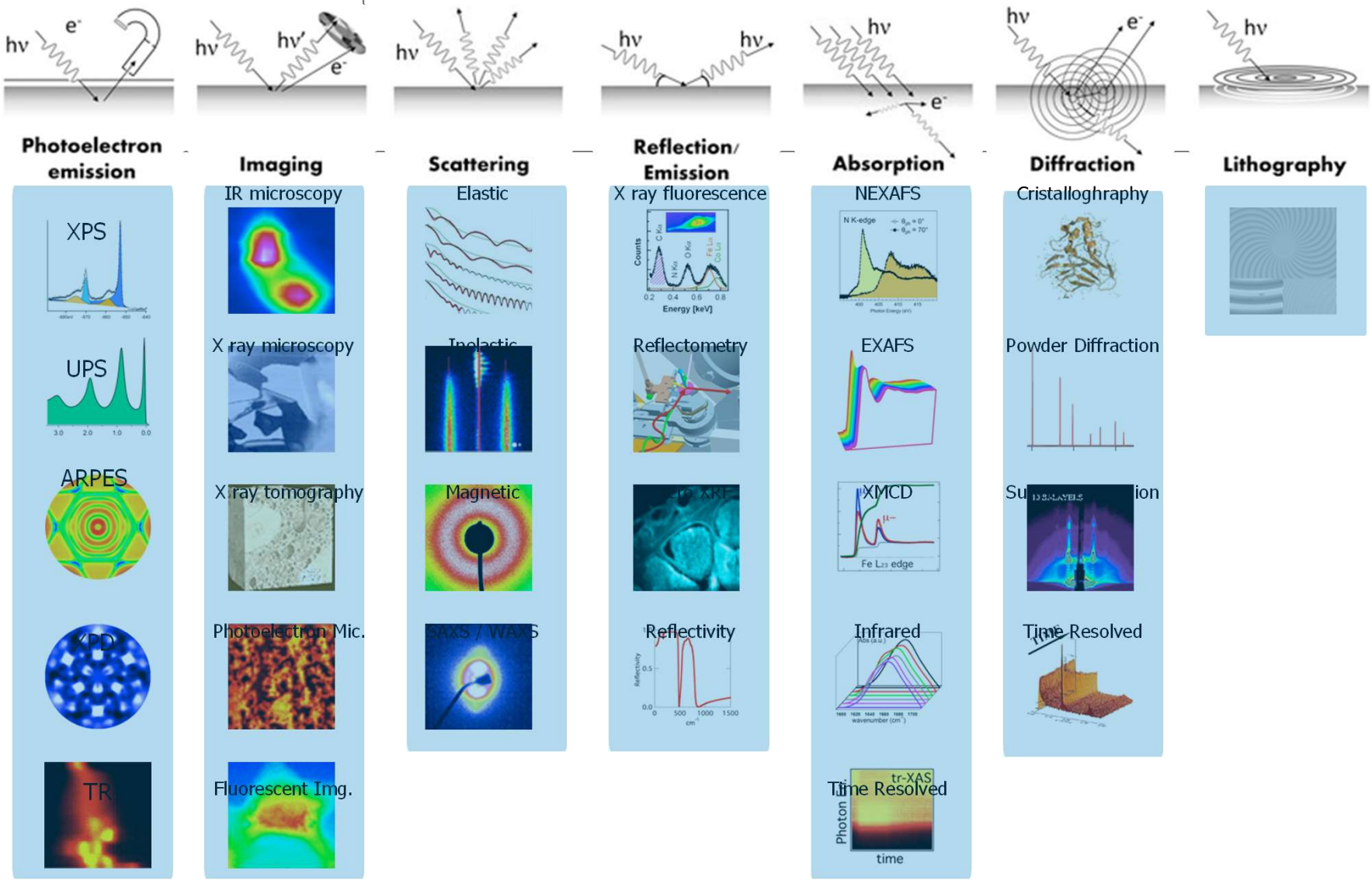
Spokespersons and telephone extensions Calendar

1.1L	TwinMic
1.2L	Nanospectroscopy
1.2L	NanoESCA
1.2R	FEL
2.2L	ESCA Microscopy
2.2R	SuperESCA
3.2L	Spectromicroscopy
3.2R	VUV Photoemission
4.2	GiPo
5.2L	SAXS
5.2R	XRD1
6.1L	Materials Science
6.1R	SYRMEP
6.2R	GasPhase



MCX	7.1
ALOISA	7.2
BEAR	8.1L
LILIT	8.1R
BACH	8.2
SISSI	9.1
APE	9.2
X-Ray Fluorescence	10.1L
DXRL	10.1R
IUVS	10.2L
BaDElPh	10.2R
XAFS	11.1R
XRD2	11.2C
Xpress	11.2R

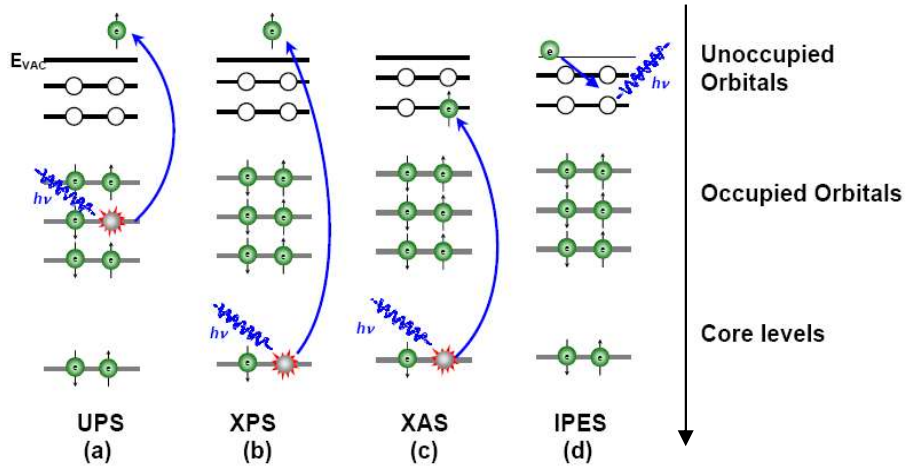
Available techniques of analysis at ELETTRA



