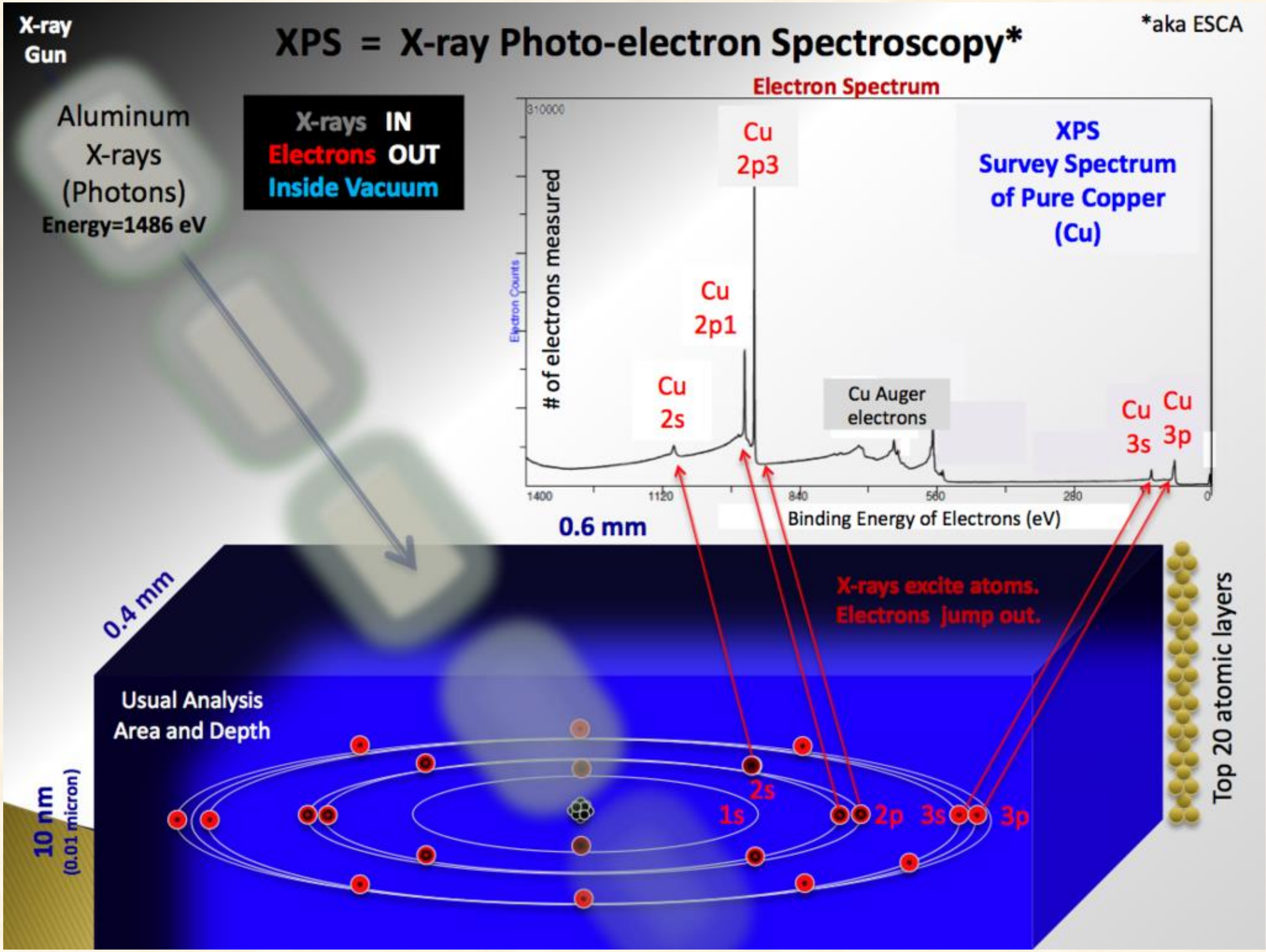
Towards Ångström Laser @ FREIA

I. XPS jouney & X-ray technology
II. Bringing X-ray laser to a lab
III. A taste of fs XPS science

Vitaliy Goryashko
on behalf of FREIA

2021, UU

X-ray Photo-electron Spectroscopy (XPS)



Wikipedia

XPS from the historical Swedish perspective

- Nobel Prize 1924, Manne Siegbahn "for his discoveries and research in the field of **X-ray spectroscopy**."

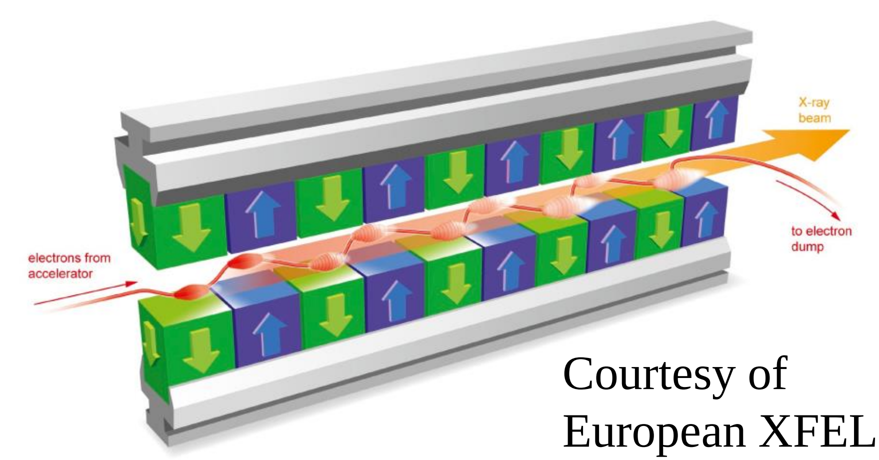
"*Siegbahn has in the course of ten years' assiduous and systematic labour devised a series of improvements and new designs dealing with almost every detail of the various apparatus and so constantly increased the exactitude of his measurements*"

- Nobel Prize 1981, Kai M. Siegbahn "for his contribution to the development of **high-resolution electron spectroscopy**."

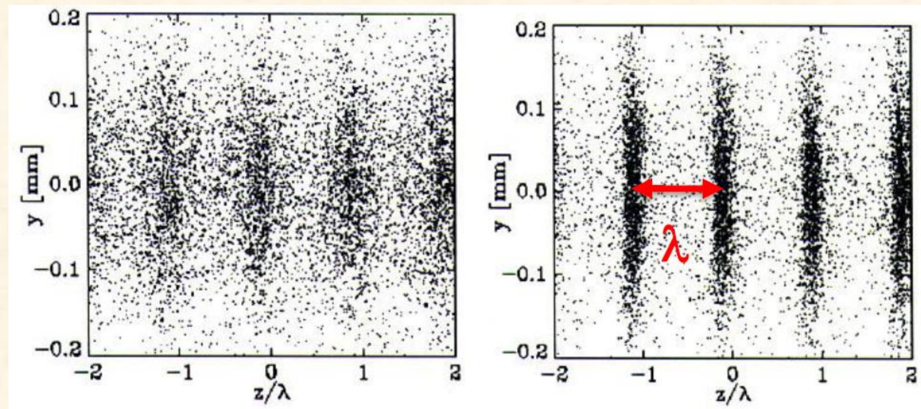
"*The decisive step at that time was taken when Kai Siegbahn together with his co-workers began to analyse photo-electrons with the aid of a high-resolution, double-focusing spectrometer*."

