The Free Electron Laser EuPRAXIA@SPARC_LAB

Augusto MARCELLI
on behalf …

marcelli@lnf.infn.it

Funded by the European Union

XLS Users Meeting

Geneva, November 27-28, 2018

Compact

Scientific case of the EUPRAXIA@SPARC_LAB

Istituto Nazionale di Fisica Nucleare

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What new should be really done?

- **attempts exist to investigate light-light interaction phenomena**

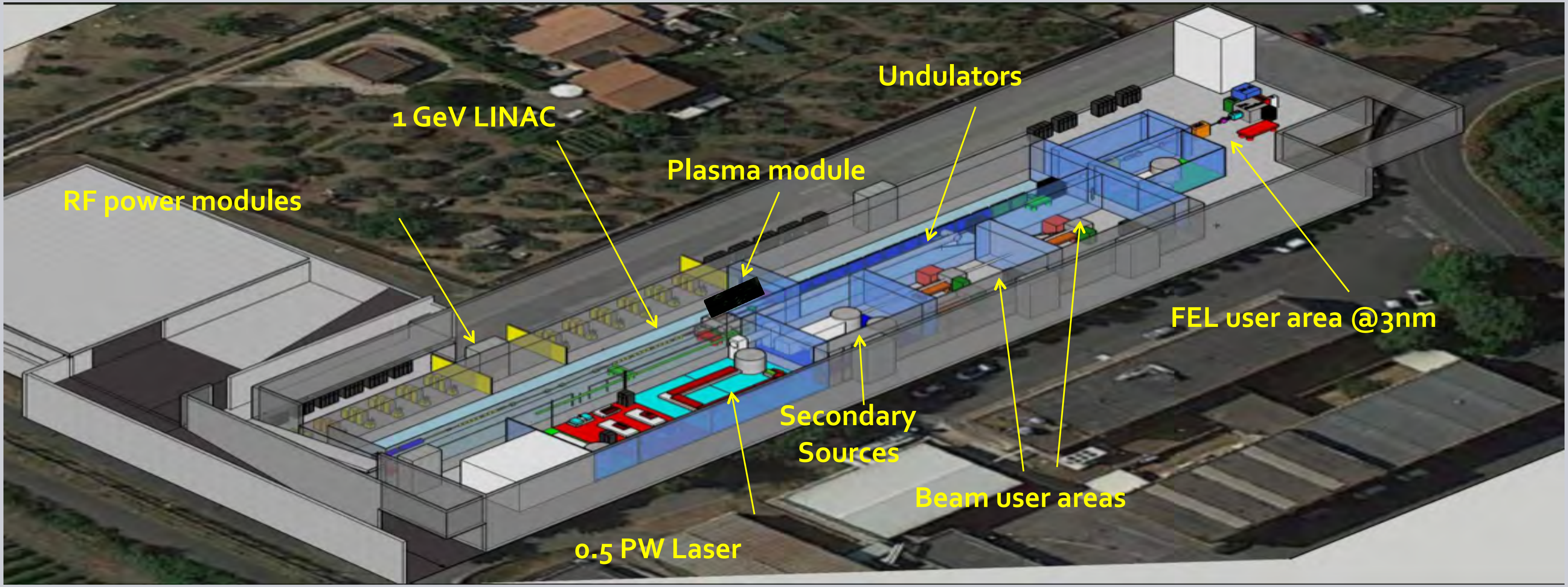
- **light does not interact with light at low energy density in vacuum**

(in the soliton hypothesis at least ~10^{33} W/cm^2 is required!!)
World most powerful laser is ~10^{14} W!

- **Efforts exist to induce and observe light-light interaction at a lower density to use photons to control photons (quantum communications, quantum computing, quantum optics, etc.)**

Osaka, March 5, 2011

EuPRAXIA@SPARC_LAB



http://www.lnf.infn.it/sis/preprint/pdf/getfile.php?filename=INFN-18-03-LNF.pdf

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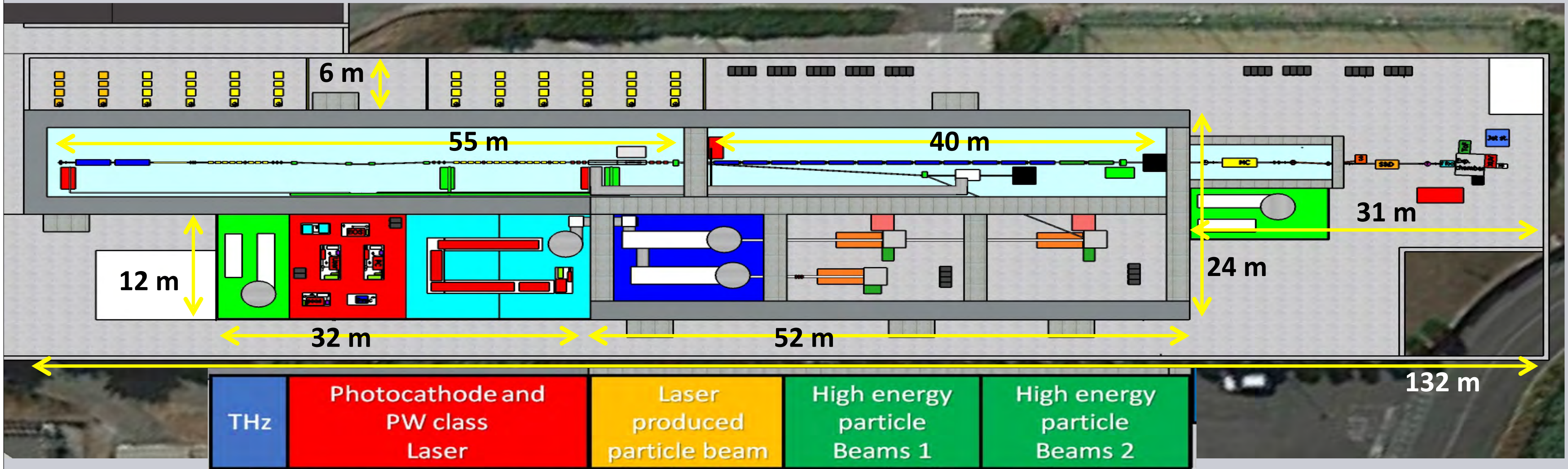
D. Alesini[a], M. P. Anania[a], M. Artioli[b], A. Bacci[c], S. Bartocci[d], R. Bedogni[a], M. Bellaveglia[a], A. Biagioni[a], F. Bisesto[a], F. Brandi[e], E. Brentegani[a], F. Broggi[c], B. Buonomo[a], P. Campana[a], G. Campogiani[a], C. Cannaos[d], S. Cantarella[a], F. Cardelli[a], M. Carpanese[f], M. Castellano[a], G. Castorina[g], N. Catalan Lasheras[h], E. Chiadroni[a], A. Cianchi[i], R. Cimino[a], F. Ciocci[f], D. Cirrincione[j], G. A. P. Cirrone[k], R. Clementi[a], M. Coreno[l], R. Corsini[h], M. Croia[a], A. Curcio[a], G. Costa[a], C. Curatolo[c], G. Cuttone[k], S. Dabagov[a], G. Dattoli[f], G. D'Auria[l], I. Debrot[c], M. Diomede[a,g], A. Drago[a], D. Di Giovenale[a], S. Di Mitri[l], G. Di Pirro[a], A. Esposito[a], M. Faiferri[d], M. Ferrario[a], L. Ficcadenti[g], F. Filippi[a], O. Frasciello[a], A. Gallo[a], A. Ghigo[a], L. Giannessi[f,l], A. Giribono[a], L. A. Gizzi[e], A. Grudiev[h], S. Guiducci[a], P. Koester[e], S. Incremona[a], F. Iungo[a], L. Labate[e], A. Latina[h], S. Licciardi[f], V. Lollo[a], S. Lupi[g], R. Manca[d], A. Marcelli[a,m,n], M. Marini[d], A. Marocchino[a], M. Marongiu[g], V. Martinelli[a], C. Masciovecchio[l], C. Mastino[d], A. Michelotti[a], C. Milardi[a], M. Migliorati[g], V. Minicozzi[i], F. Mira[g], S. Morante[i], A. Mostacci[g], F. Nguyen[f], S. Pagnutti[f], L. Palumbo[g], L. Pellegrino[a], A. Petralia[f], V. Petrillo[o], L. Piersanti[a], S. Pioli[a], D. Polese[d], R. Pompili[a], F. Pusceddu[d], A. Ricci[m], R. Ricci[a], R. Rochow[l], S. Romeo[a], J. B. Rosenzweig[p], M. Rossetti Conti[o], A. R. Rossi[c], U. Rotundo[a], L. Sabbatini[a], E. Sabia[f], O. Sans Plannell[a], D. Schulte[h], J. Scifo[a], V. Scuderi[k], L. Serafini[c], B. Spataro[a], A. Stecchi[a], A. Stella[a], V. Shpakov[a], F. Stellato[i], P. Tomassini[e], E. Turco[d], C. Vaccarezza[a], A. Vacchi[j], A. Vannozzi[a], G. Vantaggiato[e], A. Variola[a], S. Vescovi[a], F. Villa[a], W. Wuensch[h], A. Zigler[q], M. Zobov[a]