Absorption and Electron spectroscopies

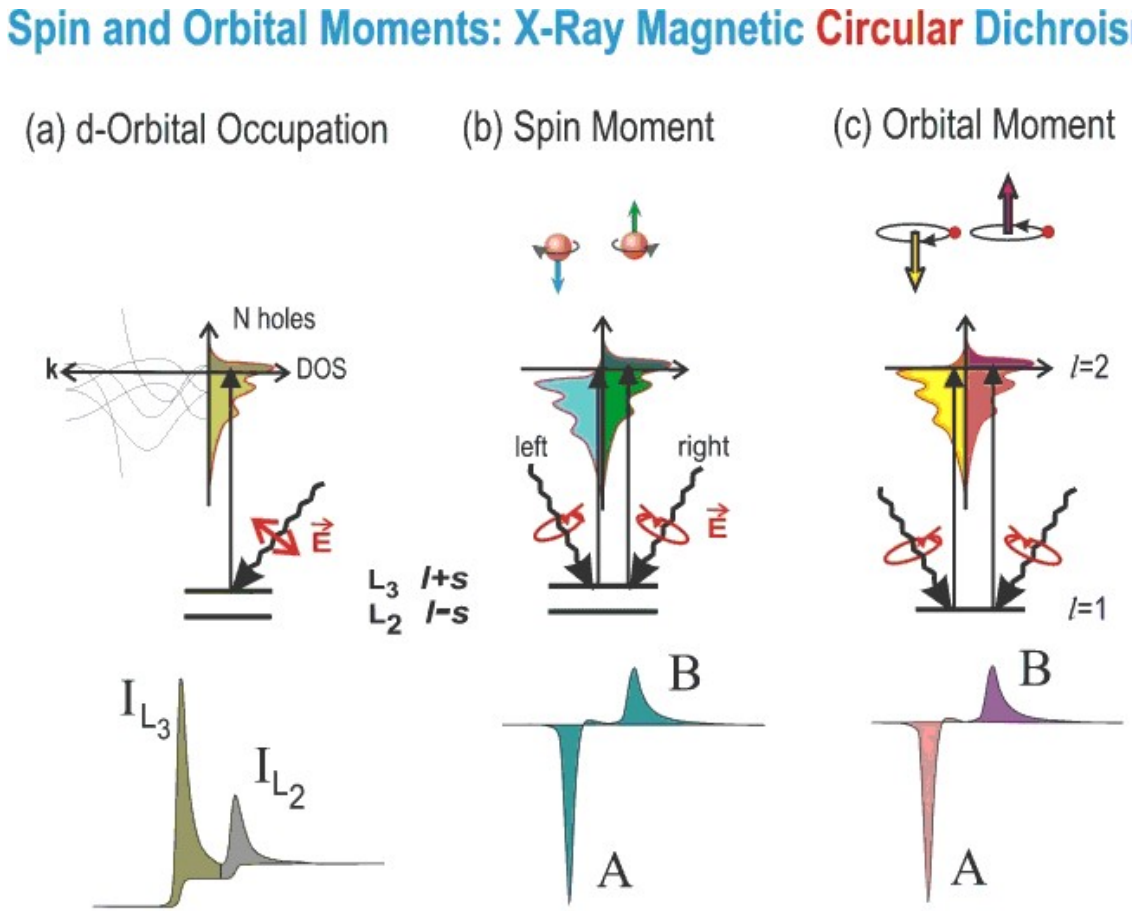
Linear response theory models the spectrum

Final state differs from the ground state



Method	Particle In	Particle Out	Information	Technique
Photoemission	Photon	Electron	Filled core states	XPS
Photoemission	Photon	Electron	Filled valence states	UPS
Inverse photoemission	Electron	Photon	Empty states	IPES
Electron energy loss	Electron	Electron	Electronic & vibrational transitions	EELS, HREELS
Auger	Electron	Electron	Filled states	AES
Absorption / emission*	Photon	Photon	Electronic transitions, filled states	UV-Vis, XRF
Core XAS	**Photon**	**photon**	**empty el states Structure**	**EXAFS/NEXAFS**
			Spin/magnetic orbitals	**XMCD**

X-Ray Magnetic Circular Dichroism (XMCD) spectroscopy
Magnetic properties of materials



Electronic transitions in conventional L-edge x-ray absorption (a), and x-ray magnetic circular x-ray dichroism (b,c), illustrated in a one-electron model.

The transitions occur from the spin-orbit split 2p core shell to empty conduction band states. In conventional x-ray absorption the total transition intensity of the two peaks is proportional to the number of d holes.

By use of circularly polarized x-rays the spin moment (b) and orbital moment (c) can be determined from linear combinations of the dichroic difference intensities A and B, according to other sum rules.

Planning an experiment

- Main Questions : structure, electronic properties, magnetic properties, functionality, etc…..
- Sample and sample environment
- Which technique is feasible?
- Which techniques provide complementary info?
- Optimization of the signal: which apparatus/beamline
- Where? (collaborations, facilities, user support, ….)
- Can you model the future results?

"Science is the belief in the ignorance of the experts." — Richard Feynman

pedio@iom.cnr.it

Access to a synchrotron facility: proposal submission

Before starting to prepare the proposal it is necessary to understand:

A) which is the best technique for my scientific problem?
B) which is the instrument better suited to my problem?

Once defined the technique, the facility and the instrument, it is good practice to contact the scientist in charge of the beamline. He/she can immediately tell you if the experiment is reasonable, can provide you with valuable information concerning the feasibility of the experiment, and also suggest alternatives.

There is high competition for beam time

Proposal must be scientifically compelling and competitive!

Courtesy Roberto Felici

Plannig experiment & References

Choosing the Info requested and the Suitable Characterization Techniques

- Sample environment/dimension/damage ←→ **choose the end station**
- Sensitivity vs. Chemical Selectivity ←→ photon flux, resolution, polarization: **choose the beamline**
- Technique, for example Core Level elemental Chemical Selectivity in Core Level Spectroscopy **choose the end station and the techniques**
  - Broadening Gaussian&Intrinsic Lifetime of Core Levels (Lorentzian $\Gamma=2\pi/\tau$)
- Detection details: Probing Depths of Electrons and Photons, geometries, ..
- Cross Sections and Dipole Selection Rules of the levels-technique
- Merge of the multitechnique information to get a coherent framework of results

LdS Booklet http://cxro.lbl.gov/x-ray-data-booklet

Lifetimes of core levels Journal of Physical and Chemical Reference Data **8, 329 (1979)**

Cross sections Atomic Data and Nuclear Data Tables **32, 1 (1985),** https://cross-sections.lbl.gov/

Mean free paths NIST database: https://www.nist.gov/srd/nist-standard-reference-database-71

Binding Energies of elements https://srdata.nist.gov/xps/main_search_menu.aspx

Beamline staff is available to provide this information

Path of a proposal

A) Submission of the proposal **within the deadline**. Normally there are two calls per year in Spring and in Autumn.

B) After the deadline, the beamline scientists perform the technically feasibility. If a proposal is considered not feasible is out.

C) Committees meet and rank all the proposal. This ranking is a suggestion to the directors, who are the final responsible for the ranking.

D) The final ranking, after directors' modifications, is presented to the Scientific Council of the facility for approval.

E) The final ranking is made public.

The members of the committees are expert in different fields in order to provide to the committee a knowledge wide enough to cover all the scientific fields of interest for the committees.
They are nominated by the directors of the facility after consultation with the scientific advisory committees of the facility and the beamline scientists.

The proposal template depends on the facility.
No a standard form.

However, the information which should be included in the text is standard

Examples

ELETTRA: New material characterization by photoemission and XAS

ESRF: X-ray magnetic circular dichroism (XMCD) applied to nanostructured paramagnetic systems

ELETTRA

2 parts:
- a module to be filled at the facility site,
including abstract and details on the beamline-end station and safety form
-two pages for background, goal of the proposal, experiment description, expected results

https://www.elettra.eu/userarea/apbt.html

EXAMPLE: Characterization of a new material

ELETTRA PROPOSAL DESCRIPTION
Proposal number 20220363:
Title: Characterization of amourphous hydrogenated silicon as ionizing radiation sensitive material

Proposer: Francesca Peverini
Beamline(s) requested: CIPO
Shifts requested: 18
Abstract: Aim of the proposal is the characterization of samples involved in devices based on a-Si:H for application as a detection material for ionizing radiation of different types. The quantity of Si-H bond and the morphology of the films strongly affects the electronic properties and consequently the devices performance. Previous Photoemission and X-ray absorption data demonstrate the spectral features of hydrogenation. Here we plan to correlate the proposed measurements with the ex-situ Infrared, AFM and electrical characterization.

