Science at the SXP instrument

Manuel Izquierdo
Head SXP group

Patrik Grychtol
Laser specialist

David Doblas
Data Analyst

Vahagn Vardanyan
Mechanical Eng.

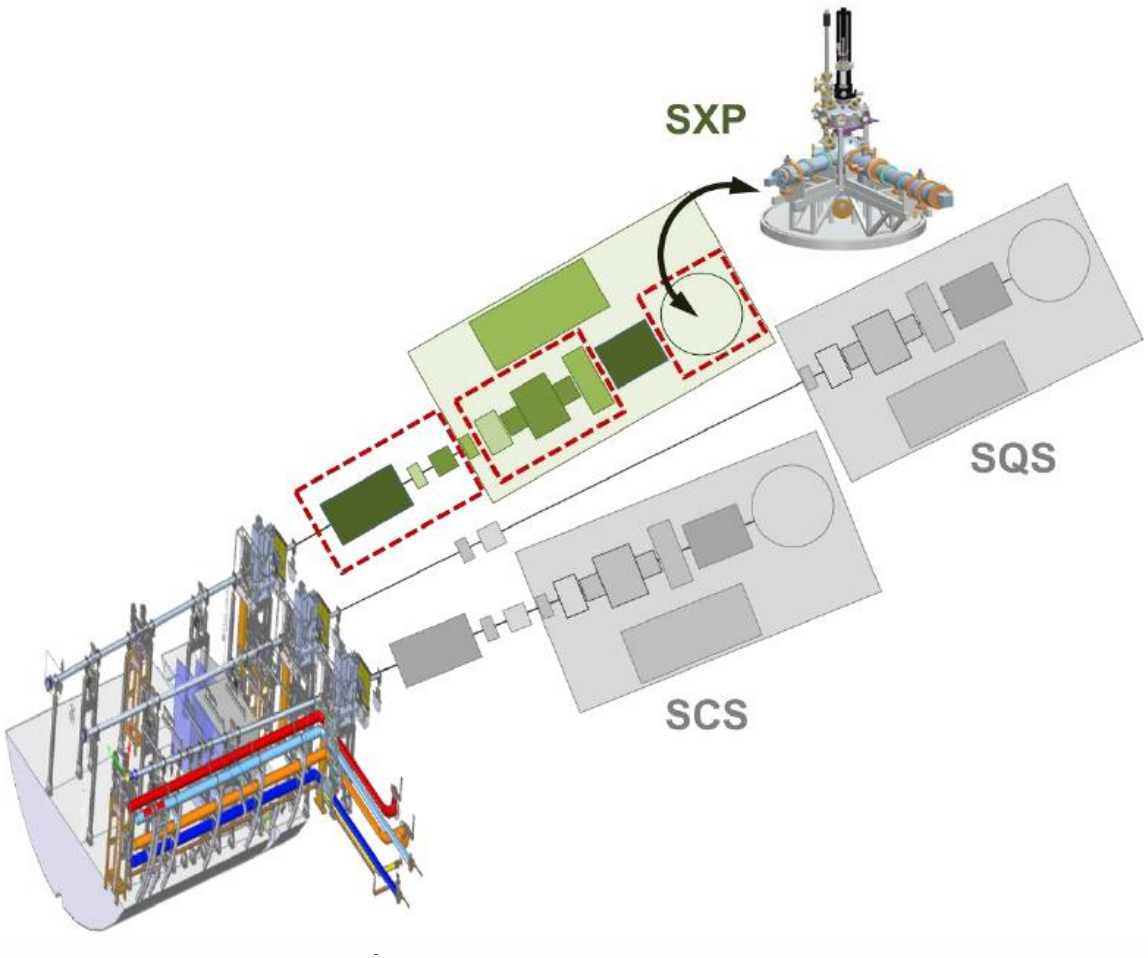
Ekaterina Tikhodeeva
PhD

Joshua Ohnesorge
Vacuum Eng. (1/3)

Maria Peter
Adm. Assistant

The 7th instrument SXP (Soft X-ray Port)

GL: Manuel Izquierdo

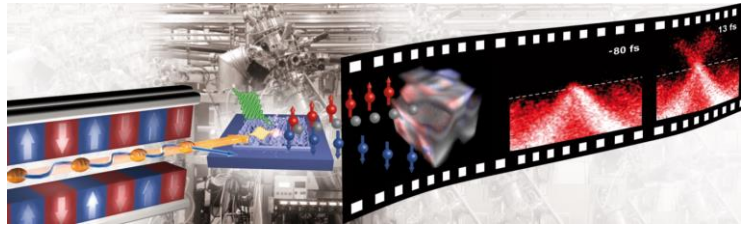


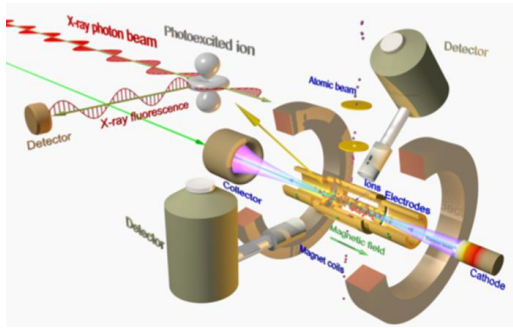
Complete Time-resolved X-ray Photoelectron spectroscopy

TR-XPES

K. Rossnagel
(Uni-Kiel/DESY)

G. Schönhense
(Uni. Mainz)





Laboratory for Astrophysics, atomic physics, fundamental research with highly charged ions

HCI

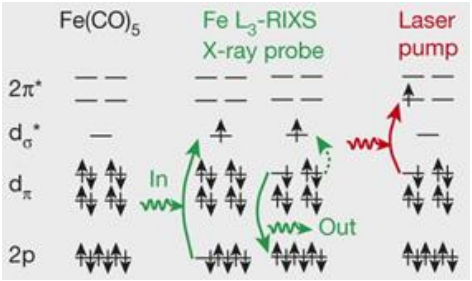
J. Crespo (MPI Heidelberg)

M. Meyer, T. Baumann (EuXFEL)

Understanding Catalysis and biochemistry by studying Chemical Bond Activation

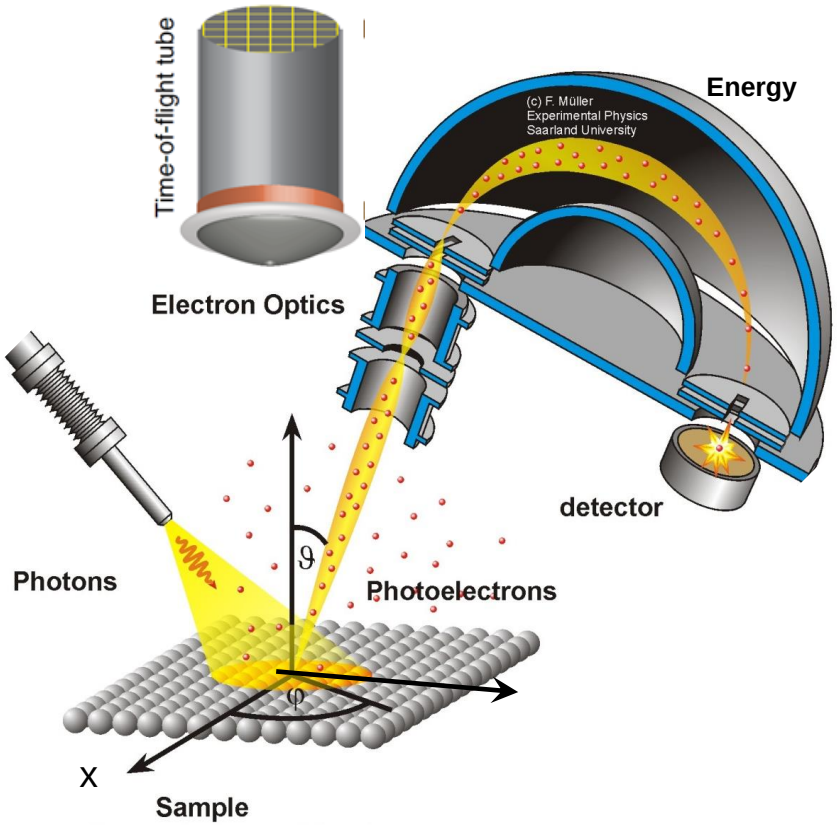
CBA

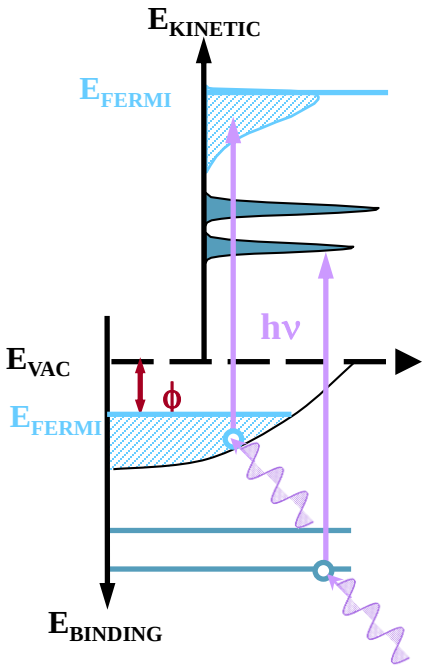
P. Wernet (Uni. Uppsala)

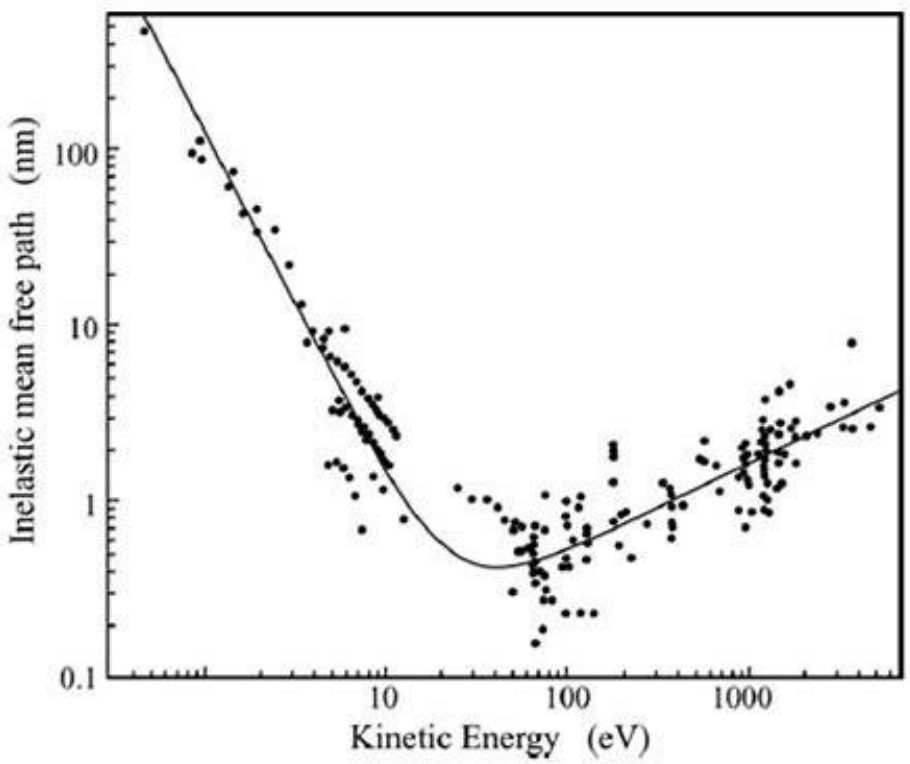


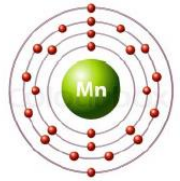
https://xfel.tind.io/record/2647?ln=en

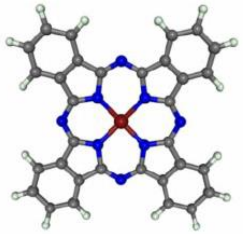
Photoelectron spectroscopy

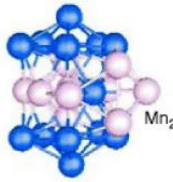


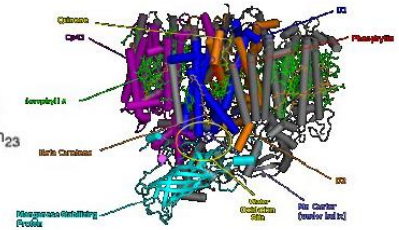


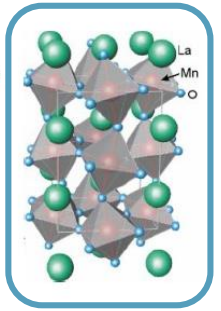










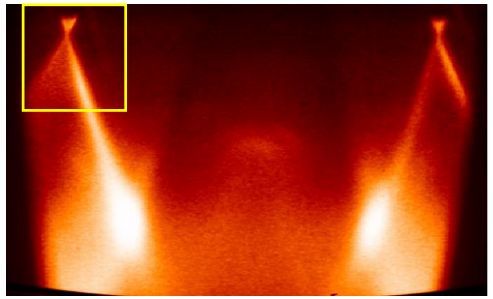


- Photoelectric effect $E_{kin} = h\nu - \Phi$
- A. Einstein: Nobel Prize Physics 1921