[a] *INFN - Laboratori Nazionali di Frascati, via E. Fermi 40, 00044 Frascati, Italy*
[b] *ENEA - Centro Ricerche Bologna, Via Martiri Monte Sole 4, 40129 Bologna, Italy*
[c] *INFN - Milano section, Via Celoria 16, 20133 Milan, Italy*
[d] *Universitá degli Studi di Sassari, Dip. di Architettura, Design e Urbanistica ad Alghero, Palazzo del Pou Salit - Piazza Duomo 6, 07041 Alghero, Italy*
[e] *Intense Laser Irradiation Laboratory (ILIL), Istituto Nazionale di Ottica (INO), Consiglio Nazionale delle Ricerche (CNR), Via G. Moruzzi 1, 56124 Pisa, Italy and INFN Pisa section, Pisa, Largo Pontecorvo 3, 56127 Pisa, Italy*
[f] *ENEA - Centro Ricerche Frascati, Via E. Fermi 45, 00044 Frascati, Italy*
[g] *Sapienza University of Roma and INFN, P.le Aldo Moro 2, 00185 Rome, Italy*
[h] *CERN, CH-1211 Geneva 23, Switzerland*
[i] *Universitá degli Studi di Roma Tor Vergata and INFN, Via della Ricerca Scientifica 1, 00133 Rome, Italy*
[j] *INFN - Trieste section, Via Valerio 2, 34127 Trieste, Italy*
[k] *INFN - Laboratori Nazionali del Sud, via S.Sofia 62, 95123 Catania, Italy*
[l] *Elettra-Sincrotrone Trieste, Area Science Park, 34149 Trieste, Italy*
[m] *RICMASS, Rome International Center for Materials Science Superstripes, 00185 Rome, Italy*
[n] *ISM-CNR, Basovizza Area Science Park, Elettra Lab, 34149 Trieste - Italy*
[o] *Universitá degli Studi di Milano and INFN, Via Celoria 16, 20133 Milan, Italy*
[p] *Department of Physics and Astronomy, University of California Los Angeles, Los Angeles, California 90095, USA*
[q] *Racah Institute of Physics, The Hebrew University of Jerusalem, 91904 Jerusalem, Israel*

- LNF candidate to host EuPRAXIA (1-5 GeV)
- FEL user facility (1 GeV – 3 nm)
- Advanced Accelerator Test facility (LC) + CERN



- 500 MeV by RF Linac + 500 MeV by Plasma (LWFA or PWFA)
- 1 GeV by X-band RF Linac only
- Final goal: a compact 5 GeV accelerator

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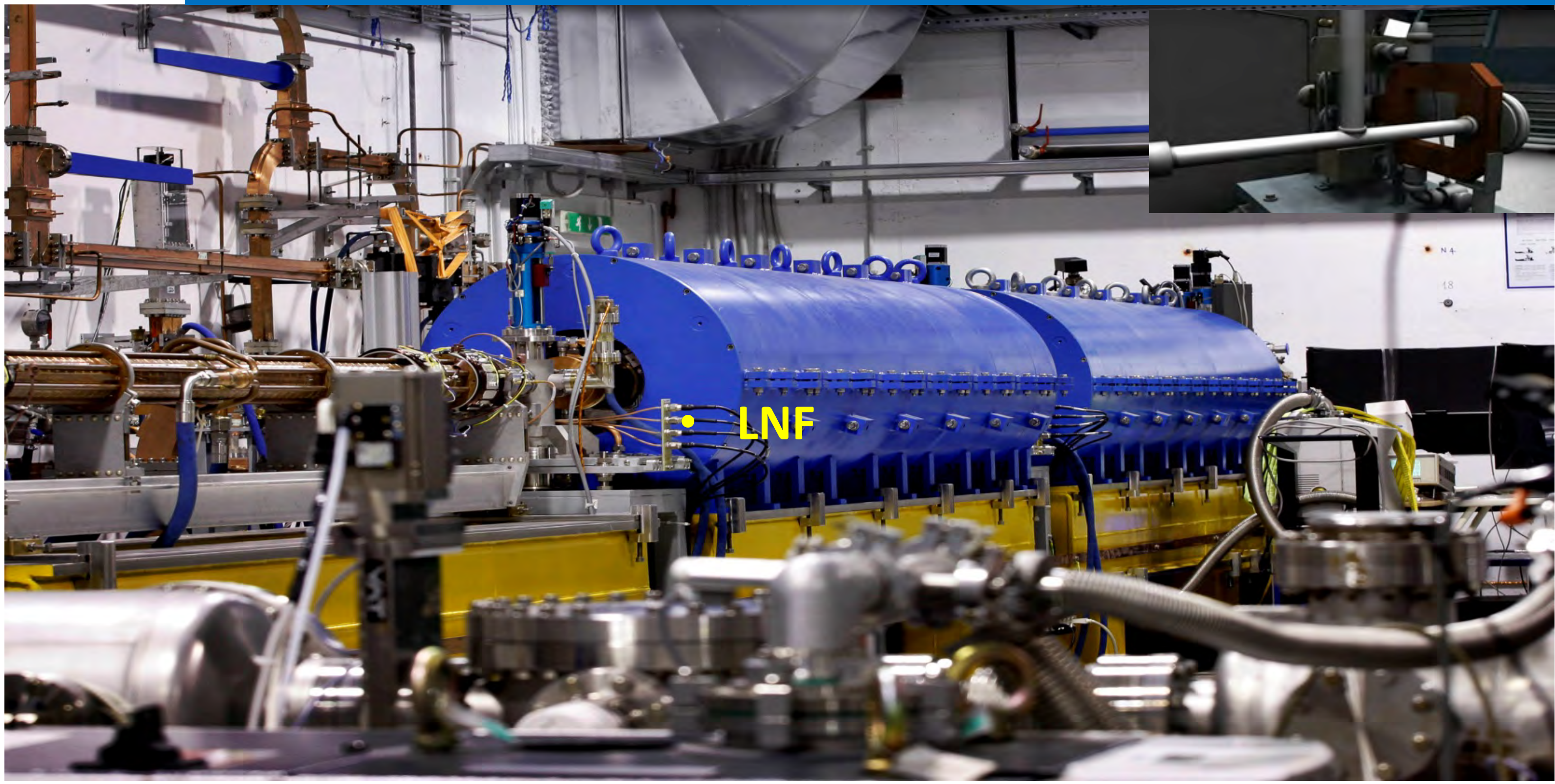
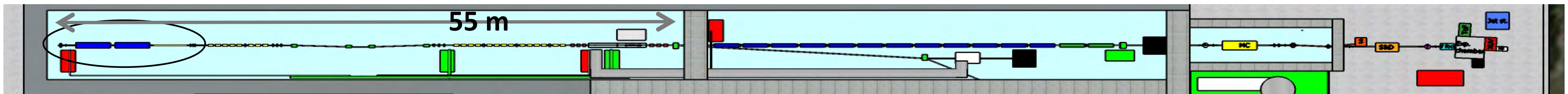
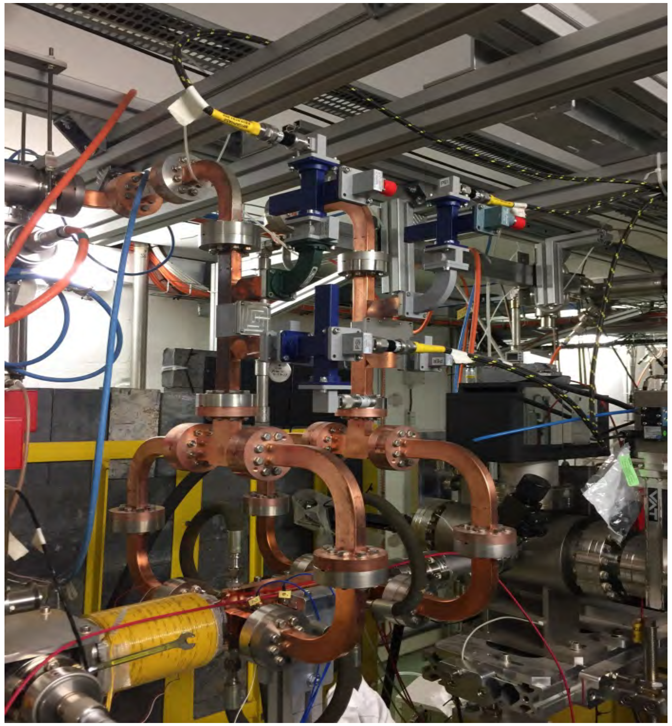
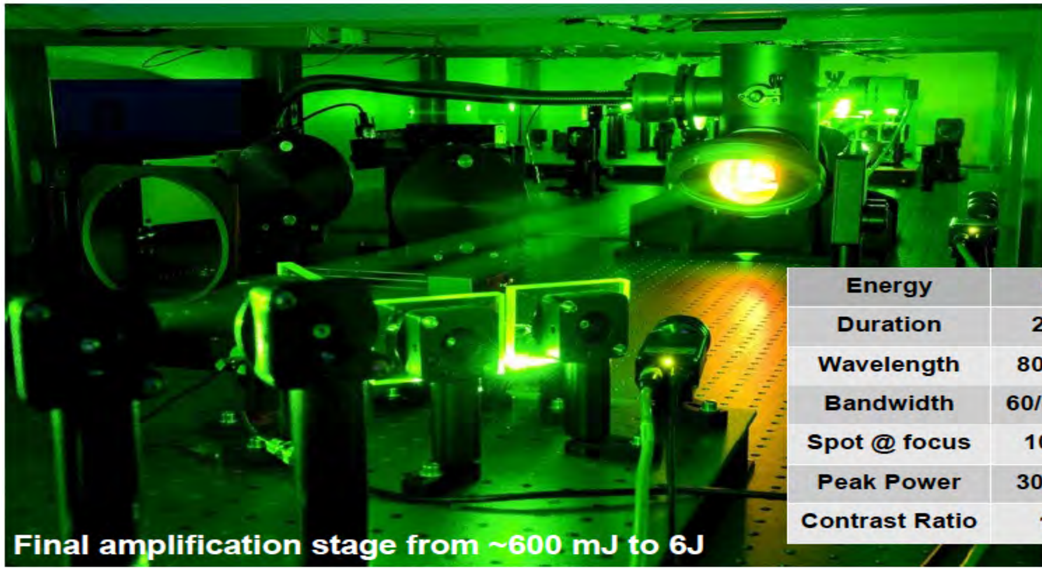
SPARC_LAB HB photo- injector