_____do not change anything above this line_____

STRONGLY RECOMMENDED FLOW CHART:

1. Scientific background
Films formed by Amorphous Hydrogenated Silicon (a-Si:H) received renewed interest in the last few years since the material in itself is very radiation-resistant, could be deposited as a thin layer of few micrometres over many substrates, including flexible ones allowing for a much greater variety of shapes.
The defining property of amorphous silicon in contrast to its well-known crystalline form is the absence of long-range order in the atomic positions, this aspect alone leads to the prominent electronic features such as dangling bonds in the band gap and exponentially decaying band tails which may cause anomalous electrical behavior.
This material can be passivated by hydrogen (Fig1) [1], which can reduce the defects density by several orders of magnitude, so a-Si:H has a sufficiently low amount of defects to be used within devices.
Its characteristics make this material a good candidate for many important applications, such as: beam monitoring of clinical and non-clinical accelerators, detection of cosmic radiation in space and neutron detection: its intrinsic non-crystalline nature that offers a natural resistance to the radiation damage, and is possibile to grow it in a very thin layer and wide surfaces.
Nevertheless, the properties of a-Si:H are intimately related to changes in its structure, compositional disorder, and H concentration, subtle details in the H fraction can change drastically the band gap of a-Si:H as also simulated by theoretical Density of States (DOS) (Fig2) [1], for this reason we want to investigate experimentally how the electronic properties in the gap evolve with H content.

2. Motivation for the proposal

The proponent group is participant to the HASPIDE project (Hydrogenated Amorphous Silicon DEtectors) which aims to study the possibility of using a-Si:H thin films as ionizing radiation sensitive material and to investigate the applications to some use-cases. In order to reach the goals of the project, several steps need to be accomplished, first of all we want to characterize the material basic physical, electrical and charge collection performances. a-Si:H sensor has already been used to monitor therapeutic beam at CNAO [2], and we have already carried out some preliminary studies, the results look encouraging (Fig.3, 4). The proposal aims at the detailed characterization of the a-Si:H electronic properties related to different growth samples a-Si:H onto Silicon and Kapton substrates.

The information that we will obtain from this type of measurements will be used as input parameters of TCAD simulations in order to model the material and its electrical characteristics. Sensors will be fabricated using different deposition technologies, for each of which, we should proceed to the characterization, to do this we must know very well all the properties of the material, since we know for example that the transport gap and in particular the valence band of a-Si:H strongly depends on the amount of Si-H bond within the amorphous silicon film.

The characterization and test of the materials and the design of dedicated structures is ongoing. We have already characterized case samples of a-Si and a-Si:H using photoemission spectroscopy to probe the sample, this technique was chosen because it provides direct information about the energy distribution of occupied states, which is essential to study the electronic structure and microscopic bonding. The feasibility of the photoemission and X-ray absorption spectra have been conducted at CIPO beamline of the Elettra synchrotron, thanks to these measurements on a-Si and a-Si:H samples and it was possible to obtain information on the fingerprint of such materials, and to quantify the defect states featured at the Valence Band Maximum.

The next step is to investigate systematically new samples already tested with AFM, electrical and InfraRed measurements (that provide the number of Si-H bonds) in campus. We want to identify and study defect-induced states on a-Si:H and the chemical environments of Si atoms, in order to quantify the number of dangling bonds and of Si–H bonds.

Moreover, the characterization of their damage induced by ex situ strong irradiation (Hard X or neutron irradiation (10^{16} neq/cmsq)) is a further issue of our research together with the recovering of the electronic properties of the a-Si:H films after annealing, for which we expect to observe a decrease in material defects.

3. Experimental plan
The Circular Polarization (CiPo) beamline at ELETTRA is equipped with an electromagnetic elliptical undulator/wiggler that provides a wide range of photon energies (10-800 eV) monochromatized by using both a Grazing Incidence Monochromator (40-800 eV) and a Normal Incidence one to cover the 10-40 eV energy range. We will investigate the valence photoelectron distributions and core level signals at normal emission by using the UHV photoemission chamber equipped with the OMICRON 125 electron analyzer. The raw samples will be introduced in the UHV chamber and sputtered in order to remove the topmost coating (10 nm SiO_2). Photoemission Si 2p core at hv=700 eV will be taken at different sputtering stages. The valence band spectra will be measured at 700 eV and 15 eV of photon energy in order to enhance the defect featured at the Valence Band Maximum. The EF will be taken on a reference Au polycrystalline in contact with the sample.
Subsequently the samples will be annealed in the preparation chamber at 100 °C for 12 hours and the measurements will be repeated, including ex-situ IR, AFM and electrical characterizations.

4. Justification of beamline(s) and beamtime requested

The photon energy range provided by the beamline allow core level photoemission, Si L23 XAS and low energy Valence Band photoemission. Feasibility has been checked in collaboration with CIPO staff

5. Results Expected & Impact
Improvement of devices of interest

6. Pictures

Include picture(s) if needed

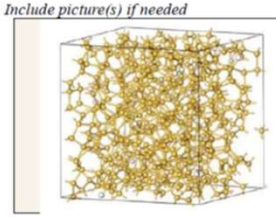


Figure 1: Structural models for 512 Si atoms with (a) 14% H concentration in saturated a-Si: H

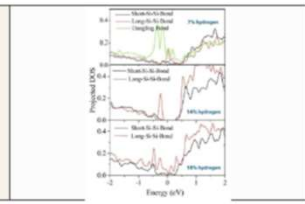


Figure 2: Projected density of states of (a) unsaturated (7%), (b) saturated (14%), and (c) oversaturated (18%) of a-Si:H.

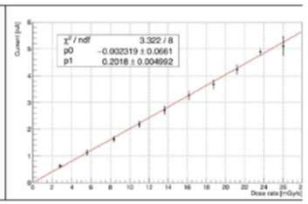


Figure 3: Current VS Dose Rate for device built with a-Si:H vertical diode structure: Bias 60 V; Dimensions: 0.5 x 0.5 x 0.01 mm3

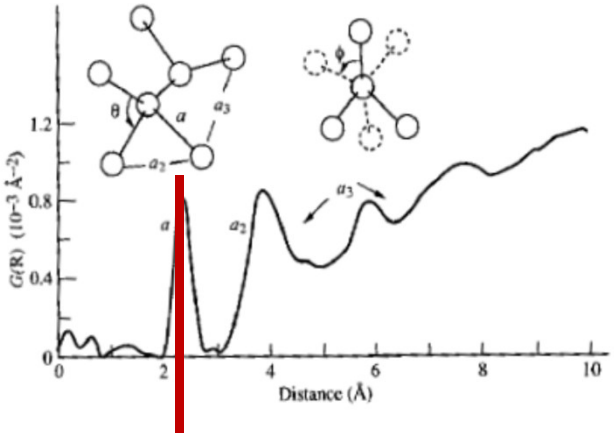
7. References related to the proposal scientific text

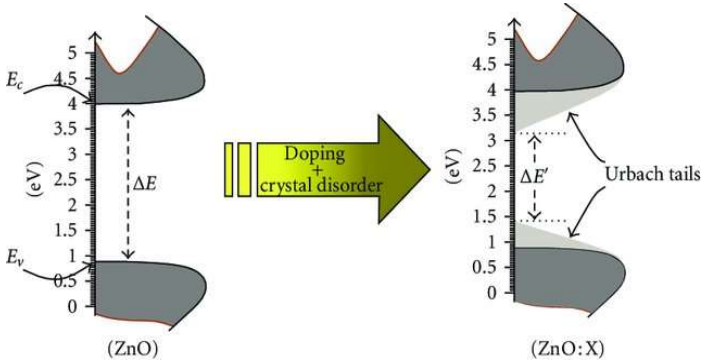
[1] Merid Legesse, Michael Nolan, and Giorgos Fagas Tyndall National Institute, University College Cork, Lee Maltings, Dyke Parade, Cork, Ireland "A first principles analysis of the effect of hydrogen concentration in hydrogenated amorphous silicon on the formation of strained Si-Si bonds and the optical and mobility gaps" JOURNAL OF APPLIED PHYSICS 115, 203711 (2014).
[2] H. Caracciolo, G. Balbinot, G. Bazzano, J. Bosser, M. Caldara, A. Parravicini, M. Pullia, C.Viviani Fondazione CNAO, Pavia, Italy. BEAM DIAGNOSTICS COMMISSIONING AT CNAO, Proceedings of IPAC2011, San Sebastian, Spain.
[3] M. Menichelli et al. "Hydrogenated amorphous silicon detectors for particle detection, beam flux monitoring and dosimetry in high-dose radiation environment." Journal of Instrumentation 15 C04005 (2020).
[4] M. Menichelli et al. "Testing of planar hydrogenated amorphous silicon sensors with charge selective contacts for the construction of 3D- detectors." Accepted for publication in "Journal of Instrumentation"

