EuPRAXIA@SPARC_LAB

Scientific Case

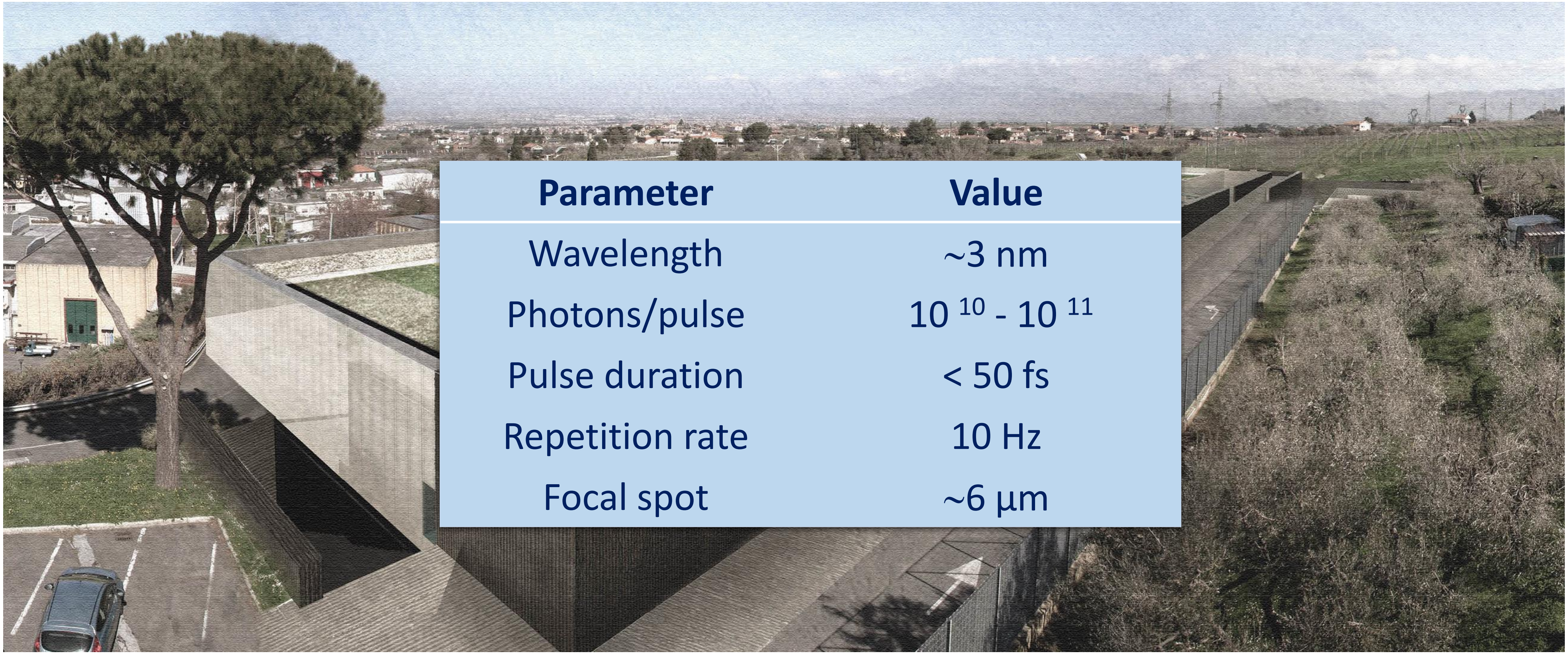
Francesco Stellato

University of Rome Tor Vergata & INFN

on behalf of the WA8 collaboration team

February 22nd, 2021

EuPRAXIA@SPARC_LAB – Where we are



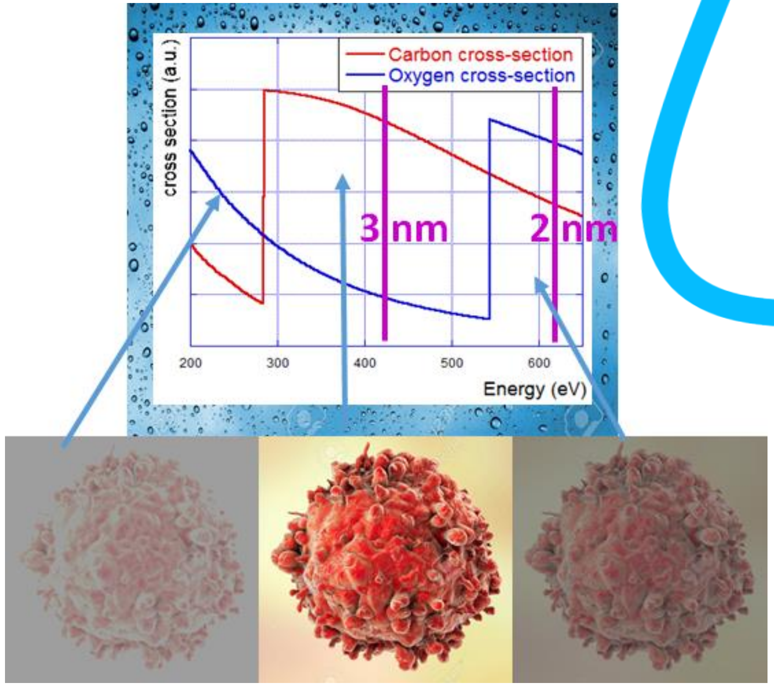
Parameter	Value
Wavelength	~3 nm
Photons/pulse	10^{10} - 10^{11}
Pulse duration	< 50 fs
Repetition rate	10 Hz
Focal spot	~6 µm

