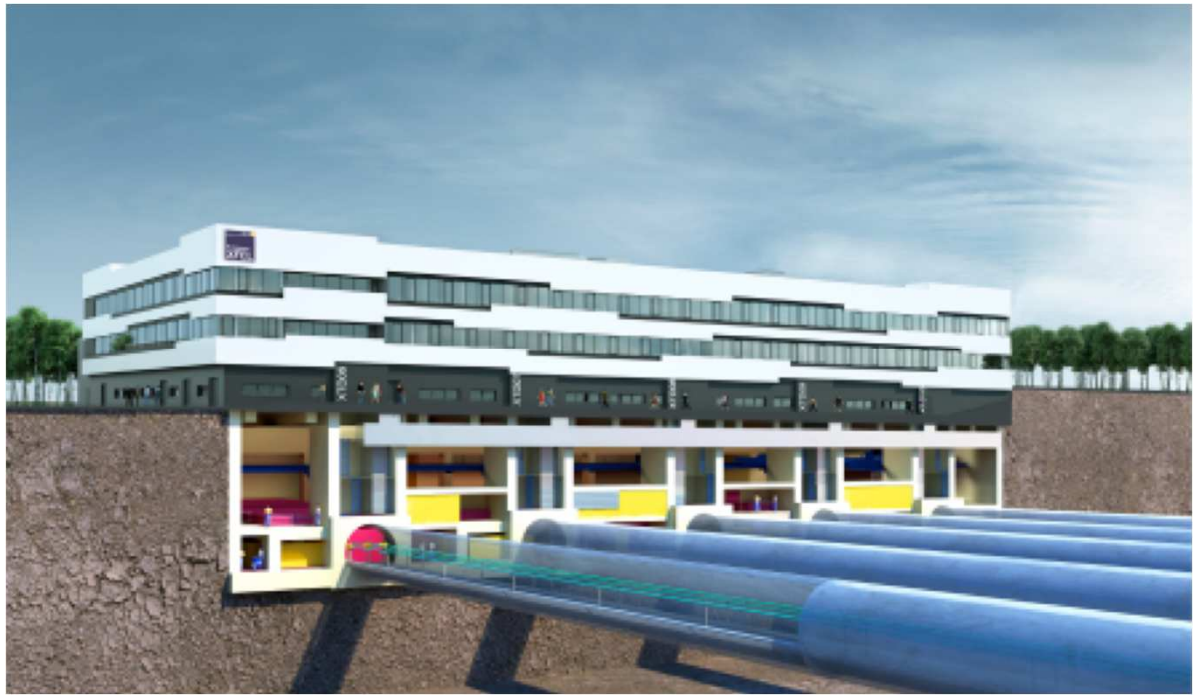
Opportunities for resonant elastic and inelastic x-ray scattering studies at the SCS instrument of European XFEL

Justine Schlappa
Spectroscopy and Coherent Scattering (SCS instrument)

Stony Brook, 26. Juni 2019

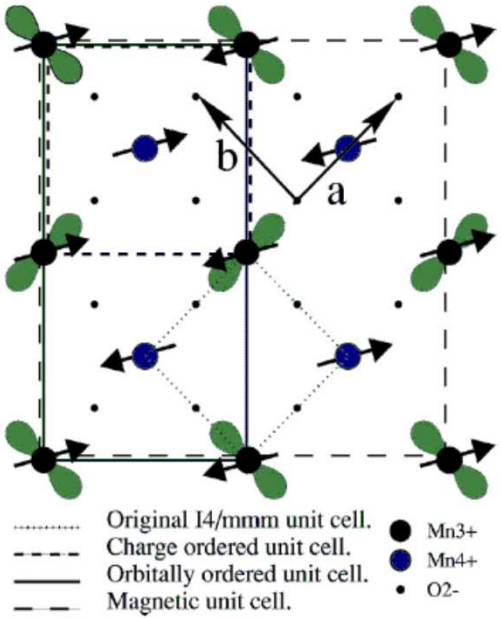


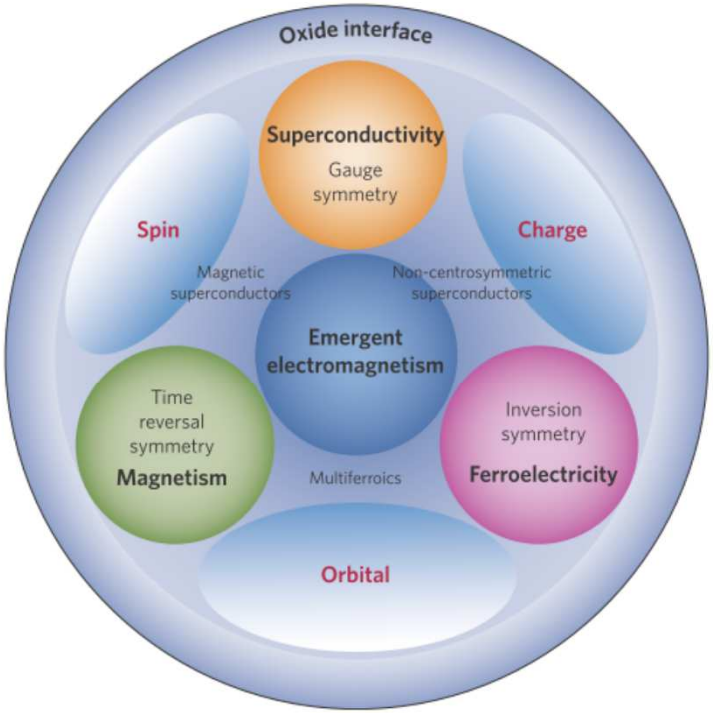
Outline

- Motivation
- Introduction to SCS instrument at SASE3
- Baseline XRD and User Consortium hRIXS setup
- First user experiment at SCS

Physics of complex materials by nuclear, charge, spin, and orbital degrees of freedom and their interplay

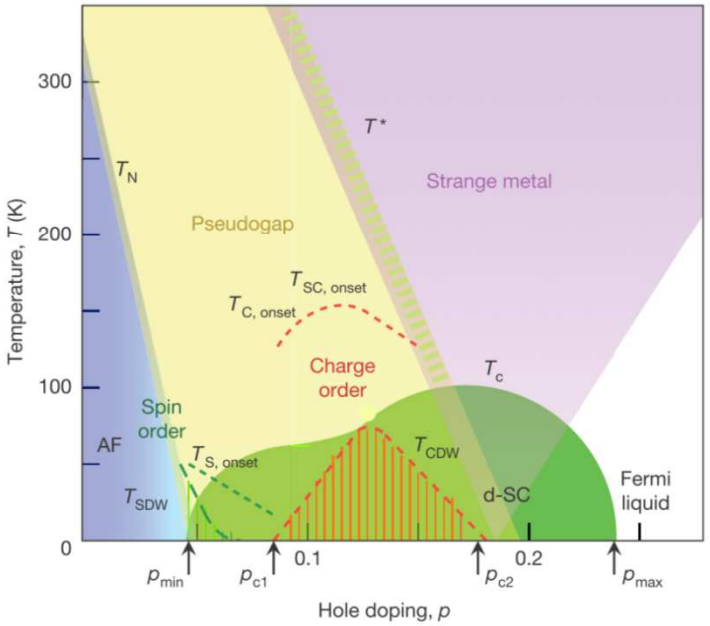
C.W.M. Castleton and M Altarelli, Phys. Rev. B 62, 1033 (2000)





H.Y. Hwang et al., Nature materials 11, 103 (2012)

B. Keimer et al., Nature 518, 179 (2015)

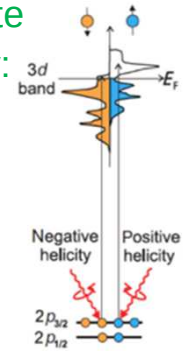


Microscopic probes

Synchrotrons:

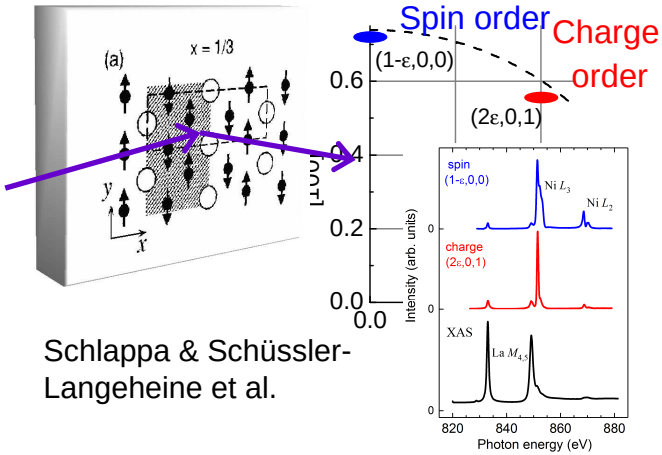
- **See the ultra small**

Atomic-site selectivity:



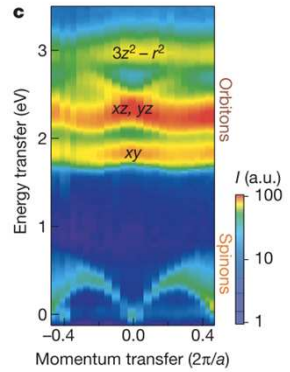
Stöhr & Siegmann, Magnetism Springer

Length scales of nm:



Schlappa & Schüssler-Langeheine et al.

Inter-particle correlations:

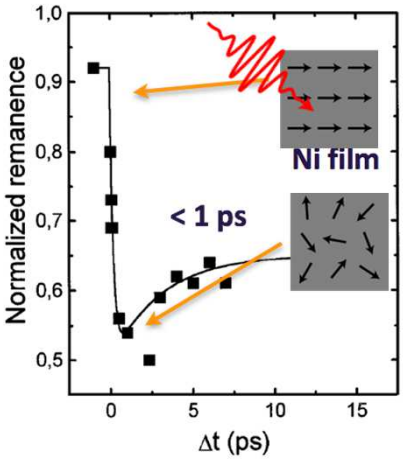


Schlappa et al., Nature (2012)

Optical Lasers:

- **See the ultra fast**

Time scales of sub-ps:

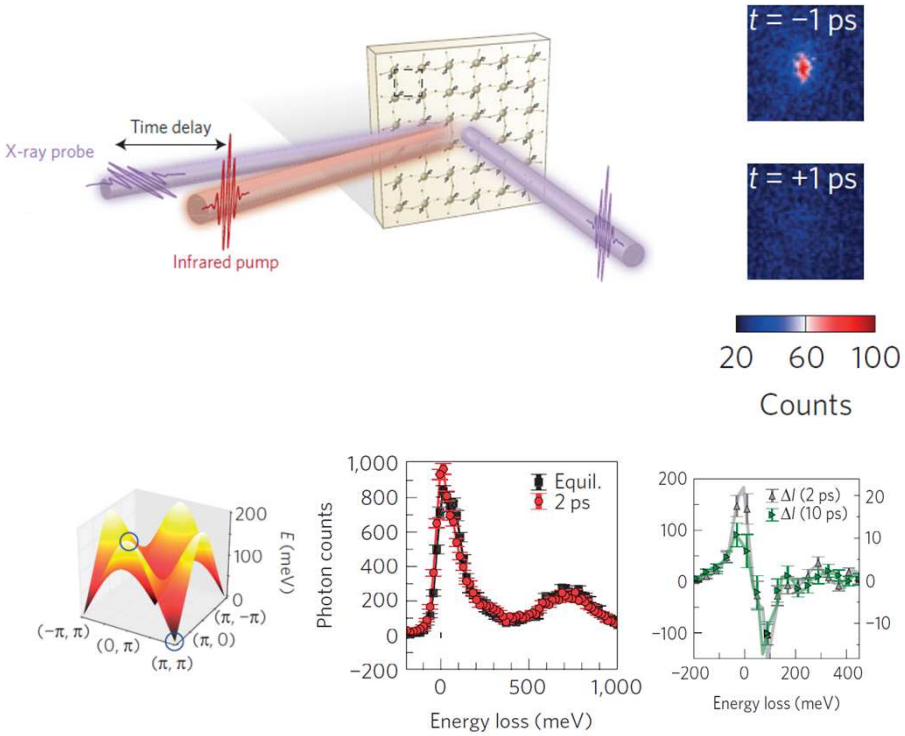


Beaurepaire et al. PRL (1996)