XPS nowadays

S.Neppl at all, J. of Electron Spectroscopy, vol. 200, April 2015, Pages 64

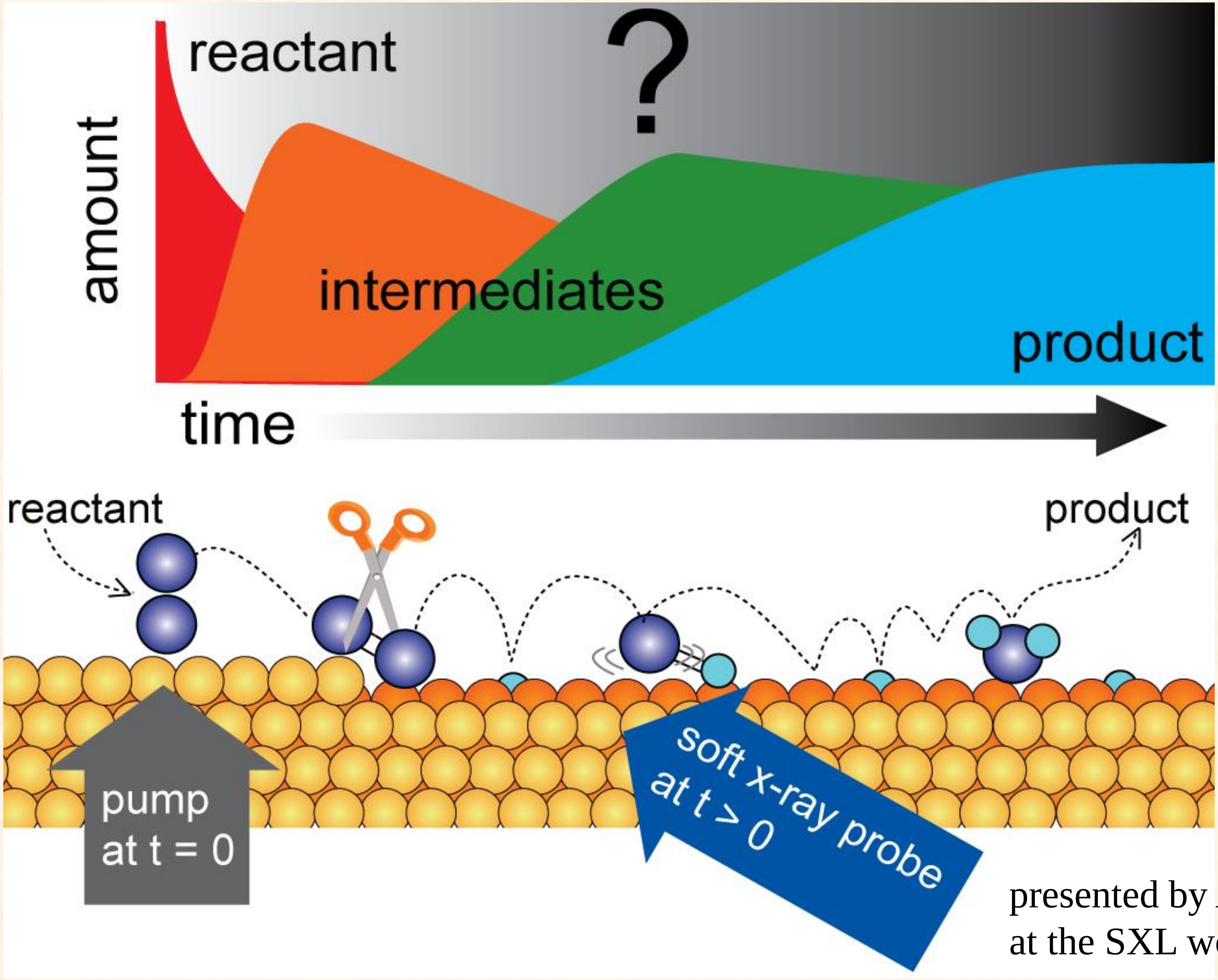


Courtesy of European XFEL



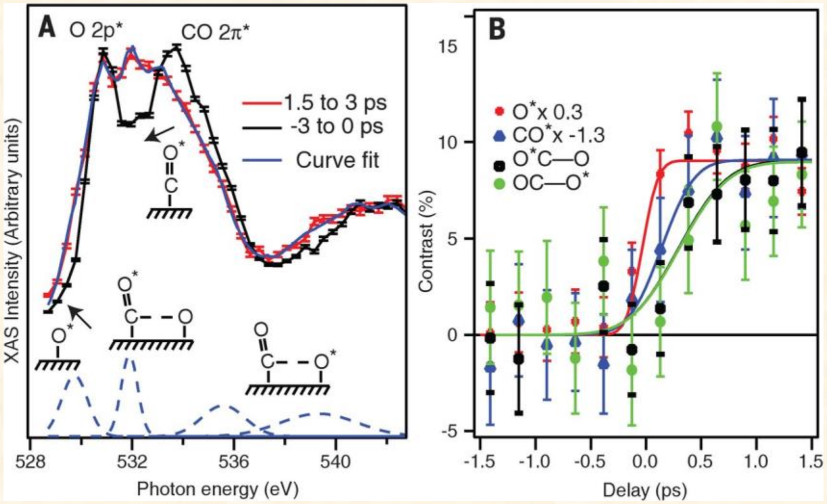
Radiation intensity $\propto N^2$

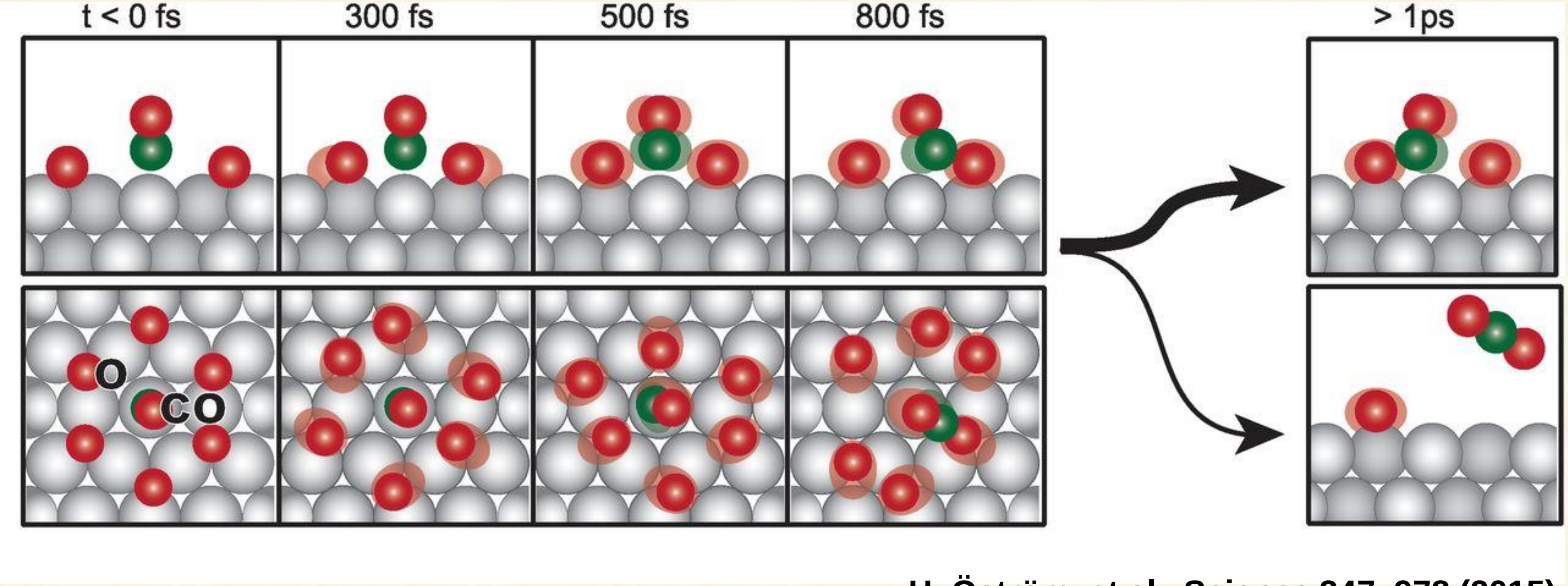
Probing Transition States in Surface Reactions



presented by A.Nilsson
at the SXL workshop

Transition state region in catalytic CO oxidation on Ru





H. Öström, et al., Science 347, 978 (2015)

Technological revolution in X-ray generation

Some historical remarks: 1944-1945

On the Maximal Energy Attainable in a Betatron

D. Iwanenko and I. Pomeranchuk
Phys. Rev. **65**, 343 – Published 1 June 1944

$$-(dE/dX) = 2/3(e^2/mc^2)^2(EH/mc^2)^2.$$

On Radiation by Electrons in a Betatron

J. Schwinger

1945

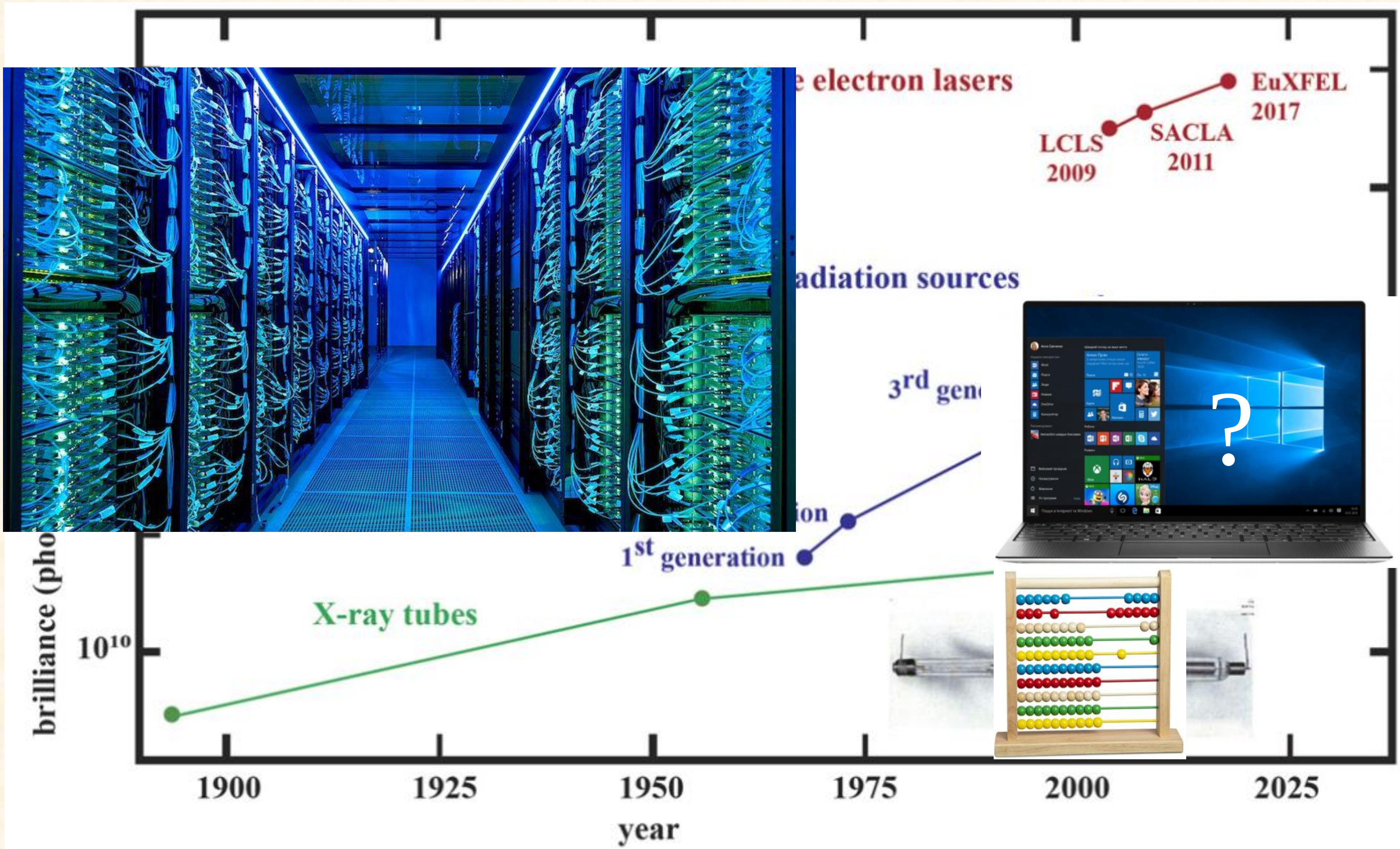
$$P_n = \frac{\omega e^2}{R}\left(\frac{n}{3}\right)^{1/3}\frac{\sqrt{3}}{\pi}\Gamma\left(\tfrac{2}{3}\right), \qquad 1 \ll n \ll n_0 .$$

The most striking thing about this result is the absence of any marked dependence on energy, at least for small n, while the total power contains the very large factor $(E/mc^2)^4$. The conclusion is irresistible that an enormous number of harmonics must contribute to the total radiation for $E/mc^2 \gg 1$. To verify

Synchrotrons worldwide

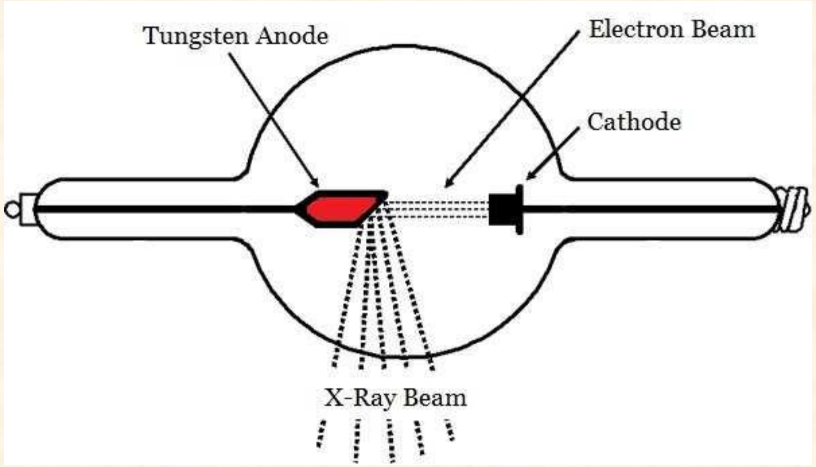
From W. Xu, Y. Liu, A. Marcelli, P.P. Shang, W.S. Liu, in Materials Today Physics, Volume 6, 2018

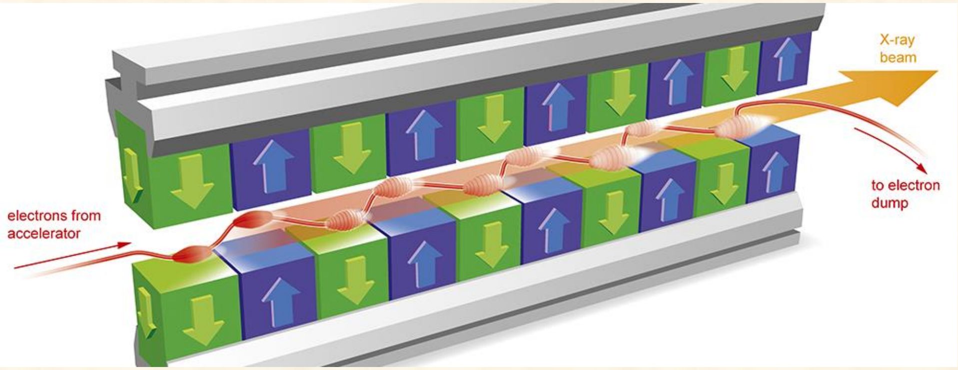
Technological revolution in X-ray generation



Valerio Cerantola et al 2021 J. Phys.: Condens. Matter 33 274003

Synchrotrons & FELs vs X-ray tubes





Synchrotrons & FELs are a fantastic tool but a high access price…

X-ray tube

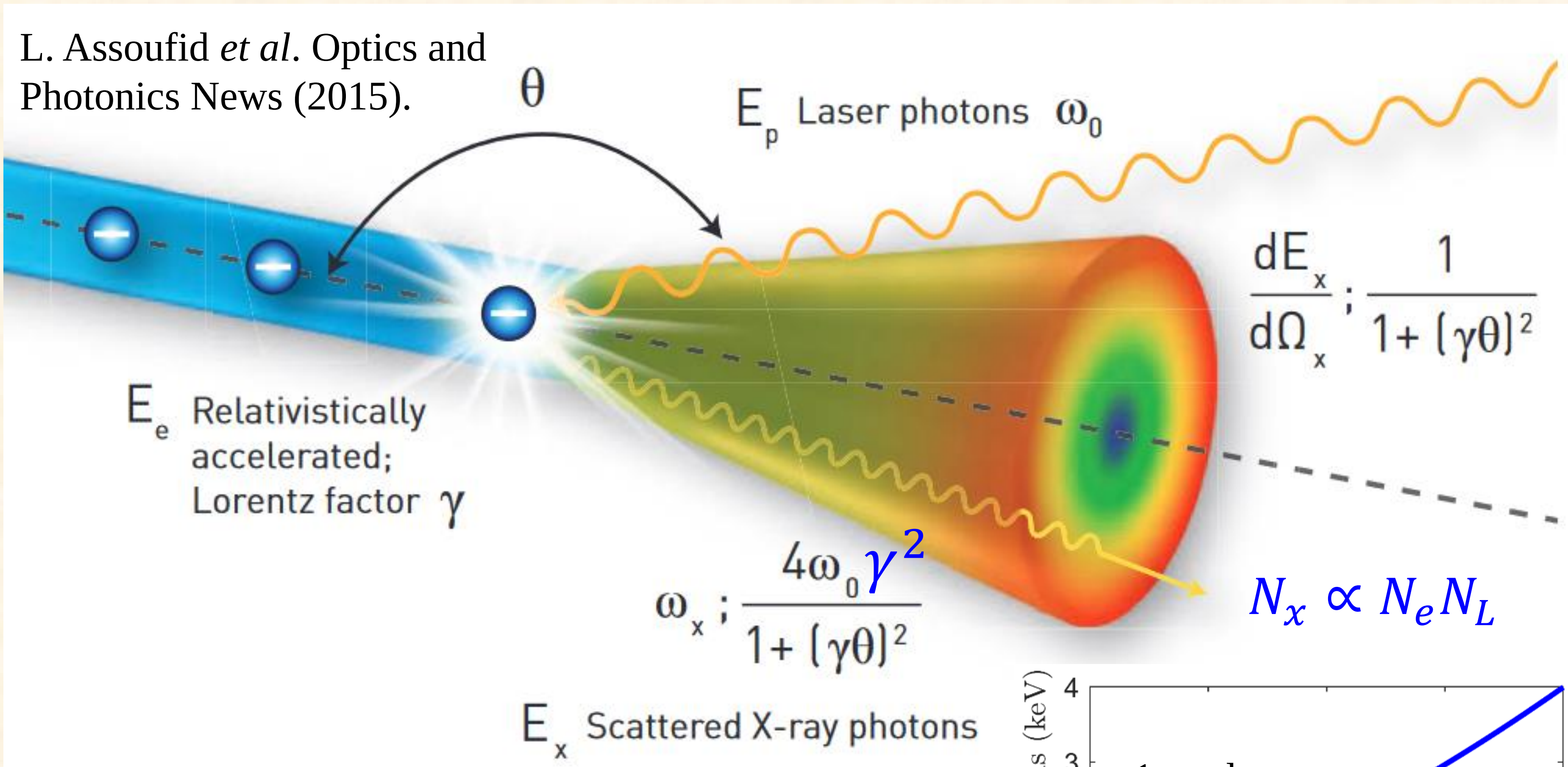
- 15 Nobel Prizes…
- wide availability
- ease of use
- capability to test new ideas without the barriers of schedule, travel and expenses