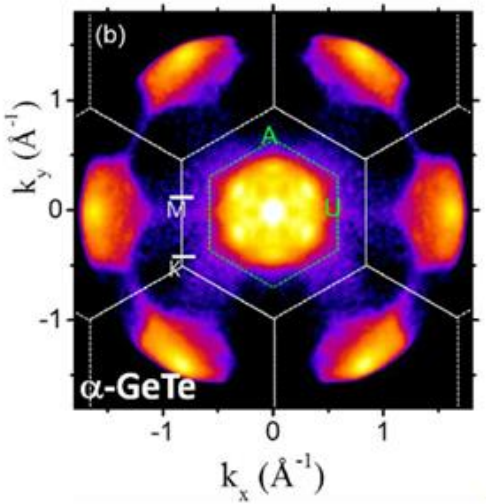
Photoelectron spectroscopy

UV regime

Band structure

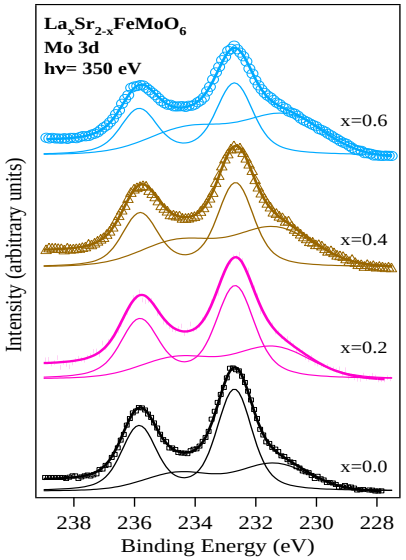


Fermi surface

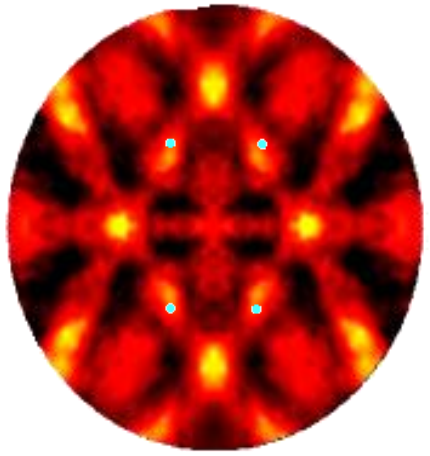


Soft X-rays

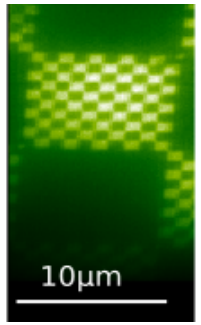
ESCA



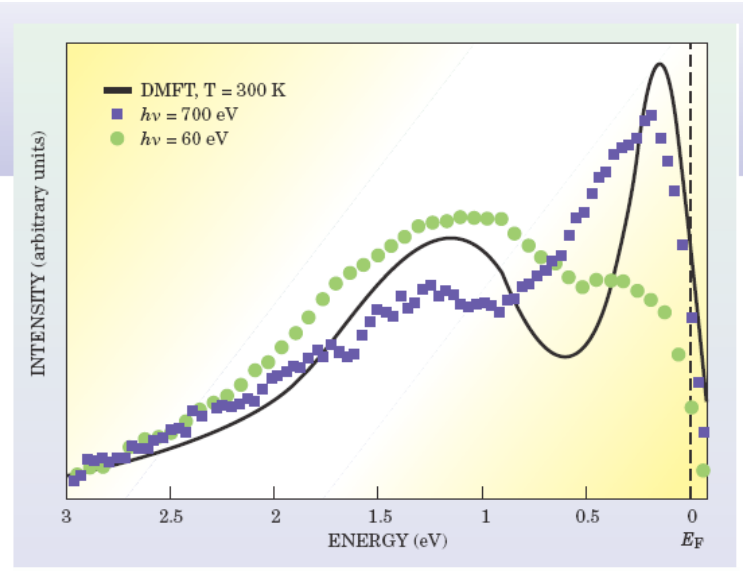
XPD



PEEM



Bulk vs surface

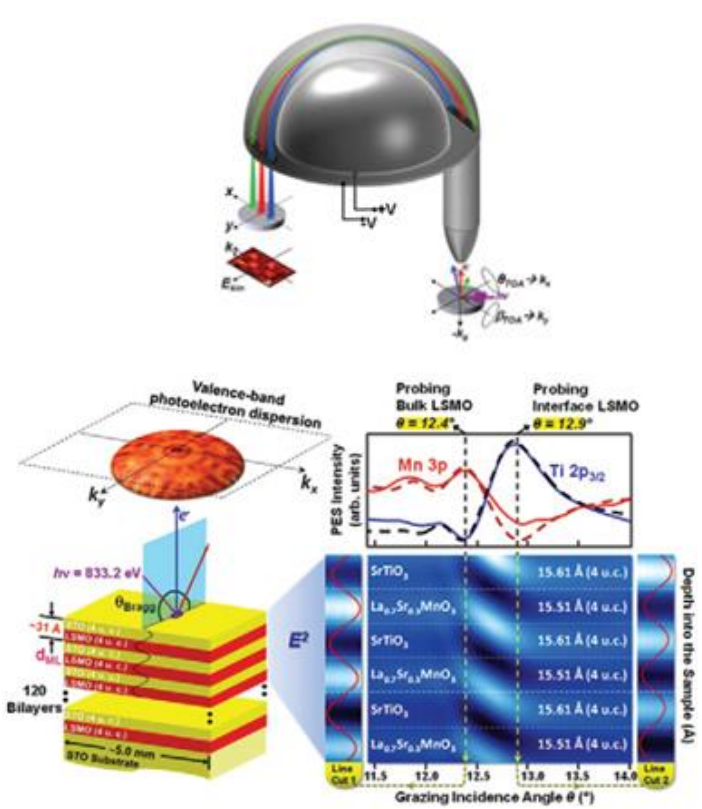


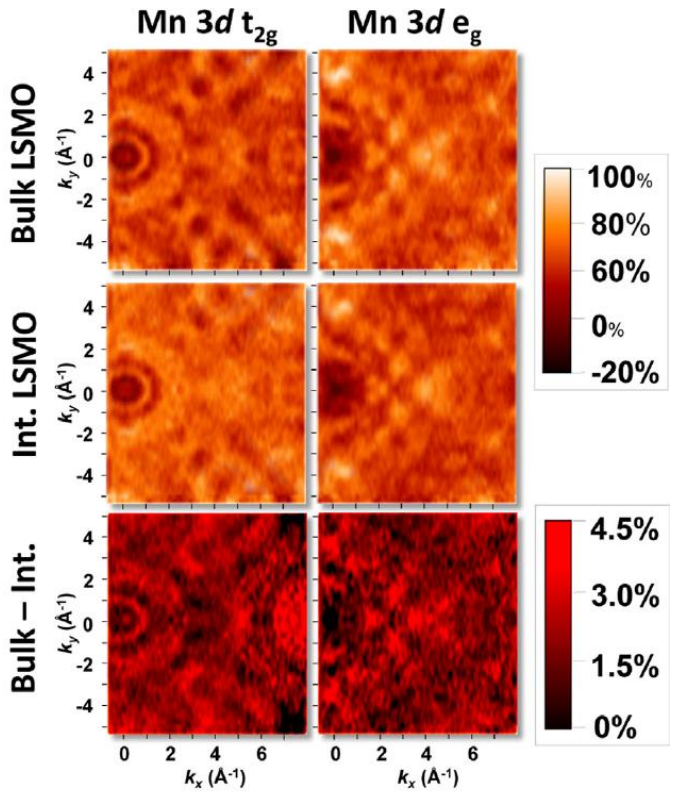
Gabriel Kotliar and Dieter Vollhardt
Physics Today 2004

Soft X-rays standing wave photoemission

Momentum-resolved electronic structure at a buried interface from soft X-ray standing-wave angle-resolved photoemission

A. X. Gray[1,2,3], J. Minár[4], L. Plucinski[5], M. Huijben[6], A. Bostwick[7], E. Rotenberg[7], S.-H. Yang[8], J. Braun[4], A. Winkelmann[9], G. Conti[1,2], D. Eiteneer[1,2], A. Rattanachata[1,2], A. A. Greer[1,2], J. Ciston[10], C. Ophus[10], G. Rijnders[6], D. H. A. Blank[6], D. Doennig[11], R. Pentcheva[11], J. B. Kortright[2], C. M. Schneider[5], H. Ebert[4] and C. S. Fadley[1,2]





ARTICLE

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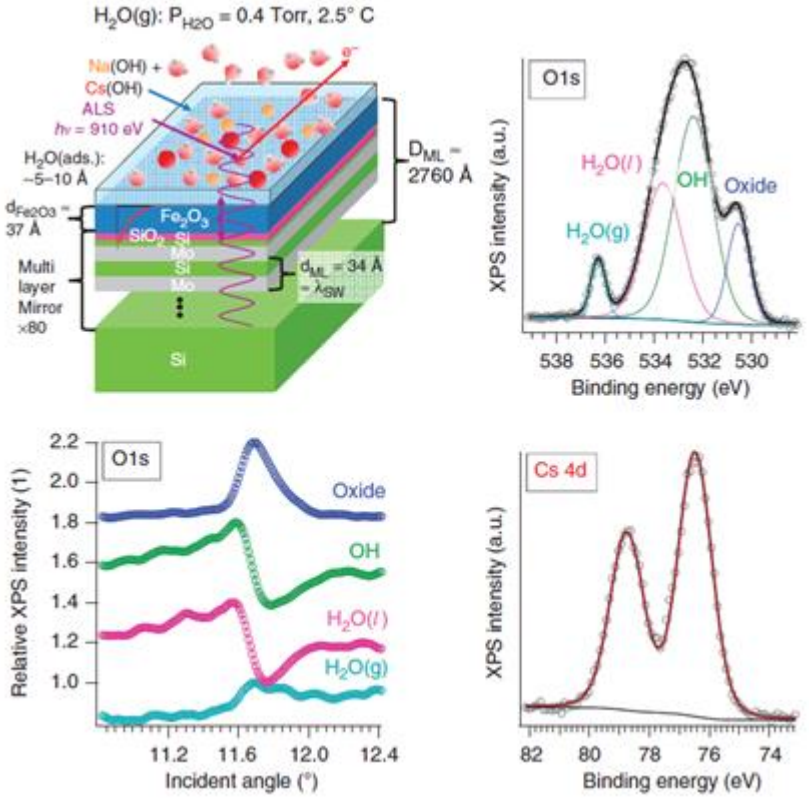
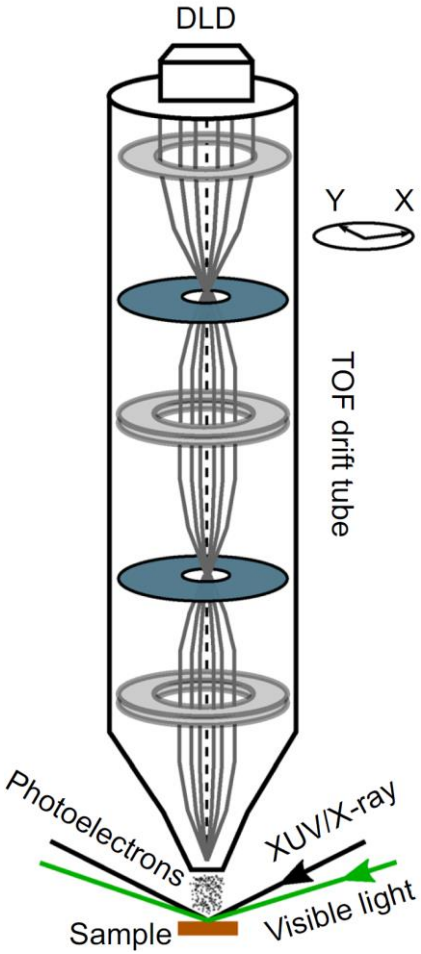
DOI: 10.1038/ncomms6441