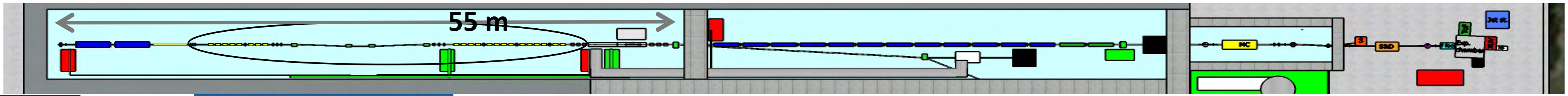


X-band Linac and High Power Laser

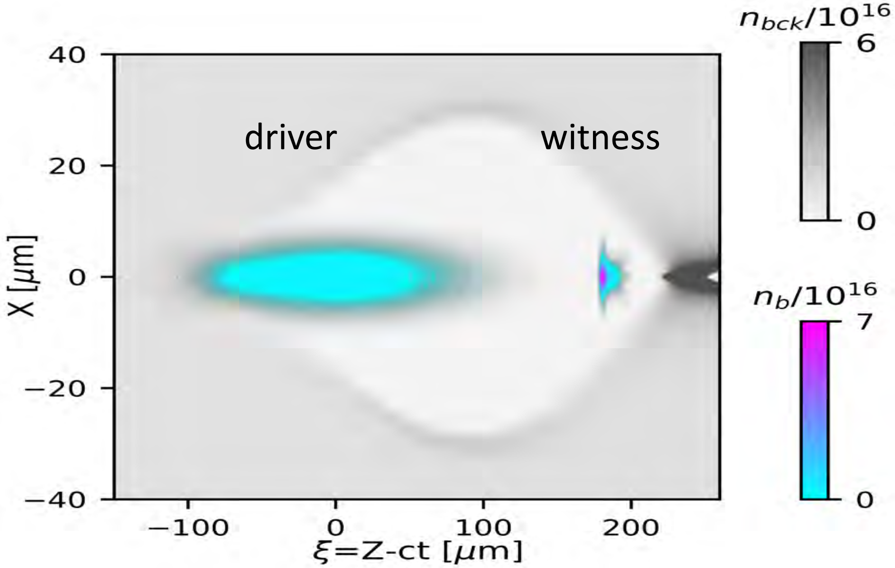


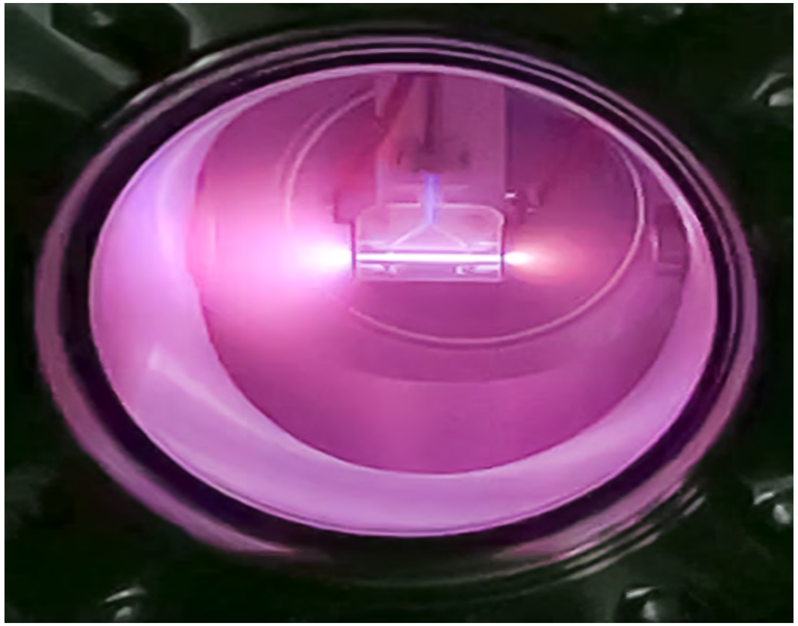


Energy	6 J
Duration	23 fs
Wavelength	800 nm
Bandwidth	60/80 nm
Spot @ focus	10 µm
Peak Power	300 TW
Contrast Ratio	10^{10}