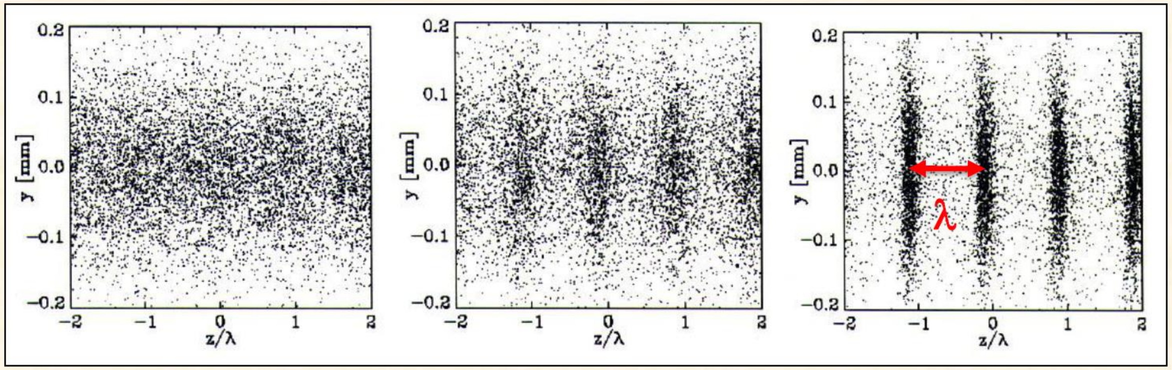
Having science without barriers calls for a femtosecond laboratory X-ray source

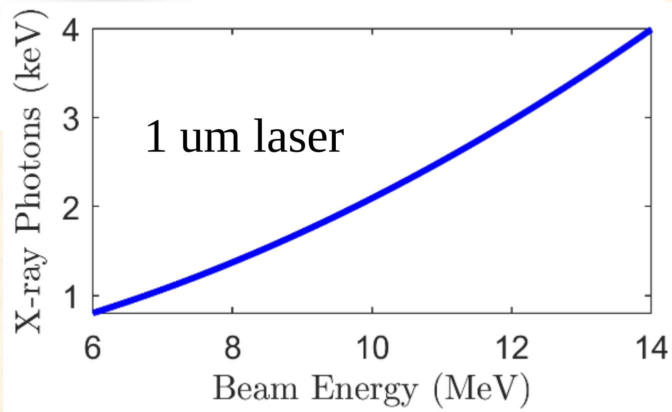
II: Can we bring the power of synchrotrons and FELs to a university lab?

Inverse Compton scattering source

L. Assoufid *et al*. Optics and Photonics News (2015).







Commercial compact synchrotron: Lyncean Tech.

Stored electron energy (max)	~100 MeV	
Optical cavity wavelength [a]	2 μm	
X-ray energy range (keV)	~30 - 90	
Brightness (1/s mrad² mm² 0.1%BW)	~4 x 10^{12} @ 90 keV	
Aperture [b]	Smaller	Larger
Divergence (mrad)	1	4
Bandwidth (FWHM)	1.5 - 2.5%	6 - 15%
Flux @ max energy (ph/s)	~4 x 10^{11}	~4 x 10^{12}

Operated at Munich university

X-ray pulse length ~50 ps

Compact synchrotron technology

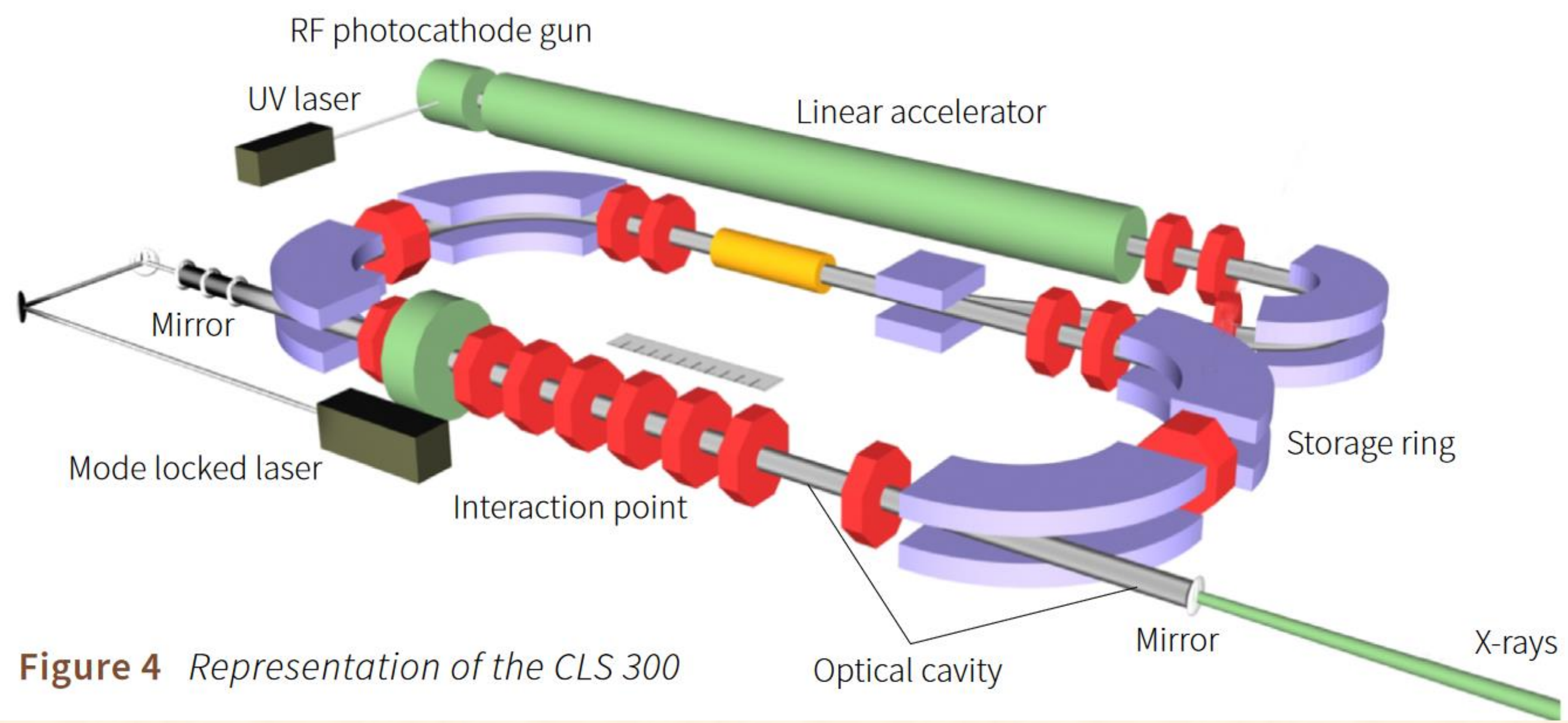
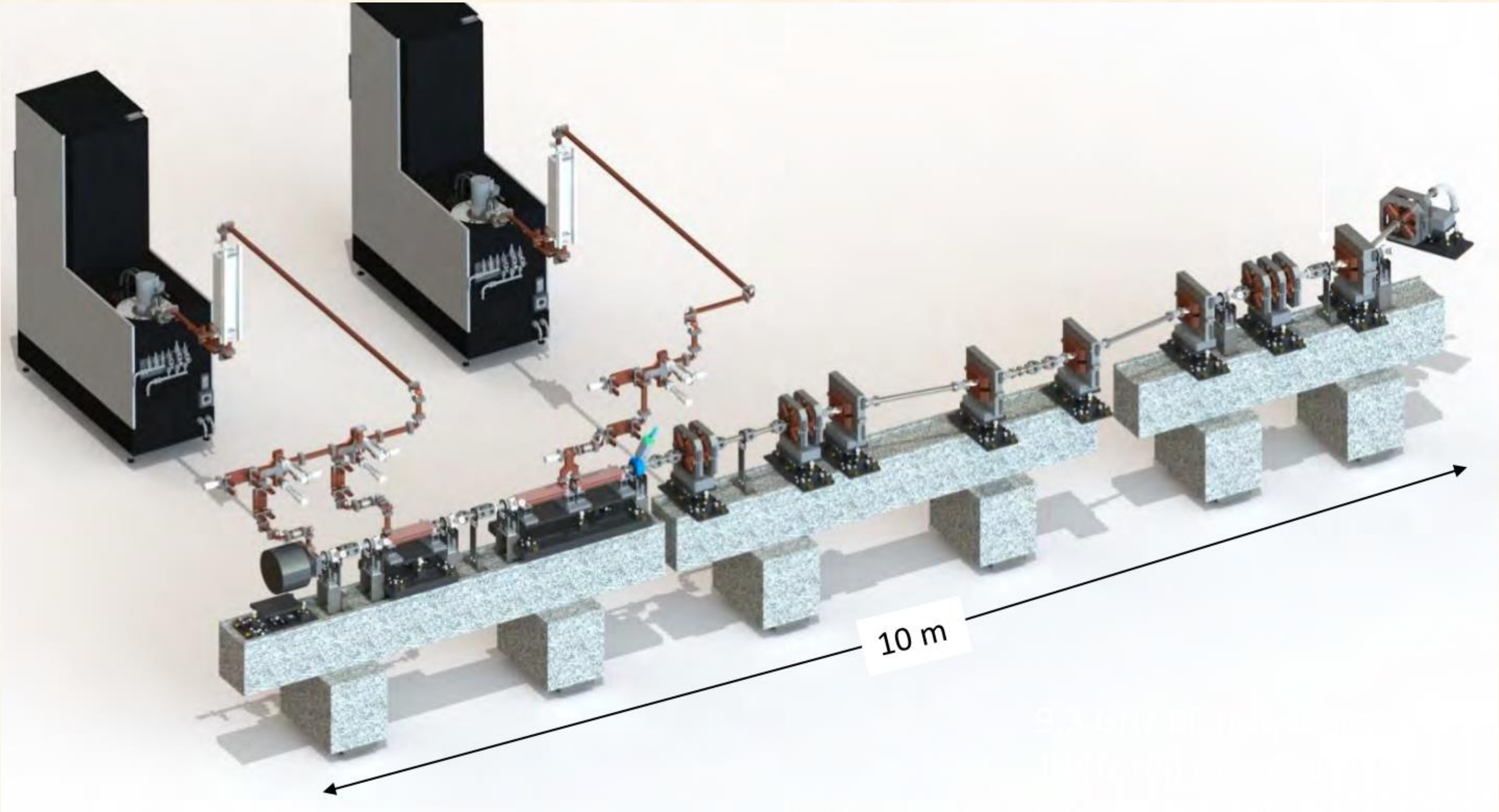