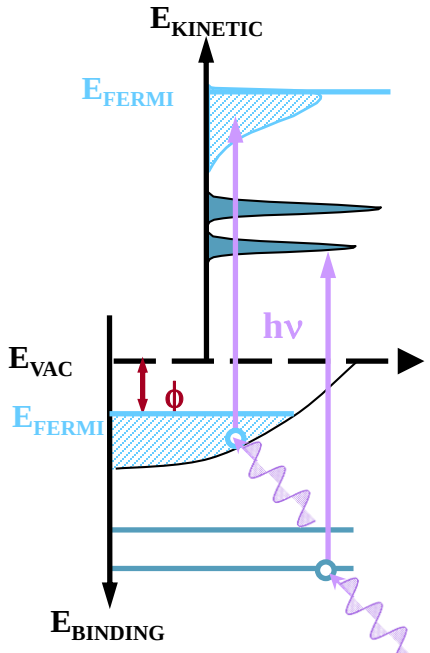
Concentration and chemical-state profiles at heterogeneous interfaces with sub-nm accuracy from standing-wave ambient-pressure photoemission

Slavomír Nemšák[1,2,†], Andrey Shavorskiy[3], Osman Karslioglu[3], Ioannis Zegkinoglou[3], Arunothai Rattanachata[1,2], Catherine S. Conlon[1,2], Armela Keqi[1,2], Peter K. Greene[1], Edward C. Burks[1], Farhad Salmassi[2], Eric M. Gullikson[2], See-Hun Yang[4], Kai Liu[1], Hendrik Bluhm[3] & Charles S. Fadley[1,2]



Femtosecond time-resolved photoelectron spectroscopy





$1T\text{-}TaS_2$

Valence electrons
trARPES
Nat. Commun. **3**, 1069 (2012)

+

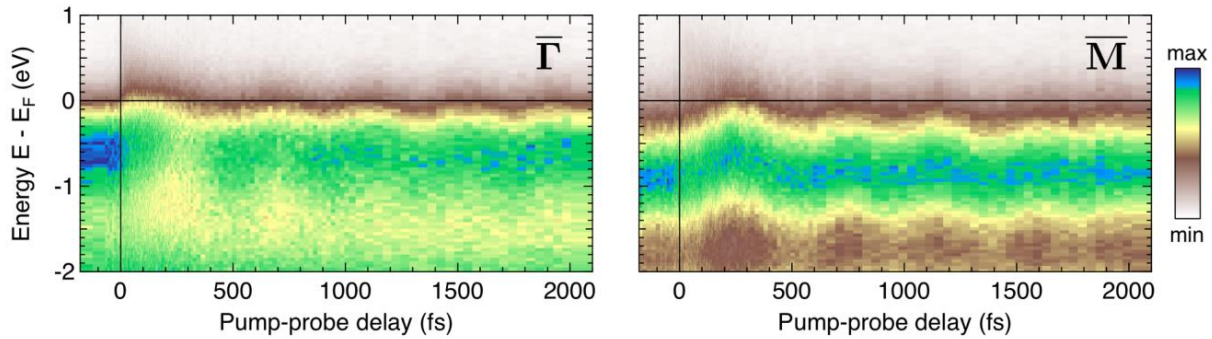
Core electrons
trXPS
PRL **105**, 187401 (2010)

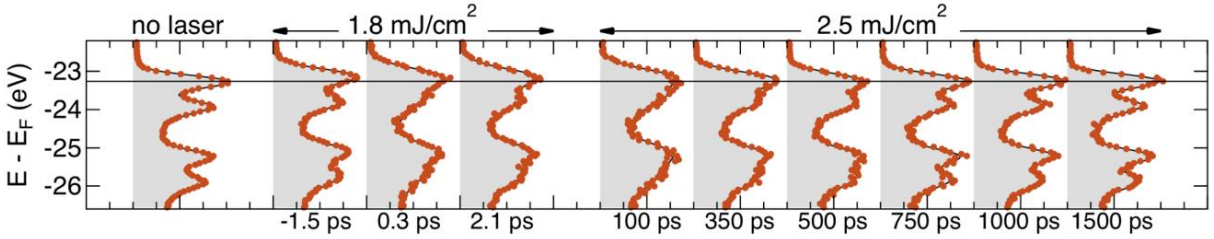
+

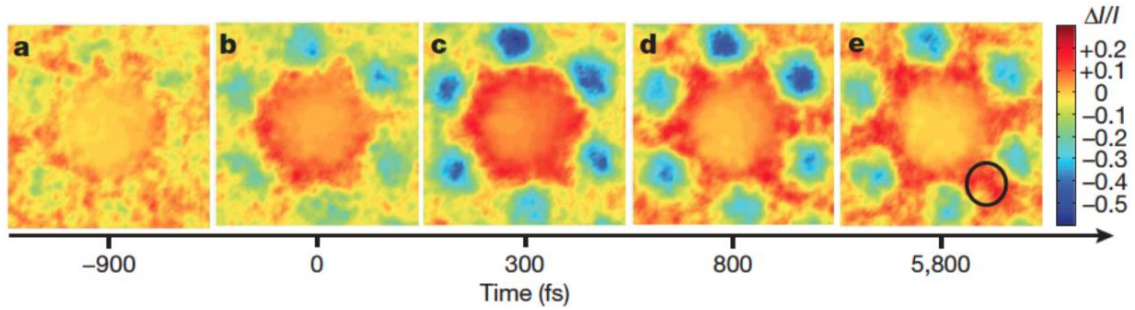
Atomic lattice
trXPD (UED)
Nature **468**, 799 (2010)

+

Spins







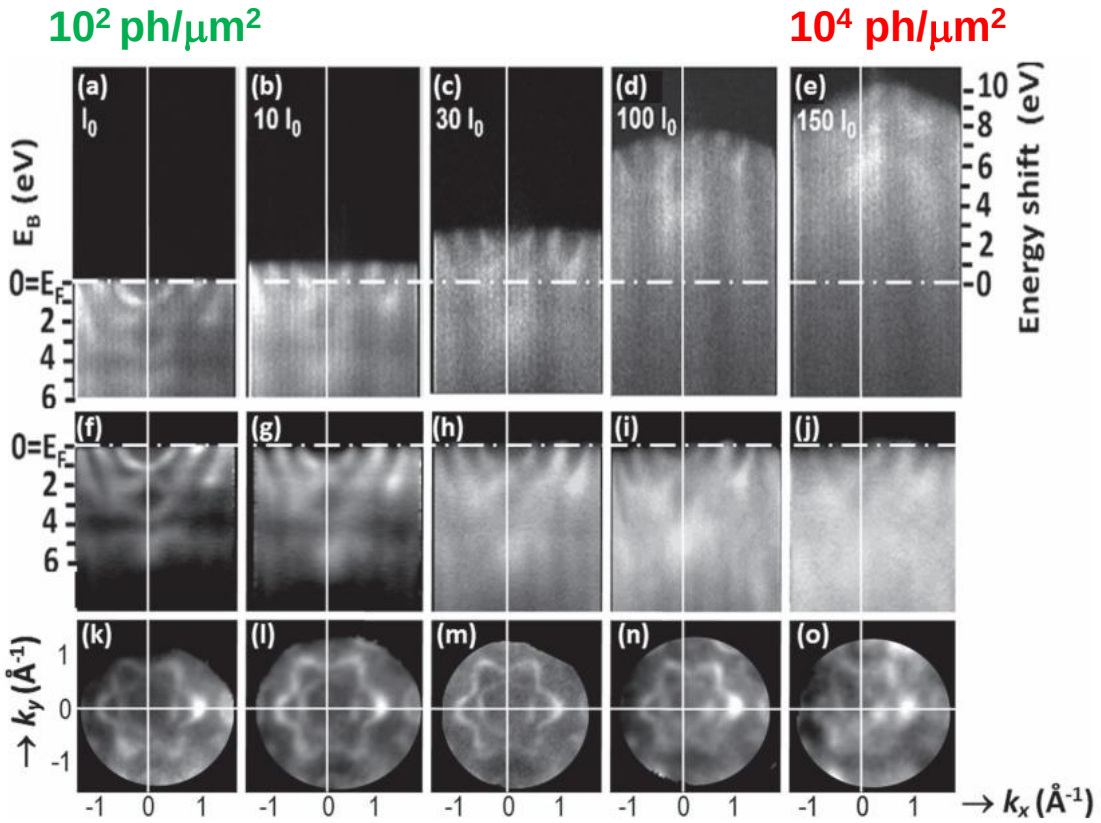
on an homogeneously excited sample !

Source requirements for photoelectron spectroscopy on solids

- High fluence induce non-linear effects (space charge)
- Spot size is limited to ~ Ø 30 μm

Ideal source

- As many pulses as possible: MHz, CW
- Moderate flux: 10^6 ph/s @ 1 MHz



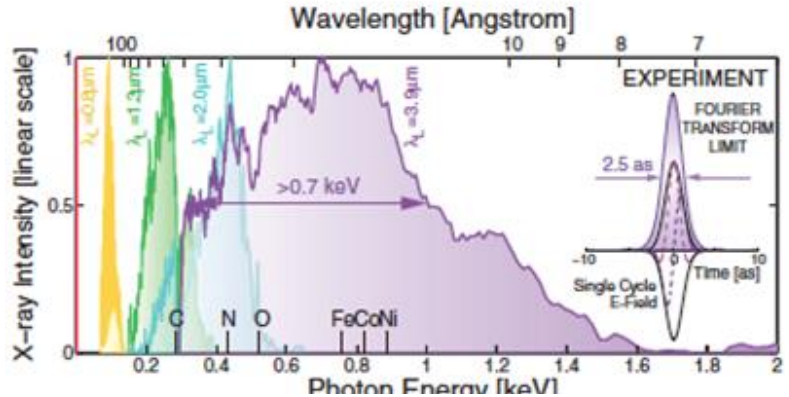
Gerd Schönhense et al.