EuPRAXIA@SPARC_LAB conceptual design report
Ferrario *et al.* Nucl. Instr. Met. (2018)
Villa *et al.* Nucl. Instr. Met. (2018)

CDR Scientific case

A scientific case @ 3 nm
«ACQUA»
has been assembled and published.

Contributions from ~15 different institutions



Article

MDPI

The potential of EuPRAXIA@SPARC_LAB for radiation based techniques

Antonella Balerna[1], Samanta Bartocci[2], Giovanni Batignani[3], Alessandro Cianchi[4,5], Enrica Chiadroni[1], Marcello Coreno[1,6], Antonio Cricenti[6], Sultan Dabagov[1,7,8], Andrea Di Cicco[9], Massimo Faiferri [2], Carino Ferrante[3,10], Massimo Ferrario[1], Giuseppe Fumero[3,11], Luca Giannessi[12,13], Roberto Gunnella[9], Juan José Leani[14], Stefano Lupi[3,15], Salvatore Macis[4,5], Rosa Manca[2], Augusto Marcelli[1,6], Claudio Masciovecchio[12], Marco Minicucci[9], Silvia Morante[4,5], Enrico Perfetto[4,16], Massimo Petrarca[3,15], Fabrizio Pusceddu[2], Javad Rezvani[1], José Ignacio Robledo[14] , Giancarlo Rossi[4,5,17], Héctor Jorge Sánchez[14,18], Tullio Scopigno[3,10], Gianluca Stefanucci[4,5], Francesco Stellato[5], Angela Trapananti[9], and Fabio Villa[1]

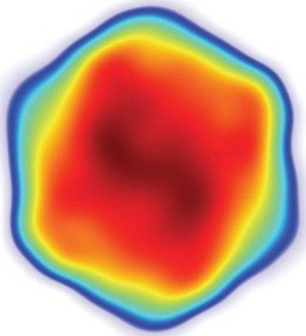
Balerna *et al.* Condensed Matter 4, 30 (2019)

Water-window: 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)