X-ray Lasers: • See the ultra small
• See the ultra fast

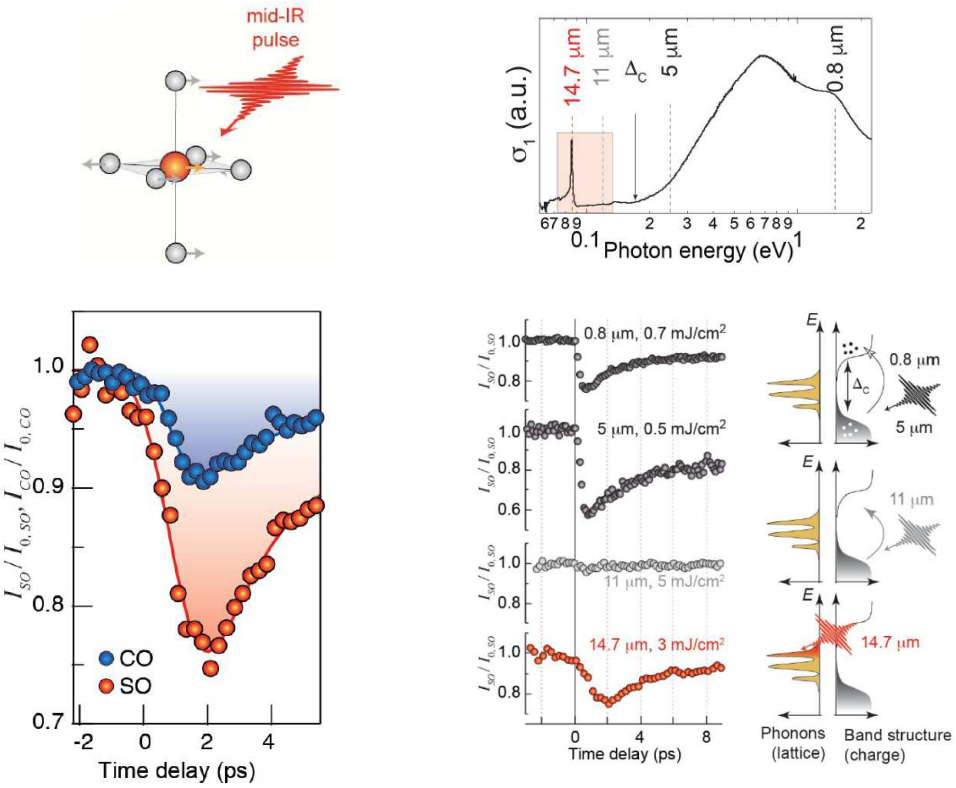
X-ray free-electro laser: examples

Magnetic correlation dynamics in 3D and 2D:



M. Dean et al., Nature Mat 15, 601 (2016).

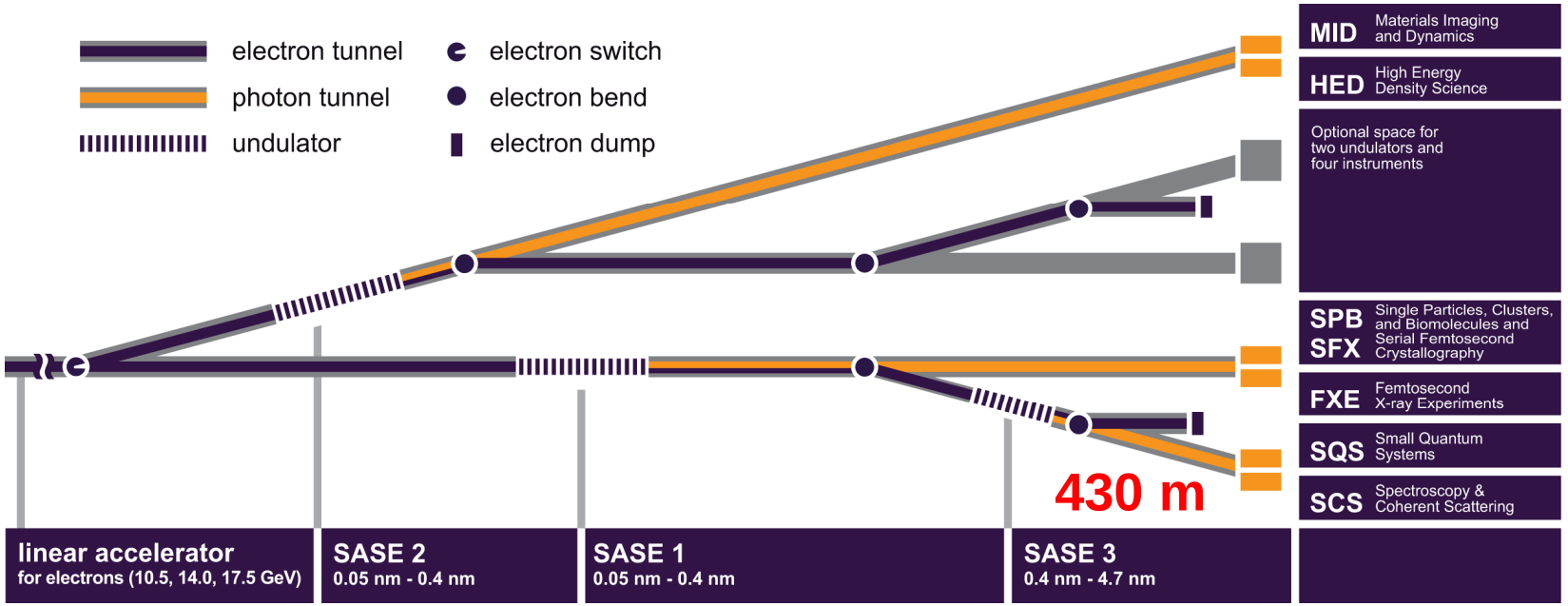
Resonantly driven dynamics:



W.S. Lee et al., Phys. Rev. B 95, 121105 (2017).

European XFEL: Photon beam transport system

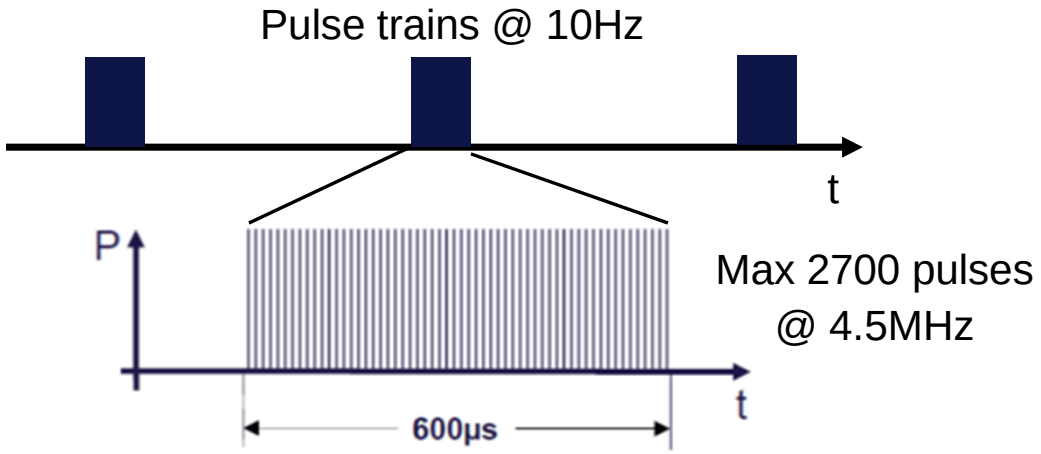
Undulator Segment	FEL radiation energy [keV]	Wavelength [nm]
SASE 1	3 - over 24	0.4 - 0.05
SASE 2	3 - over 24	0.4 - 0.05
SASE 3	0.27 - 3	4.6 – 0.4



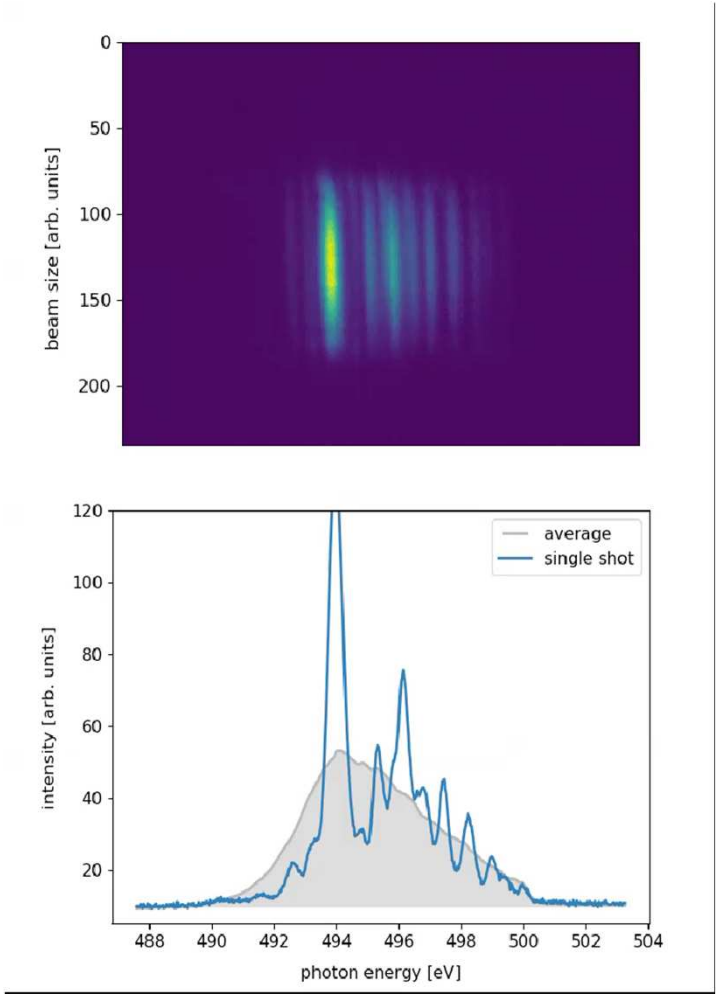
Orange color: X-ray optics & Beam Transport