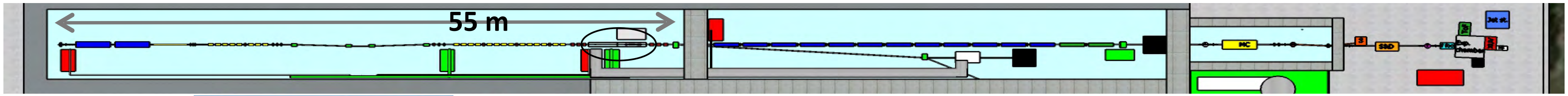


Plasma WakeField Acceleration – External Injection

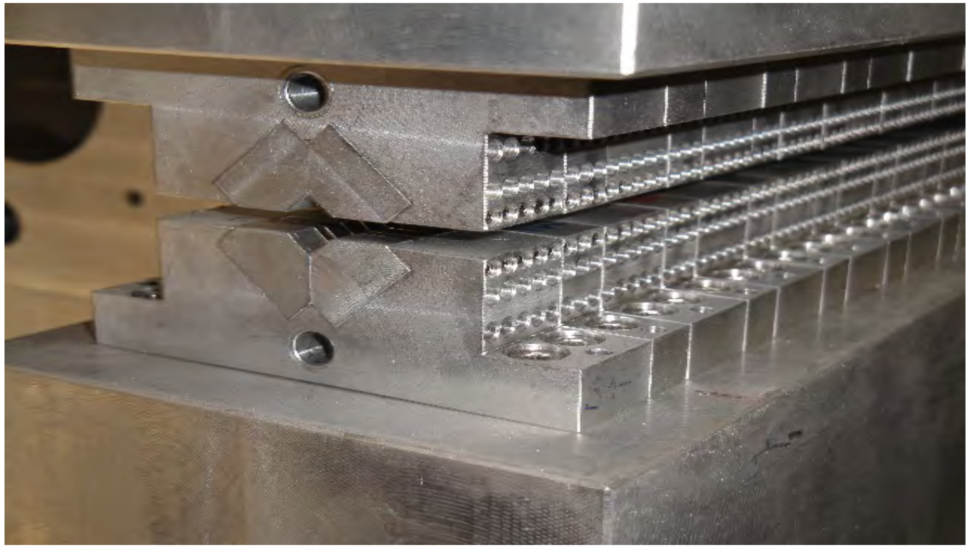


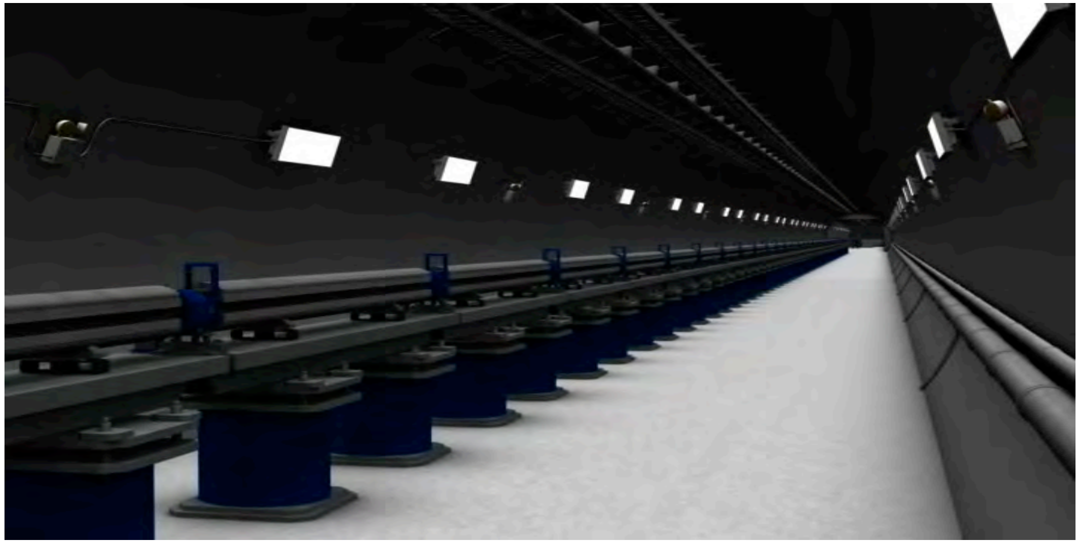


Capillary discharge at SPARC_LAB

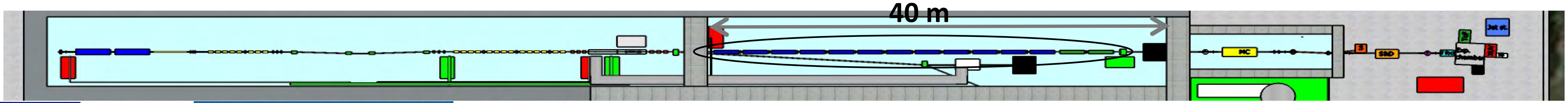


Undulators



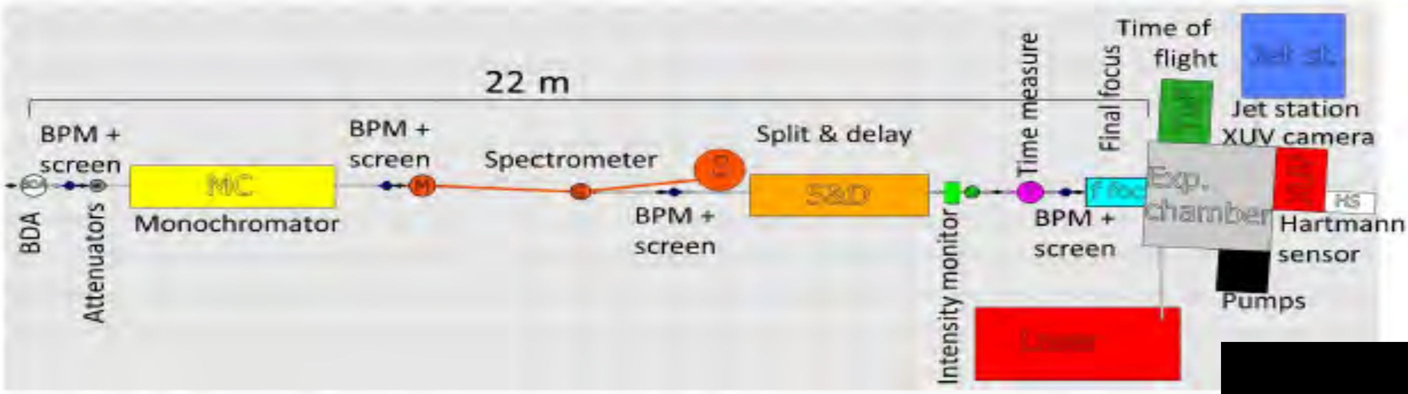


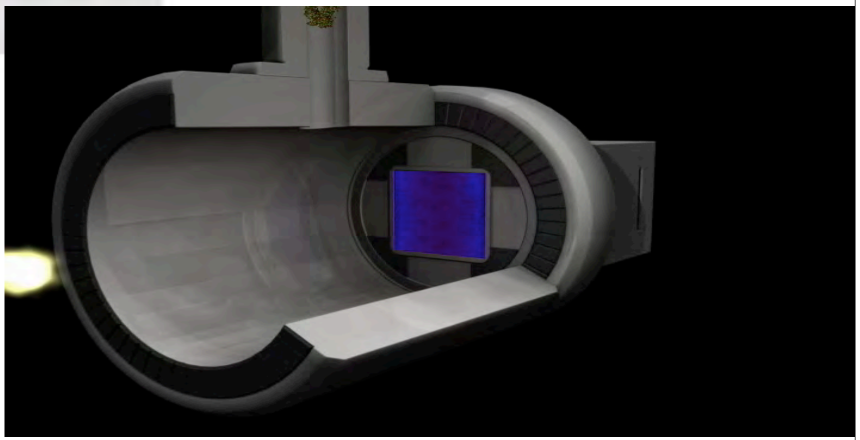
KYMA Δ udulator at SPARC_LAB: λ=1.4 cm, K1



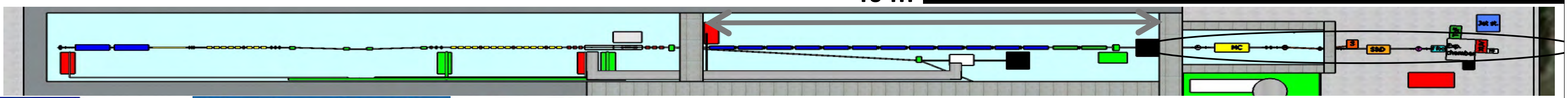
	Units	Full RF case	Plasma case
Electron Energy	GeV	1	1
Bunch Charge	pC	200	30
Peak Current	kA	2	3
RMS Energy Spread	%	0.1	1
RMS Bunch Length	fs	40	4
RMS matched Bunch Spot	µm	34	34
RMS norm. Emittance	µm	1	1
Slice length	µm	0.5	0.45
Slice Energy Spread	%	0.01	0.1
Slice norm. Emittance	µm	0.5	0.5
Undulator Period	mm	15	15
Undulator Strength K		1.03	1.03
Undulator Length	m	12	14
Gain Length	m	0.46	0.5
Pierce Parameterρ	x 10^{-3}	1.5	1.4
Radiation Wavelength	nm	3	3
Undulator matching β_u	m	4.5	4.5
Saturation Active Length	m	10	11
Saturation Power	GW	4	5.89
Energy per pulse	µJ	83.8	11.7
Photons per pulse	x 10^{11}	11	1.5

