



Istituto Nazionale di Fisica Nucleare





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UPPSALA UNIVERSITET

# The EuPRAXIA users' facilities

Francesco Stellato

University of Rome Tor Vergata & INFN

on behalf of the EuPRAXIA collaboration team



# (not only) photon sources @ EuPRAXIA

• EuPRAXIA-PP

Photon and particle sources based on novel (plasma) acceleration techniques

- Free Electron lasers: EuPRAXIA@SPARC\_LAB AQUA – water window FEL beamline ARIA - VUV FEL beamline
- Betatron source



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# The EuPRAXIA users' program

- Electrons (0.1-5 GeV, 30 pC)
- Positrons (0.5-10 MeV, 10<sup>6</sup>)
- Positrons (GeV source)
- Lasers (100 J, 50 fs, 10-100 Hz)
- X-band RF Linac (60 MV/m , up to 400 Hz)
- Plasma Targets
- Betatron X rays (1-10 keV, 10<sup>10</sup>)
- FEL light (0.2-36  $\rightarrow$  200 nm, 10<sup>9</sup>-10<sup>13</sup>)



### https://www.eupraxia-pp.org/

Courtesy M. Ferrario





# **Building up a users' community**

Collecting needs of the future users' community (both on the scientific and on the organization side)





Please do help us by filling this survey

https://surveys.infn.it/index.php/718177



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# **FEL Photon beams parameters**

**AQUA** 

Parameter	Value
Wavelength*	~4 nm
Photons/pulse	10 <sup>10</sup> - 10 <sup>11</sup>
Pulse duration	< 50 fs
Repetition rate**	10 Hz

### ARIA

Parameter	Value
Wavelength	50-180 nm
Photons/pulse	10 <sup>13</sup> - 10 <sup>14</sup>
Pulse duration	20/200 fs
Repetition rate**	10 Hz

\*Running at longer wavelength (~10 nm) is within the reach of the machine \*\* Options to run @ 400 Hz are being explored





# **AQUA** - Techniques & Samples in the water window

**Experimental techniques and typology of samples** 



Proteins Viruses Bacteria Cells Metals Semiconductors Superconductors Magnetic materials Organic molecules Organometallic compounds

### Ion Spectroscopy → Destruction without diffraction ???



# ARIA - Techniques & Samples @ 50-180 nm

### **Experimental techniques and typology of samples (and applications)**



Villa et al. Cond. Mat. 2022



# **Experimental Techniques**



# Experimental Techniques Coherent imaging

The water window is a «sweet spot» for imaging of biological samples in their native environment.

The expected resolution is tens of nanometers However, only room-temperature measurements of fully hydrated samples allow aquiring 2D images of **living cells** and of **organelles** in their native state

Single-shot 3D imaging of not-reproducible samples







# Experimental Techniques Coherent imaging

# Images of living bacteria have been acquired at SACLA (*S. aureus*, 5.5 keV)

Fan, J., Sun, Z., Wang, Y., Park, J., Kim, S., Gallagher-Jones, M., ... & Jiang, H. (2016). Single-pulse enhanced coherent diffraction imaging of bacteria with an X-ray free-electron laser. *Scientific Reports*, *6*(1), 34008.

#### and LCLS (C. gracile, 517 eV)

Van Der Schot, G., Svenda, M., Maia, F. R., Hantke, M., DePonte, D. P., Seibert, M. M., ... F. Stellato, ... & Ekeberg, T. (2015). Imaging single cells in a beam of live cyanobacteria with an X-ray laser. *Nature communications*, *6*(1), 5704.







# Experimental Techniques Coherent imaging



Yeast Nuclei 0.3  $\mu$ m < diameter < 2  $\mu$ m

LCLS experiments (still) unpublished data



520 eV (2.4 nm) photons 3x2 μm<sup>2</sup> focus - 2 μJ



A yeast nucleus diffraction pattern exhibiting clearly visible speckles



# Experimental Techniques Coherent imaging

Imaging can be also performed on inorganic samples.





Nanotubes, nanoparticles, combustion products (soot)

Again, high time-resolution pump-probe studies are the target.