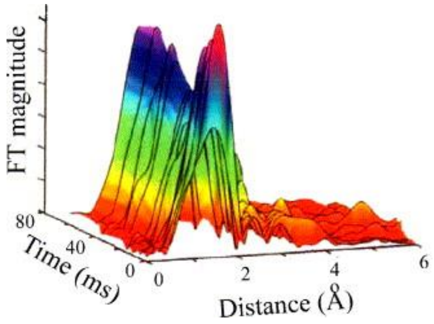
ACQUA - Techniques & Samples @ 3 nm

Experimental techniques and typology of samples

Coherent imaging



X-ray absorption spectroscopy



Raman spectroscopy

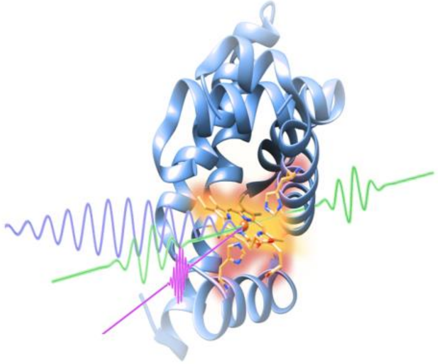
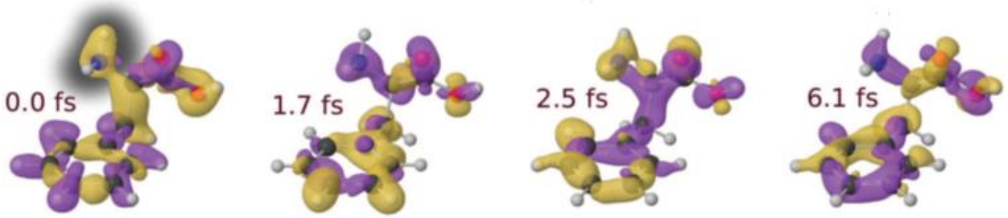
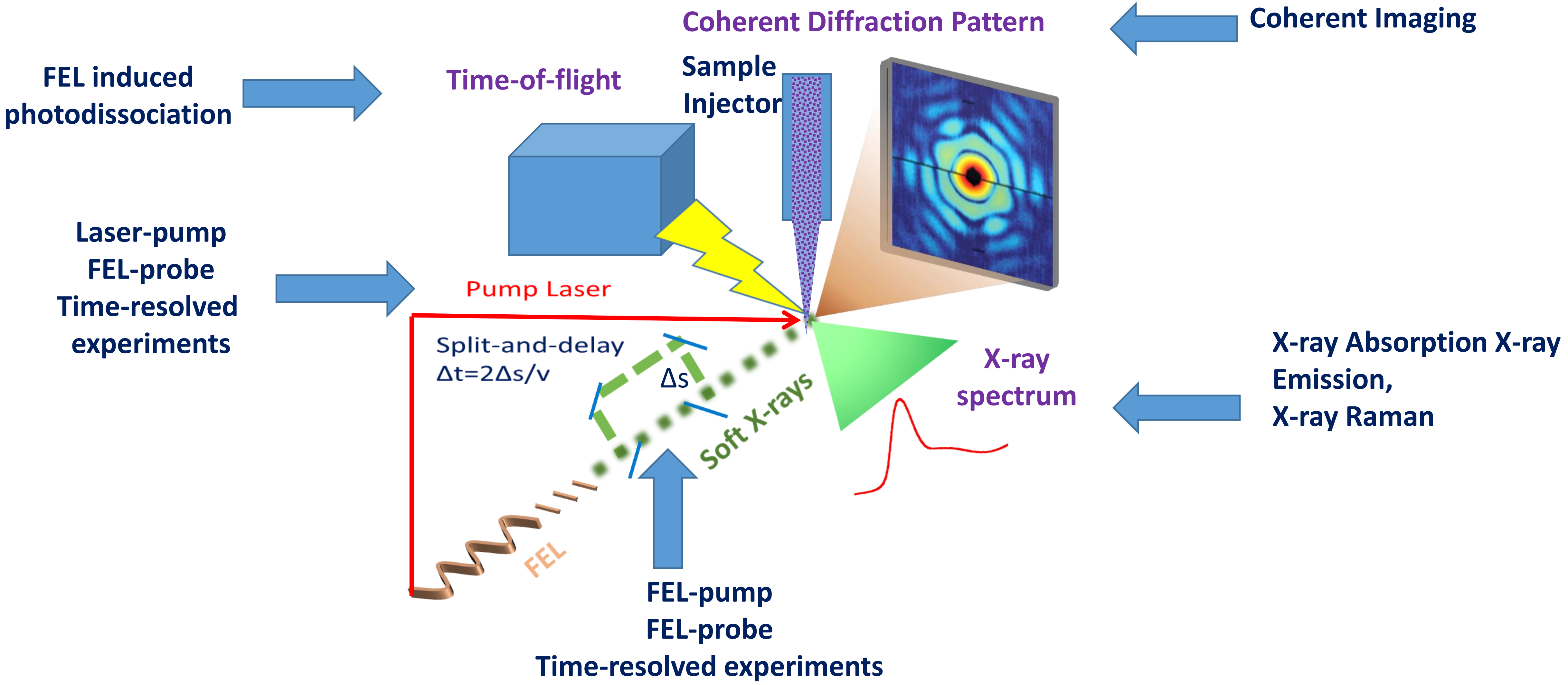


Photo-fragmentation of molecules



Proteins
Viruses
Bacteria
Cells
Metals
Semiconductors
Superconductors
Magnetic materials
Organic molecules

ACQUA - Techniques & Samples @ 3 nm



EuPRAXIA@SPARC_LAB –
Where we might go (beyond the baseline)

Parameter	Value
Wavelength	~3 nm
Photons/pulse	10^{10} - 10^{11}
Pulse duration	< 50 fs
Repetition rate	10 Hz
Focal spot	~6 µm

+

Parameter	Value
Wavelength	50-180 nm
Photons/pulse	10^{13} - 10^{14}
Pulse duration	20/200 fs
Repetition rate	10 Hz
Focal spot	~6 µm

Not only brilliance:
Seeded FEL, Polarization, first and second order coherence (i.e. stability and reproducibility in terms of pulse & photon energy), multiple colors and multiple pulses schemes, phase control