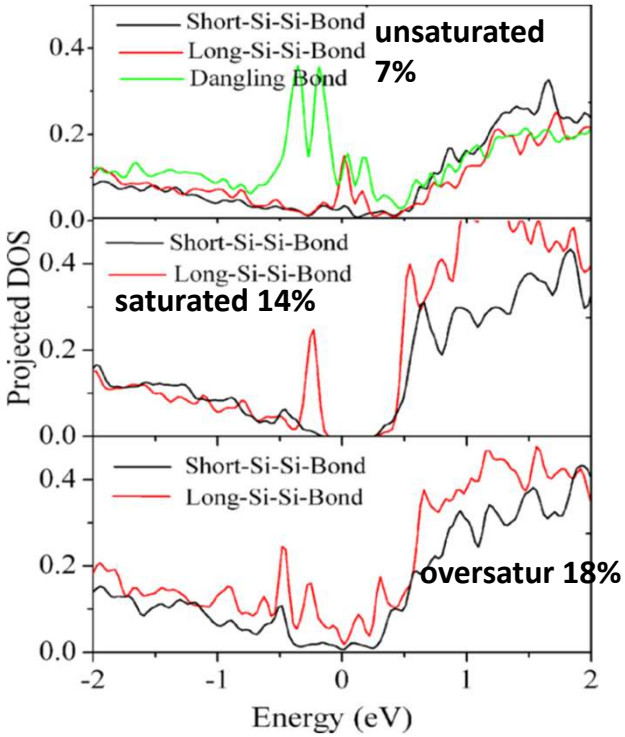
https://www.elettra.eu/userarea/apbt.html

a-Si:H properties











Density Functional Theory DFT calculations DOS vs Si-H bonds *Legesse et al 2014*

The specific band gap structure depends on the deposition conditions and film treatments (contacts, irradiation etc)

Impact on the device performance

View Proposal

Facility	Elettra
Proposer	(175604) PEVERINI Francesca
Proposal Number	20220363
Proposal Title	Characterization of amourphous hydrogenated silicon as ionizing radiation sensitive material
Proposal Abstract *(min 30 characters)* *max 3000 characters*	Aim of the proposal is the characterization of samples involved in devices based on a-Si:H for application as a detection material for ionizing radiation of different types. The quantity of Si-H bond and the morphology of the films strongly affects the electronic properties and consequently the devices performance. Previous Photoemission and X-ray absorption data demonstrate the spectral features of hydrogenation. Here we plan to correlate the proposed measurements with the ex-situ Infrared, AFM and electrical characterization

probably most important part !

- equivalent to abstract of scientific paper, one paragraph
- clear statement on essence of proposal – what are you trying to do, how you intend to do it, and why you are doing it (impact, importance of study)
- reviewers should understand exactly what the proposal is about from this summary; details are given in the following sections

ELETTRA PROPOSAL DESCRIPTION
Proposal number 20220363:
Title: Characterization of amourphous hydrogenated silicon as ionizing radiation sensitive material

Proposer: Francesca Peverini
Beamline(s) requested: CIPO
Shifts requested: 18
Abstract: Aim of the proposal is the characterization of samples involved in devices based on a-Si:H for application as a detection material for ionizing radiation of different types. The quantity of Si-H bond and the morphology of the films strongly affects the electronic properties and consequently the devices performance. Previous Photoemission and X-ray absorption data demonstrate the spectral features of hydrogenation. Here we plan to correlate the proposed measurements with the ex-situ Infrared, AFM and electrical characterization.

Proposal Category	
Proposal Category	New
Previous Proposal Number	
Application Category	Normal
Motivations of Long Term request	
Societal Challenge addressed by research *(if any)*	Other
Research Area	Condensed matter - Electronic and Magnetic Structure
Discipline	Physics
Specific discipline	Hard condensed matter - electronic properties
Financial support request	No
Financial support is crucial?	No
Financial Support Received	
ICTP-Elettra Users Programme support request	No
ICTP-Elettra Users Programme supported	No
Elettra-CNR project	No
Does this proposal have any industrial involvement or sponsorship?	No
Industrial involvement or sponsorship optional text	

Experimental Requirements	
Electron Beam Requirements	Multi Bunch
Beamline requested	
Alternative beamline requested	
Photon Energy (eV)	20-700eV
Shifts requested	18
Should the restrictions continue due to the pandemic, I am available to perform the measurements remotely in sample mail-in mode	Yes
Photon Energy Resolution (eV)	
Other requirements	UHV end stationed electron analyser

You cannot enter new shipments, because there are no other scheduled beamtimes starting from today's date.

Participants			
Participant	Institute	Address	Country
(175644) MENICHELLI Mauro	I.N.F.N. - Istituto Nazionale di Fisica Nucleare - Perugia	Via Alessandro Pascoli, 23c	ITALY
(956) PEDIO Maddalena	CNR - IOM - Consiglio Nazionale delle Ricerche - Istituto Officina dei Materiali - Sezione di Trieste	c/o "Elettra" - S.S. 14, Km. 163,5 in AREA Science Park	ITALY

give scientific drivers; single proposer unlikely to perform experiment single-handedly
only include beamline staff if they are one of scientific drivers; ask permission

Experimental Requirements

Experimental Requirements	
Electron Beam Requirements	Multi Bunch
Beamline requested	
Alternative beamline requested	
Photon Energy (eV)	20-700eV
Shifts requested	18
Should the restrictions continue due to the pandemic, I am available to perform the measurements remotely in sample mail-in mode	Yes
Photon Energy Resolution (eV)	
Other requirements	UHV end stationed electron analyser

Beamline, Scientific Area, Societal Theme and Type of Science

- careful and informed choice
- correct beamline (target the proposal) and correct beam time in shifts
- scientific area, societal themes and science type are all fed back to funding partners to monitor Facility activity

Ask beamline scientists

1. Scientific background

Films formed by Amorphous Hydrogenated Silicon (a-Si:H) received renewed interest in the last few years since the material in itself is very radiation-resistant, could be deposited as a thin layer of few micrometres over many substrates, including flexible ones allowing for a much greater variety of shapes. .....

set the scene for the interest of your research

- reviewers from many different backgrounds
- indicate fundamental and societal importance of your work
- lead to the open question stated in the summary
- refer to any previous measurements or preliminary characterization

2. Motivation for the proposal

The proponent group is participant to the HASPIDE project (Hydrogenated Amorphous Silicon DEtectors) which aims to study the possibility of using a-Si:H thin films as ionizing radiation sensitive material and to investigate the applications to some use-cases. In order to reach the goals of the project, several steps need to be accomplished, first of all we want to characterize the material basic physical, electrical and charge collection performances. a-Si:H sensor has already been used to monitor therapeutic beam at CNAO [2], and we have already carried out some preliminary studies, the results look encouraging (Fig.3, 4). The proposal aims at the detailed characterization of the a-Si:H electronic properties related to different growth samples a-Si:H onto Silicon and Kapton substrates.

.....