# **Experimental Techniques** X-ray spectroscopy: absorption (and emission)

AQUA

No **monochromator** in phase one (but space for a monochromator foreseen) SASE w/o monochromator (ghost-spectroscopy) scheme

Klein, Y., Tripathi, A. K., Strizhevsky, E., Capotondi, F., De Angelis, D., Giannessi, L., ... & Shwartz, S. (2023). High-spectral-resolution absorption measurements with free-electron lasers using ghost spectroscopy. *Physical Review A*, *107*(5), 053503.

Downstream spectrometer for X-ray emission measurements

#### ARIA

Seeded w/o monochromator scheme with short (20 fs) pulses for VUV spectroscopy

Seeded with monochromator scheme with long (200 fs, 10<sup>14</sup> photons/pulse) pulses for VUV spectroscopy



# Experimental Techniques X-ray spectroscopy

<u>J Synchrotron Radiat.</u> 2013 Jul 1; 20(Pt 4): 614–619. Published online 2013 May 30. doi: <u>10.1107/S0909049513003142</u> PMCID: PMC3682637 PMID: 23765304

Hydrocarbons, aminoacids

Al to K L-edges

C K-edge

Alloys, warm-dense matter (pump-probe)

Soft X-ray absorption spectroscopy and resonant inelastic X-ray scattering spectroscopy below 100 eV: probing first-row transition-metal *M*-edges in chemical complexes

Hongxin Wang,<sup>a,b,\*</sup> Anthony T. Young,<sup>c</sup> Jinghua Guo,<sup>c</sup> Stephen P. Cramer,<sup>a,b</sup> Stephan Friedrich,<sup>d</sup> Artur Braun,<sup>e</sup> and Weiwei Gu<sup>b</sup>

JURNAL OF THE AMERICAN CHEMICAL SOCIETY

Tabletop Femtosecond M-edge X-ray Absorption Near-Edge Structure of FeTPPCI: Metalloporphyrin Photophysics from the Perspective of the Metal

Cu to Ru M-edges

Samples: cuprates, porphyrins, metalloproteins

Sb to Ne L-edges

Lanthanides superconductors, catalysts





# **Experimental Techniques** X-ray spectroscopy

Angewandte International Edition Chemie GDCh A Journal of the German Chemical Society

Communication 🗇 Open Access 🕼 😧

Chasing the Elusive "In-Between" State of the Copper-Amyloid  $\beta$ Complex by X-ray Absorption through Partial Thermal Relaxation after Photoreduction

Enrico Falcone, Germano Nobili, Michael Okafor, Olivier Proux, Giancarlo Rossi, Silvia Morante, Peter Faller 🔀, Francesco Stellato 🔀

First published: 03 March 2023 | https://doi.org/10.1002/anie.202217791

Cu to Ru M-edges

Samples: cuprates, porphyrins, metalloproteins

Sb to Ne L-edges

Lanthanides superconductors, catalysts



Perspective of the Metal



### WA 8 – Users



# **Experimental Techniques** Small (and wide) Angle X-ray Scattering

Small angle scattering measurements provide lowresolution structural information

The ultra-short FELs allows time-resolved pumpprobe measurements

At both AQUA and ARIA, these measurements are @ reachable camera lengths





# **Experimental Techniques** Small (and wide) Angle X-ray Scattering

Pump-probe schemes allow to exploit SAXS (and WAXS) to track fast structural changes in catalysts, superconductors, photo-sensitive biological molecules, ...



Communication

*Operando* Resonant Soft X-ray Scattering Studies of Chemical Environment and Interparticle Dynamics of Cu Nanocatalysts for CO<sub>2</sub> Electroreduction

Yao Yang, Inwhan Roh, Sheena Louisia, Chubai Chen, Jianbo Jin, Sunmoon Yu, Miquel B. Salmeron, Cheng Wang,\* and Peidong Yang\*



Photo-excitation of proteins monitored by SAXS & WAXS Arnlund *et al.*, Nat Methods 2014 Levantino *et al.*, Nat Comm 2014



# **Experimental Techniques** Raman Spectroscopy

FEL pulses can be exploited as pump pulse for stimulating chemical reactions or for generating coherent excitations, and, on the other hand, they can be used as selective probe to monitor the evolution from reactant to photoproduct.