SASE3 parameter

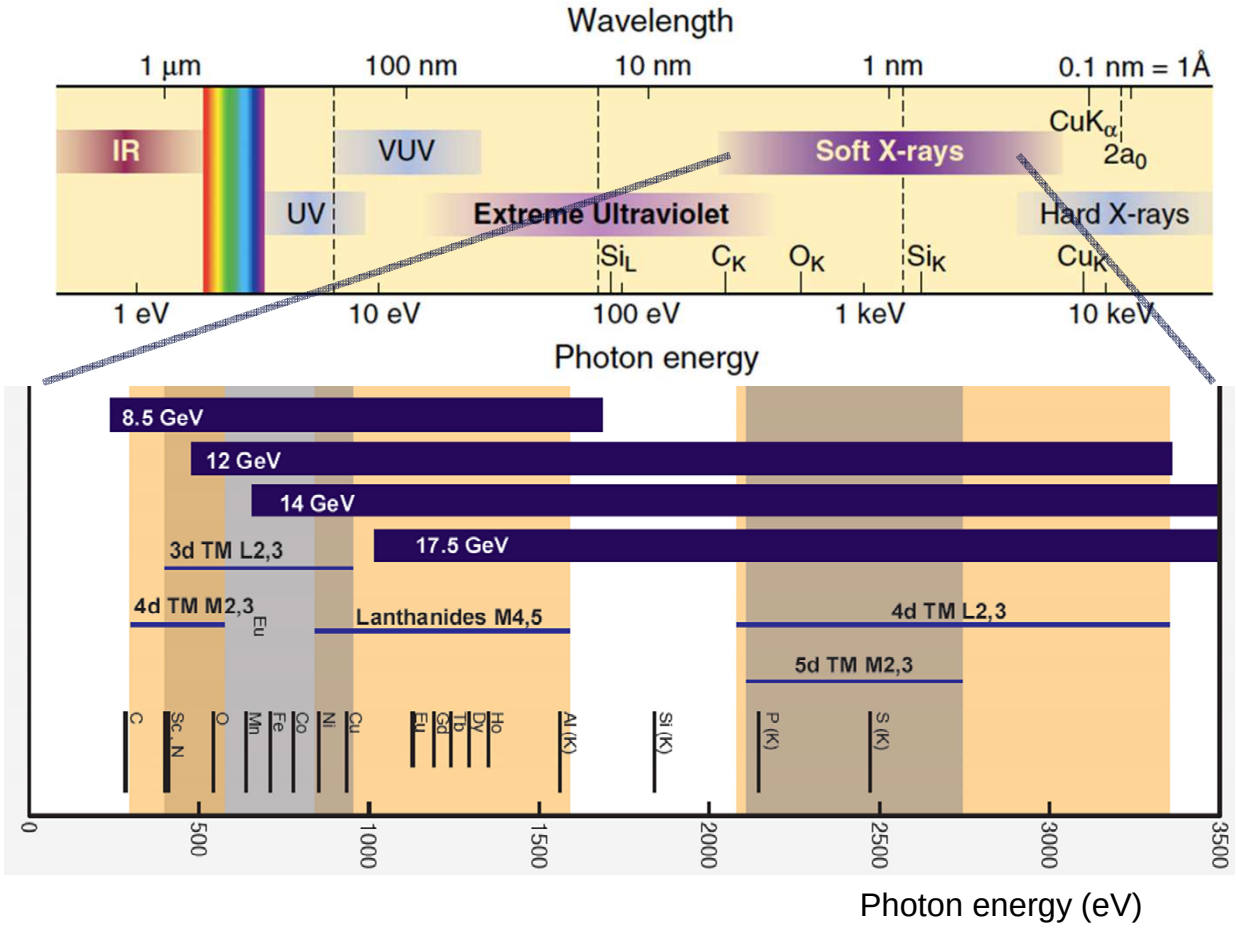
Photon beam parameters	
Photon energy	0.25 – 3.0 keV
Bandwidth	0.5 – 1.0 %
X-ray pulse energy	0.5 - 3 mJ
X-ray pulse duration	25 fs
Mono resolving power	2500-5000 @ 1 keV



Max 2700 pulses
@ 4.5MHz

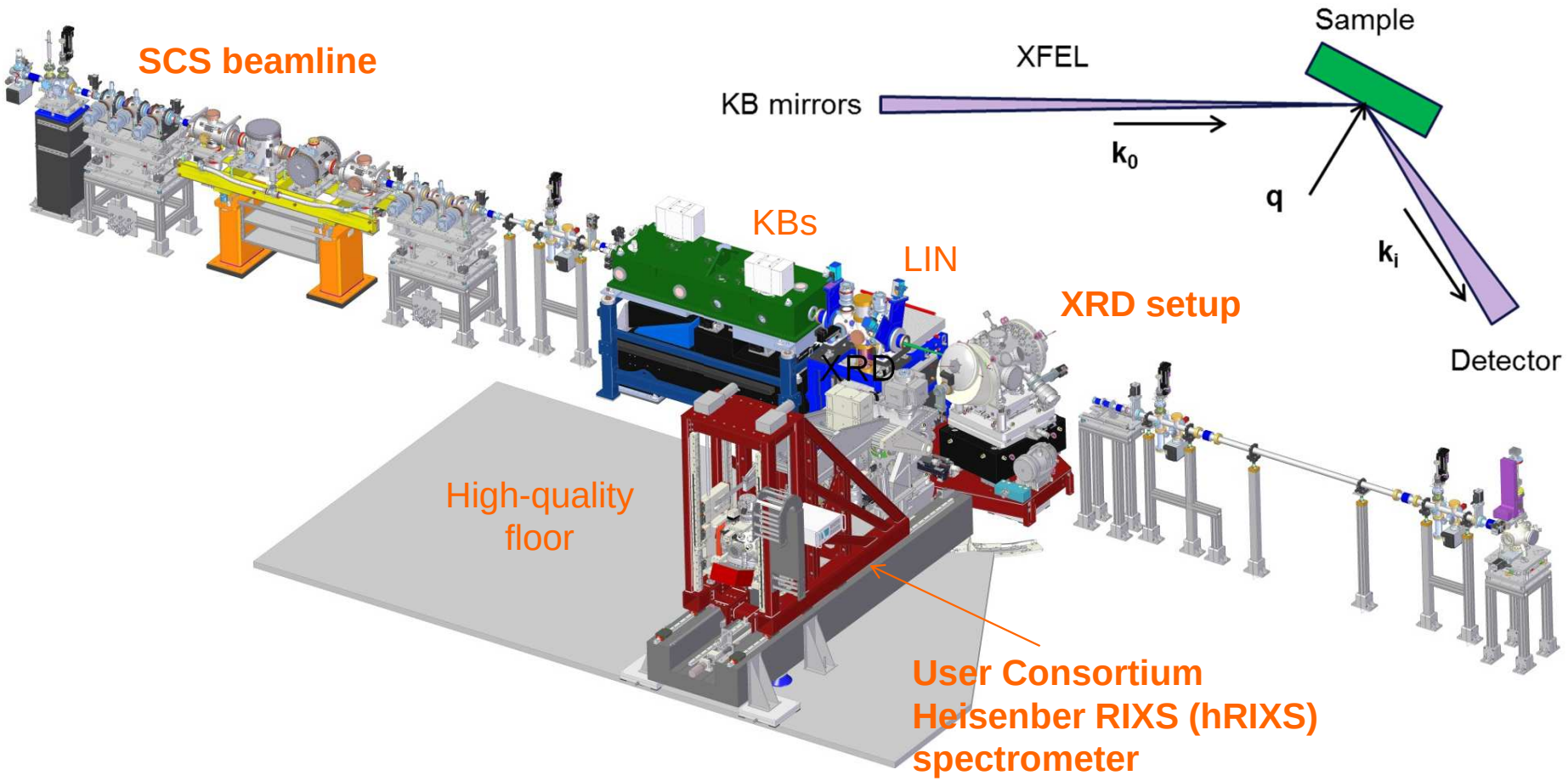


Soft X-ray region: probing electronic structure on nanometer length scales

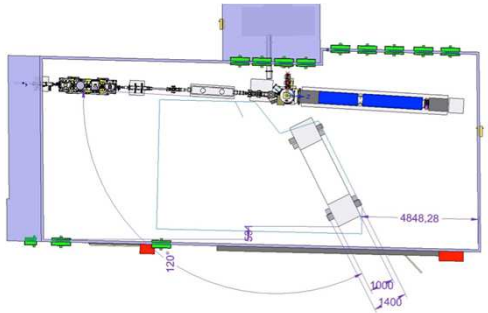


- Absorption resonances to probe the electronic states with elemental, chemical and magnetic sensitivity
- Wavelength to probe the electronic structure at nanometer length scales
- Nondestructive spectroscopy mode on solids to study repeatable dynamics
- Destructive single shot modes to probe nonlinear X-ray matter interactions and dynamics that cease to be repeatable

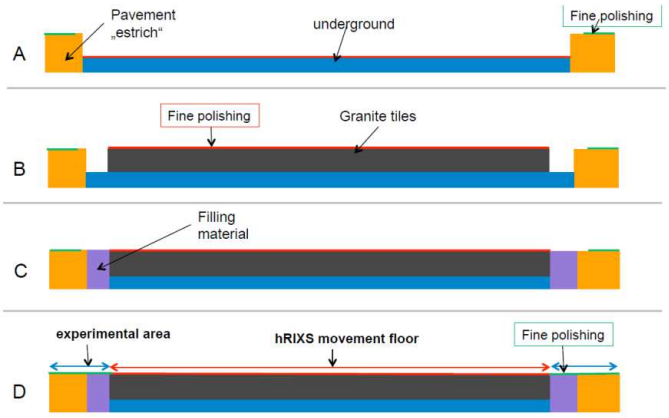
Elastic and inelastic x-ray scattering at SCS instrument



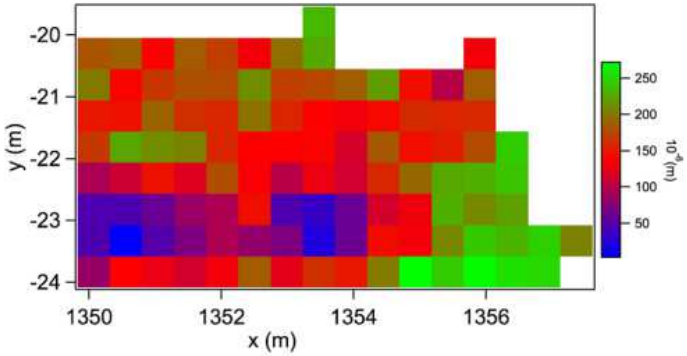
SCS high-quality floor:



Installed in October 2015:

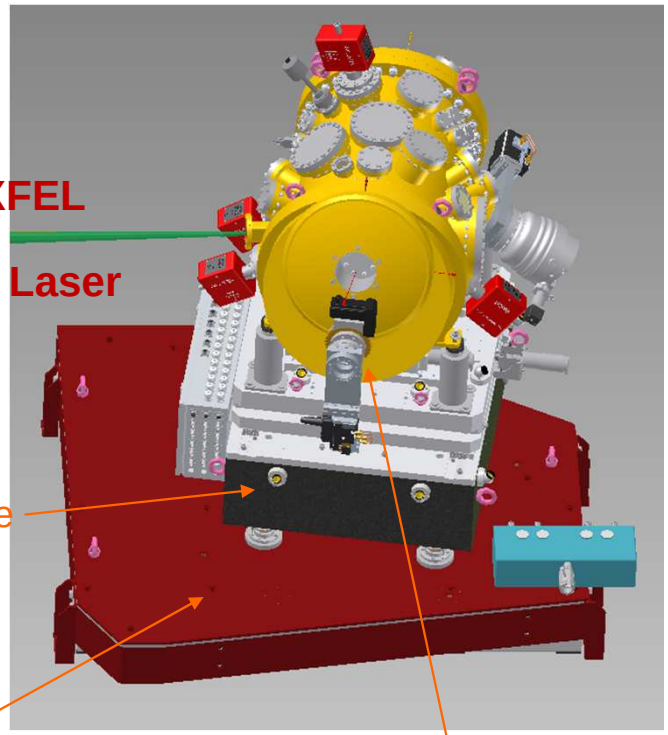


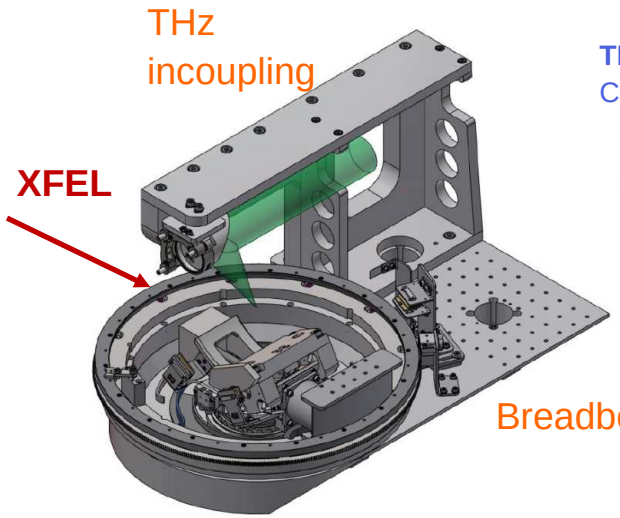
Deviation from average height:



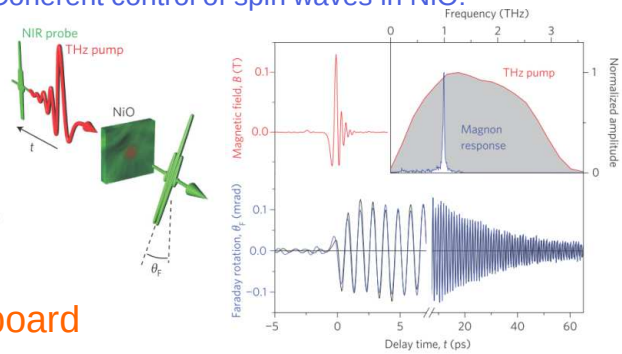
→ Average planarity over 1 m^3: 54 µm

Baseline setup for X-ray Resonant Diffraction (XRD setup)





THz pump:
Coherent control of spin waves in NiO:

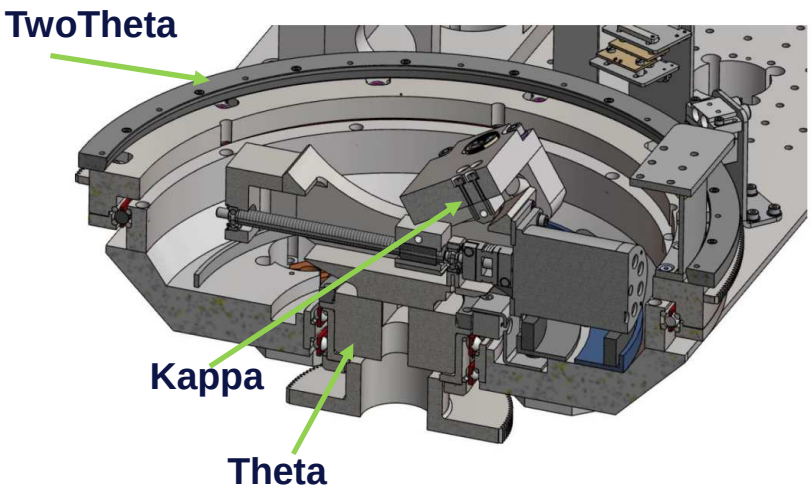


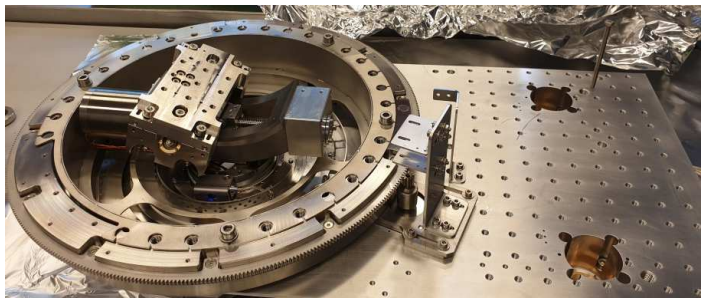
T. Kampfrath *et al.*, Nature Photon. 5, 31 (2012).

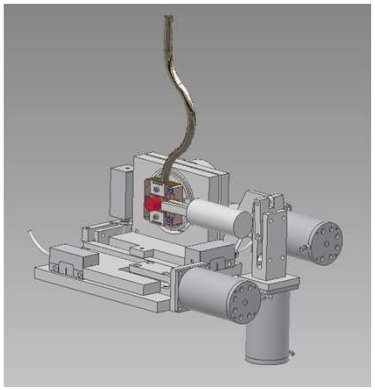
- UHV ($p < 10^{-9}$ mbar)
- Triple rotating flange: 60 deg ≤ 2Θ ≤ 150 deg, angular acceptance: 5 deg x 2.8 deg (H x V)
- 3-circle diffractometer, 6 DOF of motion for sample
- Mirror + Bradboard for THz + off-collinear laser incoupling
- High stability of entire inner mechanics

BESTEC

Baseline XRD setup inner mechanics







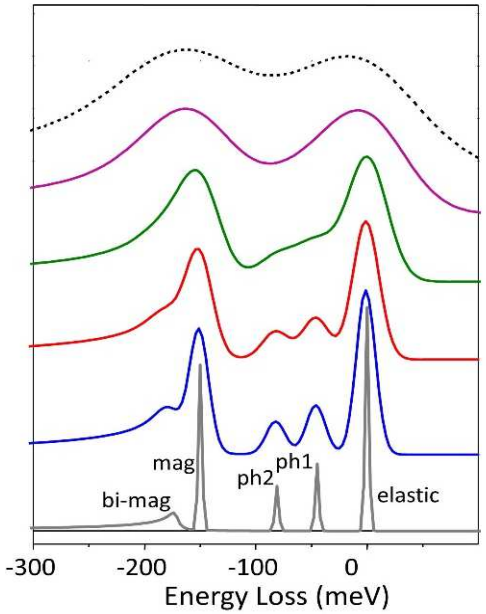
Sample stage

- 3-circle diffractometer: sphere of confusion < 25 µm
- Sample stage: 3 translations + 1 rotation
- Cryogenic studies down to at least 20 K
- Sample transfer system, sample garage with 10 places

Motion	Range	Repeability
TwoTheta	± 180 deg	< 0.002 deg
Theta	± 180 deg	< 0.002 deg
Kappa	± 30 deg	< 0.002 deg
Azimuth	± 90 deg	< 0.1 deg
TX	± 5 mm	< 0.5 µm
TY	± 5 mm	< 0.5 µm
TZ	± 5 mm	< 0.5 µm

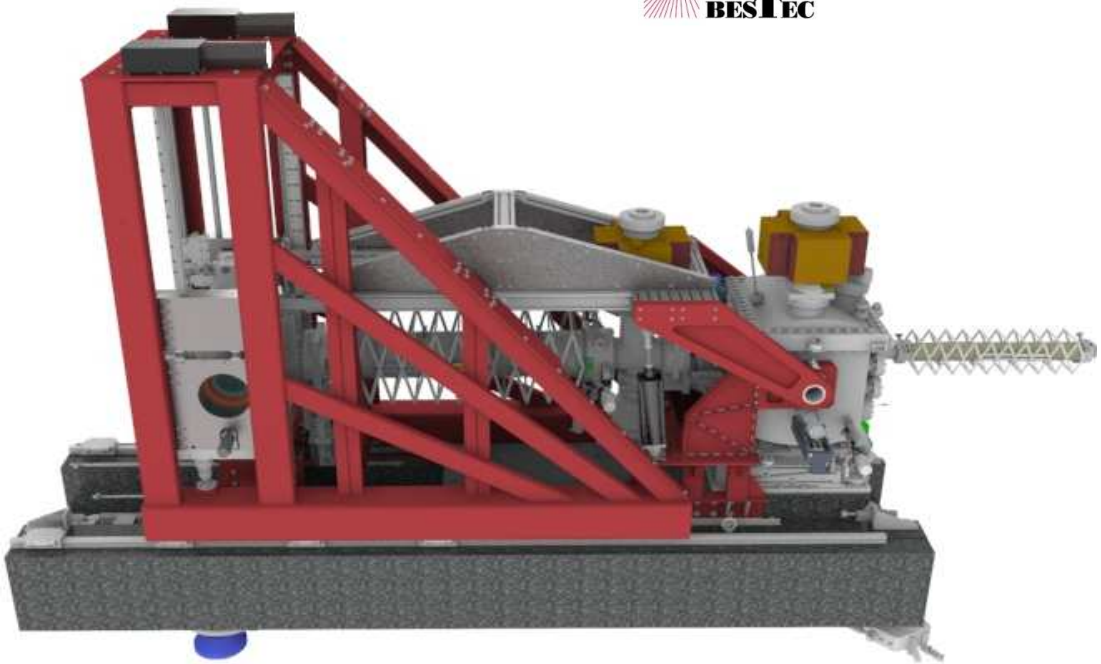
hRIXS: Heisenberg RIXS User Consortium spectrometer

Time-resolved RIXS at the transfer limit:



E/ΔE	Δt (fs)@ 1 keV	Δt (fs)@ 300 eV
7000	28	93
10000	41	137
20000	82	273
30000	123	410
40000	165	550
∞		