Photon beam line





40 m



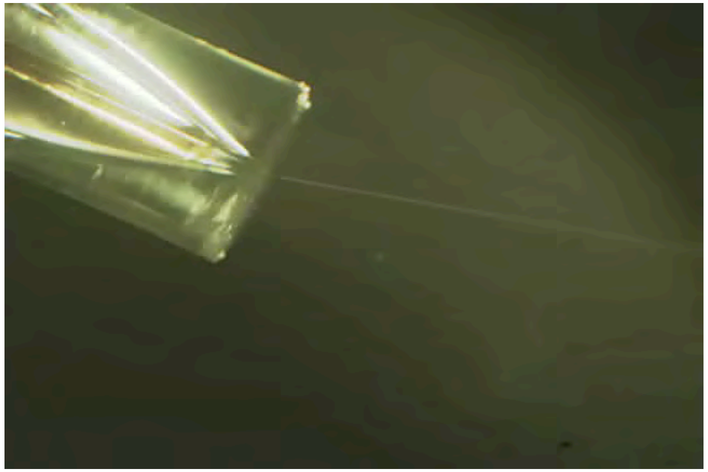
Water Window Coherent Imaging

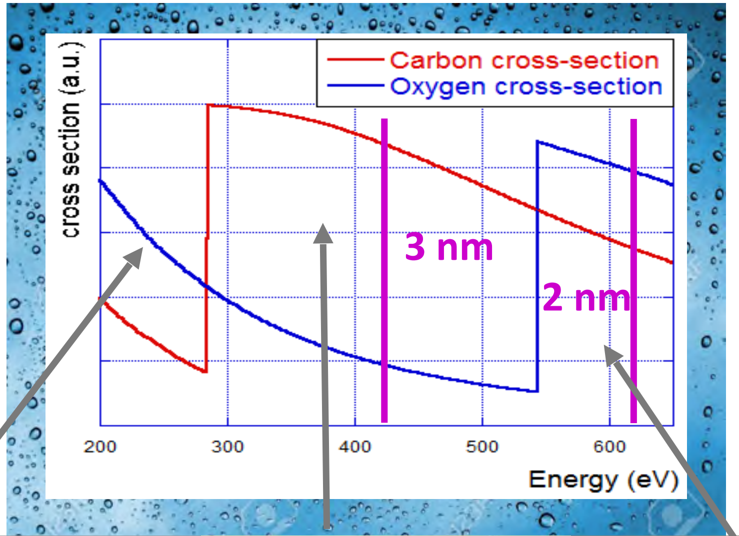
Energy region between oxygen and
carbon K-edge 2.34 nm – 4.4 nm (530 eV - 280 eV)

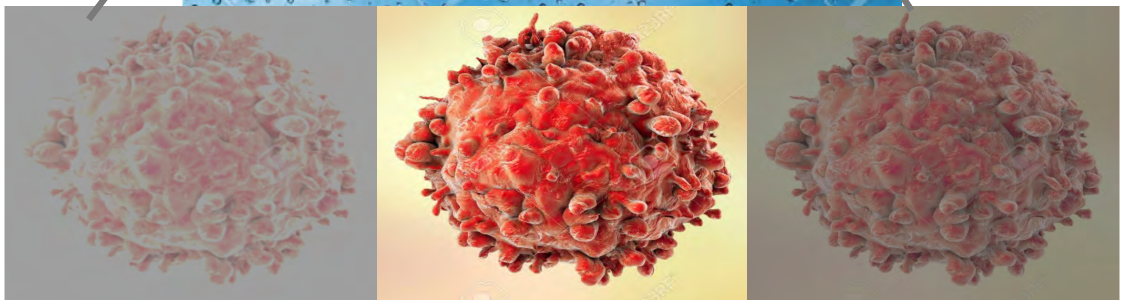
Water is almost transparent to radiation in this range while nitrogen and carbon are absorbing (and scattering).

Coherent Imaging of biological samples living in their native state.

Possibility to study dynamics







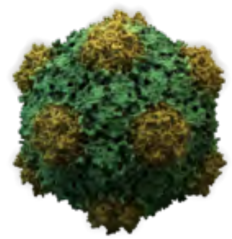
R&D perspectives

- X-band RF technology implementation → CompactLight => CERN collaboration
- Science with short wavelength Free Electron Laser (FEL)
- Physics with high power lasers and secondary particle source
- R&D on compact radiation sources for medical applications
- Detector development and test for X-ray FEL and HEP
- Science with THz radiation sources
- Nuclear photonics with γ-rays Compton sources
- R&D on polarised positron sources
- R&D in accelerator physics and industrial spin – off

The scientific case
one beamline, one class of experiments

Coherent Imaging Experiments

Biological samples (cells, viruses), nanomaterials, sooth, ashes



Seibert *et al* Nature (2011)
Single mimivirus particles intercepted and imaged with an X-ray laser.

Starodub *et al* Nature Communications (2012)
Single-particle structure determination by correlations of snapshot X-ray diffraction patterns.

Hantke *et al* Nature Photonics (2014)
High-throughput imaging of heterogeneous cell organelles with an X-ray laser.

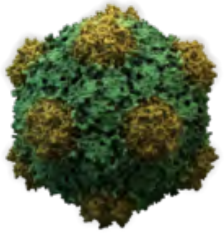
Van Der Schot *et al* Nature Communications (2014)
Imaging single cells in a beam of live cyanobacteria with an X-ray laser.

Ekeberg *et al* Physical Review Letters (2015)
Three-dimensional reconstruction of the giant mimivirus particle with an x-ray free-electron laser.

Reddy *et al* Scientific Data (2017)
Coherent soft X-ray diffraction imaging of coliphage PR772 at the Linac coherent light source.

Huang *et al* Nanoscale (2018)
Free-Electron-Laser Coherent Diffraction Images Individual Drug-Carrying Liposome Particles in Solution

The (extended) scientific case
Soft- and hard-matter science with a soft X-ray/EUV FEL