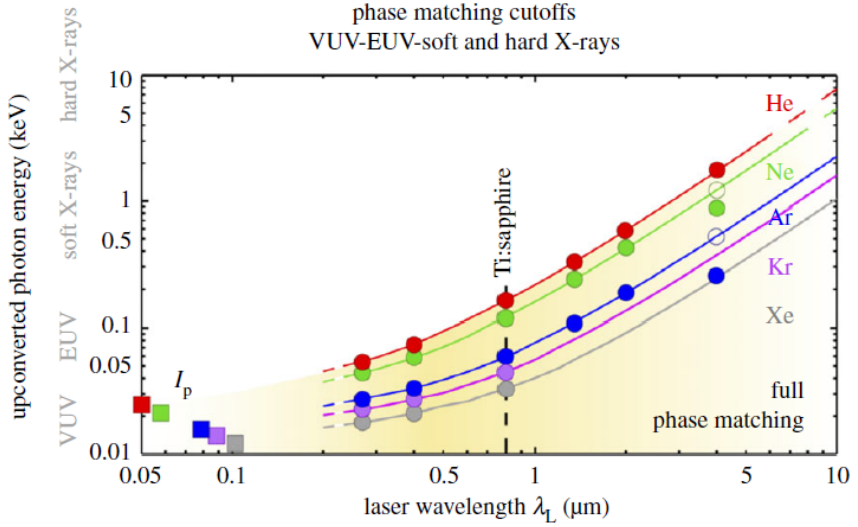
Available sources for femtosecond time-resolved photoelectron spectroscopy

- At synchrotrons ➔ Time resolution limited to the ps
- With Laser sources ➔ Energy range limited to 100 eV
- Warm LINAC FELs ➔ Repetition rate limited to 100s of Hz

Current alternative ➔ SC-MHz FELs

- MHz FELs
  - FLASH, DESY: 23 eV – 0.3 keV, ~1 keV (3rd harmonic)
  - SASE3 (EuXFEL): 0.3 – 3 keV
  - LCLS-II (SLAC): 0.3 – 1.5 keV (2024)
  - SHINE (2025)





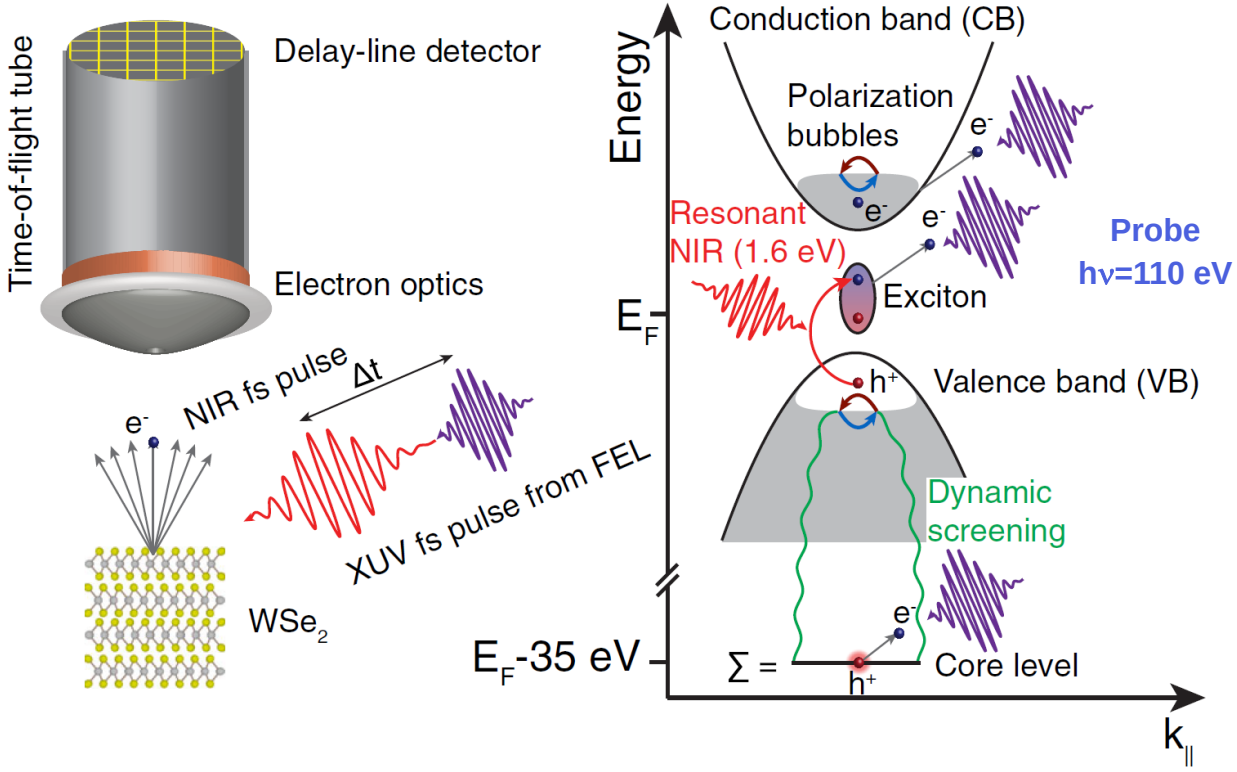
T. Popmintchev *et al.* Science 335, 1287 (2012)

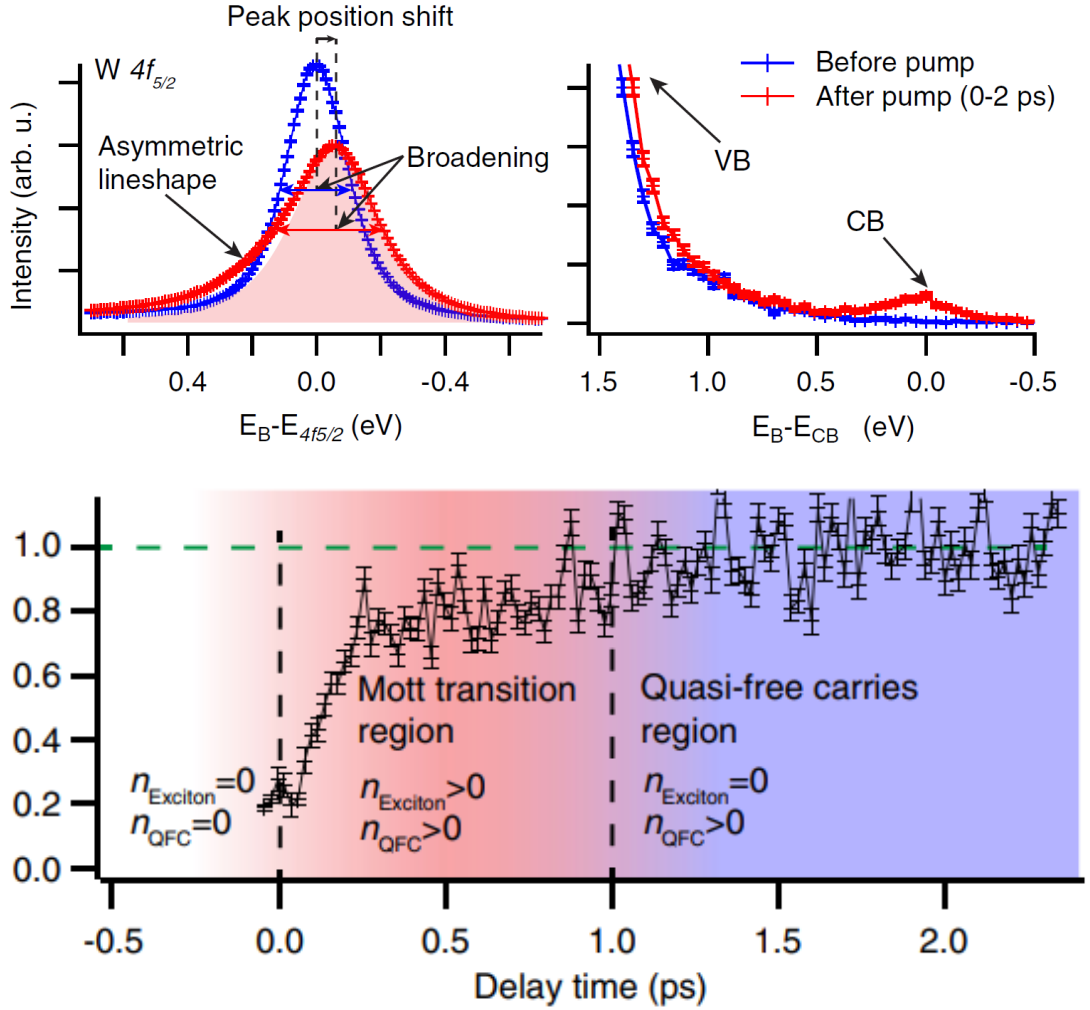
Femtosecond time-resolved experiments at FELs above 100 eV

Observation of an Excitonic Mott Transition through Ultrafast Core-*cum*-Conduction Photoemission Spectroscopy

Maciej Dendzik, R. Patrick Xian, Enrico Perfetto, Davide Sangalli, Dmytro Kutnyakhov, Shuo Dong, Samuel Beaulieu, Tommaso Pincelli, Federico Pressacco, Davide Curcio, Steinn Ymir Agustsson, Michael Heber, Jasper Hauer, Wilfried Wurth, Günter Brenner, Yves Acremann, Philip Hofmann, Martin Wolf, Andrea Marini, Gianluca Stefanucci, Laurenz Rettig, and Ralph Ernstorfer

Phys. Rev. Lett. **125**, 096401 – Published 24 August 2020



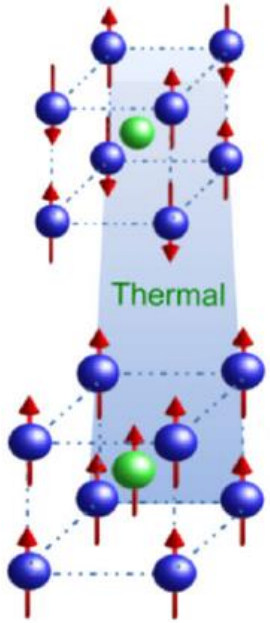


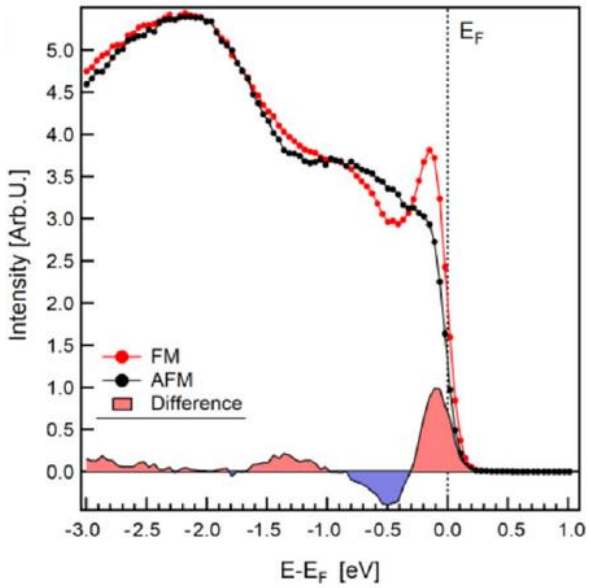
Femtosecond time-resolved experiments at FELs above 100 eV

Subpicosecond metamagnetic phase transition in FeRh driven by non-equilibrium electron dynamics

Federico Pressacco, Davide Sangalli, Vojtěch Uhlíř, Dmytro Kutnyakhov, Jon Ander Arregi, Steinn Ymir Agustsson, Günter Brenner, Harald Redlin, Michael Heber, Dmitry Vasilyev, Jure Demsar, Gerd Schönhense, Matteo Gatti, Andrea Marini, Wilfried Wurth & Fausto Sirotti