$\Delta t = h/\Delta E$



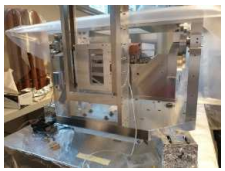
BESTEC

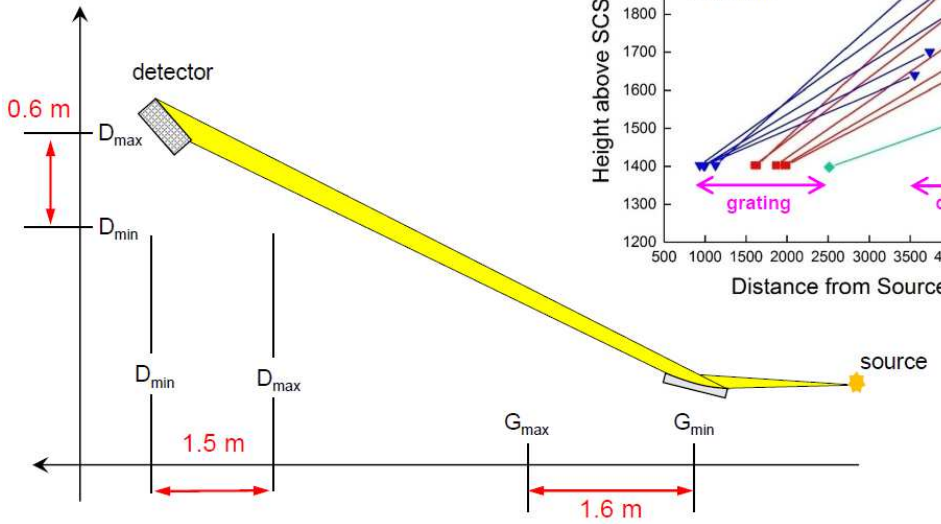
HELMHOLTZ ASSOCIATION

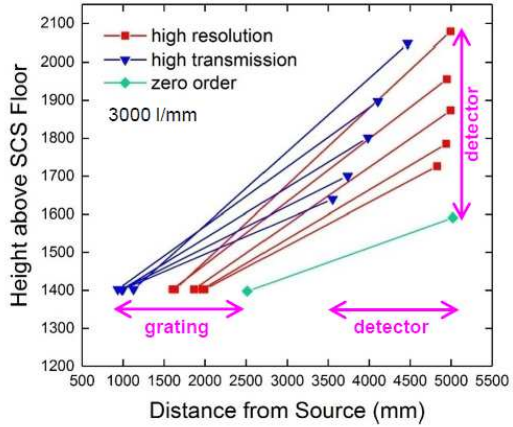
erc European Research Council

FIRI FINNISH RESEARCH INFRASTRUCTURES

hRIXS spectrometer: optical & mechanical design



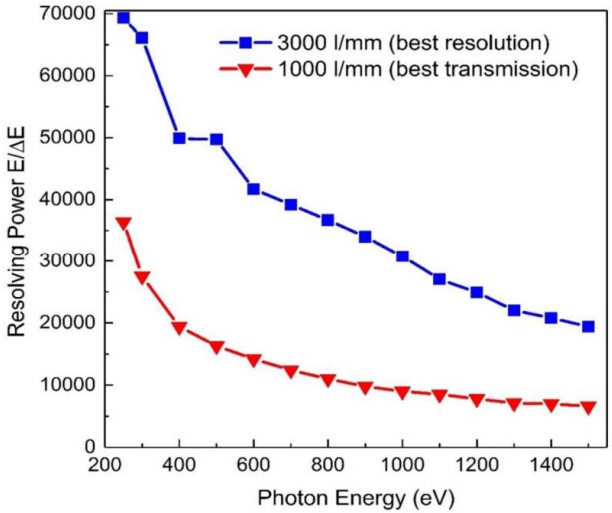


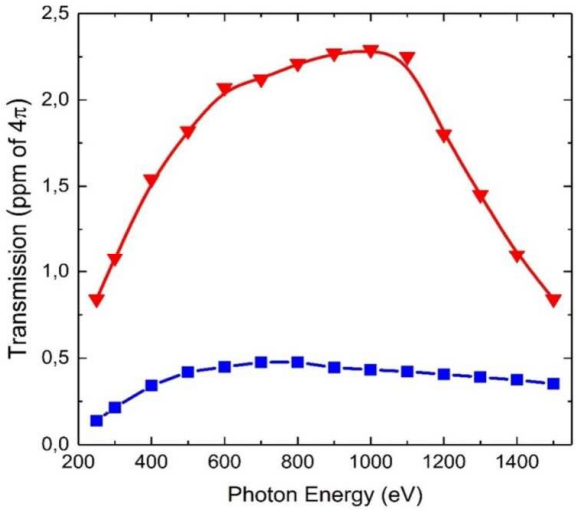


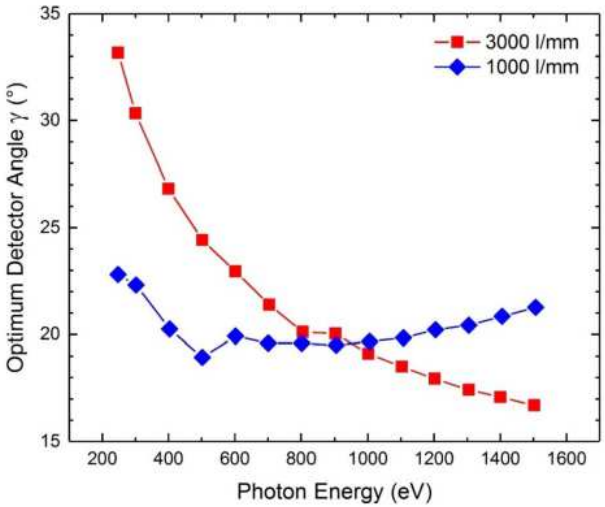
- Single optical element -> ease of alignment and operation
- Constrained VLS parameters
- optimisation for working range: 270 – 1500 eV with one grating
- Large mechanical travel range, high precision and stability

G. Ghiringhelli, Y.Y. Peng, F. Senf

hRIXS spectrometer performance







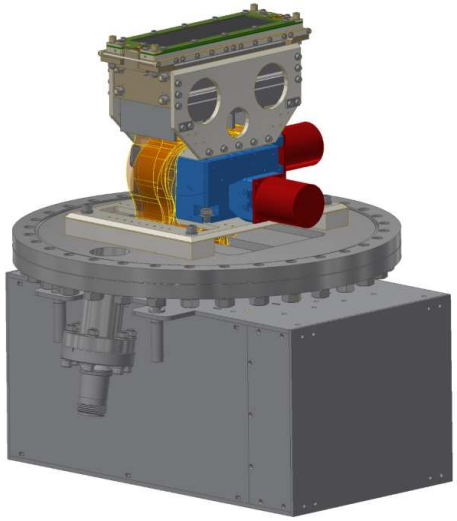
Ray tracing results for 5 µm vertical spot size and 10 µm effective spatial detector resolution

- Two gratings: 1000 l/mm and 3000 l/mm
- Laminar profile, Gold-coated
- Grating size: 40 x 200 mm^2

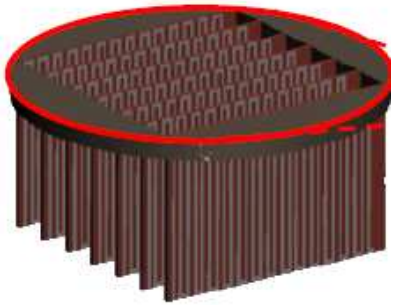
G. Ghiringhelli, Y.Y. Peng, F. Senf

Detectors

Pulse-resolved multi-hit detector:



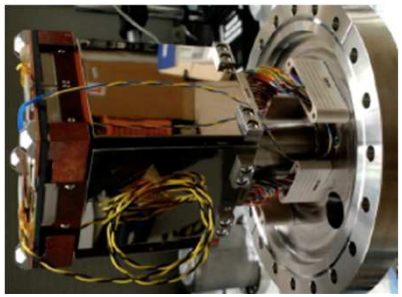
128-fold multi-DLD



- sensor area: 160 x 50 mm^2
- spatial resolution: 30-50 µm
- temp. resolution: < 200 ps

Pulse-integrated SCS detector:

Fast CCD:

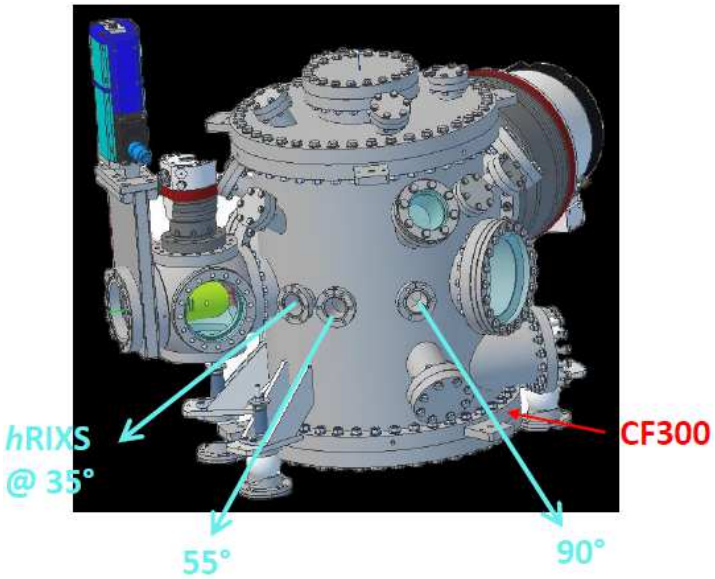


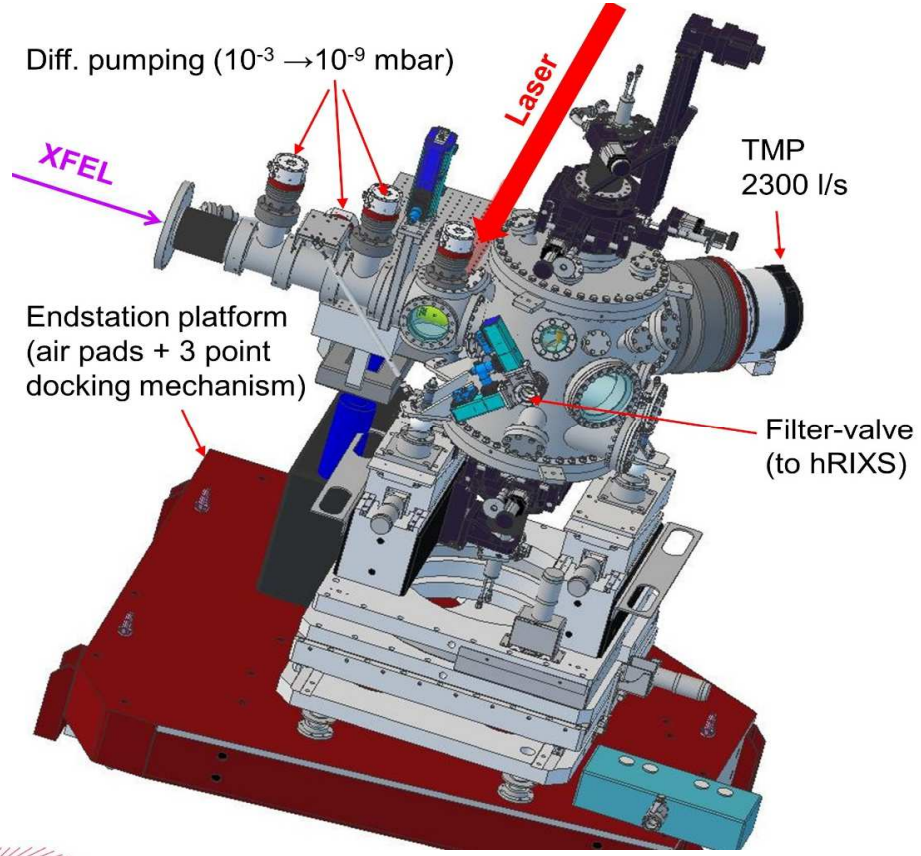
- sensor area: 58 x 29 mm^2
- spatial resolution: 30 µm
- Max. frame rate: 60 Hz
- Dynamical range: 10^3

Commercial detectors:

- 2D Delay-line (pulse-resolved)
- in-vacuum CCD (higher spatial resolution)