Figure 4 *Representation of the CLS 300*

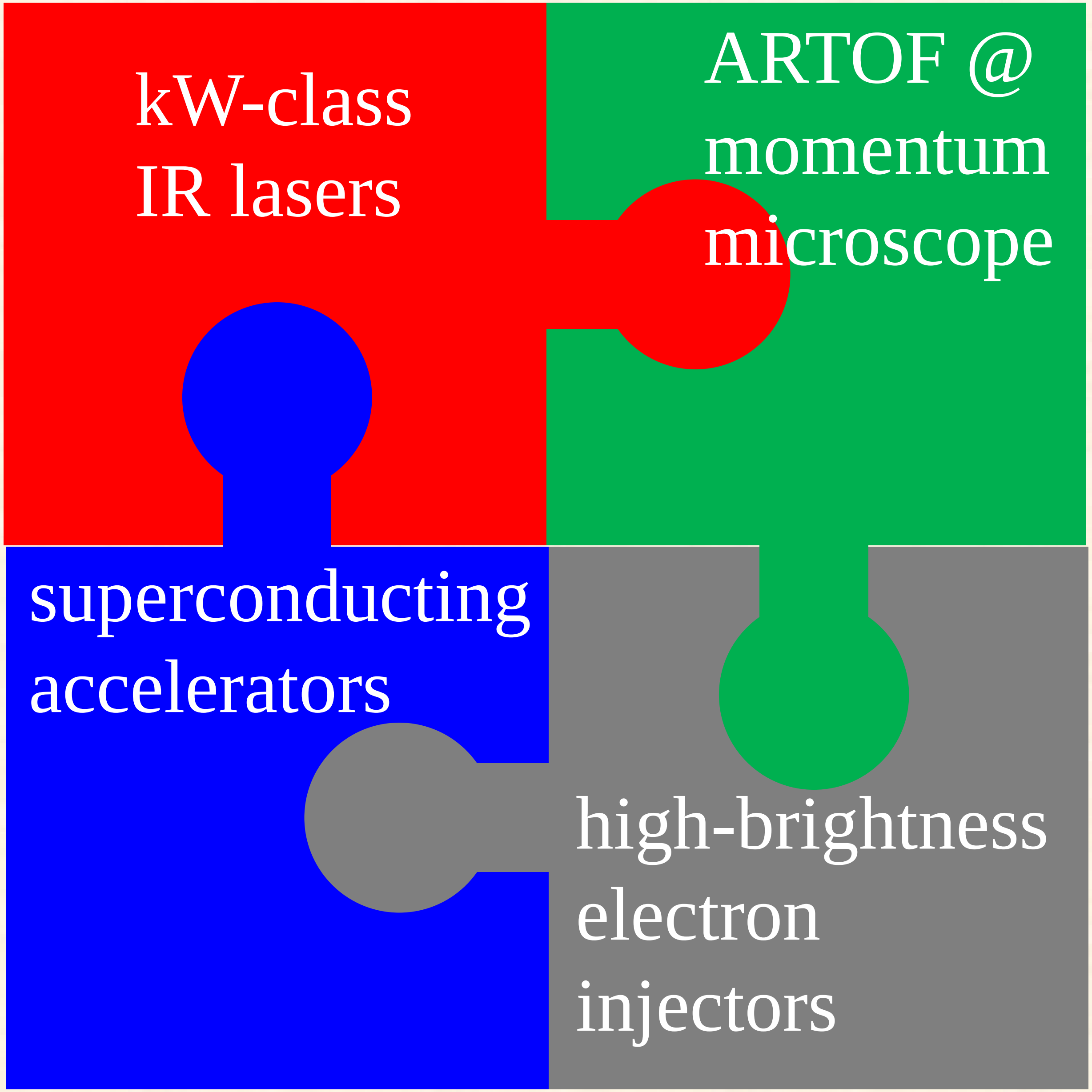
Courtesy Lyncean Technology

Project at Arizona State University



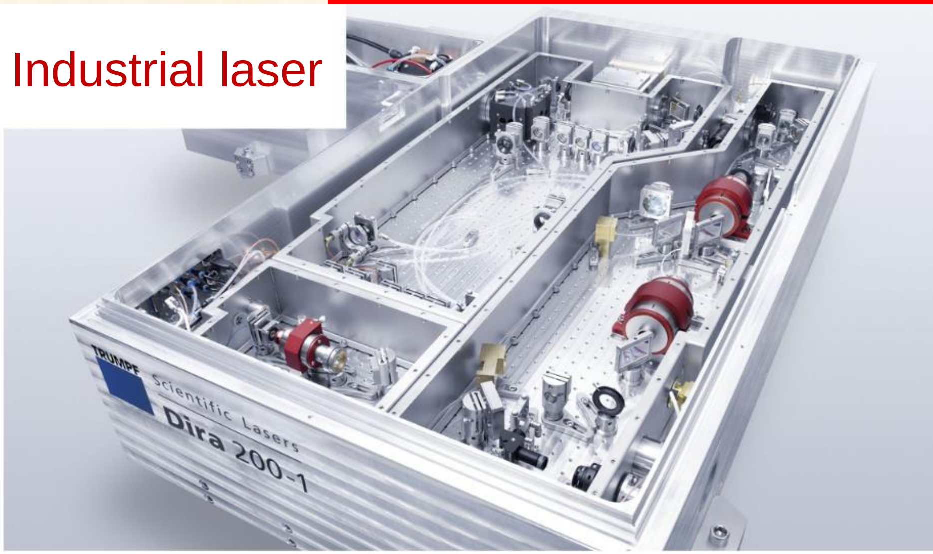
Can we make a step further to a develop a high-repetition-rate fs X-ray laser?

Enabling technologies for a compact X-ray laser

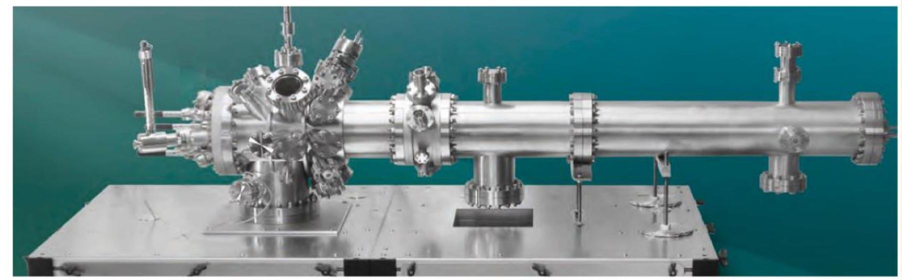


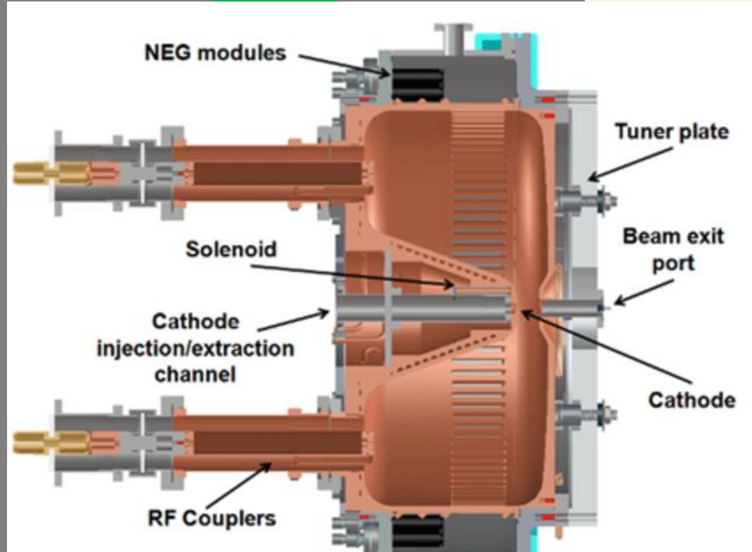
Enabling technologies for a compact X-ray laser