Nature Communications **12**, Article number: 5088 (2021) | Cite this article

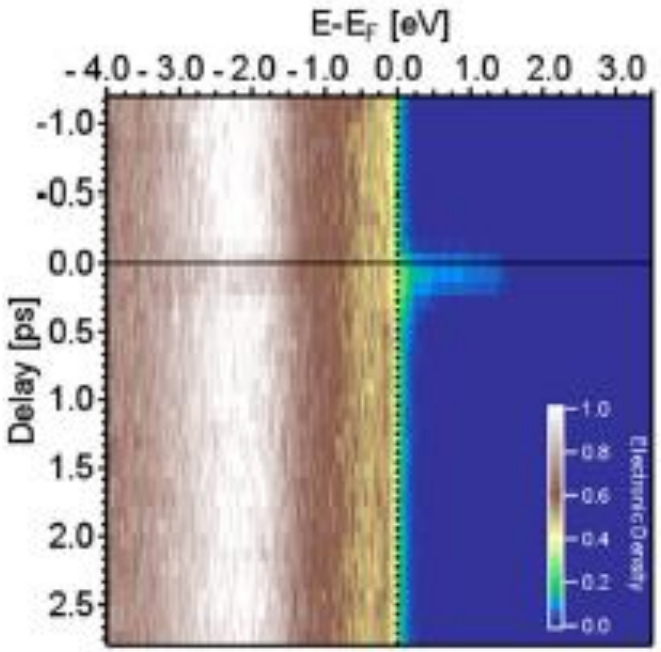


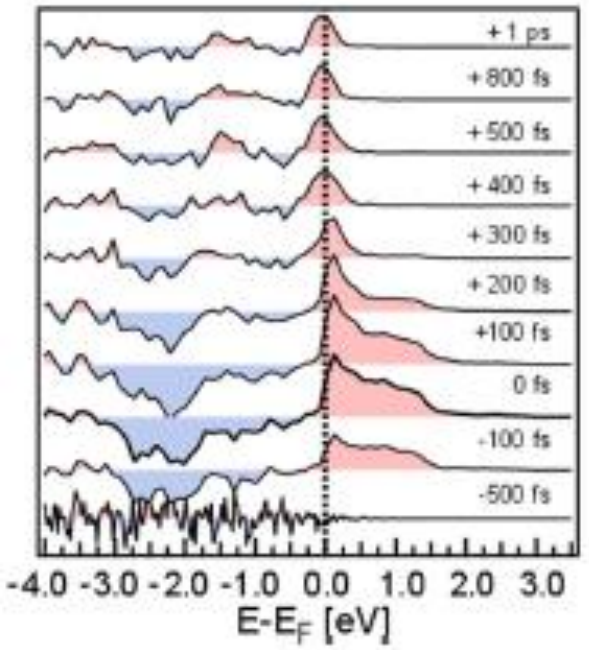


Dynamics

Pump hν=1.55 eV

Probe hν=123.5 eV



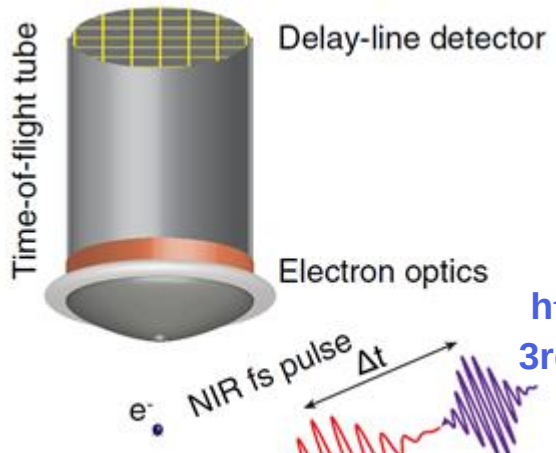


Soft X-ray femtosecond time-resolved photoemission

Ultrafast Real-Time Dynamics of CO Oxidation over an Oxide Photocatalyst

Michael Wagstaffe, Lukas Wenthaus, Adrian Dominguez-Castro, Simon Chung, Guilherme Dalla Lana Semione, Steffen Palutke, Giuseppe Mercurio, Siarhei Dziarzhytski, Harald Redlin, Nicolai Klemke, Yudong Yang, Thomas Frauenheim, Adriel Dominguez, Franz Kärtner, Angel Rubio, Wilfried Wurth, Andreas Stierle, and Heshmat Noei*

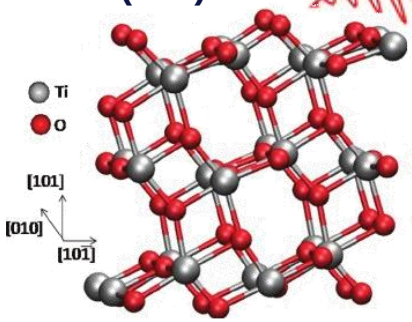
Cite This: ACS Catal. 2020, 10, 13650−13658 Read Online



Probe
hν=647.9 eV
3rd harmonic

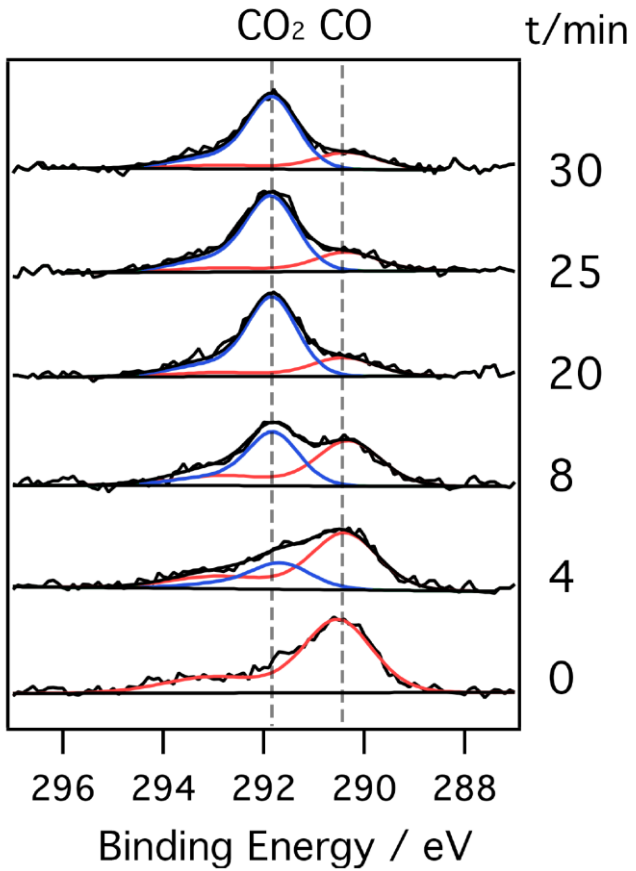
Pump
hν=1.6 eV

TiO_2: Anatase (101)

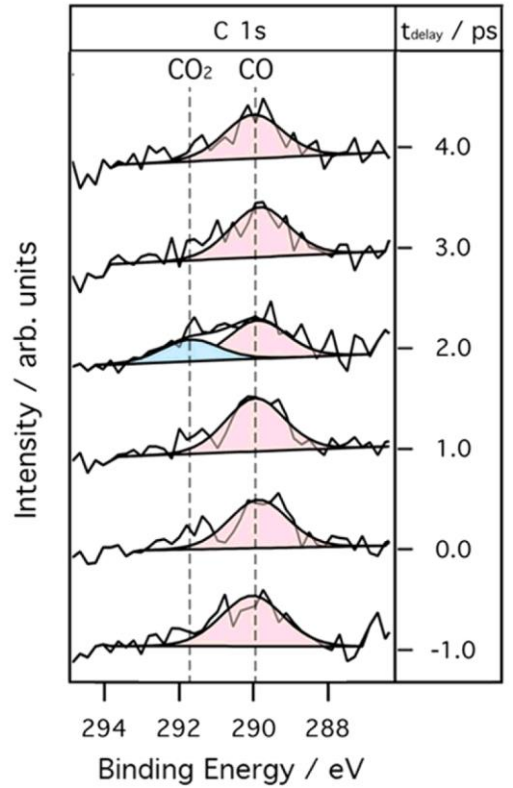


CO: $3 \cdot 10^{-8}$ mbar
O_2 : $3 \cdot 10^{-8}$ mbar

Static photo-excitation



Time-resolved



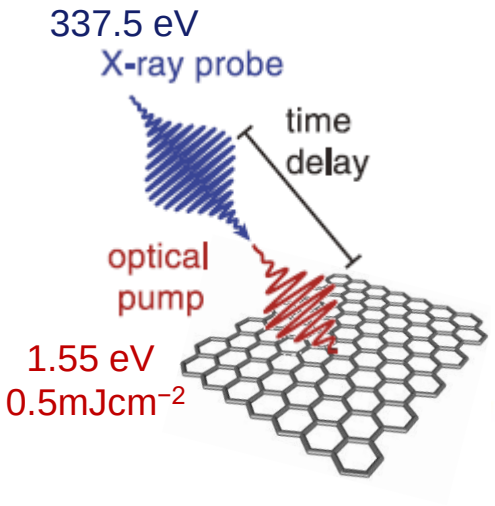
Femtosecond time-resolved photoelectron diffraction

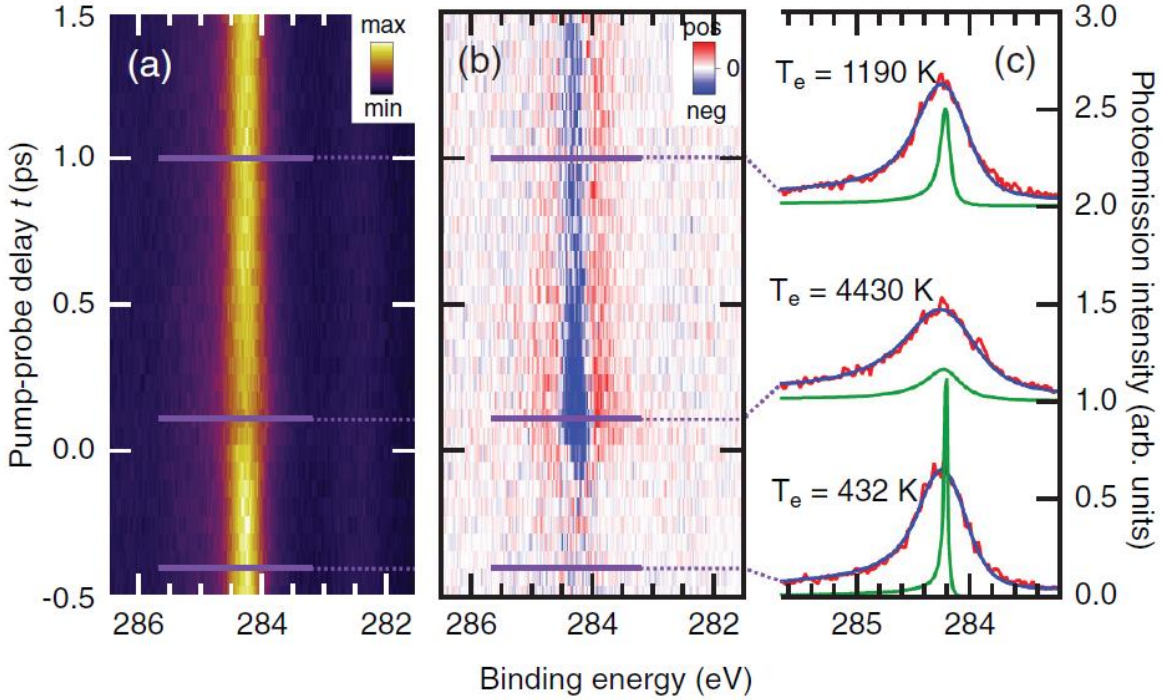
PHYSICAL REVIEW B **104**, L161104 (2021)