Chemistry chamber of Heisenberg RIXS UC





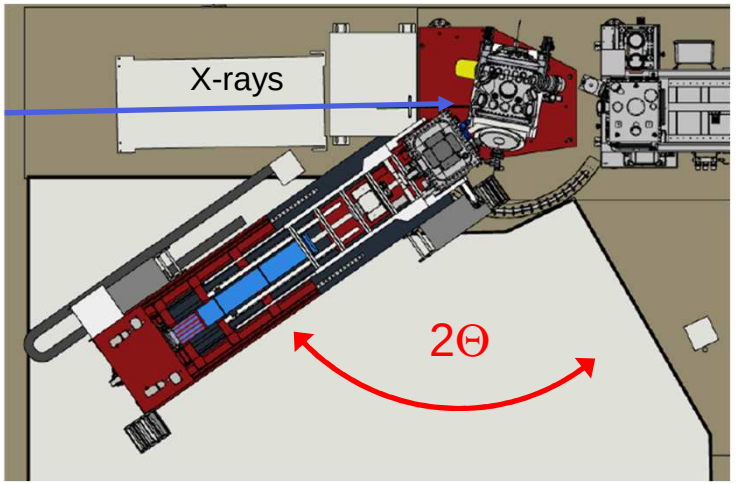
- Base pressure: 10^{-3} - 10^{-9} mbar
- Three fixed scattering angles: 90, 125 and 145 deg
- Liquid jet system + catcher / cryotrap
- Optional horizontal mount of liquid jet
- Differential pumping unit

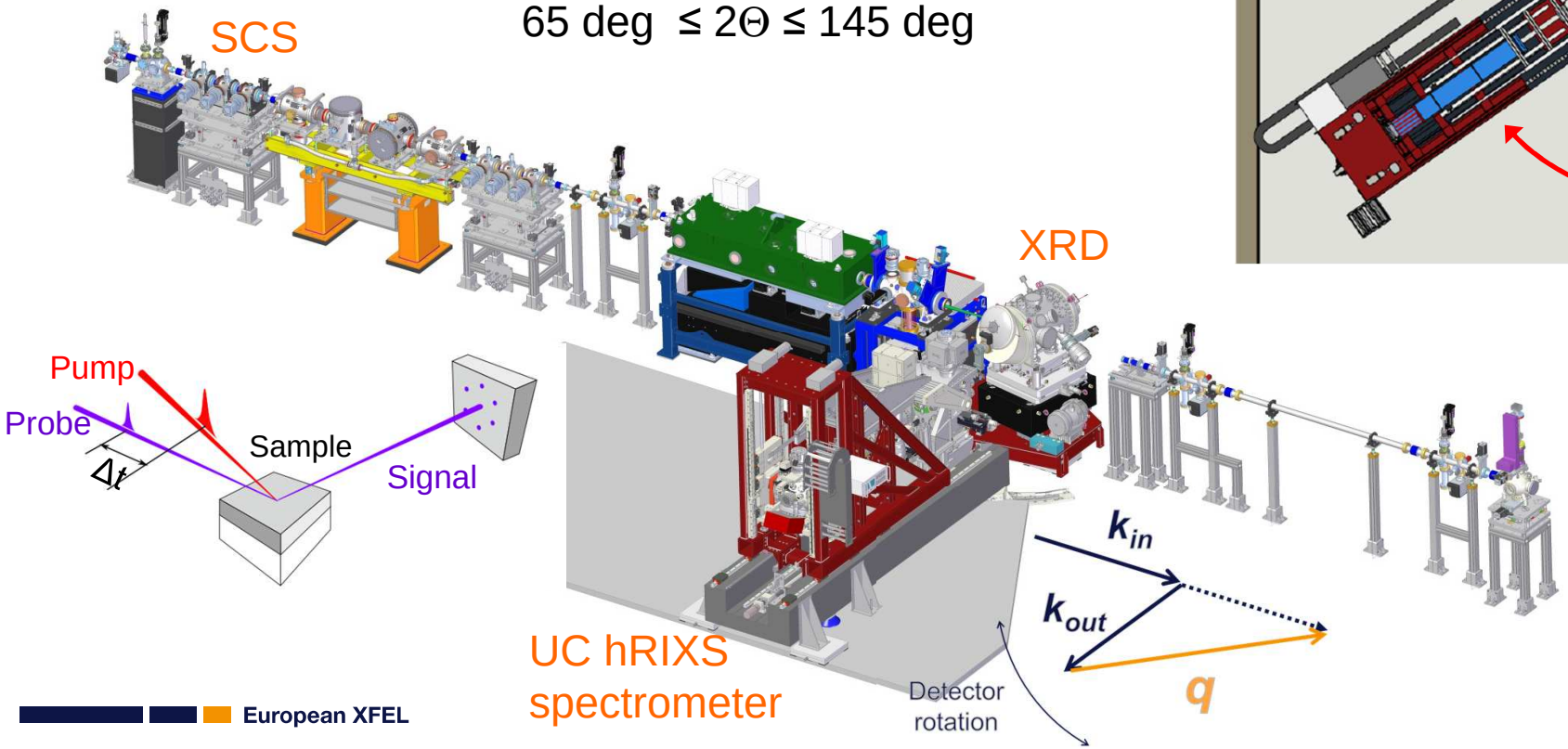
BESTEC

Momentum- and time-resolved RIXS at SCS instrument:

Combined continuous motion
in the scattering plane:

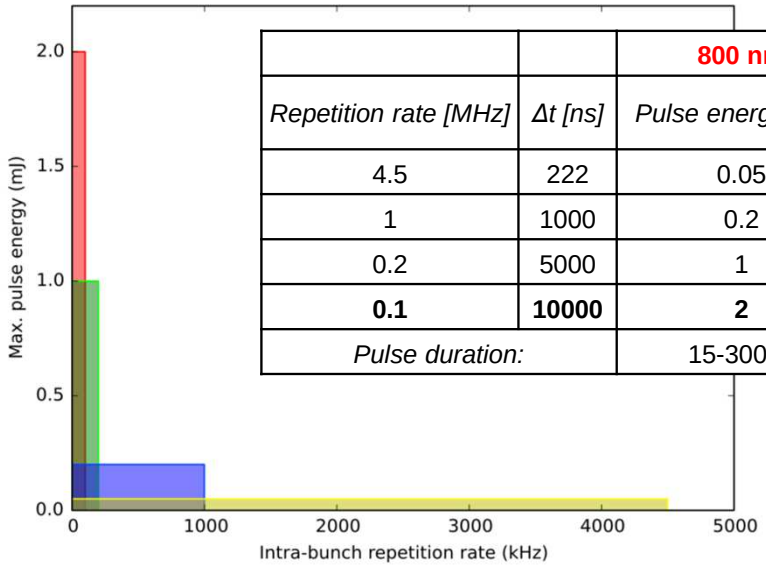
65 deg ≤ 2Θ ≤ 145 deg



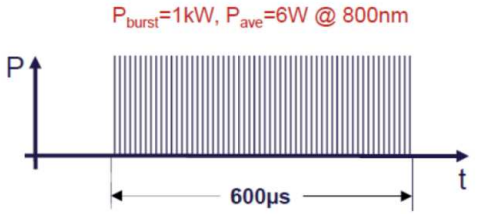


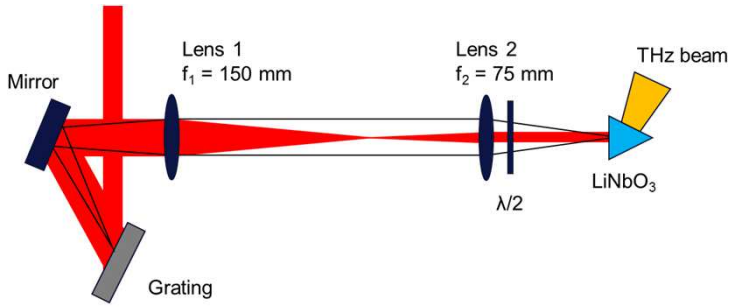
Pump-probe lasers at SCS:

- Fundamentals:
  - 800 nm and higher harmonics, down to 15 fs
  - 1030 nm and higher harmonics, above 400 fs
- Variable wavelengths:
  - TOPAS OPA: 250 nm – 10 µm
- THz:
  - Generation close to the sample, eg. LiNbO3 or DAST

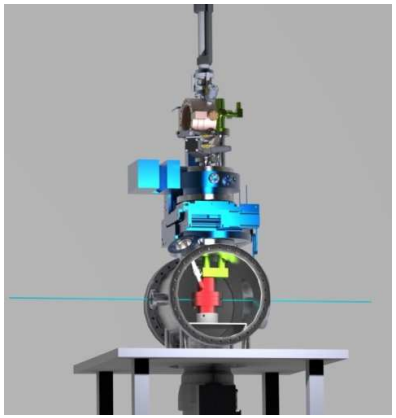


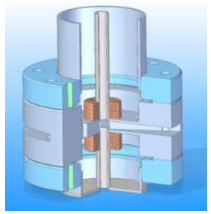
		800 nm	1030 nm
Repetition rate [MHz]	*Δt [ns]*	*Pulse energy [mJ]*	*Pulse energy [mJ]*
4.5	222	0.05	1
1	1000	0.2	4
0.2	5000	1	20
0.1	**10000**	**2**	**40**
Pulse duration:		15-300 fs	<1ps or 400 fs





In the near future: R&D setup

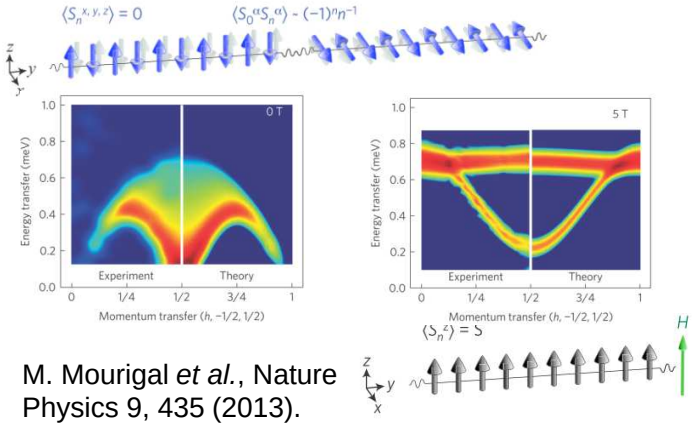




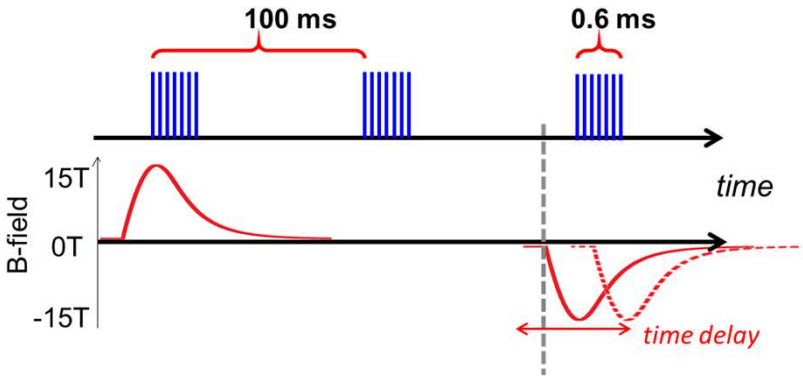
- External B-field, pulsed magnet, up to 15 T
- Cryogenic temperatures : 4–300 K
- Electrical conductivity measurements
- Specific user requirements