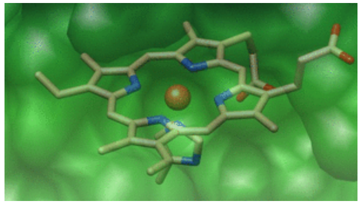


Coherent Imaging Experiments

  Biological samples (cells, viruses), nanomaterials

X-ray Absorption & Emission Experiments

  Metal compounds, semiconductors, biomolecules

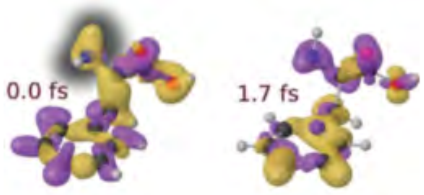


X-ray Raman experiments

  Biological molecules

FEL induced photofragmentation experiments

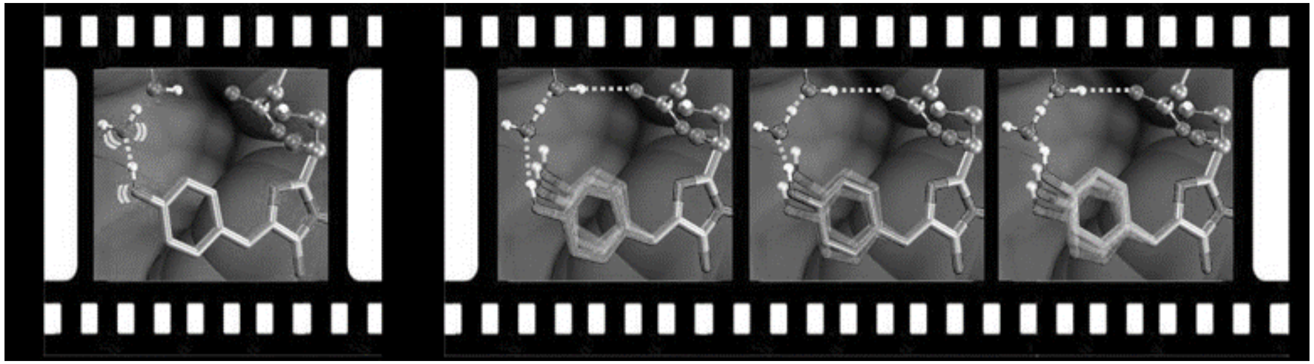
  Organic molecules



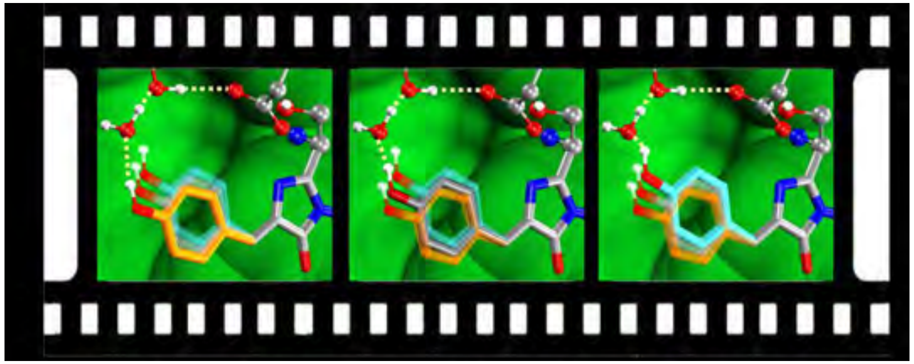
+ THz applications

A multi-dimensional molecular movie

PHOTOGRAPHY → MOVIE



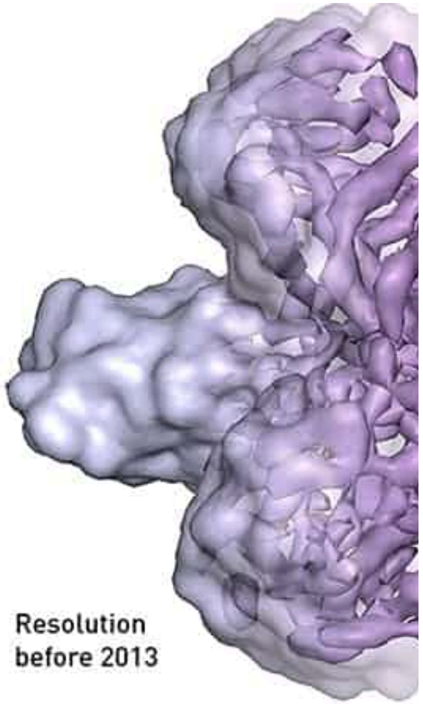
COLOUR MOVIE



Pump-probe, time resolved experiments add the time dimension to the static imaging

Spectroscopic techniques add information on chemical & electronic properties

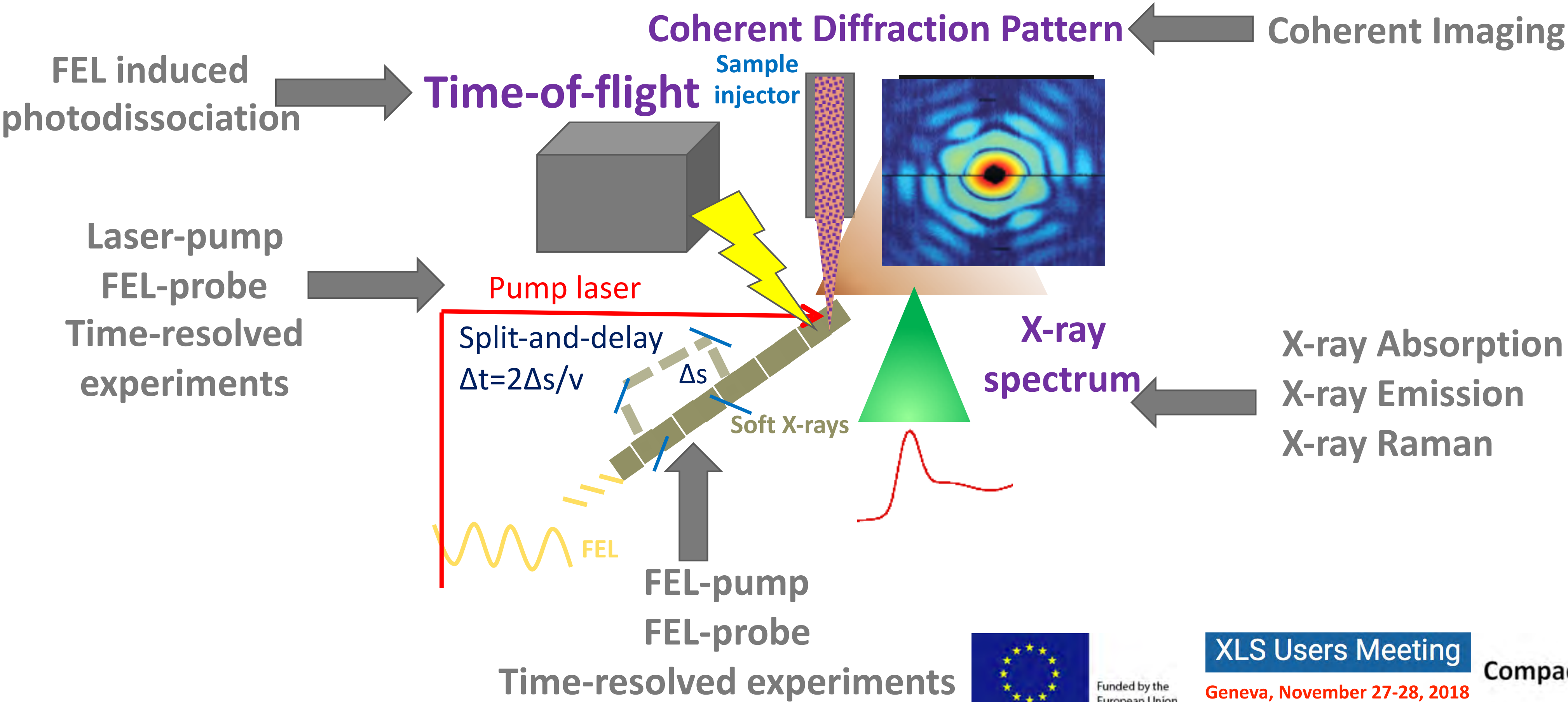
Nobel in Chemistry 2018



Jacques Dubochet, Joachim Frank and Richard Henderson received the prize for their part in developing cryo-electron microscopy (cryo-EM), a technique that fires beams of electrons at proteins that have been frozen in solution, to deduce the biomolecules' structure even in systems not suitable for X-ray crystallography.

The present

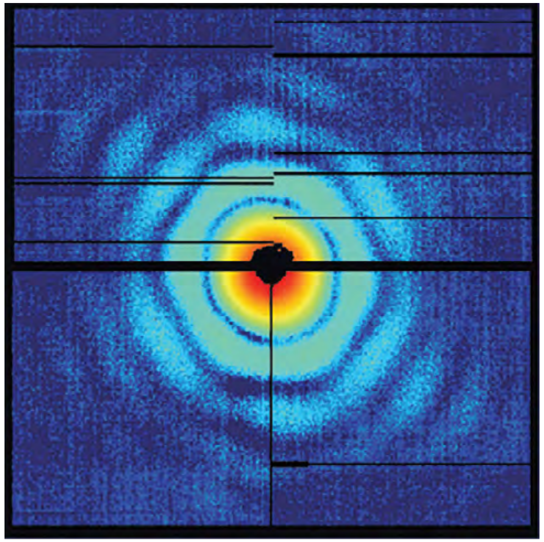
One beamline – Many classes of experiments



Coherent imaging

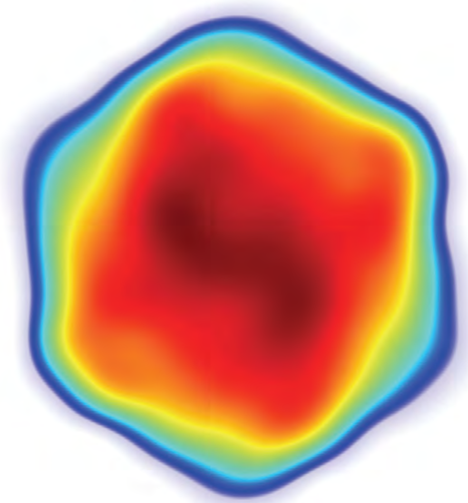
When the FEL photons hit the sample, a **diffraction pattern** is originated