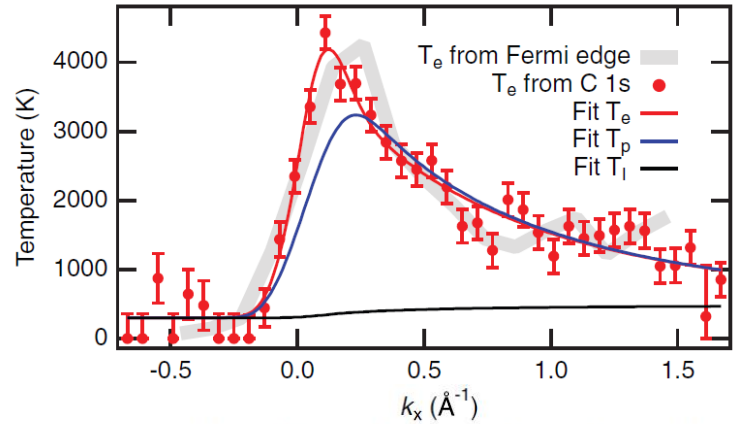
Letter

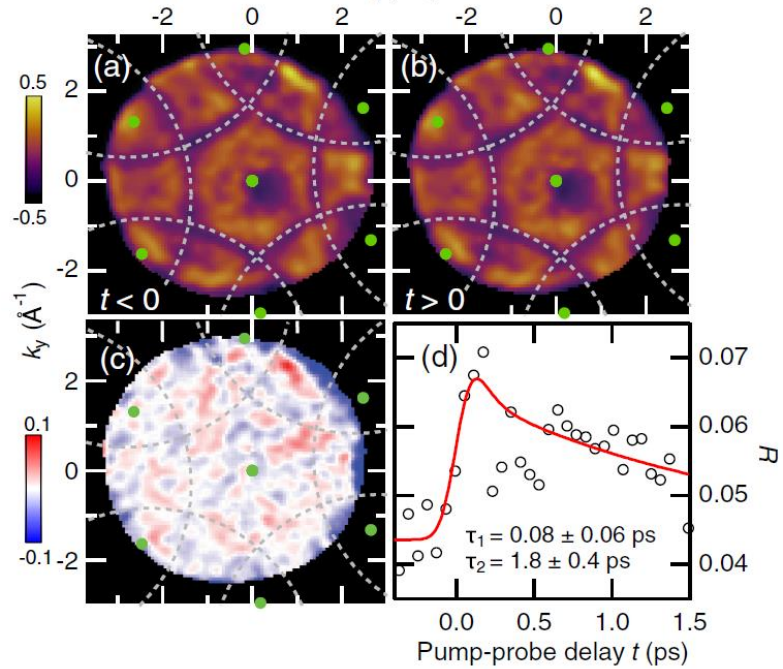
Ultrafast electronic linewidth broadening in the C 1*s* core level of graphene

Davide Curcio,[1] Sahar Pakdel,[1] Klara Volckaert,[1] Jill A. Miwa,[1] Søren Ulstrup,[1] Nicola Lanatà,[2,3] Marco Bianchi,[1] Dmytro Kutnyakhov,[4] Federico Pressacco,[4] Günter Brenner,[4] Siarhei Dziarzhytski,[4] Harald Redlin,[4] Steinn Ymir Agustsson,[5] Katerina Medjanik,[5] Dmitry Vasilyev,[5] Hans-Joachim Elmers,[5] Gerd Schönhense,[5] Christian Tusche,[6,7] Ying-Jiun Chen,[6,7] Florian Speck,[8] Thomas Seyller,[8] Kevin Bühlmann,[9] Rafael Gort,[9] Florian Diekmann,[10] Kai Rossnagel,[10,11] Yves Acremann,[9] Jure Demsar,[5] Wilfried Wurth,[4,12,*] Daniel Lizzit,[13,†] Luca Bignardi,[13,‡] Paolo Lacovig,[13] Silvano Lizzit,[13] Charlotte E. Sanders,[14] and Philip Hofmann[1]









European

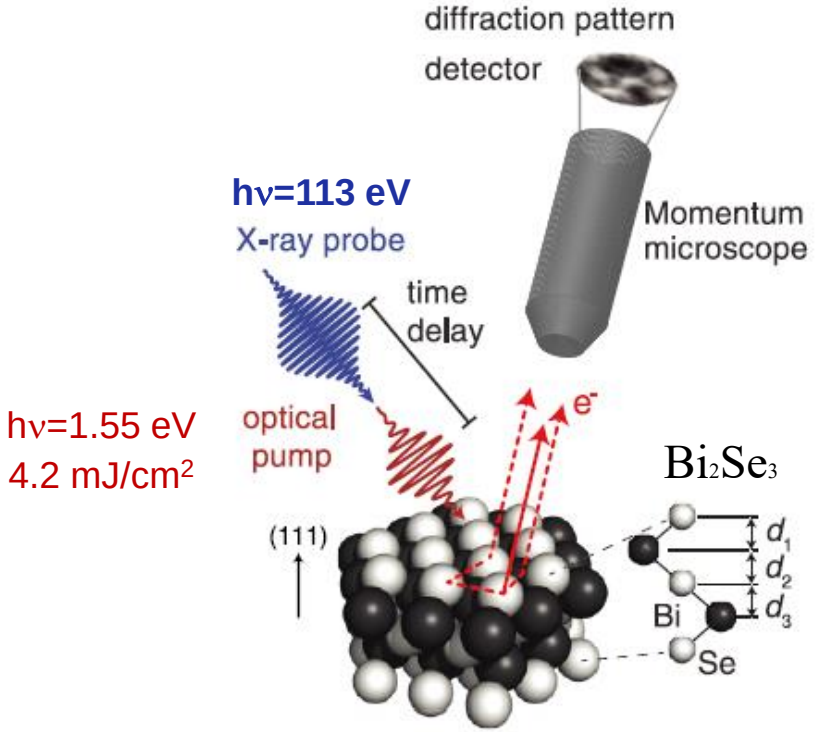
Femtosecond time-resolved photoelectron diffraction

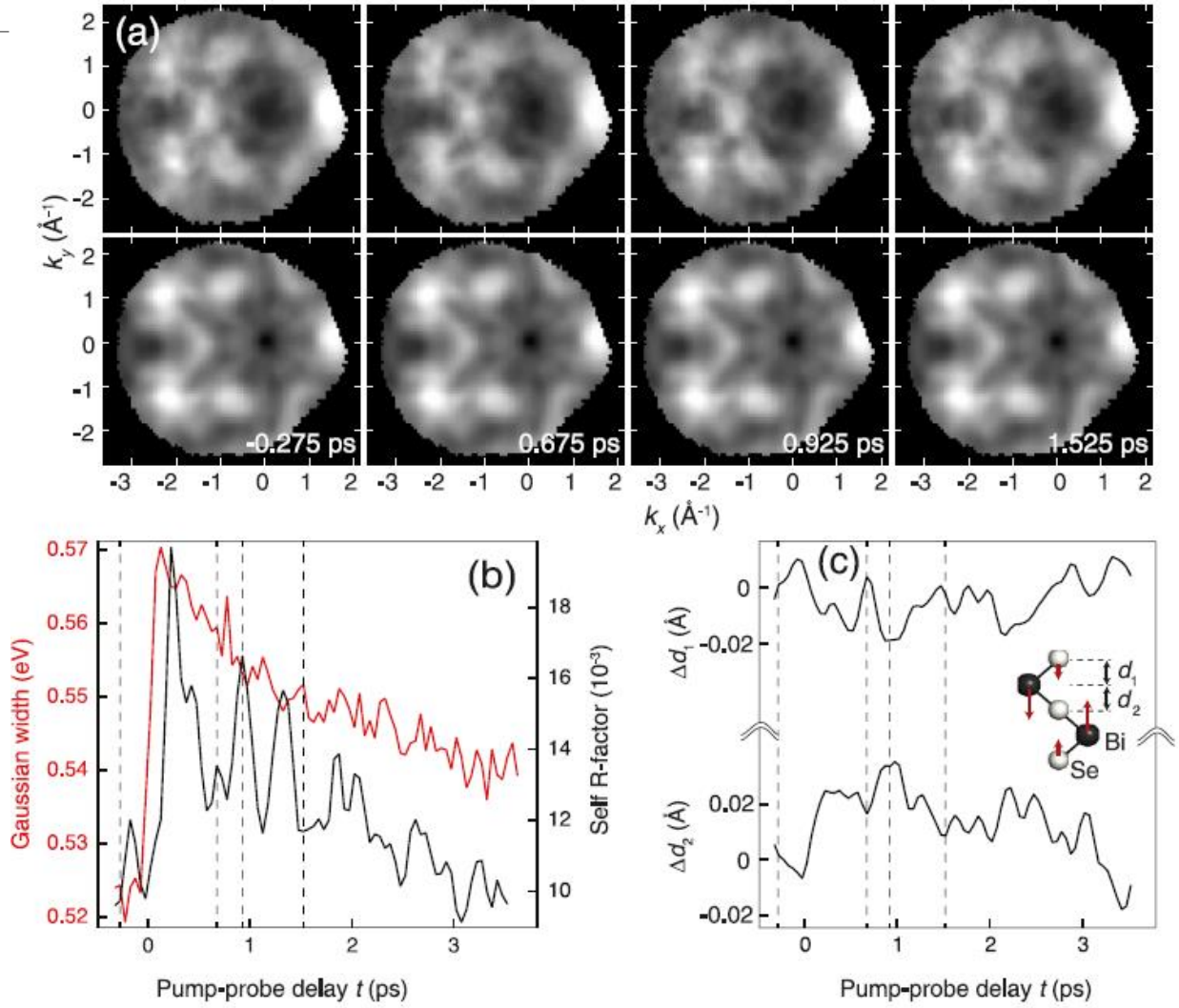
PHYSICAL REVIEW B **106**, L201409 (2022)

Letter

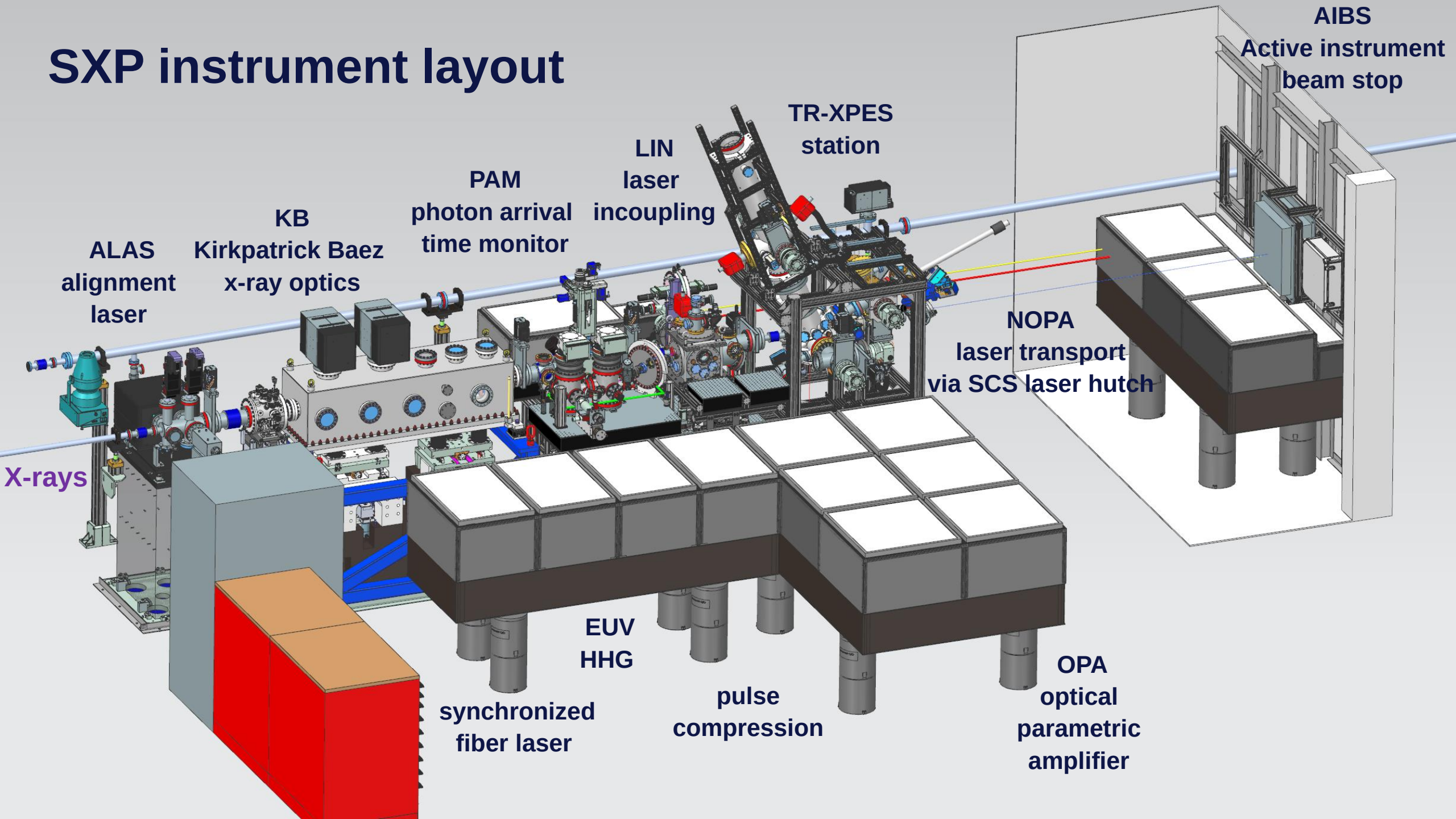
Tracking the surface atomic motion in a coherent phonon oscillation