#### ARIA

Electronic transitions for **cluster materials** such as nanocarbons and potential gap dielectrics from **metal oxides**, **nano structure**, wide band-gap materials.

#### AQUA

Electronic information on materials such as Silicon carbide SiC, boron nitride BN, Zinc sulfide ZnS, energy transfer in  $TiO_2/Ln^{+3}$  doped glass). Photocatalytic reactions  $CO_2$  and  $N_2$  reduction and  $H_2O$  oxidation







# **Experimental Techniques** Photoemission Spectroscopy

The AQUA and ARIA energy ranges are also suitable to perform Photoemission Spectroscopy (PES) experiments, in which the energy spectrum of the emitted photoelecton is measured. This provides information on the electronic structure of the samples.

PES can be performed in different schemes and it will benefit from the ultrafast structure of the FEL radiation for pumpprobe measurements.







# **Experimental Techniques** Photoemission Spectroscopy

X-ray Photon Spectroscopy C<sup>-</sup>60

Lithium Battery interface during charge/discharge



Photoelectron spectra of C60 2 at 355, 266, and 193 nm with photon fluxes of 5, 1.5, and 0.7 mJ/cm2, respectively. ( Xue-Bin Wang, 1999)



Si 2p spectrum of the pristine silicon electrode (Bertrand Philippe, 2016)

Courtesy of Federico Galdenzi

**PES** measuements of organic rings opening





# **Users' community**





# **Users' community**

EuPRAXIA@SPARC_LAB user workshop					
14-15 October 2021 Europe/Rome timezone					
Overview Timetable	Participant List 147 participants				
Registration Participant List	Last Name	First Name	Affiliation		

### The first EuPRAXIA@SPARC\_LAB user workshop

#### More than 140 registrants from 9 countries and ~30 institutions

https://agenda.infn.it/event/27926/overview



# **Users' community - Feedback**

Pros

#### **Cons (limitations)**

Limited photon flux

Energy ranges (both AQUA and ARIA) not primary for many FEL sources

Flexibility in pulse duration

Beamtime availability for long-term projects

Presence of two beamlines at very different energies

Presence of the **EuAPS** betatron source

What else?

Input from potential users still more than welcome

Limited repetition rate (mitigated if 400 Hz are reached)

Limited wavelength range (not reaching the O K-edge)



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# **EuAPS – Betatron radiation source**

Parameter	Value	unit
Photon Critical Energy	1 -10	keV
Photons/pulse	10 <sup>6</sup> -10 <sup>9</sup>	
Repetition rate	1-5	Hz
Beam divergence	3-20	mrad

Expected parameters of the EuAPS betatron radiation source



Photon science case

#### Plasma-Generated X-ray Pulses: Betatron Radiation Opportunities at EuPRAXIA@SPARC\_LAB

Francesco Stellato <sup>1,2,\*</sup>, Maria Pia Anania <sup>3</sup>, Antonella Balerna <sup>3</sup>, Simone Botticelli <sup>2</sup>, Marcello Coreno <sup>3,4</sup>, Gemma Costa <sup>3</sup>, Mario Galletti <sup>1,2</sup>, Massimo Ferrario <sup>3</sup>, Augusto Marcelli <sup>3,5,6</sup>, Velia Minicozzi <sup>1,2</sup>, Silvia Morante <sup>1,2</sup>, Riccardo Pompili <sup>3</sup>, Giancarlo Rossi <sup>1,2,7</sup>, Vladimir Shpakov <sup>3</sup>, Fabio Villa <sup>3</sup> and Alessandro Cianchi <sup>1,2</sup>





# **EuAPS – Betatron radiation source**

What are betatron pulses good for?