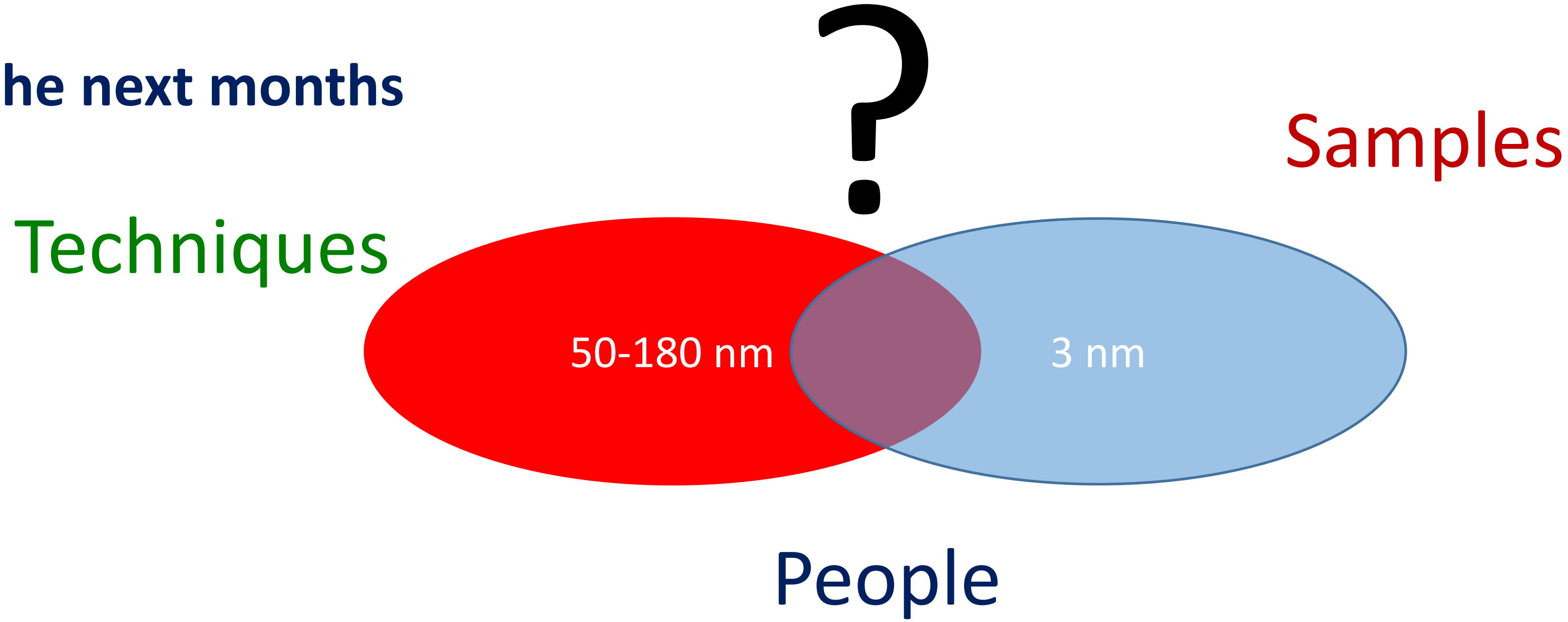
Adding a different wavelength range would open up (new) interesting scientific possibilities.

ARIA - Techniques & Samples @ 50-180 nm

A scientific case for ARIA, in the DUV (DeepUV) and VUV (VacuumUV) is (and was) there
COLLABORATIVE RESEARCH FOR A HIGH-RESOLUTION VUV FREE ELECTRON LASER USER FACILITY AT SPARC (LNF 2011)
(complementary with FEL1 @ Fermi)