Davide Curcio,[1,*] Klara Volckaert,[1,*] Dmytro Kutnyakhov,[2] Steinn Ymir Agustsson,[3] Kevin Bühlmann,[4] Federico Pressacco,[2] Michael Heber,[2] Siarhei Dziarzhytski,[2] Yves Acremann,[4] Jure Demsar,[3] Wilfried Wurth,[2,5,†] Charlotte E. Sanders,[6] and Philip Hofmann[1,‡]



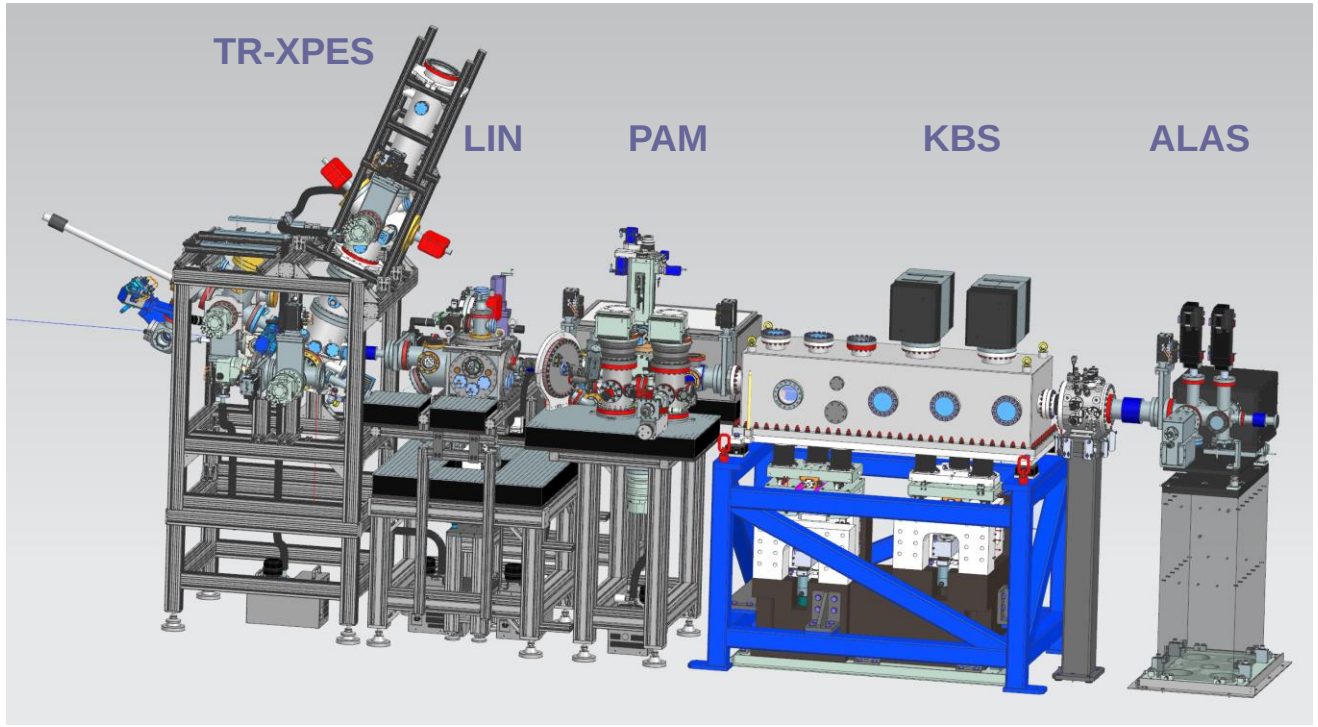


SXP instrument layout

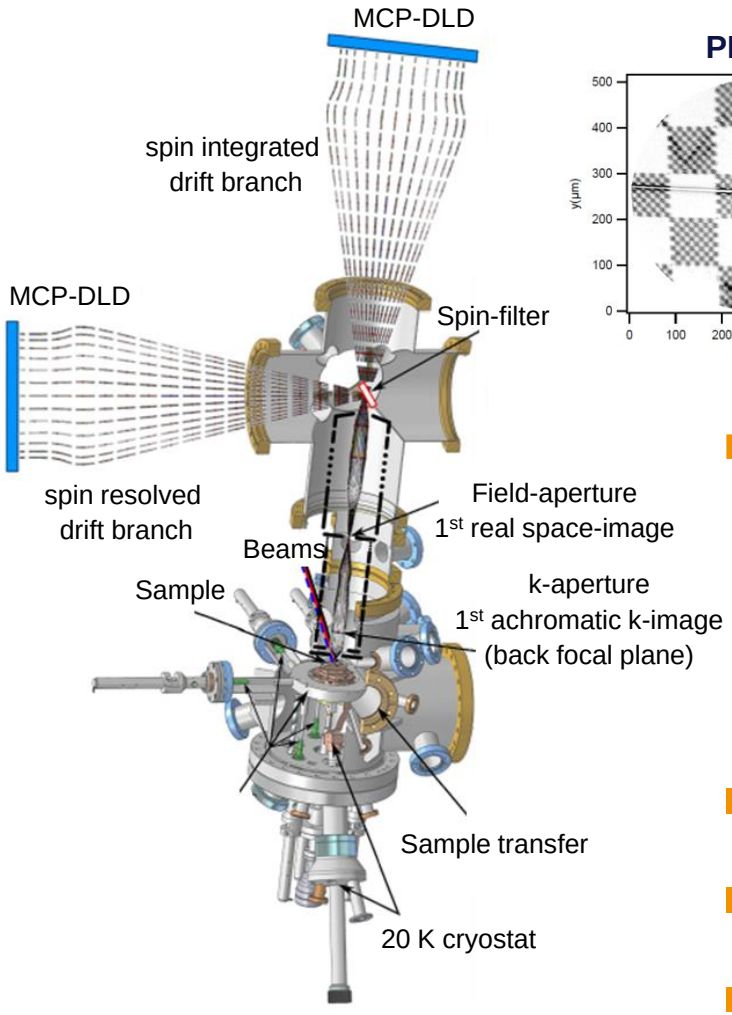


SXP instrument

- Model and real implementation of the SXP instrument
- First experiments: TR-XPES (Time-resolved photoelectron spectroscopy on solids)

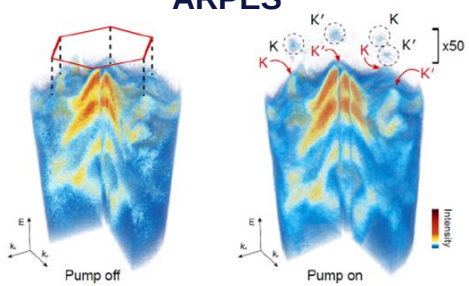


Experiment setup and laser capabilities



PEEM

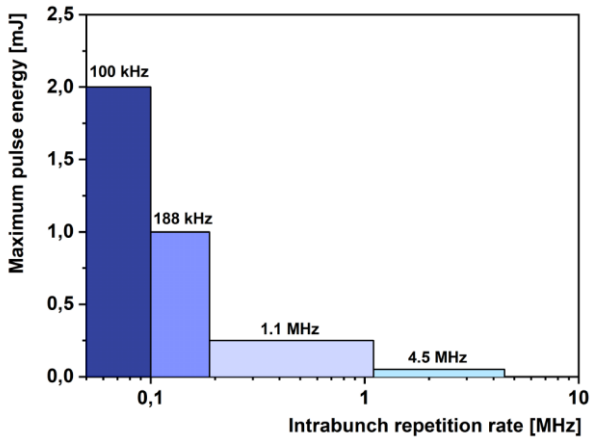
ARPES



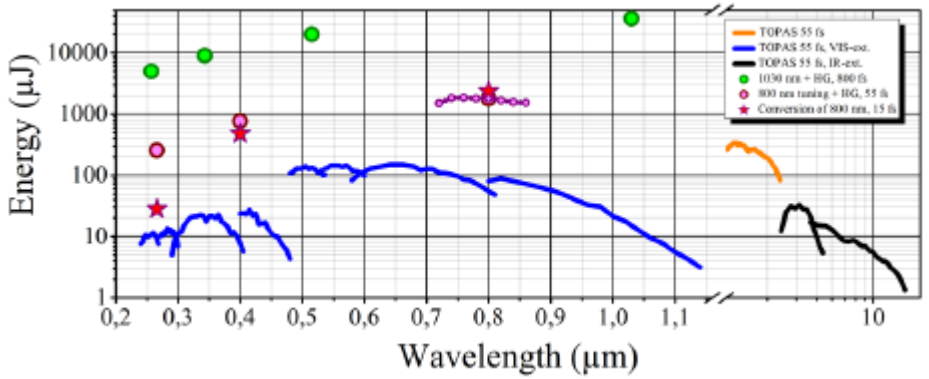
- Momentum microscope spectrometer
  - Large angular cone ~ 40º
  - MCP-DLD detector
  - $\Delta k \sim 0.06$ Å^{-1}
  - $\Delta E \sim 130$ meV
  - Spin integrated
- Omicron type mount for solid samples
- Load lock for fast sample insertion
- LEED and preparation chambers

Review of Scientific Instruments **91**, 013109 (2020)