Betatron radiation covers a broad energy range

Spectroscopic techniques

Betatron pulses are short (femtoseconds)

Pump-probe, time-resolved experiments

**Betatron** radiation is partially (spatially) coherent Phase-contrast imaging





# **Photon Science @ EuAPS**

### Ultra-fast, pump-probe time-resolved X-ray Spectroscopy

### Imaging at a small-scale source





Physics of warm-dense matter Femtochemistry of organometallic complexes Tissues Plants Cultural Heritage





# **Photon Science @ EuAPS**

### • Imaging of biological (and cultural heritage) samples

Exploits the brilliance and coherence of betatron radiation, requires small divergence and good focusing

Static X-ray Spectroscopy

Relatively easy, but does not exploit the radiation time structure

# Ultra-fast X-ray spectroscopies exploiting ultra-short betatron pulses More complicated, requires timing between pump and probe pulses, but fully exploits the fs pulse duration

### Time-resolved diffraction

Depending on the samples, likely exploiting a white beam in a Laue scheme → Serial crystallography







# **Imaging setup**

### Variable sample-detector distance

Accurate sample positioning and rotation

### Small pixel, 2D X-ray detector

### CCD or CMOS









Courtesy A. Balerna



# **Imaging – The pilot experiment**

Ministero dell'Università e della Ricerca

Italiadomani

### **Green science**

X-ray imaging of **leaves** (and **wood** → **connection with Swedish researchers**) aiming at the (tens of) microns resolution

Living plants, different hydration stares

Experiments performed with the broad radiation spectrum filtered by different materials to obtain difference maps emphasizing the presence of heavy metal contaminants  $\rightarrow$  pollution control

Reale et al. - MIDIX Soft X-rays microradiography







# **Imaging – Cultural Heritage**

# Imaging of ancient paper documents



#### В



#### Virtual unrolling and deciphering of Herculaneum papyri by X-ray phase-contrast tomography

L Bukreeva, A. Mittone, A. Bravin, G. Festa, M. Alessandrelli, P. Coan, V. Formoso, R. G. Agostino, M. Giocondo, F. Ciuchi, M. Fratini, L. Massimi, A. Lamarra, C. Andreani, R. Bartolino, G. Gigli, G. Ranocchia 🖾 & A. Cedola 🖾

Scientific Reports 6, Article number: 27227 (2016) Cite this article



### Characterization of **inks** (chemical sensitivity thanks to filters)

with Dr. Giulia Festa, Centro Studi e Ricerche Enrico Fermi





# **Time-resolved Imaging**

### Nanoparticles dynamics



#### Shock-waves in materials

#### Ultrafast Imaging of Laser Driven Shock Waves using Betatron X-rays from a Laser Wakefield Accelerator

J. C. Wood <sup>1</sup>, D. J. Chapman<sup>2</sup>, K. Poder <sup>1</sup>, N. C. Lopes<sup>1,3</sup>, M. E. Rutherford <sup>2,4</sup>, T. G. White<sup>5</sup>, F. Albert<sup>6</sup>, K. T. Behm<sup>7</sup>, N. Booth<sup>8</sup>, J. S. J. Bryant<sup>1</sup>, P. S. Foster<sup>8</sup>, S. Glenzer<sup>9</sup>, E. Hill<sup>10</sup>, K. Krushelnick<sup>7</sup>, Z. Najmudin <sup>1</sup>, B. B. Pollock<sup>6</sup>, S. Rose <sup>10</sup>, W. Schumaker<sup>9</sup>, R. H. H. Scott <sup>08</sup>, M. Sherlock<sup>10</sup>, A. G. R. Thomas<sup>7</sup>, Z. Zhao<sup>7</sup>, D. E. Eakins <sup>2,4</sup> & S. P. D. Mangles <sup>1</sup>

### Liquid jet explosion

### under X-ray beams







# **Absorption Spectroscopy**

### Single-shot XANES spectrum at the Ti K-edge

### Single-shot **EXAFS** spectrum at the Cu K-edge







# **Spectroscopy Setup**



No monochromator to maximize the photon flux on the sample





### **Ultra-fast Spectroscopy**

Optical laser pump / betatron probe experiments can follow the non-equilibrium dynamics of the copper heating process via XAS on fs timescale Mahieu *et al.* Nature Comm 2015

dall'Unione europea

Measurements of Ionization States in Warm Dense Aluminum with Betatron Radiation Mo *et al.* 2017





# Outlook

- Building up the scientific case and the users' community for plasma-based pulsed sources: from X-rays to VUV
- EuPRAXIA@SPARC\_LAB Technical Design Report Detailed definition of spaces and experimental requirements
- EuAPS

Final design of experimental chamber, getting ready for pilot experiments

• R&D: optics, sample delivery, detection schemes