Industrial laser



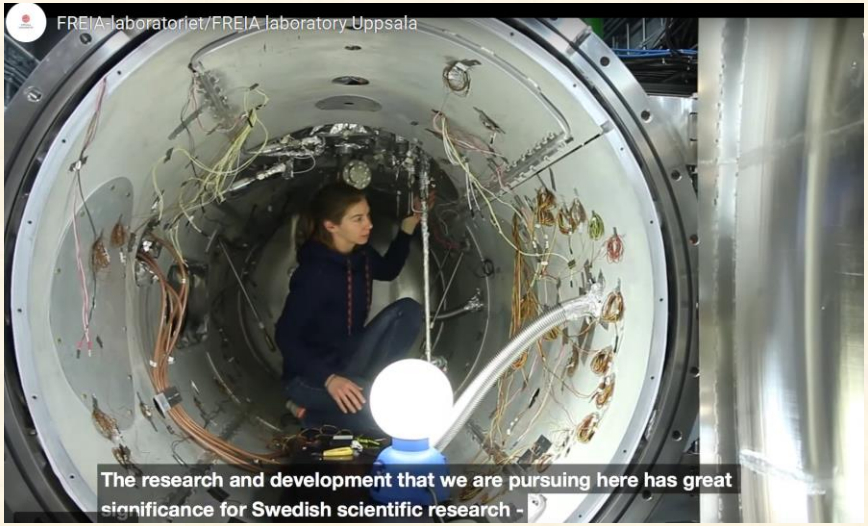
ARTOF @ momentum microscope

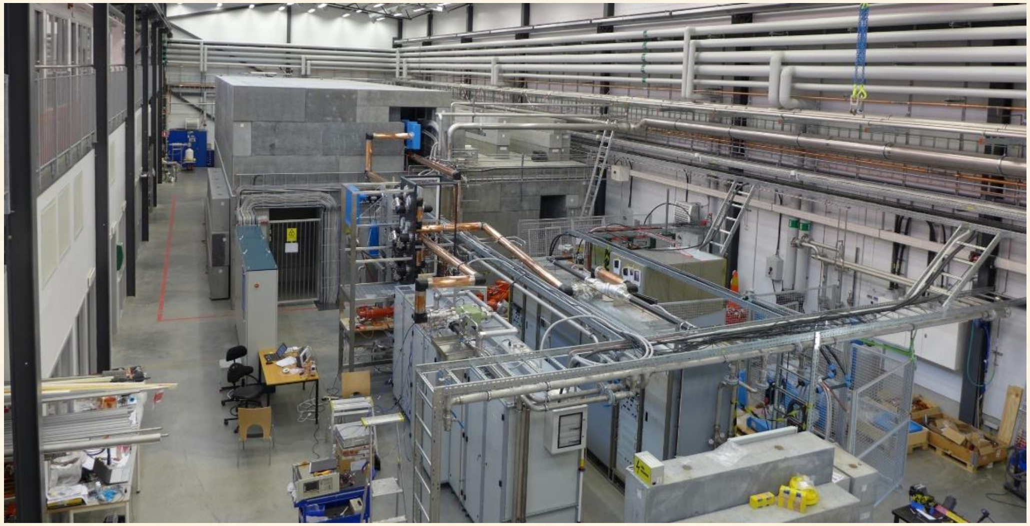


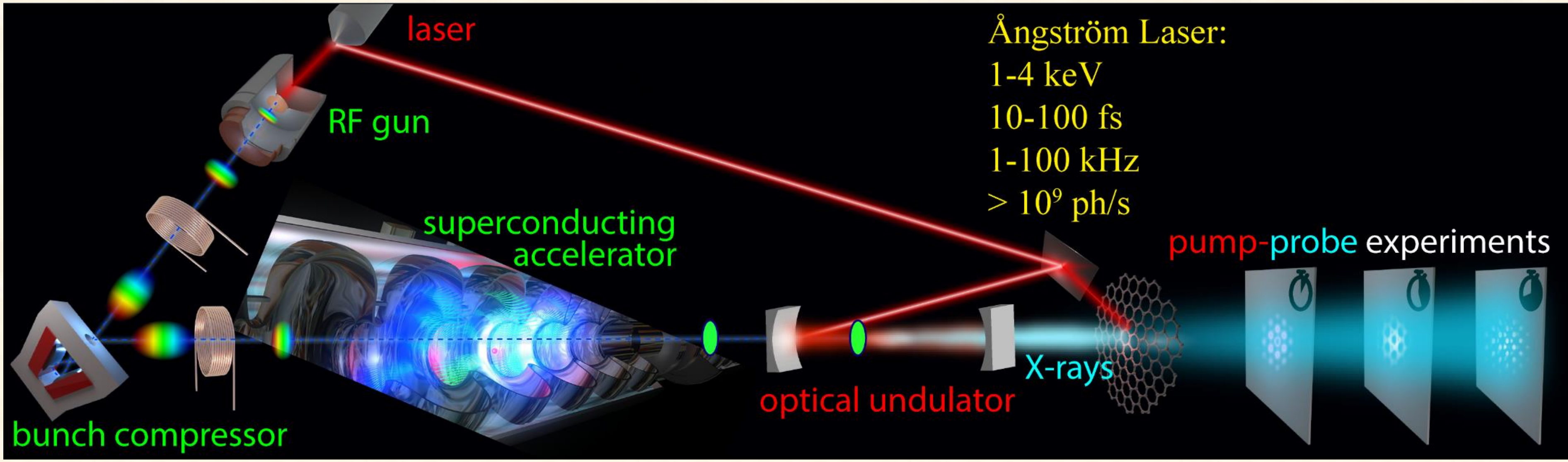


APEX VHF gun

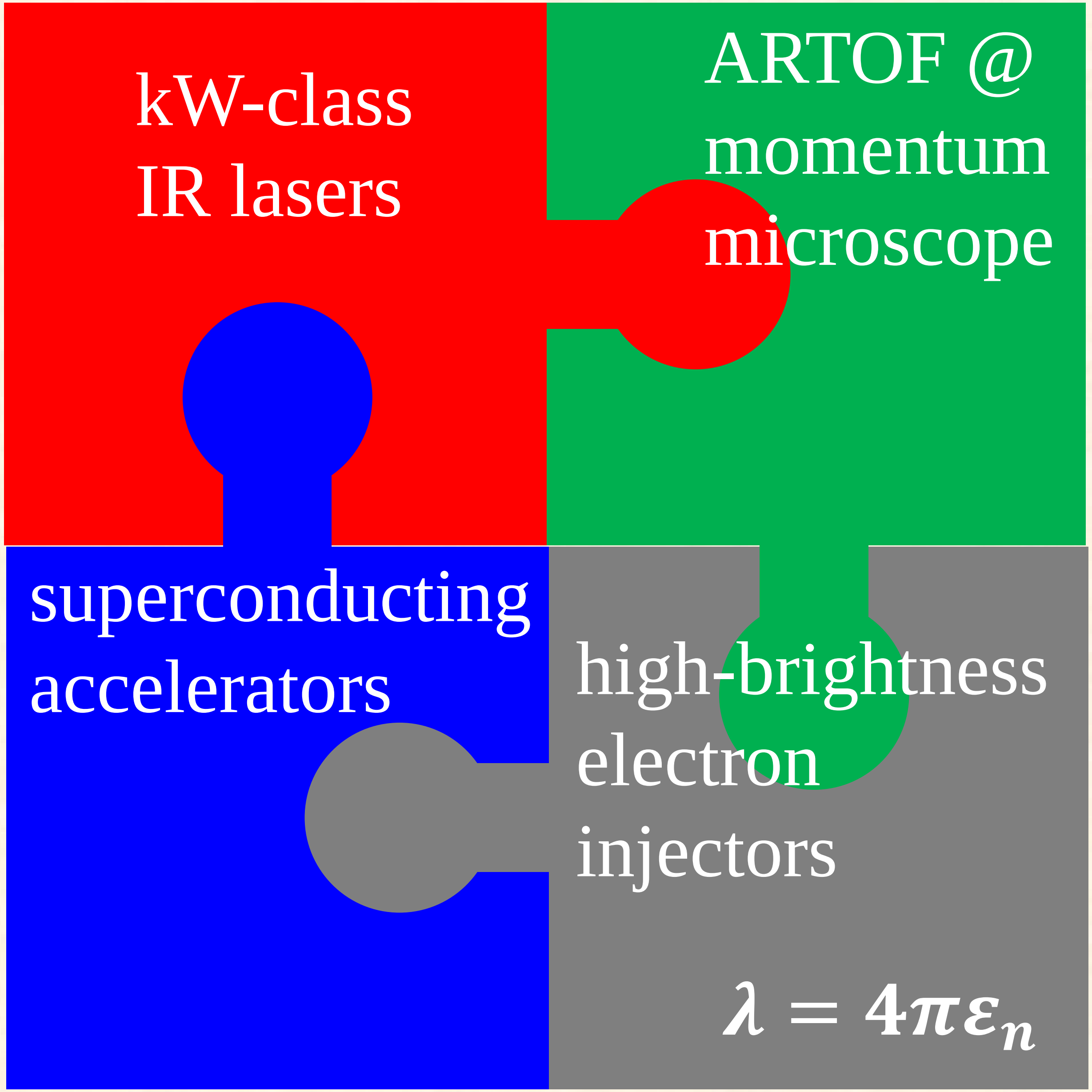
Towards Ångström Laser @ FREIA



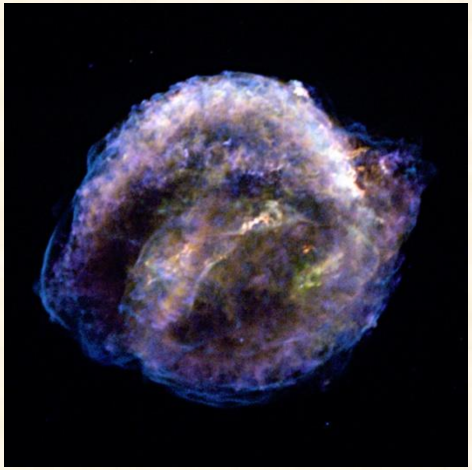




Enabling technologies for a compact X-ray laser

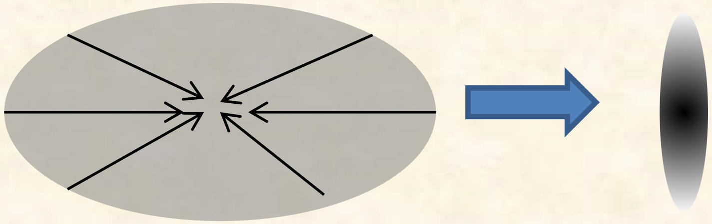


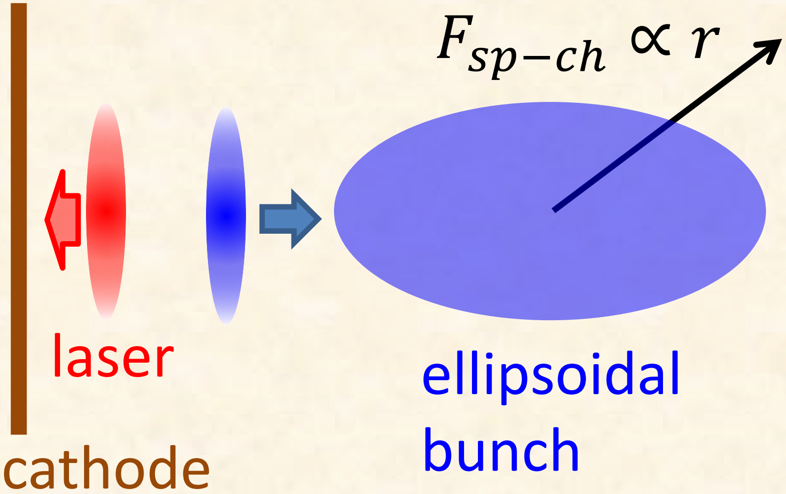
From gravitational collapse to high-brightness beams



$$V(\mathbf{x}) = -\int_{\mathbf{R}^3} \frac{G}{|\mathbf{x}-\mathbf{r}|}\, dm(\mathbf{r})$$

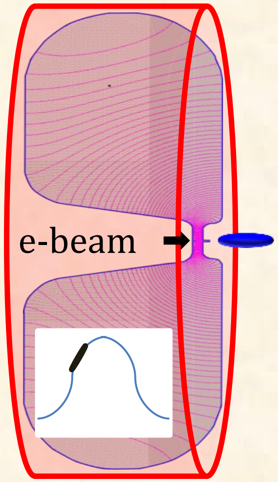
$$\rho = \sigma\delta(z)\sqrt{1 - r^2/R^2}$$





O.J. Luiten, PRL 094802 (2004)

RF gun

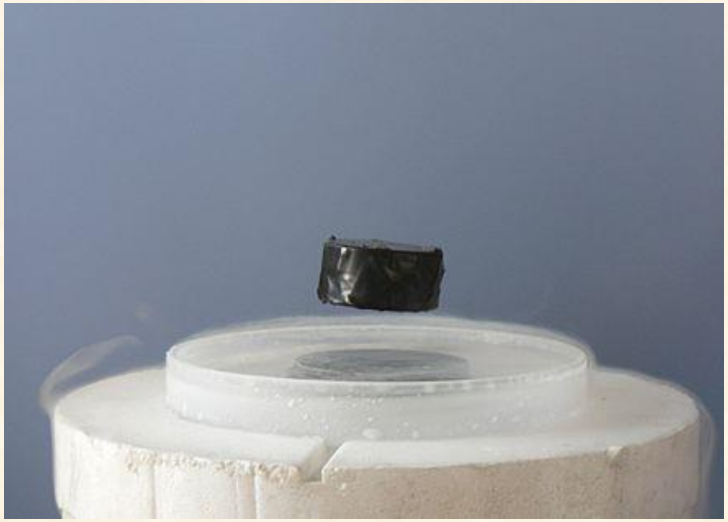


325 MHz
CW, ~ 25 kW
420 keV

A. Opanasenko et al.
arXiv:2105.07923

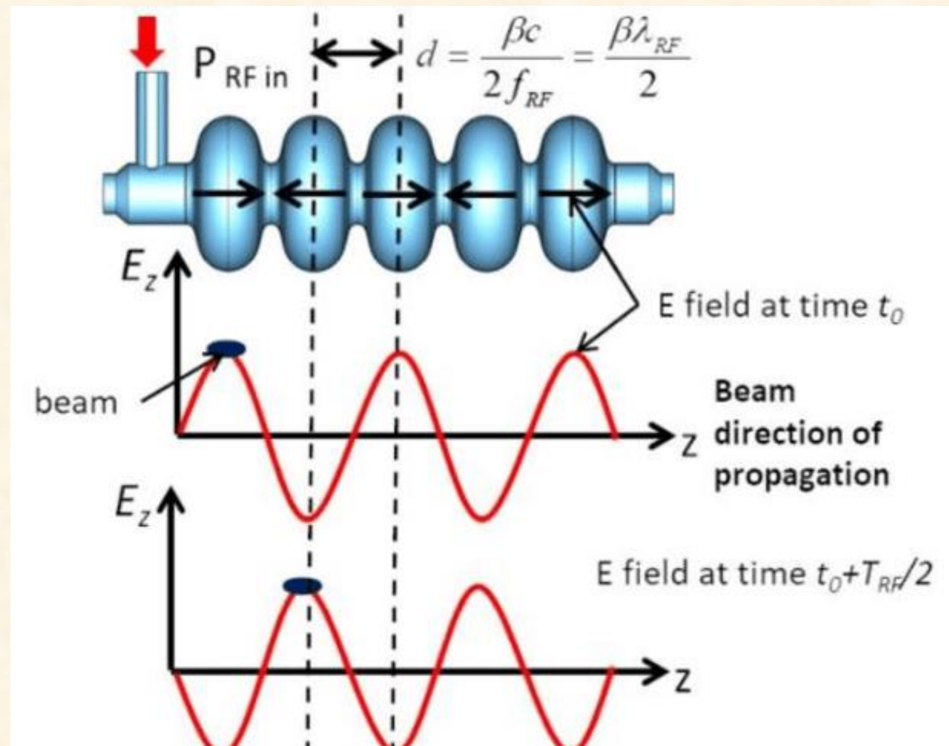
Blow-out generation of high-brightness beams