James Moore
Sample environment

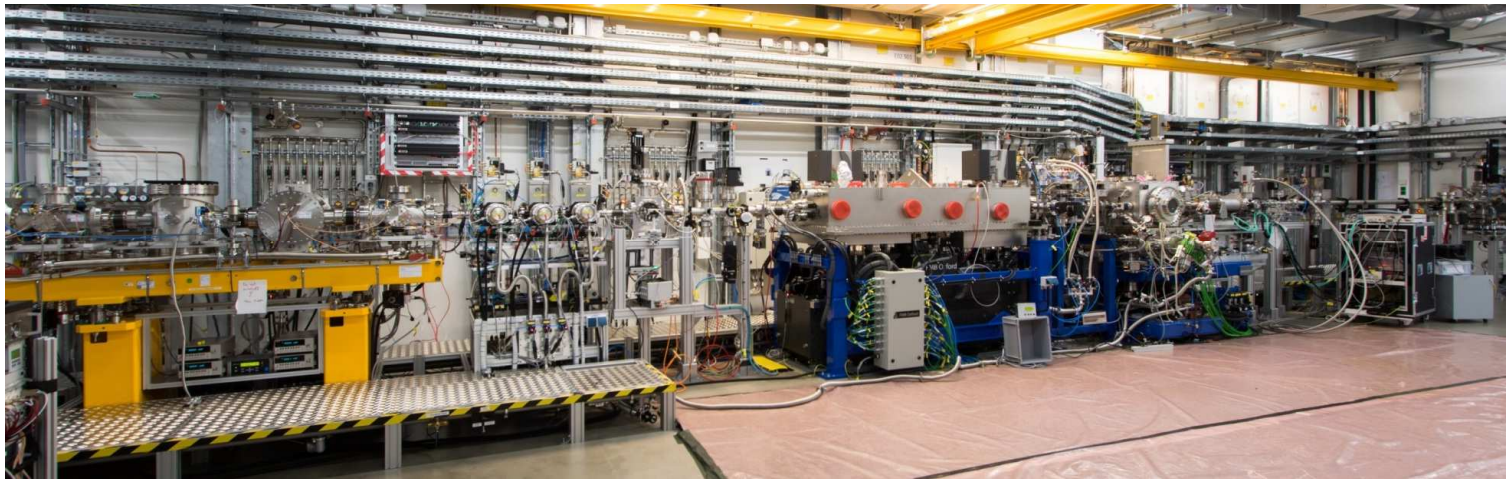
Magnetization of $CuSO_4 \cdot D_2O$:

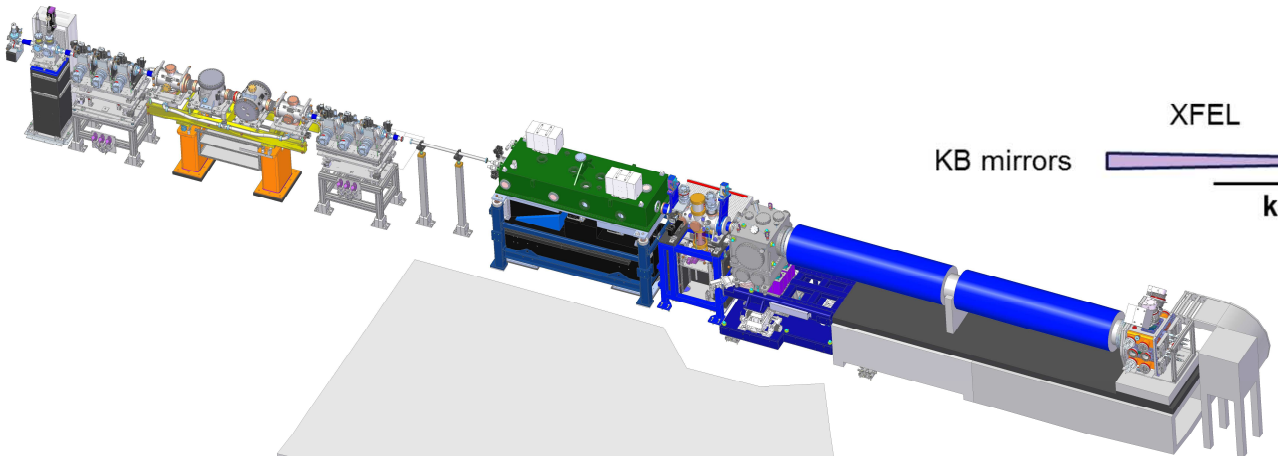


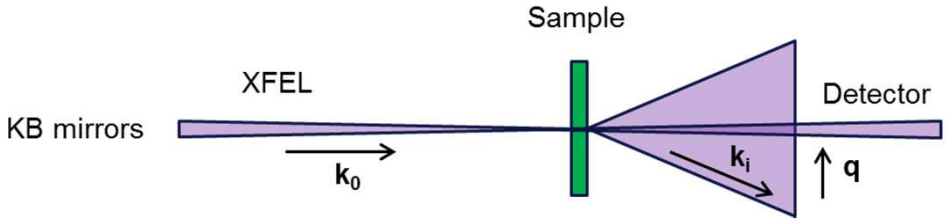
M. Mourigal *et al.*, Nature Physics 9, 435 (2013).



SCS instrument in operation for early users: since December 2018

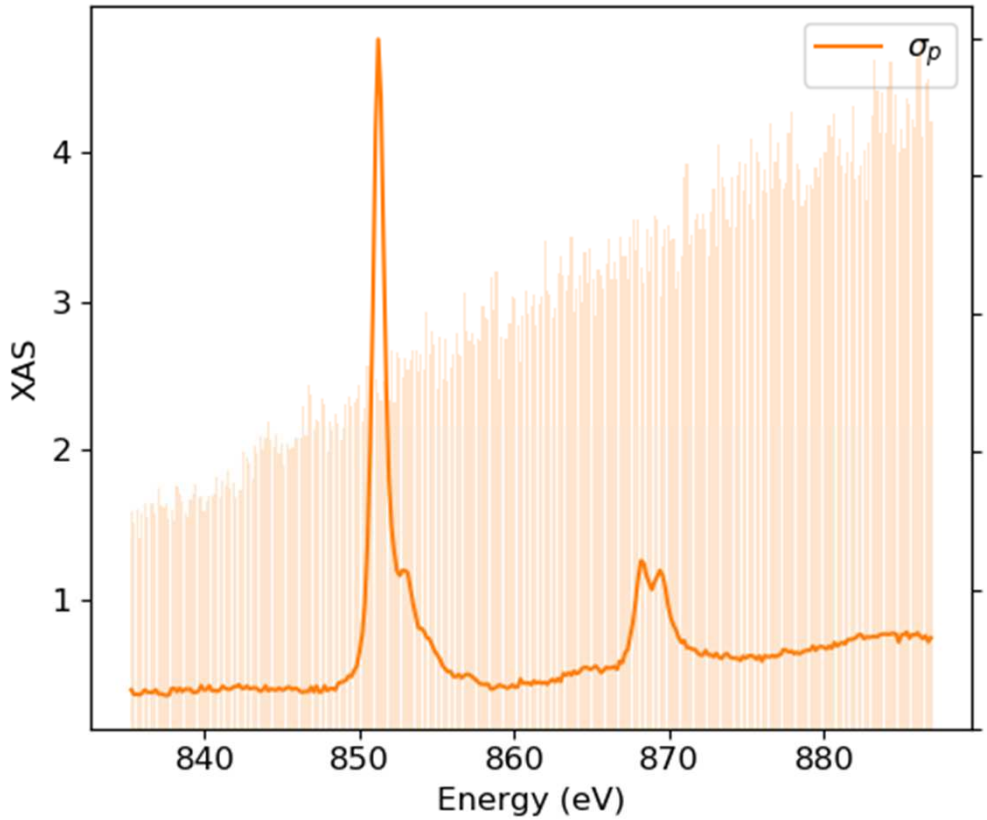






Femtosecond X-ray Absorption Spectroscopy: Monochromator and undulator gap scan

- NiO oxide
- XAS with Transmission Grating Zone Plates and Fast CCD
- transmission 0.08-0.1%
  1 pulse
- Gap scan parameters,
  grating speed: 0.00008 mm/s,
  undulators: 0.5 eV/step



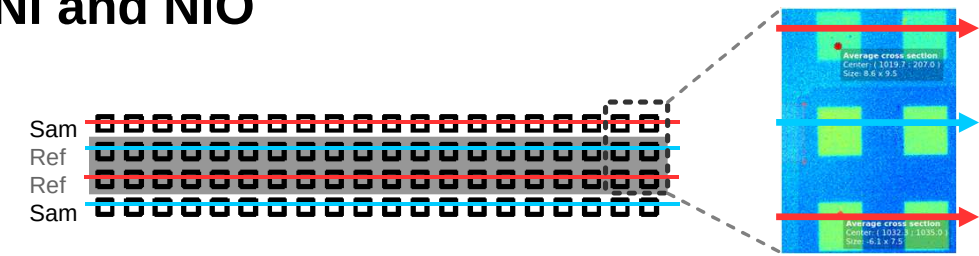
First users Dec. 5th, 2018
Open community proposal on efficient X-ray absorption spectroscopy at FELs: from nonperturbing fluences to nonlinear effects

Dr. Martin Beye (DESY)
Prof. Dr. Giacomo Ghiringhelli (Politecnico di Milano)
Dr. Christian David (Paul Scherrer Institut)
Dr. Benedikt Rösner (Paul Scherrer Institut)
Mr. Adam Kubec (Paul Scherrer Institut)
Prof. Dr. Kai Rossnagel (Univ. Kiel)
Dr. Ivan Baev (University of Hamburg (UHH))
Dr. Piter Miedema (DESY)
PD Dr. Tim Laarmann (DESY)
Dr. Michael E Stückelberger (DESY)
Prof. Dr. Simone A. Techert (DESY)
Dr. Craig Philip Schwartz (LBNL)
Prof. Dr. Jan Luning (HZB)
Dr. Katharina Ollefs (Univ. Duisburg-Essen)
Prof. Dr. Alexey Pavlovich Menushenkov (MEPhI, Moscow)
Prof. Dr. Frank de Groot (Univ. Utrecht)
Prof. Dr. Heiko Wende (Univ. Duisburg-Essen)
Prof. Dr. Uwe Bovensiepen (Univ. Duisburg-Essen)
Dr. Andrea Eschenlohr (Univ. Duisburg-Essen)
PD Dr. Gheorghe S Chiuzbaian (Lab. de Chimie Physique
Dr. Victoria Mazalova (DESY)
Prof. Dr. Peter Schwander (Univ. Wisconsin-Milwaukee)
Dr. Sam M. Vinko (Oxford Univ.)
Dr. Robert E Carley (EuXFEL)
Dr. Laurent Mercadier (EuXFEL)
Dr. Justine Schlappa (EuXFEL)
Dr. Alexander Yaroslavtsev (EuXFEL)
Dr. Giuseppe Mercurio (EuXFEL)
Dr. Natalia Gerasimova (EuXFEL)
Dr. Thomas Robert Preston (EuXFEL)
Dr. Manuel Izquierdo (EuXFEL)
Dr. Andreas Scherz (EuXFEL)
Dr. Loic Le Guyader (EuXFEL)
Prof. Dr. Artem Rudenko (Kansas State Univ.)
Prof. Dr. Jonathan Phillip Marangos (Imperial College London)
Dr. Daniel Higley (SLAC National Accelerator Lab.)
Dr. William F. Schlotter (SLAC National Accelerator Lab.)
Dr. Zhong Yin (ETH Zurich)
Dr. Marco Moretti (ESRF)
Dr. Jens Buck (Univ. Kiel)