The diffraction pattern is the |FT| of the sample electron density



Diffraction pattern
k - space

$|FT|^{-1}$



Sample image (electron density)
real space

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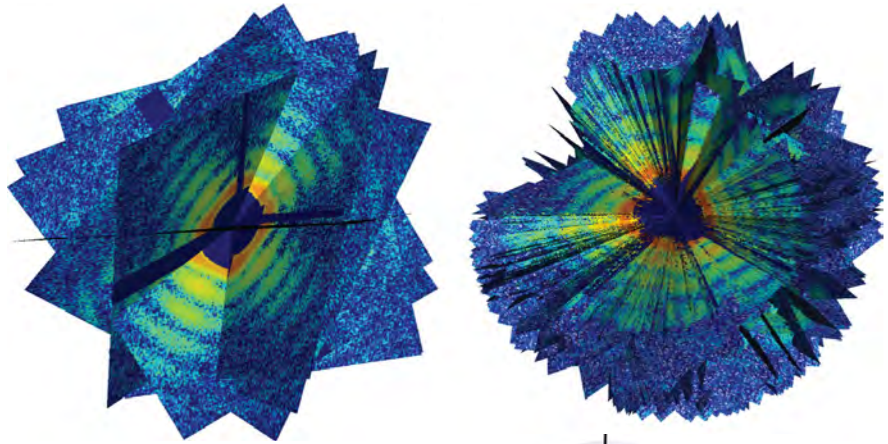
Coherent Imaging - Biosamples

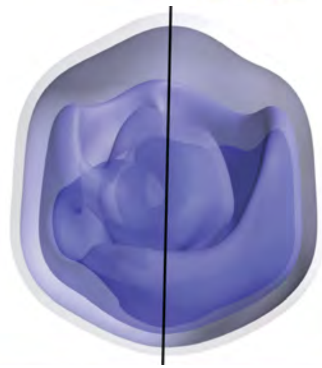
2D images can be obtained from a single shot

Cells, cell organelles
(e.g. nuclei, mitochondria, ribosomes)
viruses, protein aggregates



3D images can be obtained by merging info from several shots

Since the sample is destroyed by the
interaction with FEL photons,
many identical samples are needed



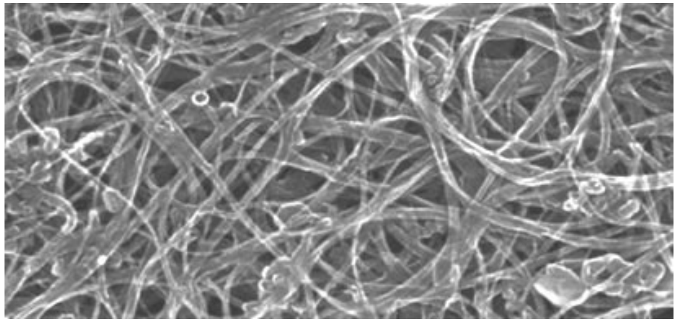
Viruses, protein fibrils, single protein molecules…

Van der Shoot, …, FS, et al., Nature Comm (2015)
Van der Shoot, …, FS, et al., Sci Data (2016)
Ekeberg et al., PRL (2015)

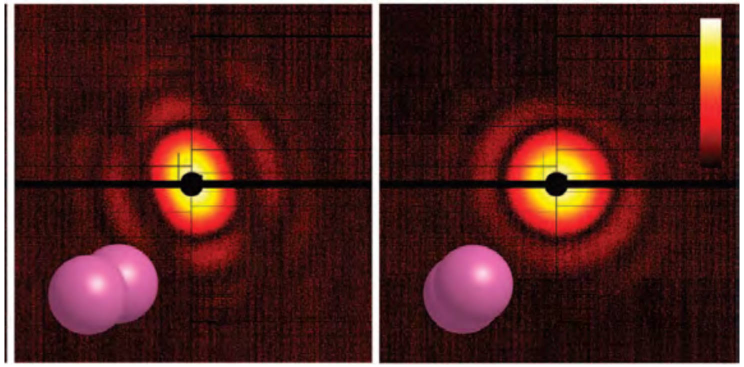
Coherent Imaging - Materials

Nanomaterials

Especially those significantly scattering in the EuPRAXIA@SPARCLAB energy range



Nanotubes
Nanoparticles
Soot (engines emissions)
Volcanic ashes



Statodub *et al.*, Nature comm (2012)

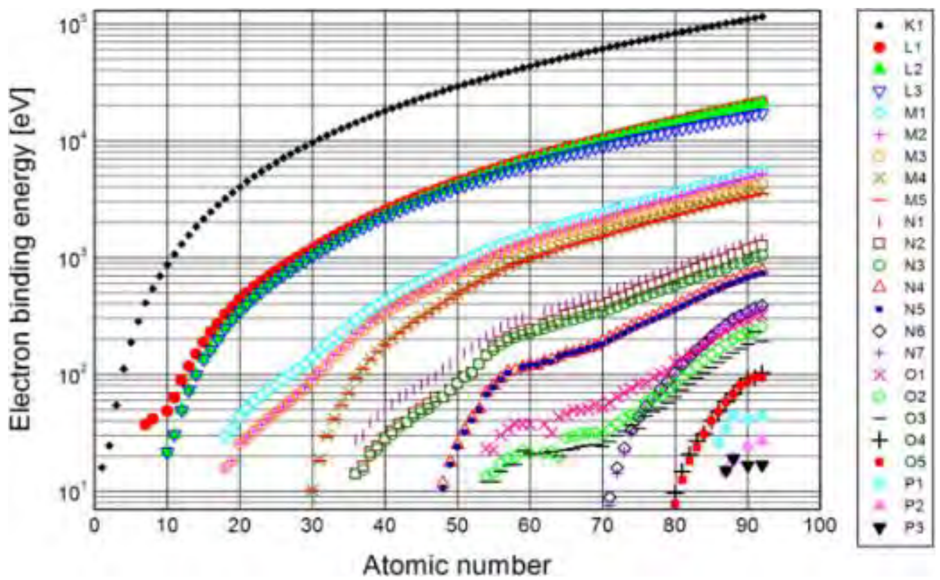
Technology development: photovoltaic, H storage
Biomedical applications: functionalized, bio-compatible materials

High time resolution pump-probe studies

X-ray Absorption & Emission

Transition metal L- and M-edge spectroscopy: ideal method to obtain detailed information on the electronic structure of a metal center.

Due to the large absorption cross sections at soft X-ray energies, the damage threshold is much lower than at hard X-ray energies and it is practically impossible to collect undamaged M- and L-edge spectra from diluted metal complexes in aqueous solution under ambient condition at SR sources.



FEL «scatter & destroy» experiments can overcome the radiation damage problem

A. Balerna & Co. @ LNF

A. Di Cicco & Co. @ Camerino

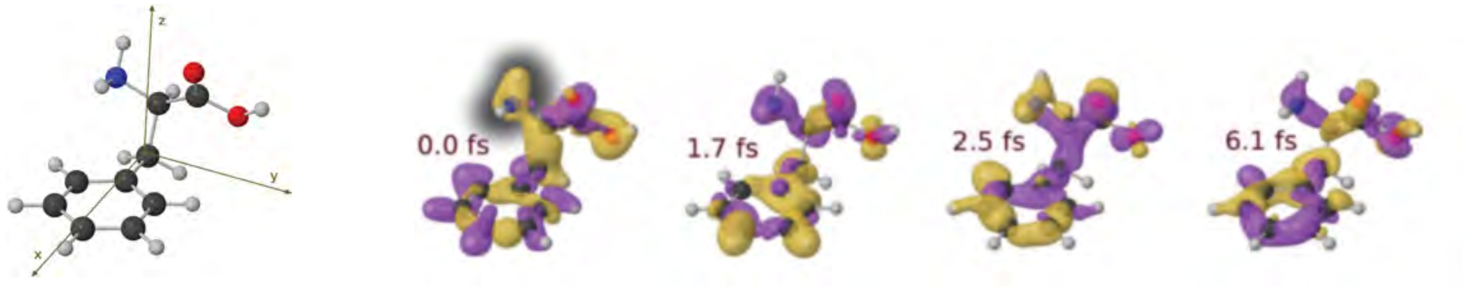
Photo-fragmentation of molecules

SCIENTIFIC GOAL

Photo-protection or photo-damage of biomolecules

FEL (or laser) pulse can be used to break molecules in controlled ways

Time-resolved, time-of-flight fragment abundance allow getting dynamic information on the excited states of the molecules and *viceversa*