Superconducting RF technology



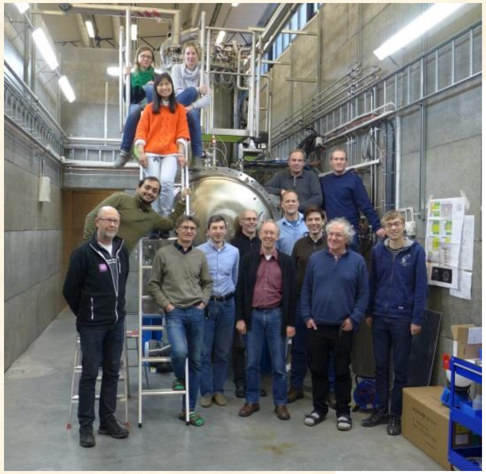
30 billion electron x volts

D. Alesini, CERN school, 2021



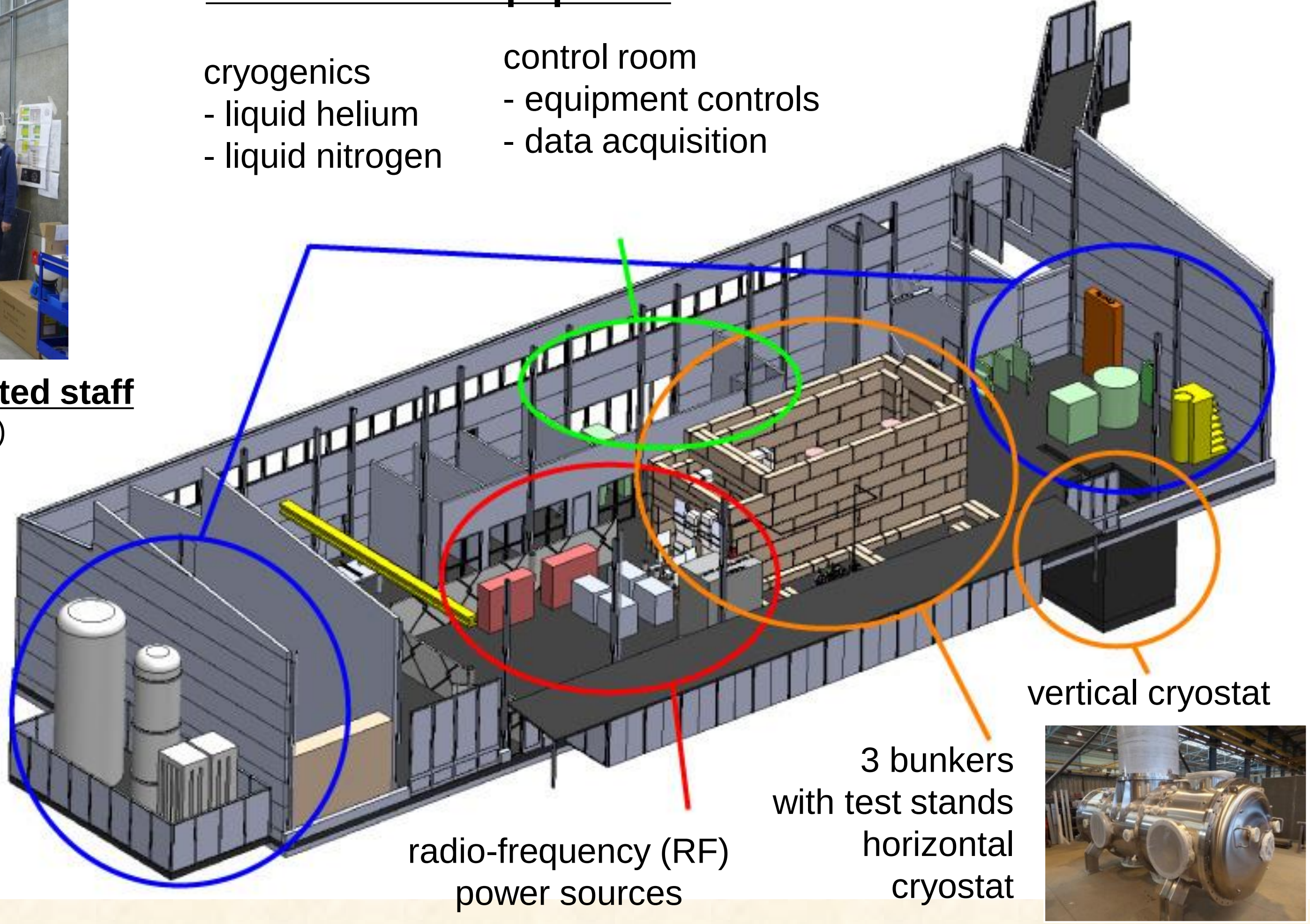
Vitaliy Goryashko

FREIA: Facility for Research Instrumentation & Accelerator Development



Competent and motivated staff
collaboration of physics (IFA)
and engineering (Teknikum).

State-of-the-art Equipment

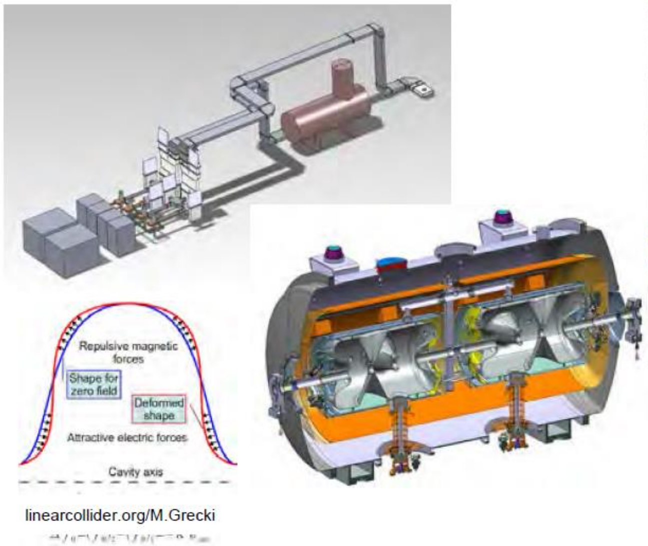


Funded by
KAWS,
Government,
Uppsala Univ.