Include motivation of the selected technique related to the information we want to get

avoid vague or too broad aims

- preliminary measurements or characterization recommended when appropriate

Crucial

3. Experimental plan

The Circular Polarization (CiPo) beamline at ELETTRA is equipped with an electromagnetic elliptical undulator/wiggler that provides a wide range of photon energies (10-800 eV) monochromatized by using both a Grazing Incidence Monochromator (40-800 eV) and a Normal Incidence one to cover the 10-40 eV energy range. We will investigate the valence photoelectron distributions and core level signals at normal emission by using the UHV photoemission chamber equipped with the OMICRON 125 electron analyzer. The raw samples will be introduced in the UHV chamber and sputtered in order to remove the topmost coating (10 nm SiO2). Photoemission Si 2p core at hv=700 eV will be taken at different sputtering stages. The valence band spectra will be measured at 700 eV and 15 eV of photon energy in order to enhance the defect featured at the Valence Band Maximum. The EF will be taken on a reference Au polycrystalline in contact with the sample.

The plan must be clear, specific and feasible in the requested time

- exact description of how are you going to carry out the experiment; strategy
- details and quantity of samples
- technique and setup; special requirements
- show reviewers you are ready and prepared
- allow beamline scientists to make a technical feasibility assessment
- prior discussion with beamline scientist is strongly advised

4. Justification of beamline(s) and beamtime requested

The photon energy range provided by the beamline allow core level photoemission, Si L23 XAS and low energy Valence Band photoemission. Feasibility has been checked in collaboration with CIPO staff

5. Results Expected & Impact

Improvement of devices of interest

what results you are expecting how these results will allow you to answer the specific question(s) stated in summary

Elettra Sincrotrone Trieste

Safety form

Proposal	20220363
Title	Characterization of amourphous hydrogenated silicon as ionizing radiation sensitive material
Proposer	Francesca PEVERINI
Beamline	CIRCULARPOLARIZATION

Sample(s) and chemical substance(s) to be used in this experiment

Substance	Silicon
Chemical formula	Si

CAS registry number		**Size**	10
Physical state	Solid	**Mass**	10 mg
Supplier	Siltronix	**Sample container**	flat plate

Only for diffraction proposals

Surface area	mm^2
Space group	
Unit cell dimensions at	T: a= b= c= alpha= beta= gamma=

Only if the physical state of the substance is gas

Volume of cylinder to be used	cm^3
Pressure of gas in cylinder	mbar

Risk in sample, preparation or equipment	No

The sample is:

Radioactive	No	**Oxidising**	No
Corrosive	No	**Combustive**	No
Contaminant	No	**Carcinogene**	No
A biological hazard	No	**Inflammable**	No
Toxic	No	**Explosive**	No

Exhaust disposal conditions	

Sample disposal	Removed by user

ESRF

2 parts:
- a module to be filled at the facility site,
including abstract and details on the beamline-end station and safety form
-two pages for background, goal of the proposal, experiment description, expected results

https://www.esrf.fr/home/UsersAndScience/Applying.html

Ref. No 39051
Final N° HC-2305

EUROPEAN SYNCHROTRON RADIATION FACILITY
INSTALLATION EUROPÉENNE DE RAYONNEMENT SYNCHROTRON

ESRF

Standard Application for Beam Time at the ESRF

Proposal Title (175 chars maximum.)
Growth and structure of ultrathin Co ferrite layers for spin-filtering: CoFe2O4/Ag(001)

Keywords
#1: Epitaxial growth #2: ferrimagnetic spinel ferrites #3: film structure #4: Surface x-ray diffraction

- **This proposal is:**
  A new proposal ☑
  A resubmission of ... A continuation of : ...
- This proposal is: Fundamental Science ☑ % 100 Applied Science ☐ % 0 Industrial Science ☐ % 0
- **Relevant reports:** *Please specify your most recent experiment(s) at ESRF, for which you have submitted report(s), and which are relevant to this new proposal.*
  #1: 32-03- 718 #2: ... #3: ...

Societal Themes

- ☐ Earth and Environment
- ☐ Health
- ☑ Information and Communication Technology (ICT)
- ☐ Other Functional Materials
- ☐ Energy
- ☐ Fundamental Science
- ☐ Other Please give keyword(s)

Scientific Area of the proposal

- ◉ HC - Hard Condensed Matter Science
- ○ MA - Applied Materials Science
- ○ ME - Engineering
- ○ CH - Chemistry
- ○ SC - Soft Condensed Matter Science
- ○ LS - Life Sciences
- ○ MD - Medicine
- ○ MI - Methods and Instrumentation
- ○ ES - Earth Sciences
- ○ EV - Environment
- ○ HG - Cultural Heritage

Beamline(s) requested:
Principal # 1 BM32
OR
(alternatives)
...
...

Number of shifts required 18 Total required shifts: 18
Preferred starting time: *Please select the period* April/May *Unacceptable dates*

Beam Requirements

- ☐ 16 Bunch Mode ☐ 4 x 10mA Mode ☑ Multi Bunch
- ☐ Circular polarization ☐ White beam ☐ Monochromatic beam
- ☑ Fixed energy [keV]: 18.0 ☑ Tunable energy [keV] from: 7.0 to: 8.0
- Beam energy resolution [meV]: 1000.0 Spot size on sample [µm]: 300.0
- Other:

Main proposer (to whom correspondence will be addressed):

Sample Environment
Items Supplied by the ESRF

- ☐ Furnace ☐ Magnet ☐ Cryostat ☐ Cryogenic gas stream ☐ Refrigerator
- ☐ Laser Class ... Wavelength [nm] ☐

……

EUROPEAN SYNCHROTRON RADIATION FACILITY
ESRF User Office
CS 40220, F-38043 GRENOBLE Cedex 9, France
Delivery address: 71 avenue des Martyrs, 38000 GRENOBLE, France
Tel: +33 (0)4 7688 2552; fax: +33 (0)4 7688 2020; email: useroff@esrf.fr; web: http://www.esrf.fr

ESRF

Application for beam time at ESRF – Experimental Method

This document should consist of a maximum of two A4 pages (including references) with a minimal font size of 12 pt.

Proposal Summary (should state the aims and scientific basis of the proposal) :
The purpose of this proposal is the growth of high quality epitaxial Co ferrite ultrathin films on a Ag(001) substrate and the study of their structure by *in situ* grazing incidence x-ray diffraction (GIXRD). Ferrimagnetic spinel layers are outstanding materials for spin-filtering applications. Their properties like the spin-dependent gap, the magnetic anisotropy and the coercivity are function of morphologic and crystallographic features. Interface sharpness, spinel inversion degree and epitaxy-induced strains are key parameter which we aim to control in this experiment. In the past we successfully employed Ag(001) for growing magnetite films of similar structure. We will also perform anomalous GIXRD at the Co K edge, which allows the determination of the inversion degree. In a second step the ferrite layer will be coupled to a magnetite electrode to realize a model device whose properties will be studied *ex situ* further on.

Scientific background :
Spintronic has its origin in the discovery of the giant

Beamline(s) and beam time requested with justification :
We ask for 18 shifts on BM32 (INS2 instrument). This beamline is well equipped for *in situ* GIXRD measurements and for sample growth requiring three different evaporators.
5 shifts will be used for beam alignment and Co ferrite growth. 4 shifts for the structural study at fixed energy (18 Kev), 3 shifts for the K edge anomalous scattering, and 6 shift for the growth and structural study of the MgO and magnetite layers.

Results expected and their significance in the respective field of research :
Co ferrite as barrier for SF in multilayered devices is studied since a few years (see for ex. [6], [7]). However a detailed knowledge of films and interfaces structure at an atomic level is missing. We expect to fill this lack, elaborating a well-defined heterostructure that could be used as input in theoretical calculations to improve the understanding of spin filtering phenomena.