Experimental techniques and typology of samples

to be detailed in the next months



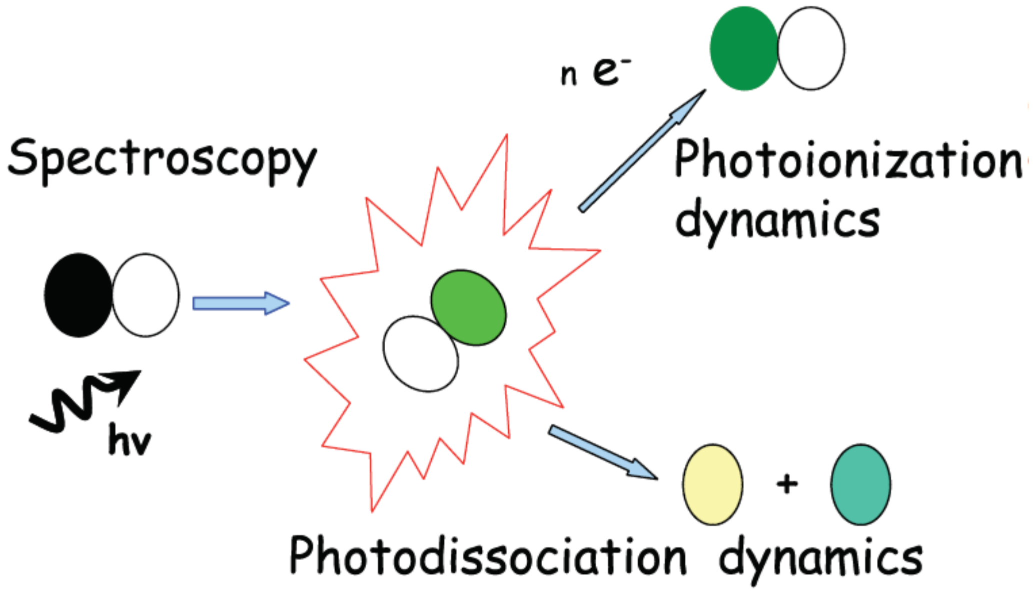
ARIA - Techniques & Samples @ 50-180 nm

Defining experimental techniques and typology of samples (and applications)

Photoemission Spectroscopy

Raman spectroscopy

Photo-fragmentation of molecules
Time of Flight Spectroscopy



Gas phase & Atmosphere (Earth & Planets)
Aerosols (Pollution, nanoparticles)
Molecules & gases (spectroscopies, time-of-flight)
Proteins (spectroscopies)
Surfaces (ablation e deposition)

ARIA - Techniques & Samples @ 50-180 nm

λ FEL (Fermi) = 64 nm

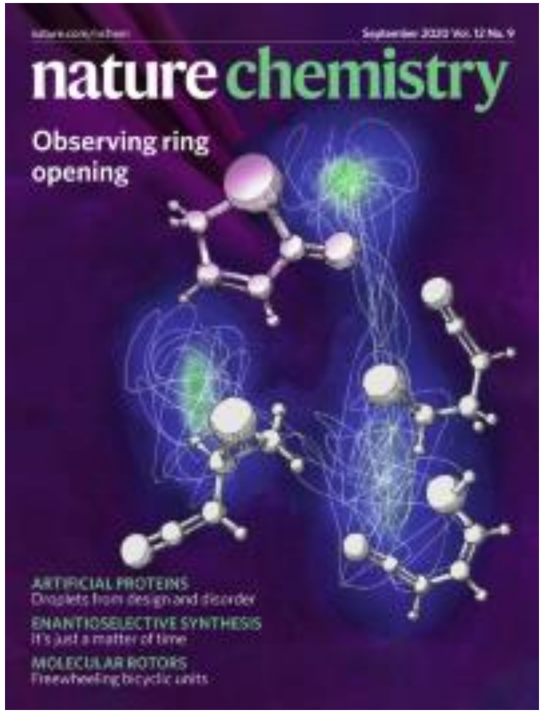
Some recent applications

Circularly polarized XUV FEL light on 1T-$TiSe_2$ while cooling it below the critical temperature results in preferential formation of one chiral domain.

Xu *et al.* Nature 2020

Observing ring opening in organic molecules

Light-induced ring-opening/closing reactions can be studied by Time-Resolved Photoemission Spectroscopy



Initial thiophenone hit by a laser and its photoproducts, with the white lines follow the smoothed paths of reaction trajectories.

Pathak *et al.* Nature Chemistry 2020

ARIA - Techniques & Samples @ 50-180 nm

A theoretical look at future applications

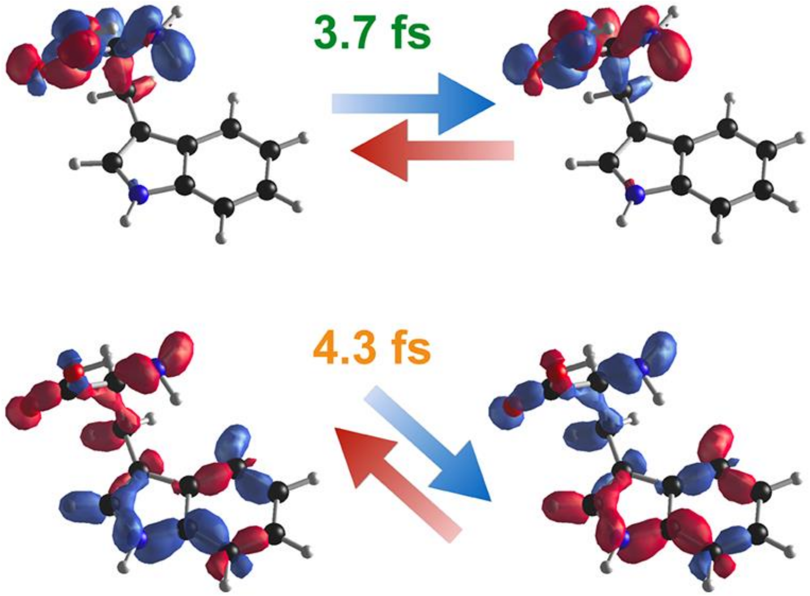
Ultrafast Quantum Interference in the Charge Migration of Tryptophan