Total budget
~200 MSEK

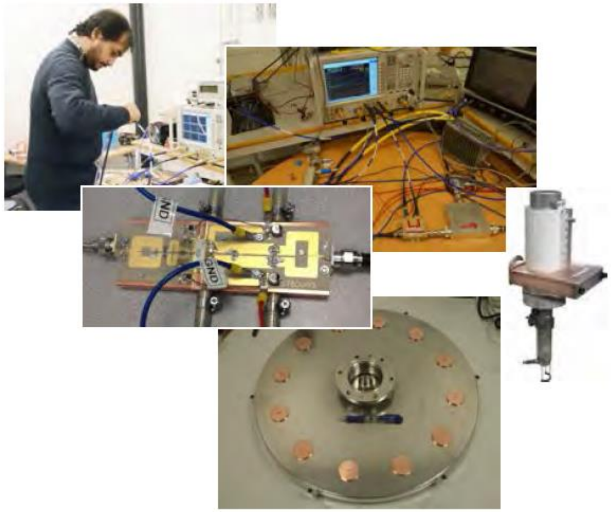
FREIA – a unique accelerator laboratory

SRF Spoke Cavities & Linac



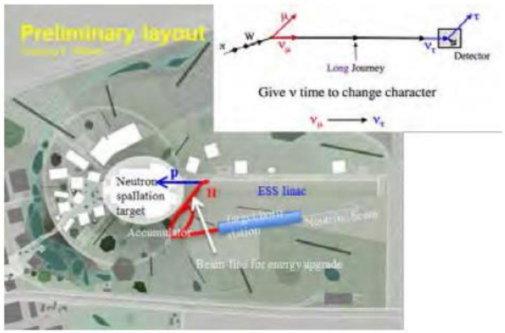
Cryogenics

High Power RF Amplifiers Solid-state & Vacuum Tube

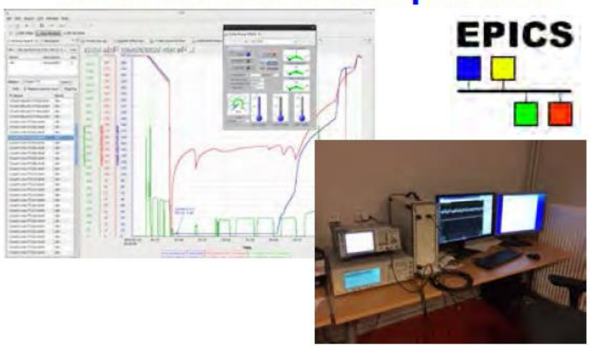


SRF Test Stand

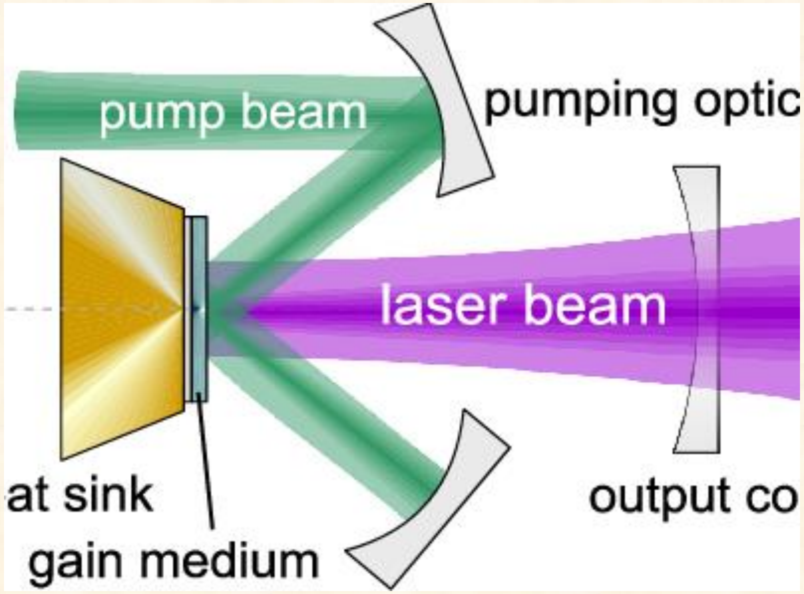
ESS neutrino Super-beam

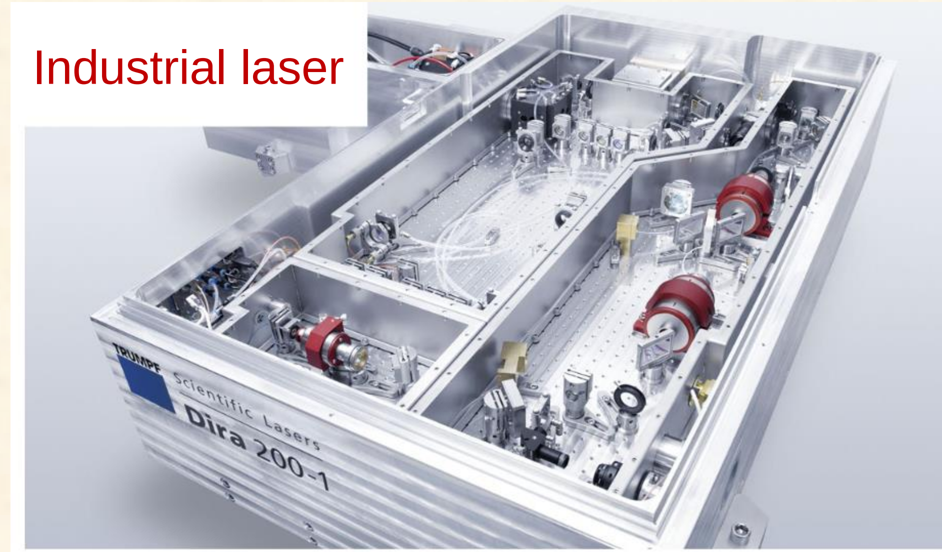


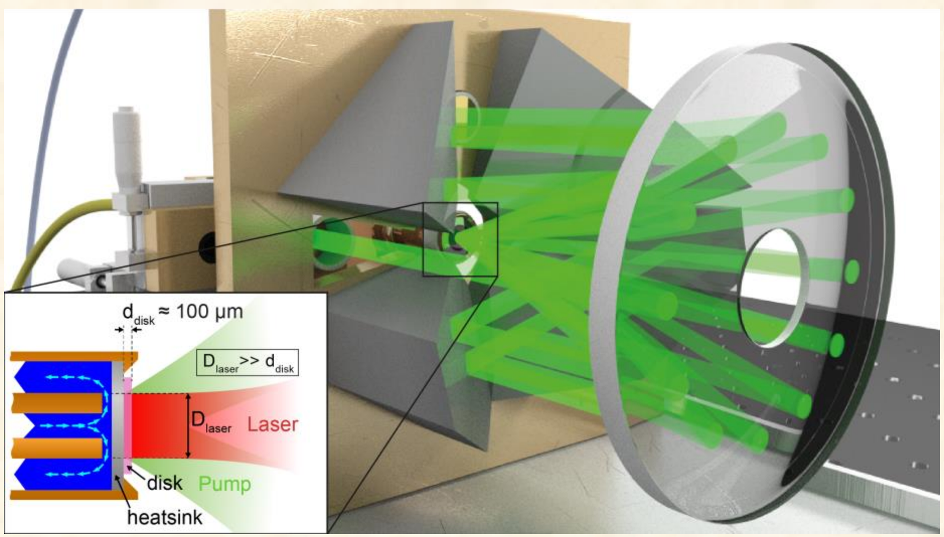
Controls & Data Acquisition



kW-class IR laser: thin-disk Yb:YAG technology





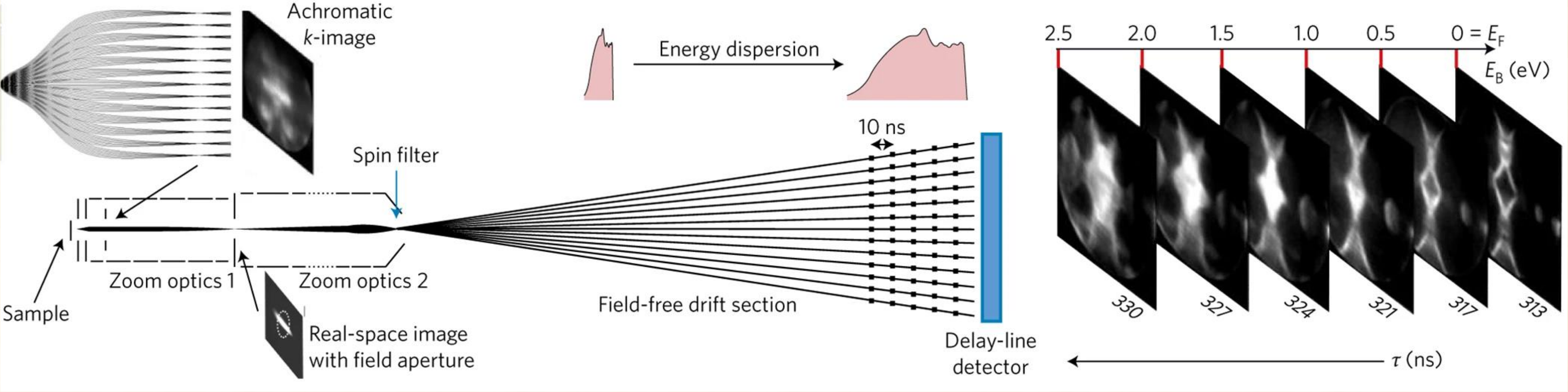


Courtesy of M. Saraceno, martin@saraceno.info

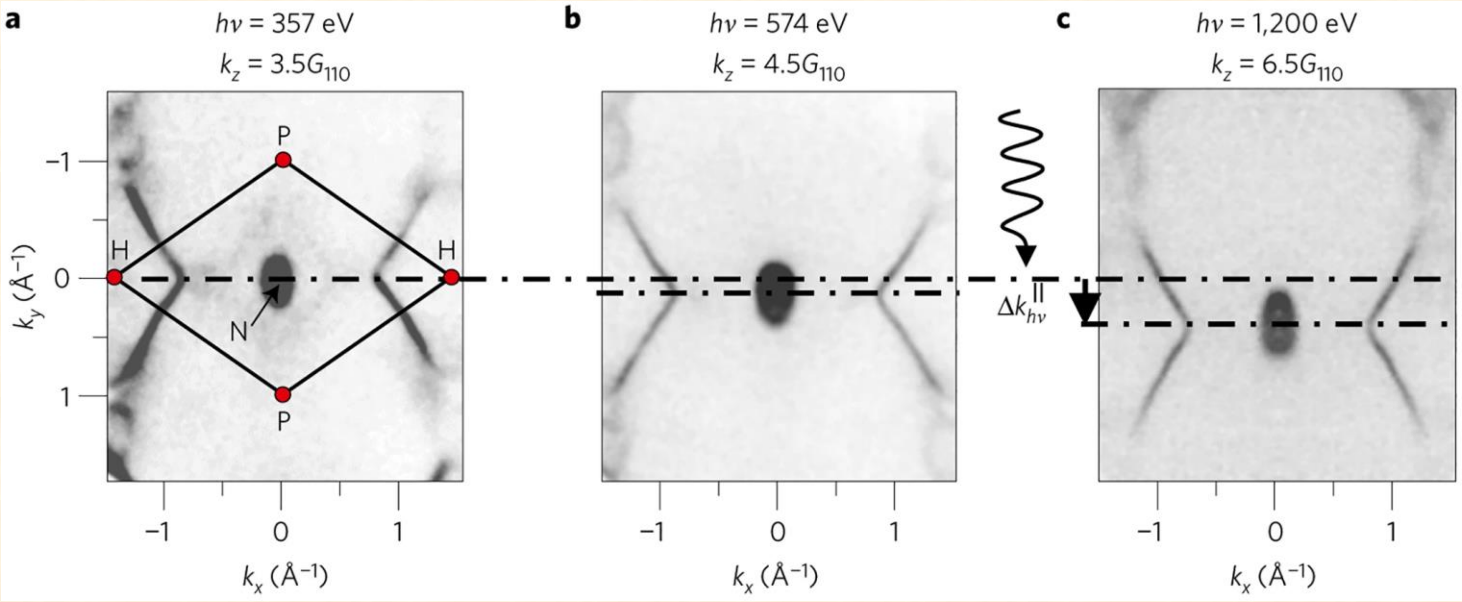
Thin-disk Yb:YAG lasers from TRUMPF at 1 um:

- Off-the-shelf: 0.75 kW, 20-100 kHz, up to 150 mJ, < 1 ps
- Demonstrated: 1.9 kW, 20 kHz, up to 95 mJ, < 1 ps
- On special order: 5 kW, 100 kHz, 50 mJ, < 1 ps

Detection of photo-electrons

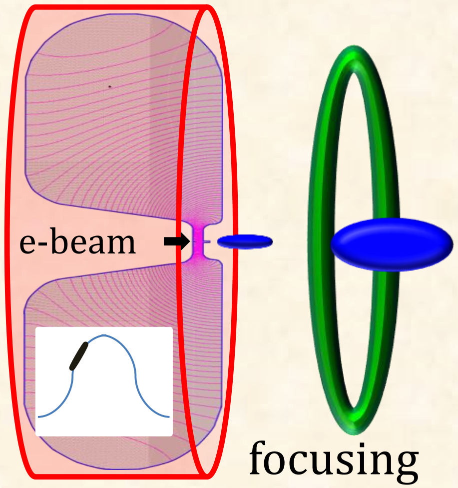


[Nature Mat. 16, 615 (2017)]



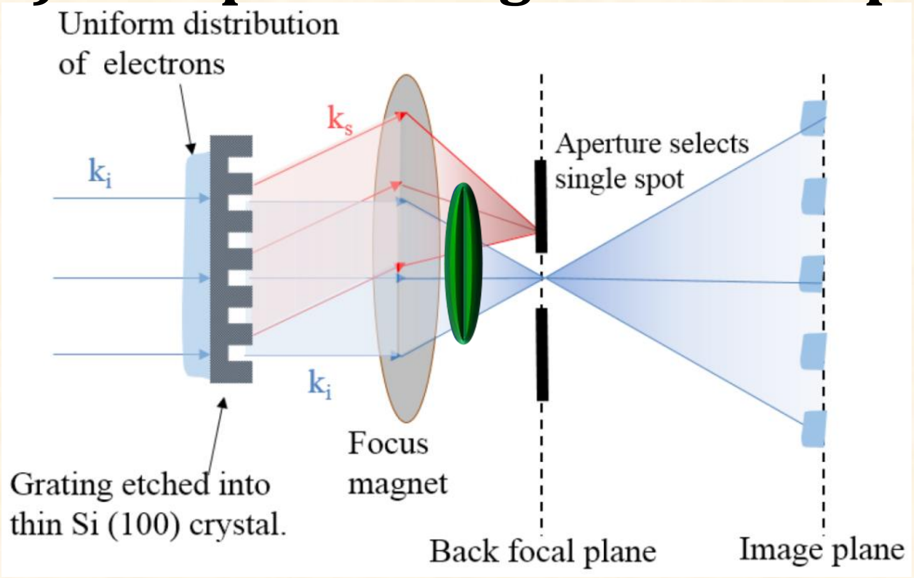
Key parts of the accelerator

(1) RF gun



325 MHz
CW, ~ 25 kW
0.4 MeV

(2) nanopatterning: ASU concept



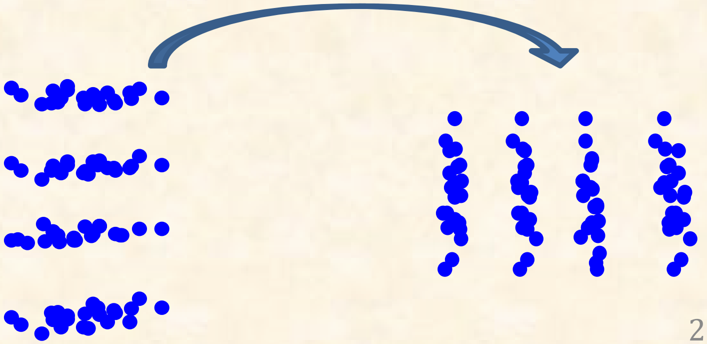
(3) booster

1.3 GHz, SC
CW, ~ 10 W
2-3 MeV

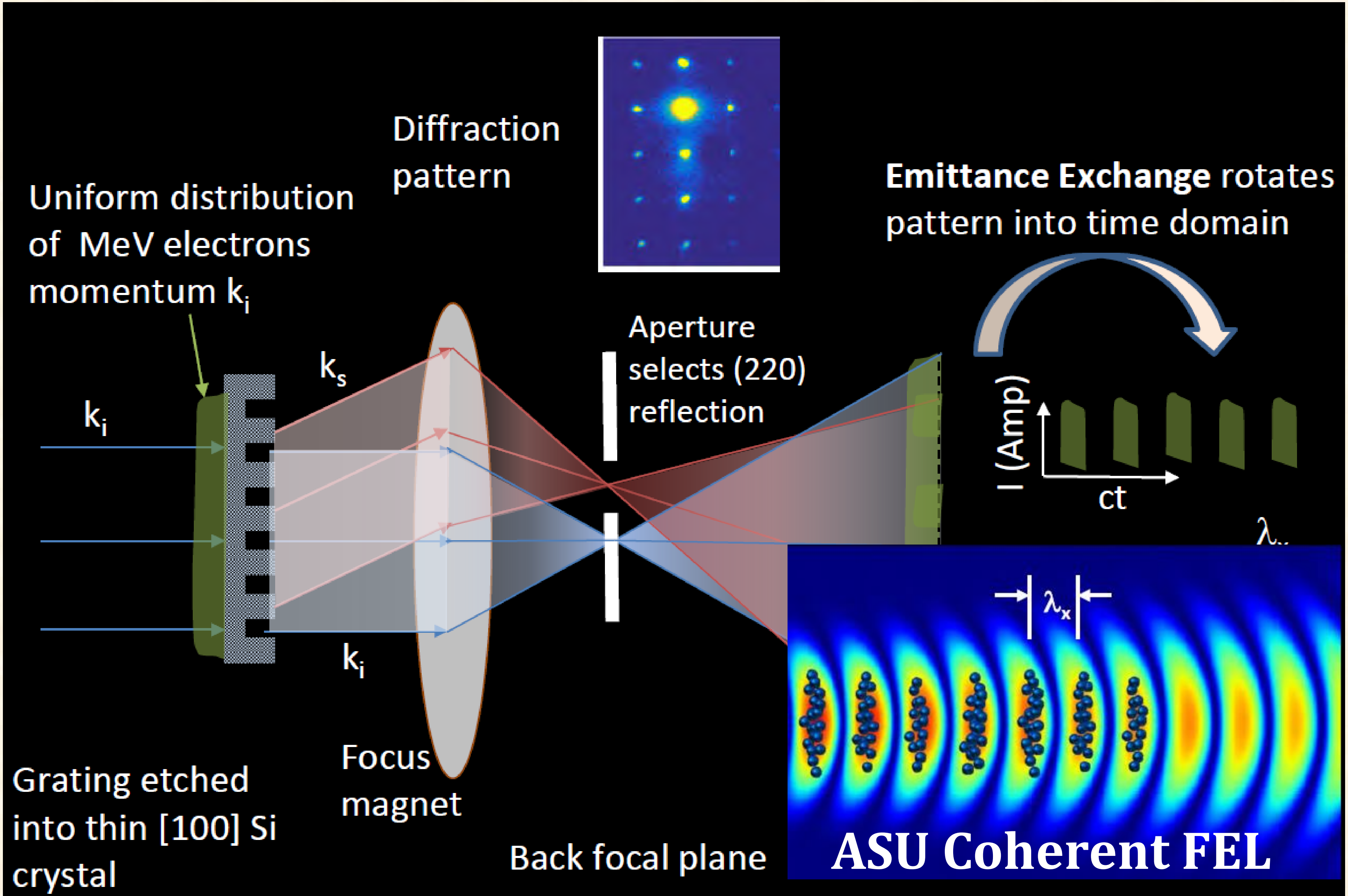
(4) main accelerator

1.3 GHz, SC CW, ~ 100 W, 7-14 MeV

(5) emittance exchange



ASU nanopatterning concept



Target parameters of our incoherent X-ray source

Electron beam parameters	electron bunch charge	Q_b	16	pC
	number of electrons	N_b	10^8	
	bunch energy	U_b	7.6	MeV
	relative energy spread	δ_γ	10^{-3}	
	rms bunch duration	τ_b	12.5	fs
	bunch emittance	ϵ_n	0.08	mm mrad
	rms bunch size	σ_b	3.5	um
	geometrical beta-function	β_g	2.3	mm
Laser beam parameters	laser wavelength	λ_L	1.0	um
	rms laser pulse duration	τ_L	1	ps
	rms laser beam size	σ_L	4.9	um
	Rayleigh length	z_R	0.3	mm
	laser pulse energy	$\mathcal{E}_L$	50	mJ
	undulator parameter	$\mathcal{K}$	0.14	
	laser rep. rate	f_L	100	kHz
X-ray yield	radiation wavelength	λ_r	1	nm
	rms X-ray pulse duration	τ_X	12.5	fs
	rms X-ray beam size	σ_X	2.9	um
	rms X-ray beam divergence	$\sigma_{X'}$	0.5	mrad
	Full bandwidth	BW	0.7%	
	X-ray photons/shot	N_{ph}	$5.9\ 10^4$	
	X-ray photons/second/0.1%BW	$\mathcal{F}_{0.1\%}$	10^9	