References
[1] I.S. Moodera et al. J. Phys.: Condens. Matter 19 (2007) 165202

…… Max 2 pages
If resubmitted, previous runs reports

Experimental report on proposal 20130289 (32-03-718)

Elaboration of an epitaxial all-oxide magnetic tunnel junction:
growth and structure of MgO/Fe_3O_4 and $MgO/Fe_3O_4/CoO$ on Ag(001)

Metal organic complexes: Phthalocyanines, Porphyrins

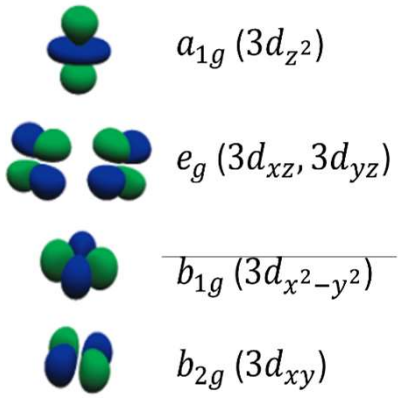
Central transition metal atom → differences in paramagnetic properties (FePc, CoPc etc)

Metal *3d* electronic configuration

Open-shell 3d^7 complexes (CoTPP, CoPc)

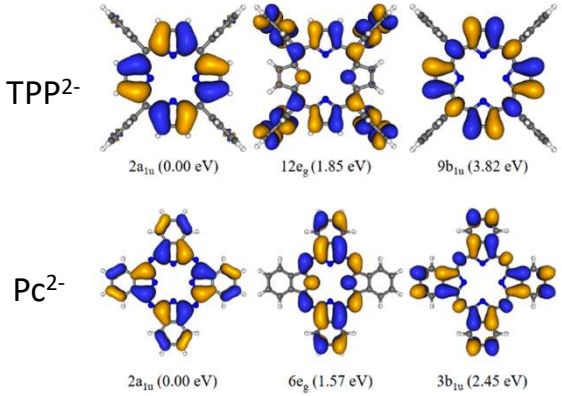
Closed-shell 3d^{10} complexes (ZnTPP, ZnPc)

D_{4h} splitting of *3d* orbitals



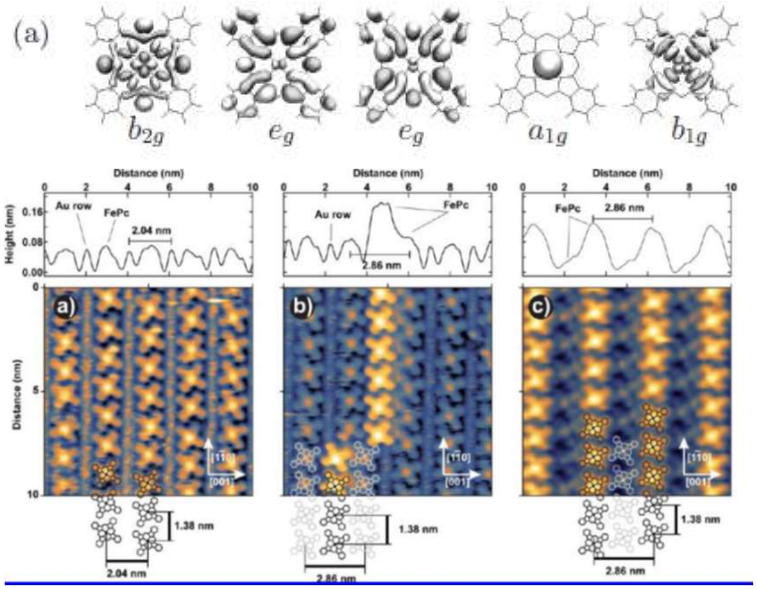
Adapted from *The Journal of Physical Chemistry C,* **2010** *114* (49), 21638-21644C

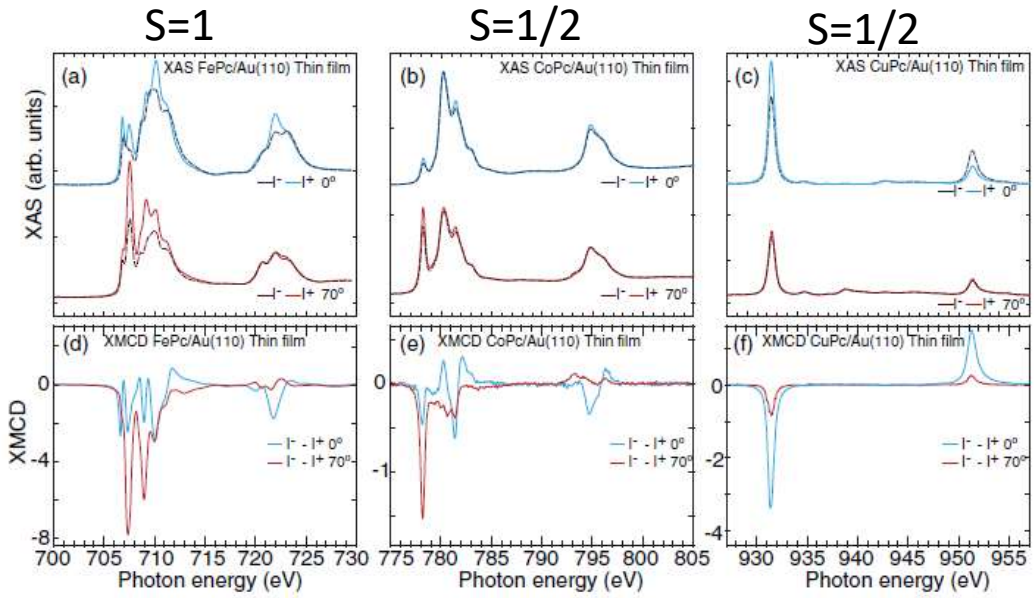
Macrocycle molecular orbitals



Phys. Chem. Chem. Phys., 2025,**27**, 11762-11779

EXAMPLE: XMCD at L2,3 Metal of paramagnetic Phthalocyanine arrays on Au(110) →Magnetic properties





FePc CoPc CuPc

Array formation on Au(110)
Proposal scientific question: how the paramagnetic properties of Phthalocyanines are changed after interaction with the substrate and array ordering formation

XMCD Results on MPc Films

$L_{2,3}$ XAS
2 p → 3d empty orbitals
2p → s 1/5 intensity

Sample environment

- Surfaces **electron** spectroscopies
  Ultra High Vacuum



- XAS Transmission and Fluorescence
  also Vacuum or Air



- Liquids samples
  - Special cells/Liquid microjets

Sample dimension

Damage

Sample Environment

Items Supplied by the ESRF

☐ Furnace ☑ Magnet ☑ Cryostat ☐ Cryogenic gas steam ☐ Refrigerator

☐ Laser Class [...] Wavelength [nm] ☐

☐ High pressure Pressure range [GPa] from ☐ to ☐

☐ Fixed temperature Temperature range [K] from 7.0 to 300.0

Detector system: TEY - drain current

Other equipment: sample preparation requires: 1) ion gun for Argon-sputtering, 2) heating capability for annealing to 750K ; STM in UHV in (or UHV connected to) preparation+analysis chamber

Items Not Supplied by the ESRF

List all equipment that you will insert into the instrument

☐ Laser Class Wavelength [nm] ☐

☐ Other equipment

Please indicate requirements for special equipment or facilities

phthalocyanine evaporators to be installed in the preparation chamber (CF40 flange)

Sample Description

Substance and formula

Au (110) and (111) xtals
Co phthalocyanine C32H16CoN8
Fe phthalocyanine C32H16FeN8

☑ Single crystal ☑ Powder ☐ Polycrystalline ☐ Multilayer ☐ Liquid ☐ Gas

☐ Nanoparticles ☐ Prepared at ESRF ☐ Other

Average size [mm] Volume [mm³] Surface area [mm²] 50

Mass [mg] 20.0 Matrix or solvent Conc.of absorb.[mmol]

Space group Cell dimensions at T= K:

a= Å b= Å c= Å alpha= ° beta= ° gamma= °

Container (capillary, flat plate, type of pressure cell, etc.)