→

TD-PES Theory

At present, 4 fs visible/near-infrared (VIS/NIR) probe pulses, in combination with mass spectroscopy

Interest to explore VIS/IR pump + high intensity UV probe



2020: Ultrafast Quantum Interference in the Charge Migration of Tryptophan. *The journal of physical chemistry letters*, *11*(3), 891-899.

ARIA - Coupling of Low-Energy Degrees of Freedom with High-Energy Excitations

When electrons are excited by a pump pulse in VIS/UV their relaxation **usually** implies the excitation of many low energy modes: Phonons, Intermolecular Vibrations, and Spin Degrees of Freedom that could be measured through a Terahertz/Infrared probe.

On the contrary, the modulation of high-energy modes through the effective excitation of low-energy degrees of freedom is rather unusual and scarcely investigated.

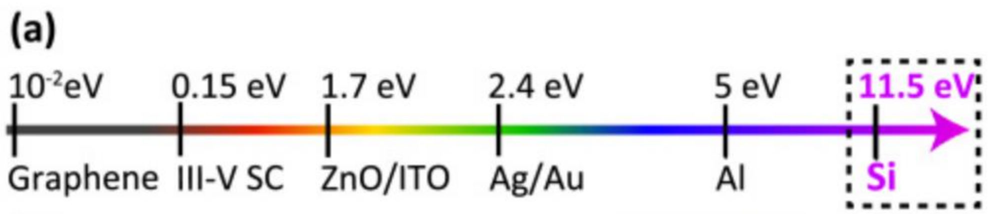
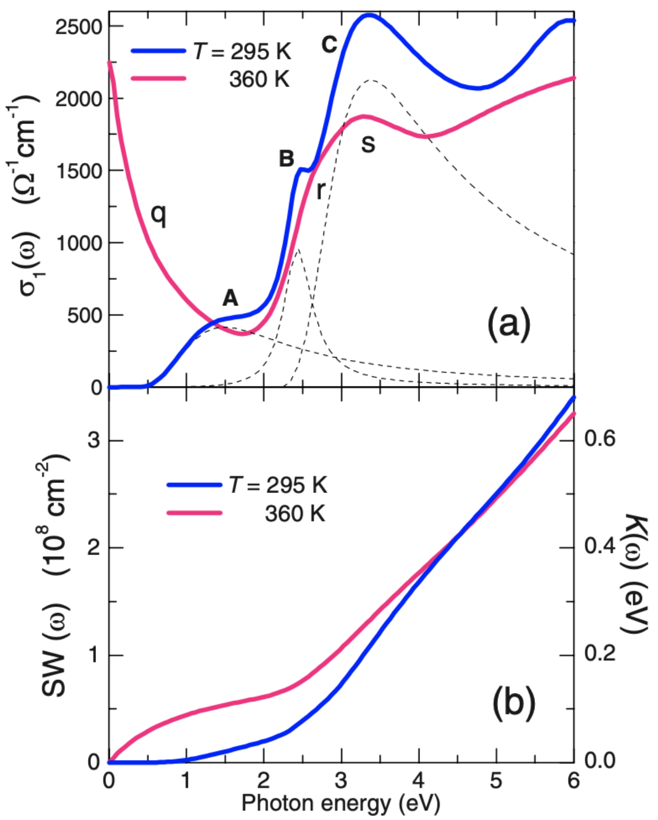