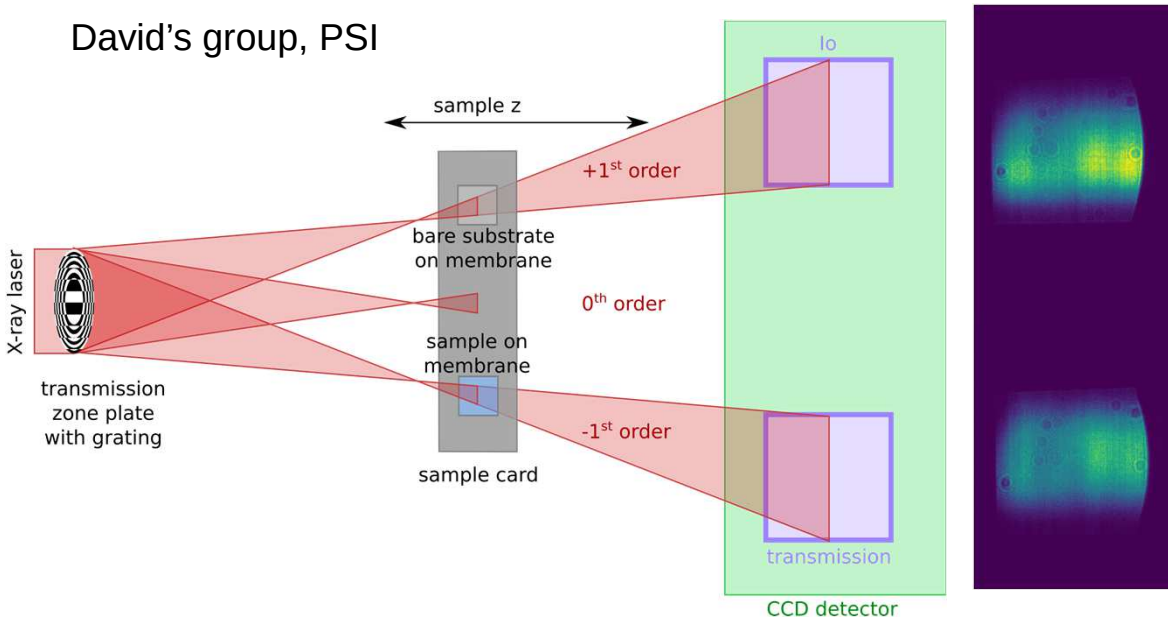
Single-shot X-ray absorption spectroscopy on Ni and NiO

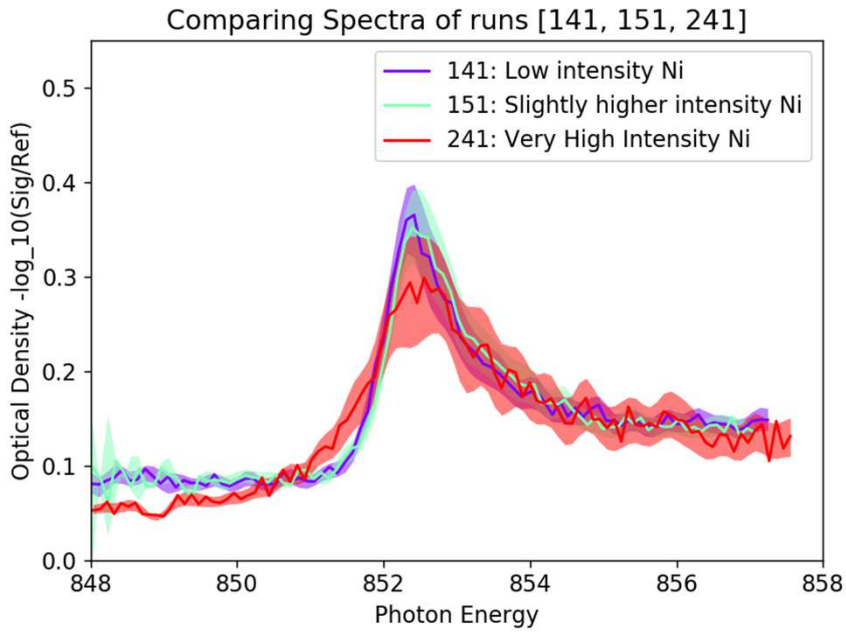
- Accurate shot-to-shot detection scheme
- Fluences from μJ/cm^2 to J/cm^2
- From non-perturbing to non-linear regimes
- Transmission grating / zone plate

  David's group, PSI



fCCD





Preliminary results !

Early User Workshop: hRIXS @ SCS, 21-22 January 2019

6 community proposals have been identified:

- Melting of stripe order in LSNO

Lead: E. Benckise, M. Minola and M. Mitrano

- Charge-transfer dynamics in NiO and CoO

Lead: T. Schmitt and J. Vale

- Spin correlations in photo-excited NiO and LCO

Lead: M. Moretti and M. Dean

- Dynamics of liquid water

Lead: J. Niskansen

- Stimulated x-ray scattering in liquids

Lead: V. Kimberg

- Ultrafast dynamics in metallic complexes

Lead: S. Neppl (HZB)

scs@xfel.eu

XRD & Chemistry stations and RIXS spectrometer
Installation and technical commissioning start 2019

Thank you!

SCS team , European XFEL: **scs@xfel.eu**

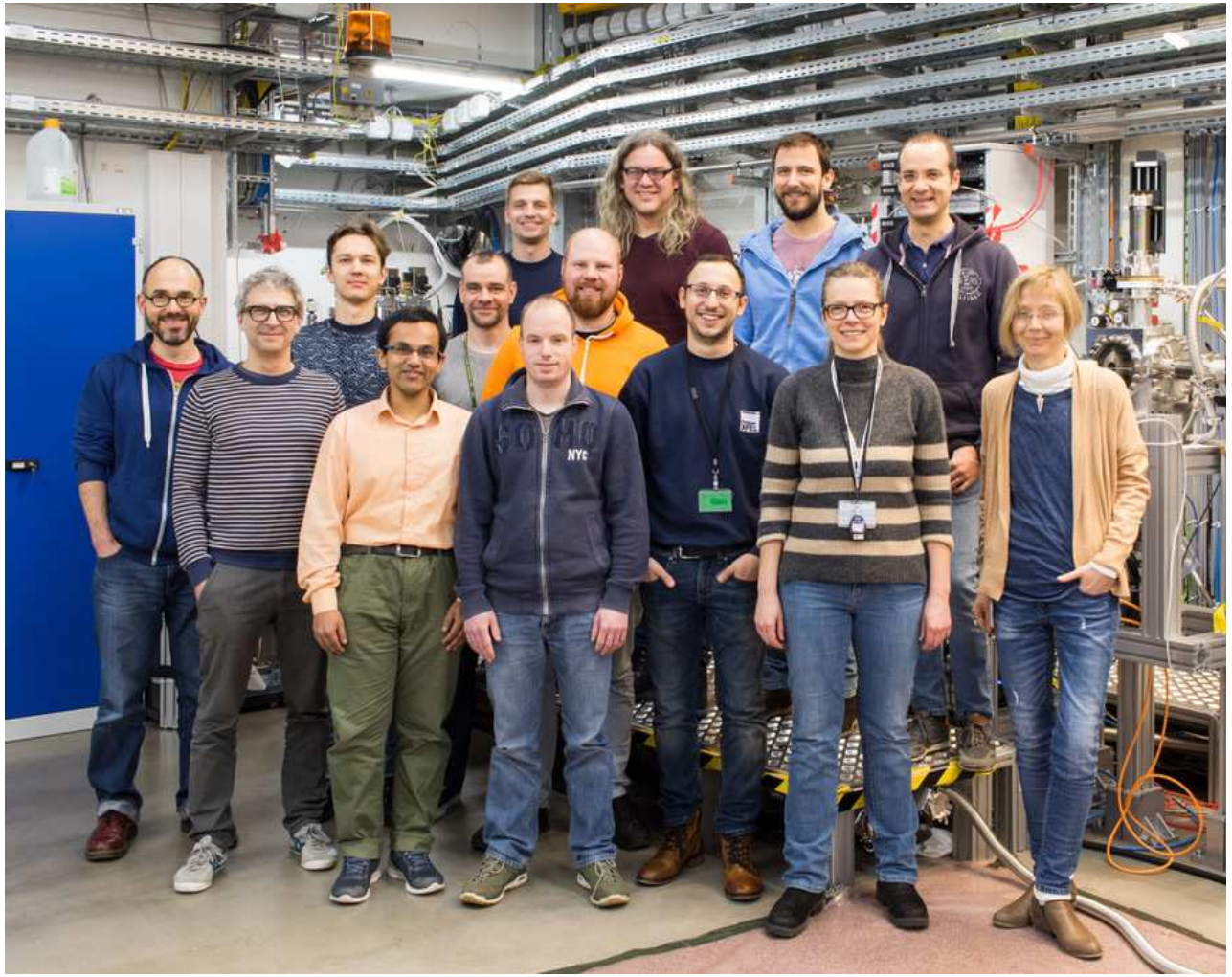
Andreas Scherz, Justine Schlappa, Robert Carley, Alexander Yaroslavtsev, Giuseppe Mercurio, Natalia Gerasimova, Loic Le Guyader, Laurent Mercadier, Manuel Izquierdo, Rafael Gort, Naman Agarwal, Martin Teichmann, Jan Torben Delitz, Alexander Reich, Carsten Broers

hRIXS User Consortium working group:

Stefan Neppl, Justine Schlappa, Jan Torben Delitz, Torben Reuss, Fred Senf, Annette Pietzsch, Tim Laarmann, Simone Techert, Simo Huotari, Giacomo Ghiringhelli, Andreas Scherz, Alexander Foehlisch

SCS team: scs@xfel.eu

Naman Agarwal
Lukas Behrens
Carsten Broers
Robert Carley
Jan Torben Delitz
Natalia Gerasimova
Rafael Gort
Loïc Le Guyader
Laurent Mercadier
Giuseppe Mercurio
Alexander Reich
Andreas Scherz
Justine Schlappa
Martin Teichmann
Alexander Yaroslavtsev



Run 5 – SCS instrument parameters

Photon beam parameters		
Photon energy	0.27 – 3.0 keV	
X-ray pulse energy	0.5 - 5 mJ (SASE3), 1-10µJ (Monochromatic)	
X-ray pulse duration	25 fs	(FWHM)
Mono resolving power	2500-5000 @ 1 keV	
Number of pulses per train	200*	(*) 200 pulses can be operated at 1.1MHz and in addition, may depend on specific conditions of operation. At reduced intra-train frequencies the pulse number reduces accordingly.
Repetition rate in pulse train	1.1 MHz	
Train repetition rate	10 Hz	
Polarization	Linear (horizontal)	
Focal spot size at sample, tunable	1-2 µm (hor, ver) up to 500µm	