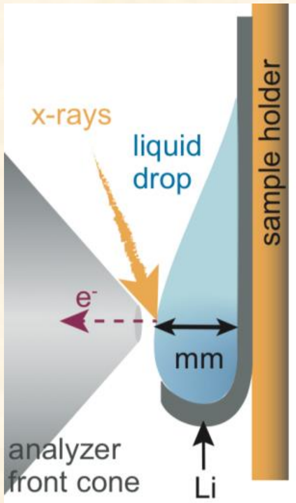
Ångström Laser

Electron beam parameters	electron bunch charge	Q_b	0.8	pC
	number of electrons	N_b	$5\ 10^6$	
	bunch energy	U_b	7.6	MeV
	relative energy spread	δ_γ	10^{-4}	
	rms bunch duration	τ_b	50	fs
	bunch emittance	ϵ_n	0.03	mm mrad
	rms bunch size	σ_b	2	um
	geometrical beta-function	β_g	2	mm
Laser beam parameters	laser wavelength	λ_L	1.0	um
	rms laser pulse duration	τ_L	1000	fs
	rms laser beam size	σ_L	4.9	um
	Rayleigh length	z_R	0.3	mm
	laser pulse energy	$\mathcal{E}_L$	50	mJ
	undulator parameter	$\mathcal{K}$	0.14	
	laser rep. rate	f_L	100	kHz
X-ray yield	radiation wavelength	λ_r	1	nm
	X-ray pulse duration	τ_X	50	fs
	rms X-ray beam size	σ_X	1.5	um
	rms X-ray beam divergence	$\sigma_{X'}$	75	urad
	X-ray photons/shot/0.01%BW	$N_{ph,0.01\%}$	$3\ 10^4$	
	X-ray photons/second/0.01%BW	$\mathcal{F}_{0.01\%}$	$3\ 10^9$	

III: a taste of fs X-ray science

Workshop program and talks are available at:
https://indico.uu.se/event/688/

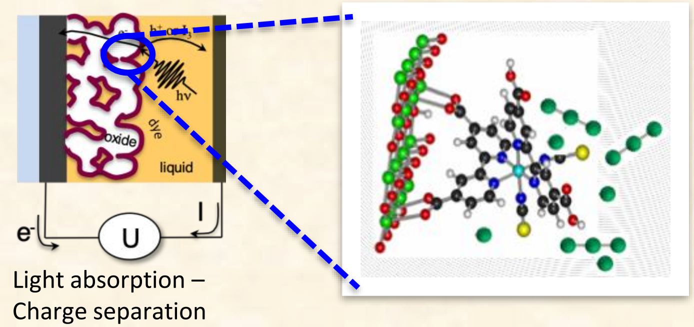
Science opportunities



X-ray photoemission provides access to bulk properties, e.g. in batteries

J. Maibach, et al., Nature Comm. **10**, 3080 (2019)

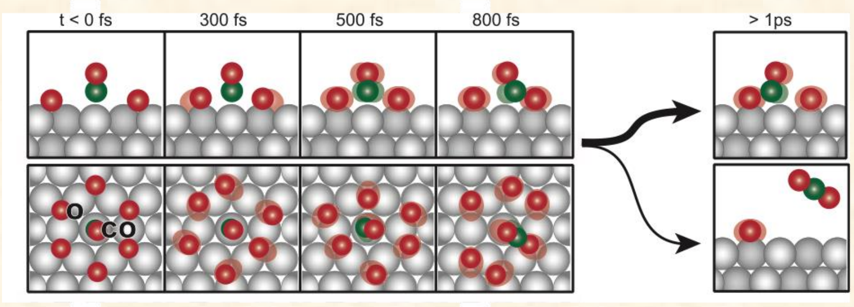
Enables probing the charge separation across buried interfaces in solar cell materials



Allows to discover novel complex functional materials

“Materials Genome” exploration of new materials

Exploring chemical reactions and catalysis at ambient conditions

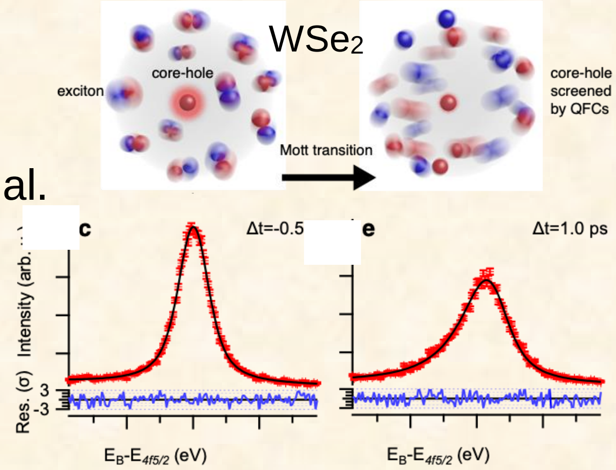


H. Öström, et al., Science **347**, 978 (2015)

Adopted from H. Durr talk

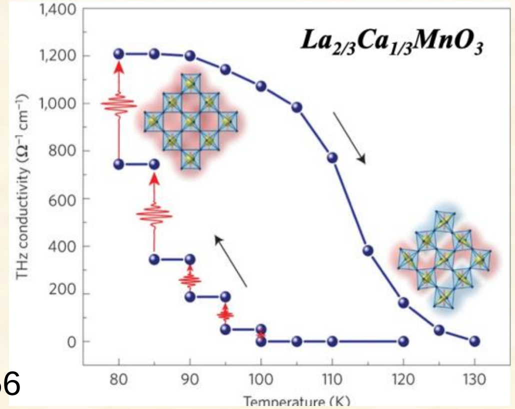
Science opportunities (continued)

Core levels are sensitive probes of electron correlations



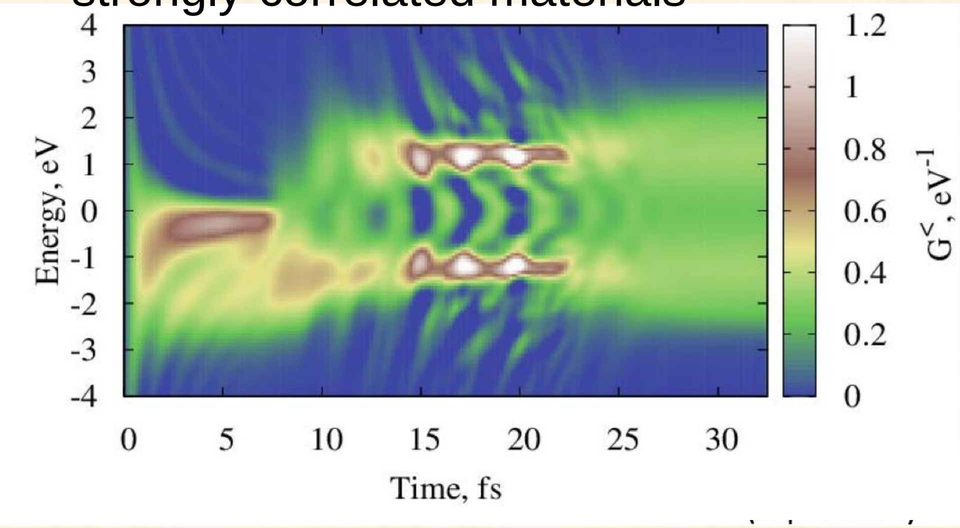
Dendzik, et al. PRL (2020)

Access new non-thermal metastable states in quantum materials

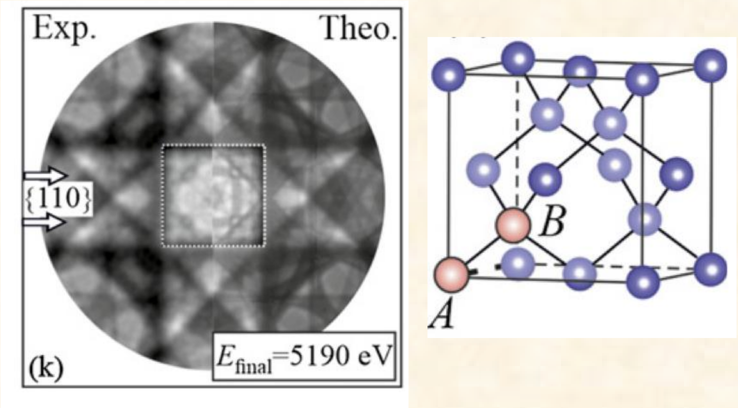


J. Zhang, et al., Nature Mat. **15**, 956 (2016)

Directly link to theory for driven strongly-correlated materials



Site-specific structural dynamics probed by photoelectron diffraction



A. Fedchenko et al. NJP **22**, 103002 (2020)

Expected science impact of a fs lab X-ray source

Impact	How?
Topological electronics	ARPES identification of the band topology of surface states of a sample right after its synthesis without breaking the ultrahigh vacuum.
Sustainable energy production	Charge-carrier in nanostructures for solar fuels.
	Angle resolved core-level spectroscopy of organic photocells (damage-sensitive samples).
Material discovery acceleration	Examining samples without leaving the ultrahigh vacuum environment.
Understanding surface contamination	Measuring the chemical states of surface species via time-resolved ARPES.
Control of energy flows	Photodriven semiconductor-to-metal phase transitions in surface layers.

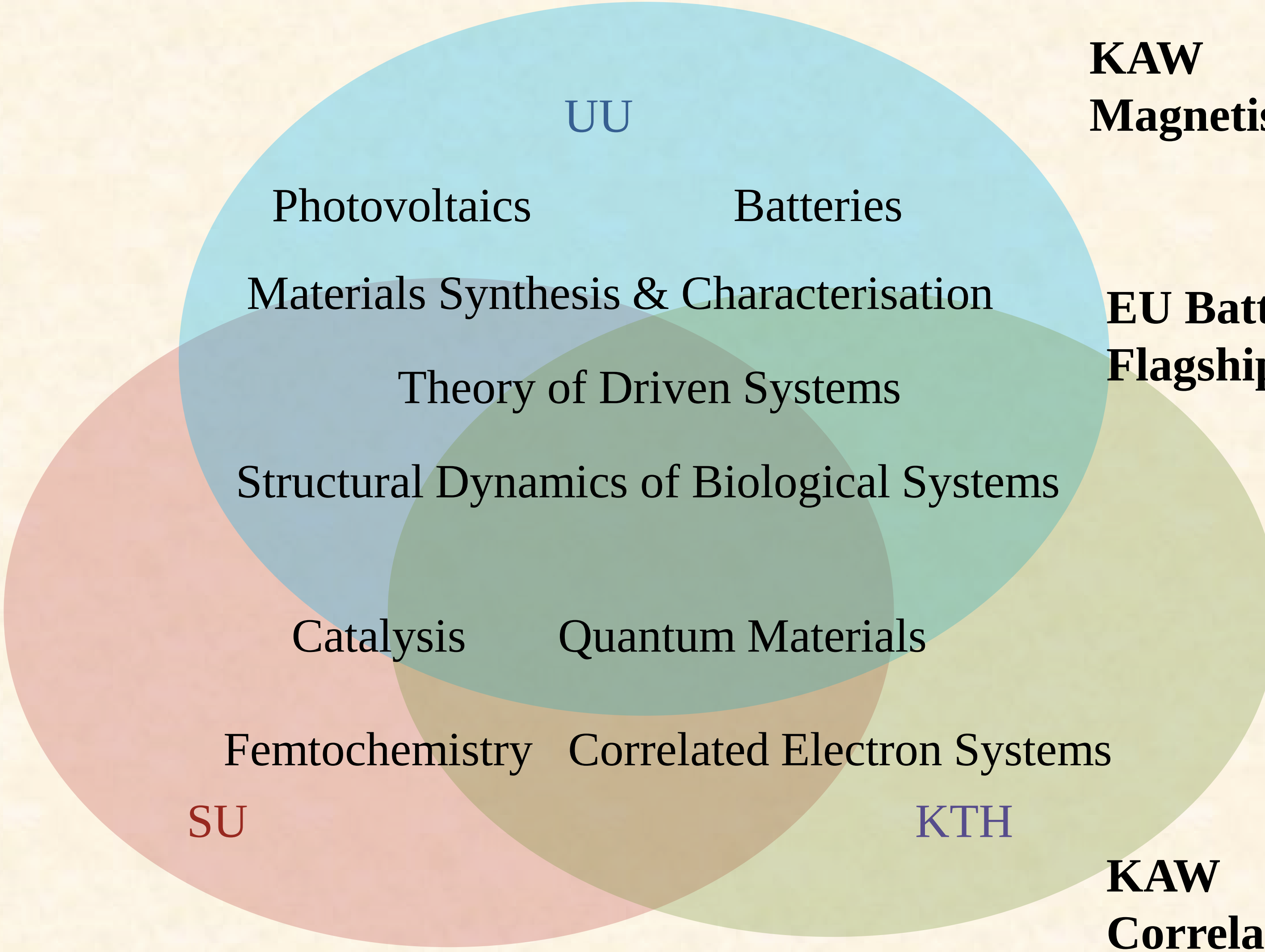
The Uppsala-Stockholm research environment

ERC
Synergy

KAW
Magnetism

KAW
Scholars

EU Battery
Flagship



KAW
Catalysis

KAW
Correlated
Electrons

Adopted from H. Durr talk

The Ångström Laser project

- Builds on the strengths of UU's instrumentation tradition

- Provides the UU and national science community with a complementary world-class research facilitiy

- Enables novel discovery science by close integration with campus activities

- Aims to be a hub for education and innovation