Fig.1 Localized Plasmon Excitations

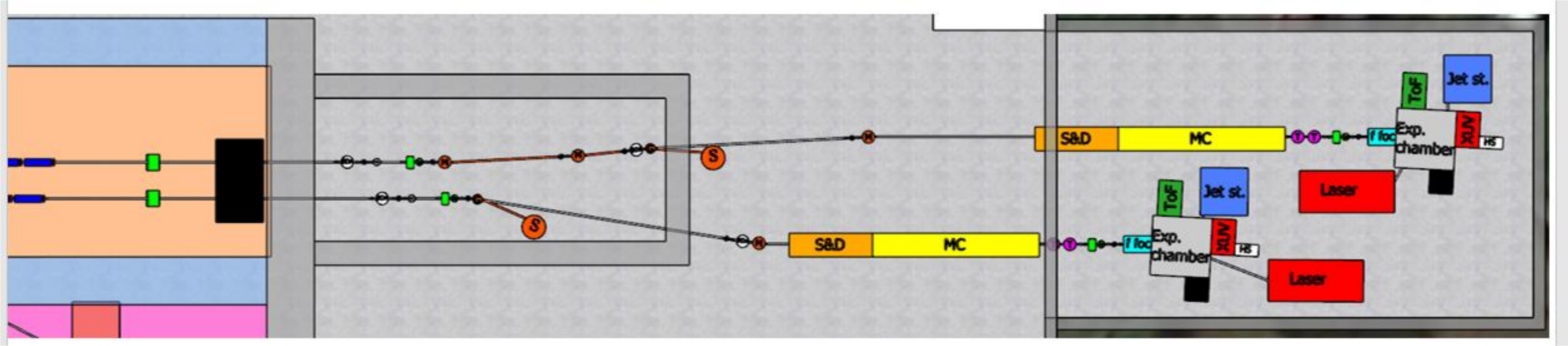
In dielectric nanoparticles decorated with metals, plasmon modes can be controlled and tuned through the excitations of dielectric phonons.



The Insulator-to-Metal Transition in many strongly correlated systems implies a strong coupling among low and high energy degrees of freedom. This is the case of VO_2 (Fig.2) and V_2O_3.

S. Lupi et al, Nature Comm. 2010

Beamlines @ 3 nm (& 50-180 nm)



Courtesy of Fabio Villa

Simple calculations confirm that there is sufficient space for hosting two beamlines. The deflection angle is actually larger for the long wavelengths and would allow a better lateral separation.

Photon & Users Beamline(s)
Intermediate Deliverables on the road to the TDR

AQUA – Photon beamline @ 3 nm (baseline)

- Photon transport study and simulations (COMSOL & ZEMAX) up to the user endstation
- Study and design of each beamline component and diagnostic (some with prototypes *):
  - Beam Defining Apertures
  - Beam Position Monitors
  - Beam Arrival Time Monitor (*)
  - Longitudinal Dimension (*)
  - Transverse Dimensions
  - Longitudinal Coherence (*)
  - Transverse Coherence (*)
  - Intensity Monitors
  - Attenuators (*)
  - Spectrometer
  - Wavefront
  - Monochromator (*)
  - Beam Polarization (*)
  - Split & Delay Line
  - Optical Transport (mirrors) (*)

ARIA – Photon beamline @ 50-180 nm (beyond the baseline)

- Photon transport study and simulation up to the user endstation
- Study and design of each beamline component and diagnostic

Scientific Case & Endstation(s)
Intermediate Deliverables on the road to the TDR

AQUA - Scientific case @ 3 nm

- User Science: fine tuning of samples & techniques
- Details of instrumentation (detector, sample delivery) for the experimental endstation @ 3 nm at a TDR level

ARIA - New perspectives @ 50-180 nm

- User Science: definition samples & techniques
- Users' community commitment
- Evaluation of instrumentation for the experimental endstation @ 50-200 nm from scratch to a TDR level

AQUA + ARIA

- Connections with correlated services (lasers and THz)
- Detailed costs evaluation

External Radiation Sources

Time-resolved pump-probe experiments require (besides split&delay) coupling to an **external radiation sources** :

Two **laser** options are being explored and will be detailed in the TDR:

1- **Tunable**, for the experiments requiring an intensity of the order of few TW (e.g. Ti:sapphire)

2- **High-power** laser (FLAME or FLAME-like, hundreds of TW)