Extra information required for Macromolecular Crystallography:

Origin and expression system

Previously observed diffraction (resolution, X-ray source, exposure/°)

Safety

Is the sample:

☐ Radioactive? ☐ Contaminant? ☐ Corrosive? ☐ Oxidizing?

☐ Explosive? ☐ Biologic? ☑ None of those

Is there any danger associated with the proposed sample, with any preparation at ESRF, or with sample equipment?

○ Yes ○ Uncertain ◉ No

If you have ticked Yes or Uncertain, you must give details of the associated risks in the box below:

Will you use live animals *on site for your experiment* ***(all kinds of animals are concerned)?*** ○ Yes ◉ No

If yes, you will later receive a special form.

After the experiment *, will the sample be:* ◉ Removed by user? ○ Stored at ESRF?

Beamline staff
+
Committee

High photon flux
Variable polarization
High resolving power
High magnetic field
UHV end station

Standard Application for Beam Time at the ESRF

Proposal Title (175 chars maximum.)

Magnetic properties of FePc and CoPc ordered arrays on Au(110): influence of 3d metal-substrate interaction

Keywords
#1: kondo resonance #2: xmcd #3: phthalocyanines #4:

- **This proposal is:**
  A new proposal ☑ A proposal relating to research in collaboration with an industrial group ☐
  A resubmission of ... ☐ A continuation of : ... ☐

Research Area of the proposal

- ☐ CH - Chemistry
- ☑ HE - Hard Condensed Matter - Electronic and Magnetic
- ☐ HS - Crystals and Ordered Systems - Structures
- ☐ HD - Disordered Systems and Liquids
- ☐ MA - Applied Materials and Engineering
- ☐ EC - Environmental and Cultural Heritage Matters
- ☐ MD - Medicine
- ☐ MI - Methods and Instrumentation
- ☐ MX - Macromolecular Crystallography
- ☐ SC - Soft Condensed Matter and Biological Materials
- ☑ SI - Surfaces and Interfaces

Other :

Beamline(s) requested: ID08 and ... / ... or ...

Number of shifts required *(1 shift is 8 hours)* 15
Preferred starting time: *Please select the period* August/September
Unacceptable dates 10-20 sept

Beam Requirements

☑ Multi Bunch ☑ 16 Bunch Mode ☐ 4 x 10mA Mode
☑ Circular polarization ☐ White beam ☑ Monochromatic beam
☐ Fixed energy [keV] : ☐ Tunable energy [keV] from: 0.3 to: 1.3
Beam energy resolution [meV]: 200.0 Spot size on sample [µm]:
Other:

Main Proposer (to whom correspondence will be addressed):

Experience with Synchrotron Radiation

What are the technical reasons which make ESRF necessary for your experiment?Why are other synchrotron radiation sources not appropriate?

The selected beamline (ID8) has the following characteristics crucial for this experiment:
Low temperature and High magnetic field for the XMCD measurements of the magnetization
High sensitivity (high S/N ratio), needed for the detection of the signal coming from sub-ML coverages
In addition, availability of an STM on-line for checking the sample preparation before the measurements.

Have you used synchrotron radiation at the ESRF? ○ No ◉ Yes

Have you used synchrotron radiation at other sources? ○ No ◉ Yes, at: Elettra (Trieste, Italy)

Have you already used synchrotron radiation for this project? ◉ No ○ Yes

Publications

Please give the references of papers published during the past 18 months as a result of experiments done at the ESRF.

Origin (1): if from data from ESRF beamlines ONLY, (2) : if from data from more than one source

	Description	Origin

Application for beam time at ESRF – Experimental Method

Proposal Summary (should state the aims and scientific basis of the proposal) :

Aim of the proposed experiment is to comparatively determine the magnetic properties of FePc and CoPc arrays on the Au(110) reconstructed channels, by X-ray Absorption Spectroscopy (XAS) and the related magnetic dichroism (XMCD). The influence of the molecule-substrate interaction on the magnetic moments will be clarified from the comparison with the results on the CoPc and FePc thick films.

Scientific background :

Organometallic molecules (OM) with magnetic properties have gained great appeal, as they offer an ideal platform to advance the fundamental understanding of magnetism at the nanoscale, and can act as templates for molecular spintronic device fabrication. Porfirines and phthalocyanines with a magnetic central atom can be used as chemical "cage" for anchoring the magnetic ion to a metal surface, and the spin-state of the central atom could be changed by modifying the molecular conformation. The ability to control and manipulate the individual spin of the metal atoms caged in the OM molecules and the coupling of single spins to their environment are at the basis of prospective quantum technologies. Recently, a Kondo resonance due to the coupling between the Fe spin state and the Au states has been observed for a Fe-phthalocyanine (FePc) deposited on Au, by scanning tunneling spectroscopy (STS) at the metal site of a single molecule[1]. The observed Kondo temperature is well above RT, in contrast to the much lower Kondo temperature for isolated Fe adatoms, showing the crucial role of the organic moiety in defining the properties of the system. However, a magnetic metal atom in the OM molecule does not guarantee that the magnetic moment be kept when the molecule is adsorbed on surfaces. This has been theoretically proved for CoPc that, when deposited on Au, does not show any Kondo resonance[2] [CoPc: free=1.09 μB, ads=0μB, (ref. 2); FePc: free=2.03μB, ads=1.05 μB (ref. 1)]. The distance between magnetic centers of MPcs and substrate[2] as well as the adsorption site[1] were found to strongly influence the Kondo temperature. All the cited experiments[1,2] did not present long-range ordered structures of the flat-lying MPc molecules and they have been investigated by means of local microscopy/spectroscopy. We recently grew highly-ordered 2D MPc single-layers (M=Zn, Cu, Ni, Co, Fe) of flat-lying molecules on the reconstructed channels of the Au(110) surface[3]: LEED patterns for the FePc and CoPc (5x3) single-layers are reported in Fig.1. Photoemission data has been collected exploiting the high energy-resolution of a SES200 analyzer at 20 K sample temperature, in the LOTUS laboratory in Rome. Preliminary data on single-layer MPcs do not show detectable interaction between the central atom and the underlying metal for NiPc, ZnPc and CuPc, while FePc and CoPc show distinct interface states, involving metal d-like orbitals.

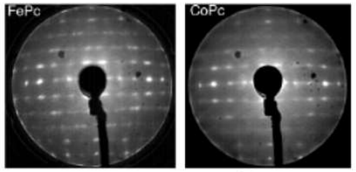


Fig. 1: LEED patterns of the (5x3) SL FePc, CoPc on Au(110)

Committee

Experimental technique(s), required set-up(s), measurement strategy, sample details (quantity...etc):

SETUP: FePc (and CoPc) powder will be brought by us into small quartz ampoules mounted on CF40 UHV standard flanges with electrical connections, and sublimated in UHV by resistive heating (sublimation temperature about 400°C). The Au(110) surface will be kept at 430 K during deposition. The Au(110) and (111) single-crystals (7x9 mm^2) will be mounted on an azimuthally turning sample holder and cleaned by sputtering and annealing cycles (1000-600 eV Ar+, 700K-400K annealing).

MEASUREMENTS: The correct sample preparation will be checked by LEED and STM. Exploiting the chemical specificity of XAS and XMCD, we shall investigate the $L_{2,3}$ edges of Fe and Co, as well as the N-edge of Au. Measurements will be performed in Total Electron Yield (TEY), at different temperatures and magnetic fields (up to 5T), at the Fe, Co $L_{2,3}$ and Au-N absorption edges on Single-Layer (SL) long-range ordered and isolated molecules of FePc, CoPc on Au (110) and (111) surfaces, as well as on FePc and CoPc multi-layers; also the K edge of nitrogen will be analyzed.