Phenylalanine electron dynamics
Science **346**, 336 (2014)

RELEVANCE

Photo-protection or photo-damage of biomolecules

Potential relevance in diagnostic, radiotherapy etc

Ultrafast electron dynamics in biological molecules initiated by a core ionisation

STATE OF THE ART

Photofragmentation chronoscopy

to study valence motion initiated by valence-shell ionisation due to a XUV pulse - *Science 346, 336 (2014)*

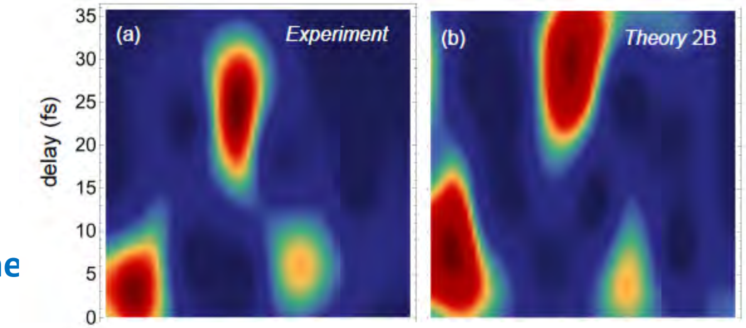
Transient photoabsorption spectroscopy

to study valence motion initiated by valence-shell ionisation due to a NIR pulse - *Nature 466, 739 (2010)*

Core ionisation (theory & experiments) are still missing !! Imaging is still in its infancy

Coherent Imaging

to directly observe the electron density – *PRL (2018????)*



A possible way to describe ab initio the core ionisation

THEORY @ Tor Vergata (G. Stefanucci, E. Perfetto)

"Charge migration in XUV photoexcited phenylalanine: a first-principles real-time Green's function study", J. Chem. Phys. Lett. 9, 1353 (2018)

"Real-time dynamics of Auger wave packets and decays in ultrafast charge migration processes", Phys. Rev. A 97, 061401(R) (2018)

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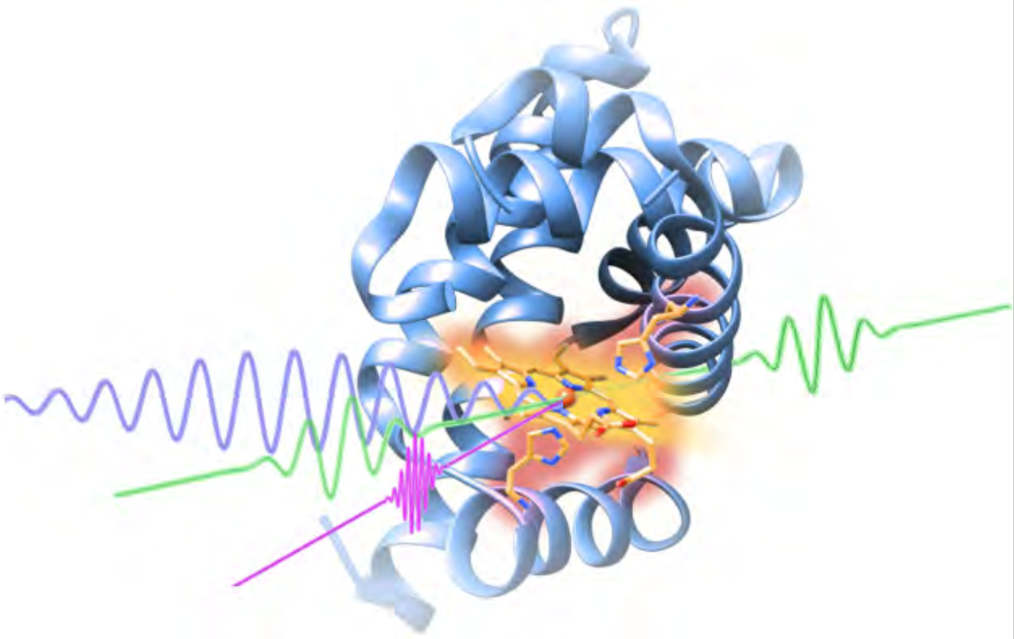
X-ray Raman + Resonant Inelastic Scattering

X-ray Raman scattering (XRS) is the scattering of X-rays from core electrons. It is analogous to Raman scattering, which is a widely used tool in optical spectroscopy, with the difference being that the wavelengths of the exciting photons fall in the X-ray regime and the corresponding excitations are from deep core electrons.



T. Scopigno & coworkers
@ La Sapienza

XRS is an element-specific spectroscopic tool for studying the electronic structure of matter. In particular, it probes the excited-state density of states (DOS) of an atomic species in a sample, including biological ones such as proteins.

J. Sanchez
@ Cordoba University

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Conclusions

Several experimental techniques
A variety of samples
Coherent imaging
Nanoparticles, cells, viruses, soot
X-ray spectroscopies
Proteins, metals, semiconductors
X-ray Raman, RIXS
Proteins, liquids, magnetic materials
Photo-fragemntation
Organic molecules

We are submitting a manuscript on a special issue of «Condensed Matter» with a description of the scientific case

I Science with Free Electron Laser

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Parameters	Expected values
Radiation wavelength	2.8 nm
Photons per pulse	> 10^{11}
Pulse length (FWHM)	10-50 fs
Repetition rate	10 Hz
Bandwidth (FWHM)	<1 %

1) Extend the range is always useful, open new spectroscopic possibilities, but for the water window nothing change.

2) Going to $10^{12} – 10^{13}$ ….. is nice. In principle we can go even to higher flux still destroying the sample, but in this way we have the possibility to increase the S/N.

3) At present this scientific case does not requires shorter PL, but photo-fragmentation experiments may exploit shorter PL with benefit.

4) Repetition – higher for sure. Continuous ? Detectors are not able to sustain rates > kHz.

5) For spectroscopy this is ok. Improve a factor 3-4 will be certainly useful for many experiments.

6) Variable polarization (linear & circular).

All parameters can be improved taking care the stability of the photon beam in term of spatial position and energy.
Spatial stability is a difficult issue to measure: we may propose few % at the exit of the undulators.

Brilliance (photons/mm^2/$mrad^2$/0.1% bw)

Outside and inside rendering

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XLS Users Meeting

Experimental hall

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Geneva, November 27-28, 2018

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dadu DIPARTIMENTO DI ARCHITETTURA, DESIGN E URBANISTICA

University of Sassari
Department of Architecture, Design and Urban planning_DADU

Team
Prof. Arch. Massimo Faiferri faiferri@uniss.it
Arch. Samanta Bartocci sbartocci@uniss.it
Arch. Fabrizio Pusceddu fapusceddu@uniss.it
Arch. Rosa Manca mancarosa@yahoo.it

EuSPARC

Urban and architectural design

People & Institutions

A. Balerna
G. Batignani
E. Chiadroni
D. Cirrincione
F. Cometto
M. Coreno
A. Cricenti
S. Dabagov
E. De Santis
A. Di Cicco
C. Ferrante
G. Fumero
L. Giannessi
R. Gunnella
A. Irizawa
J.J. Leani
S. Lupi
C. Masciovecchio
A. Marcelli
A. Minicucci
S. Morante
E. Perfetto
S.J. Rezvani
A. Ricci
J. Robledo
M. Rubio
H.J. Sanchez
V. Sbarato
T. Scopigno
G. Stefanucci
F. Stellato
A. Trapananti
A. Vacchi
F. Villa

34 researchers

12 institutions

CNR - Istituto Struttura della Materia
Elettra - Sincrotrone Trieste
Istituto Nazionale di Fisica Nucleare
Istituto Italiano di Tecnologia
Argentinian Scientific and Technical Research Council
RICMASS - Rome
Roma La Sapienza University
Roma Tor Vergata University
Camerino University
Cordoba University
Udine University
Osaka University