THz setup will also be detailed in the TDR

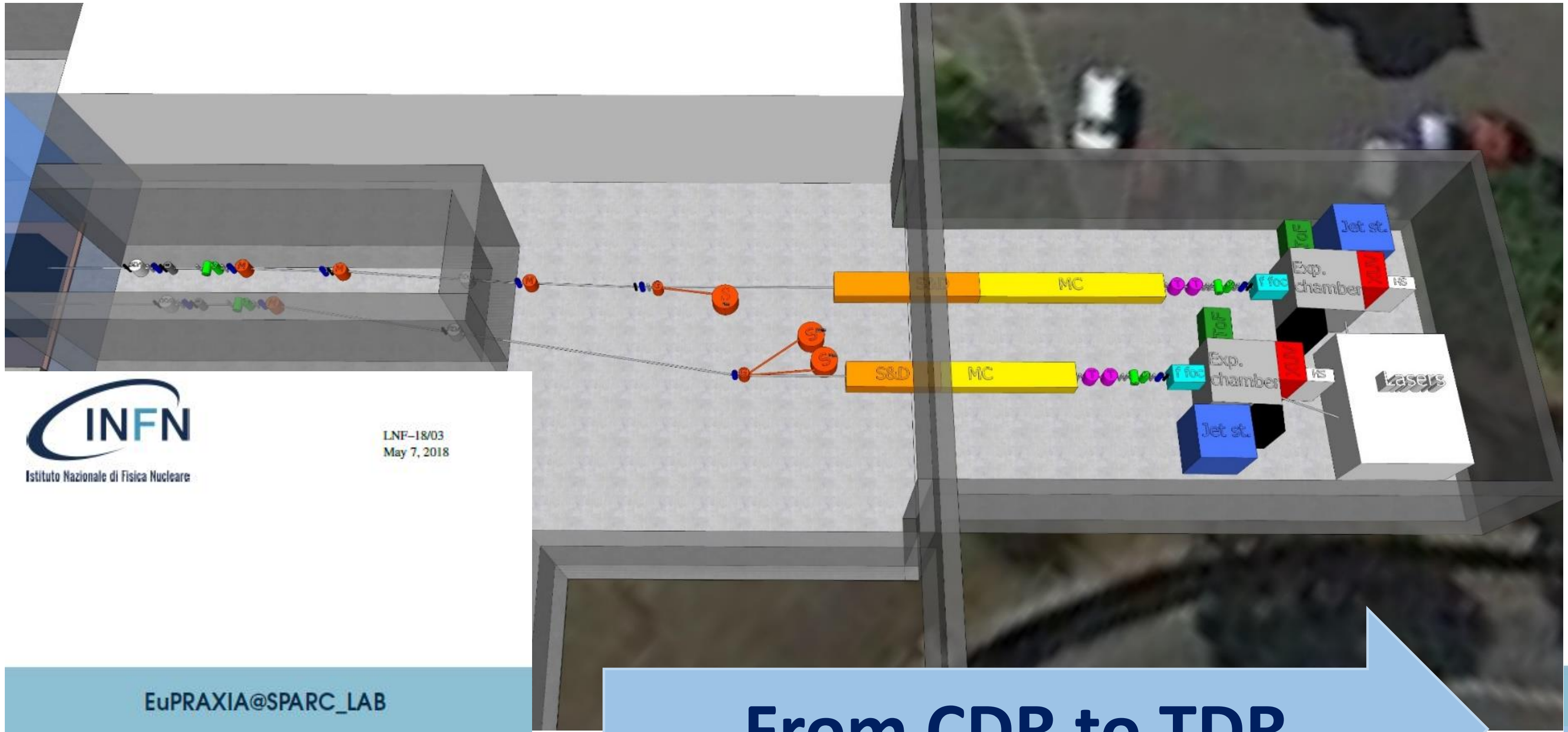
Timescale

Year 1
Inputs from (and to) FEL group
Inputs from (and to) laser group
Preliminary Beam transport & Optical elements simulations

Year 2
Optical elements & detectors (0D, 2D, ions) R&D
Beam transport & Optical elements simulations

Year 3
Beam transport & Optical elements design
Preliminary optical elements & detector tests @ other facilities
Sample delivery R&D
Mechanical components design

Bringing this picture from CDR to TDR level

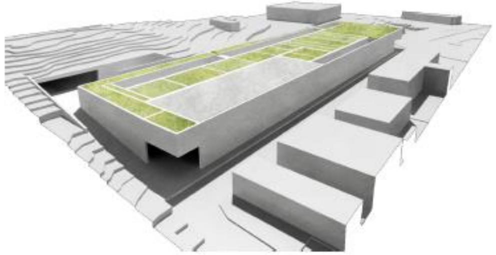


INFN
Istituto Nazionale di Fisica Nucleare

LNF–18/03
May 7, 2018

EuPRAXIA@SPARC_LAB

Conceptual Design Report



From CDR to TDR

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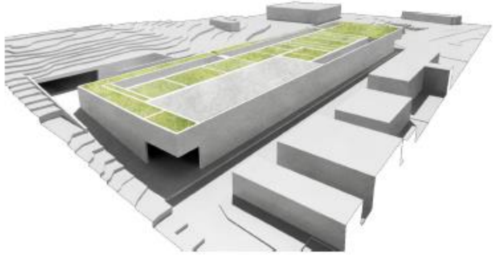
Technical Design Report



Thanks for the attention

Questions and comments are
(and will be)
more than welcome