Feasibility
Beamline staff

Beamline(s) and beam time requested with justification :

The low density of Co and Fe central metal atoms in MPc sub-monolayers requires the high sensitivity of XAS and XMCD, the high magnetic field (up to 5T) and low temperature (LHe) available at the ID8 beamline, indispensable for detecting a significant dichroic signal, as already proved by our fruitful recent experience on comparable systems[7]. This beamline also has the required photon energy range, a high signal-to-noise ratio, very good energy resolution and stability and, finally, an STM connected with the acquisition chamber, making it almost unique for the successful performing of such kind of experiment.

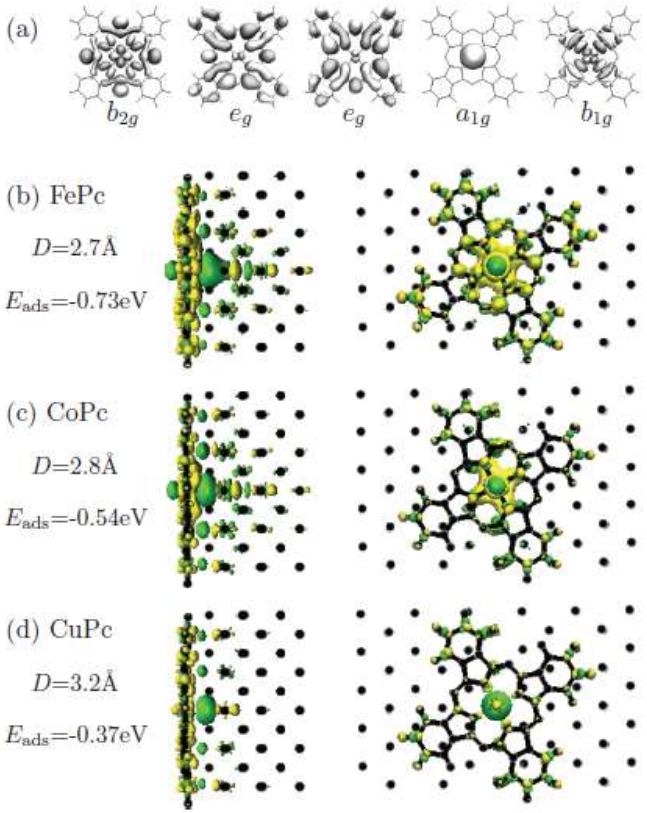
Feasibility
Beamline staff
+
Committee

Results expected and their significance in the respective field of research :

The main goal is to deduce experimentally the Fe and Co magnetic moments for a highly-ordered single-layer and isolated molecules of FePc and CoPc deposited on Au surfaces, to compare with those calculated[1,2] and the ones obtained for the corresponding multi-layers. Measurement of the magnitude and direction of the magnetic moments is very relevant for the comparison with our photoemission data and local spectroscopy[1] on single molecules, where the density of states at the Fermi level has been interpreted as a Kondo resonance.

References

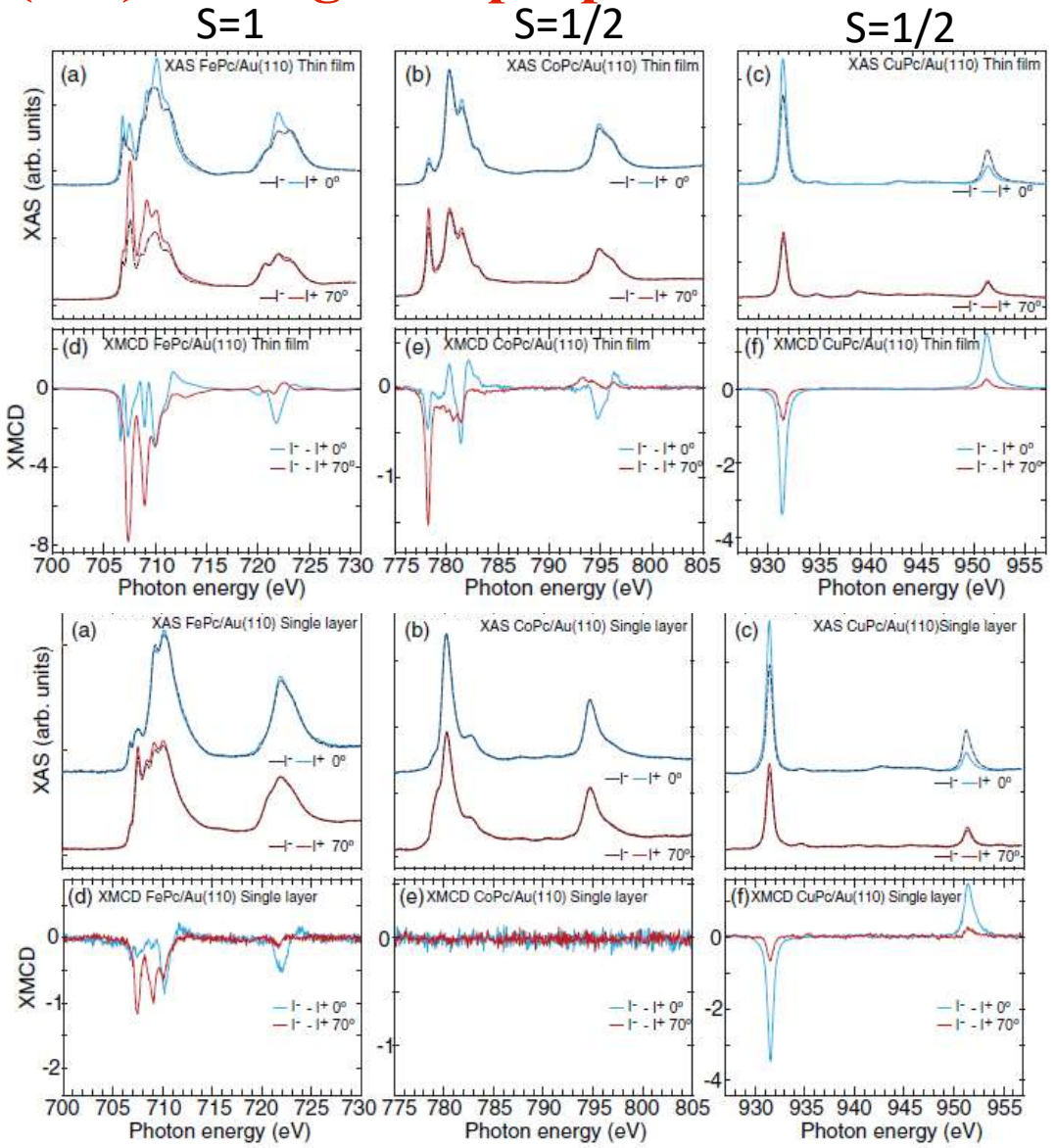
Final results XMCD at L2,3 Metal applied to paramagnetic Phthalocyanine arrays on Au(110) →Magnetic properties



$L_{2,3}$ XAS

2 p → 3 d empty orbitals

2p → s 1/5 intensity



Gargiani et al. PRB 2013

Before beamtime

- Contact staff for the schedule
- Ask details on the sample mounting, etc

- Agreement with the beamline staff:
  - Who makes the analysis?
  - Collaboration or independent publication+acknowledments

After beamtime

- Remove the samples
- Transfer data
- Control the data analysis codes and the conditions to use them
- Write the report of beamtime (1-2 month of time)

- Agreement with the beamline staff:
  - Who makes the analysis?
  - Collaboration or independent publication+acknowledments

- After publication add it to the facility database

Resubmission

Users Support Programs

Data analysis procedures and codes

Tutorials

ILL:
https://youtu.be/R3tOpLvKQm8

ESRF:
https://www.esrf.fr/files/live/sites/www/files/UsersAndScience/UserGuide/Applying/Advice_on_writing_a_good_proposal.pdf

Thanks!

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Theory

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