Pump Laser

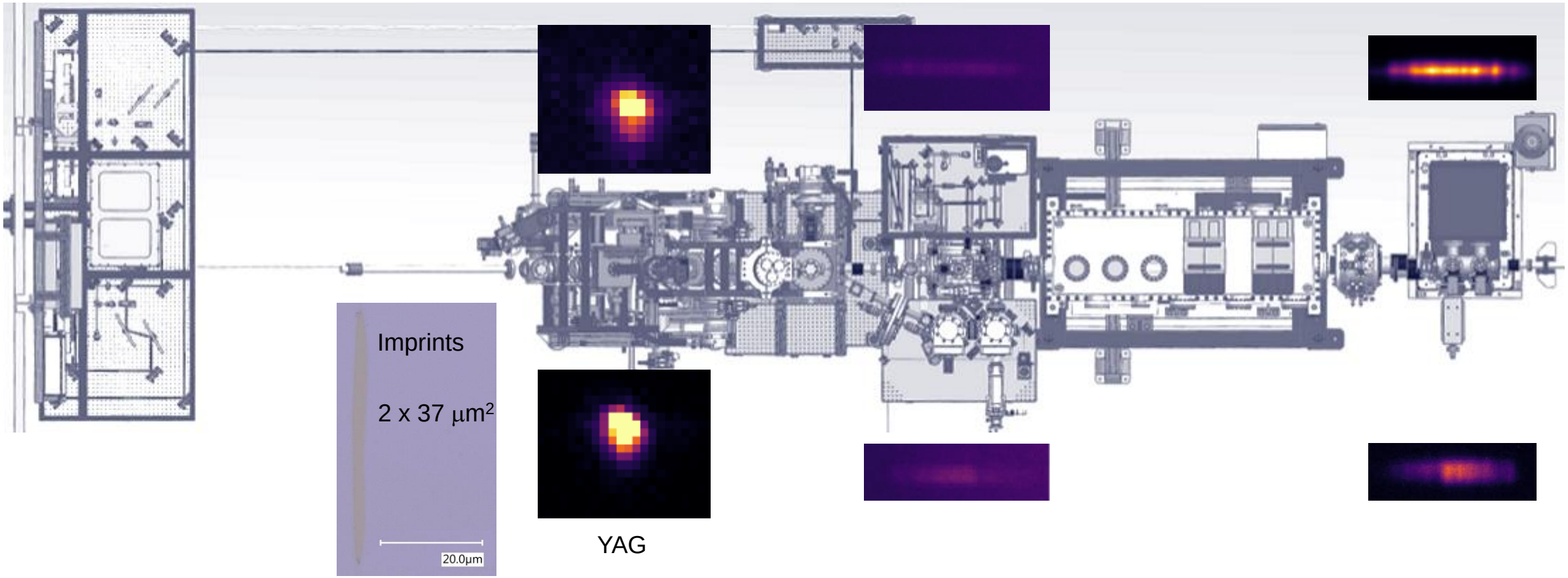


- 800 nm, 1030 nm & harmonics outputs
- OPA @ 118 KHz

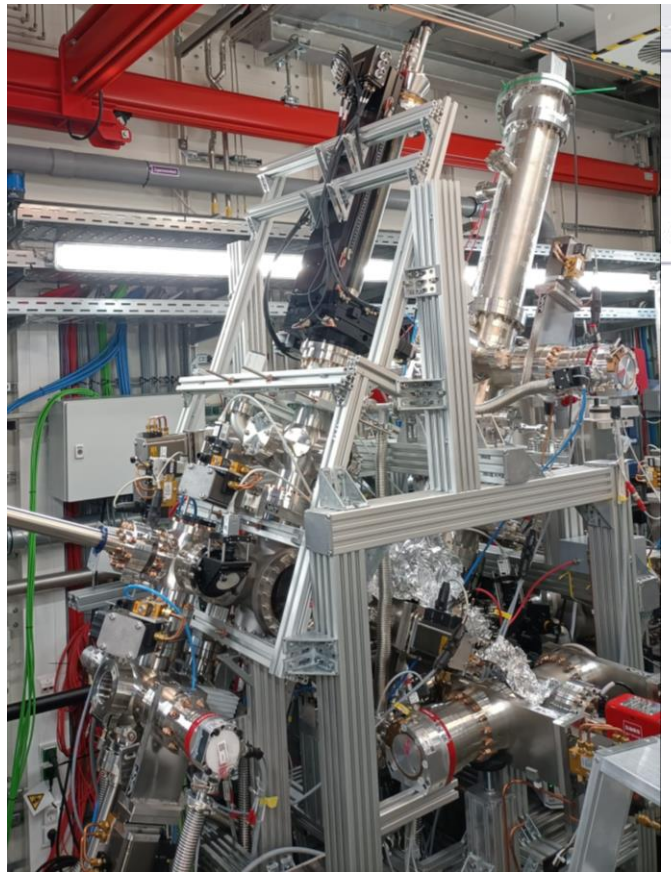


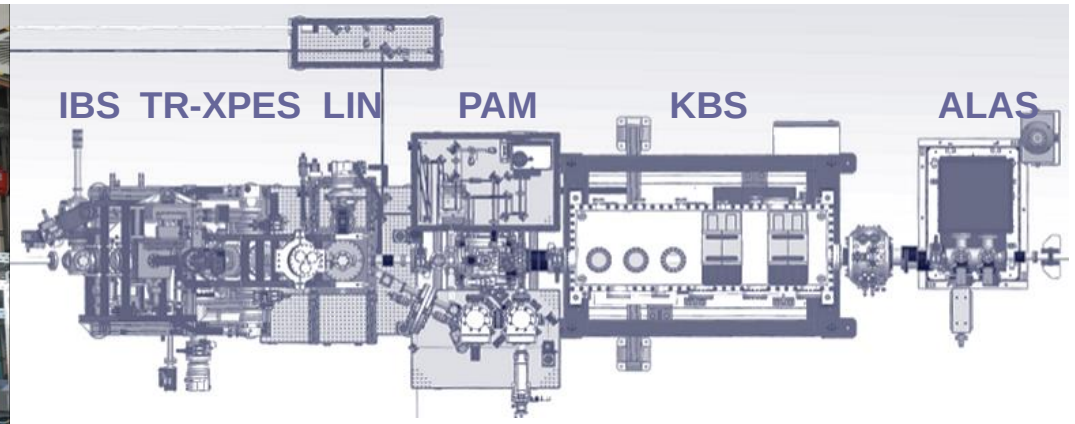
FEL commissioning

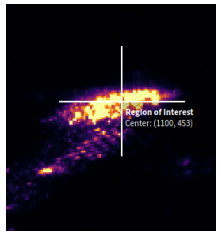
- KB focus commissioned @ 1 & 2.5 keV, best horizontal focus 10 μm

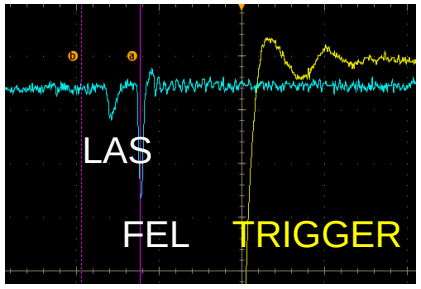


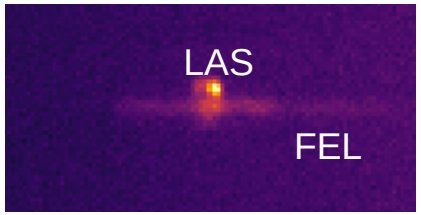
FEL, Optical Laser & momentum microscope commissioning

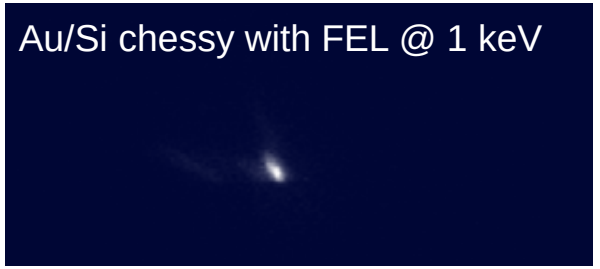










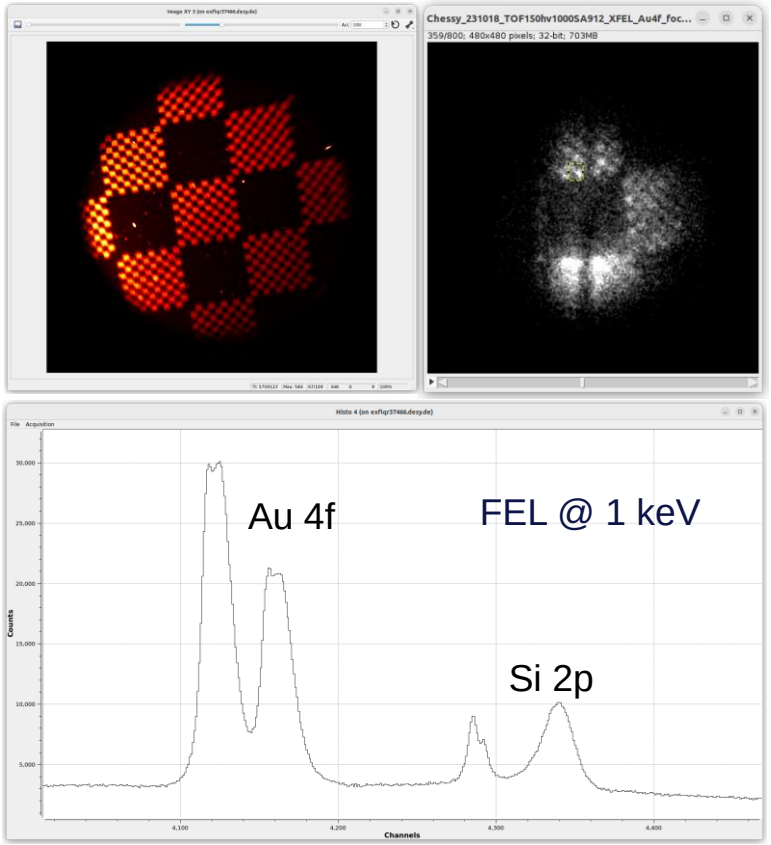


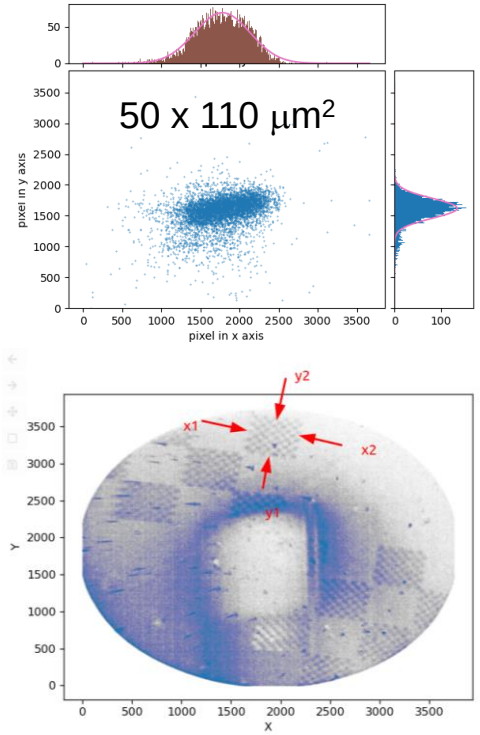
SXP first results: spatial mode

Au/Si chessboard sample

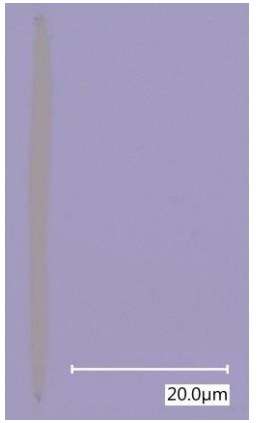
Hg lamp

FEL @ 1 keV

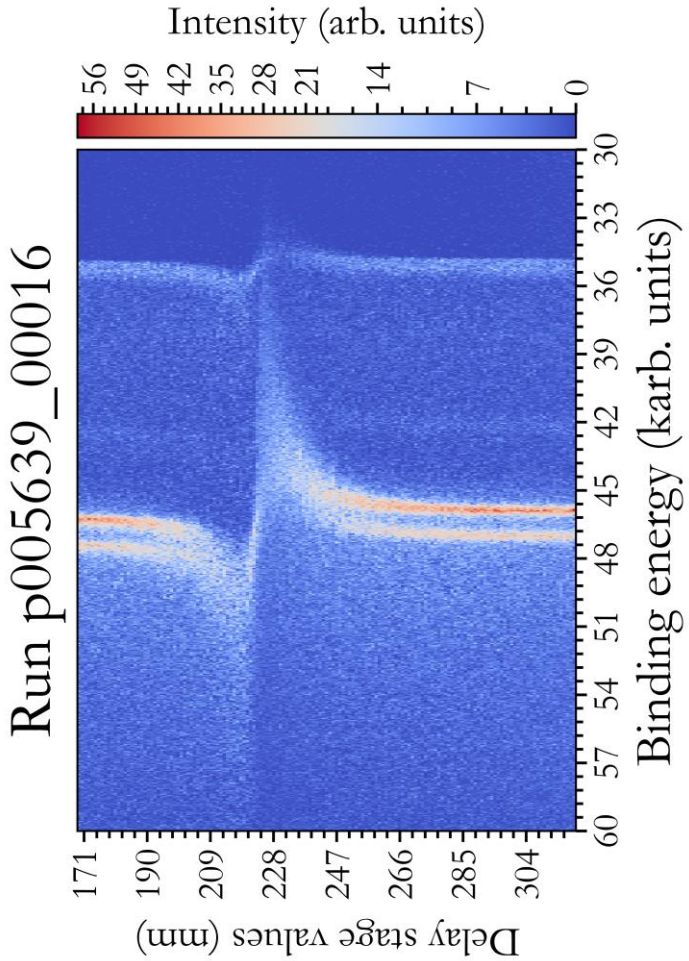




2 x 37 μm²

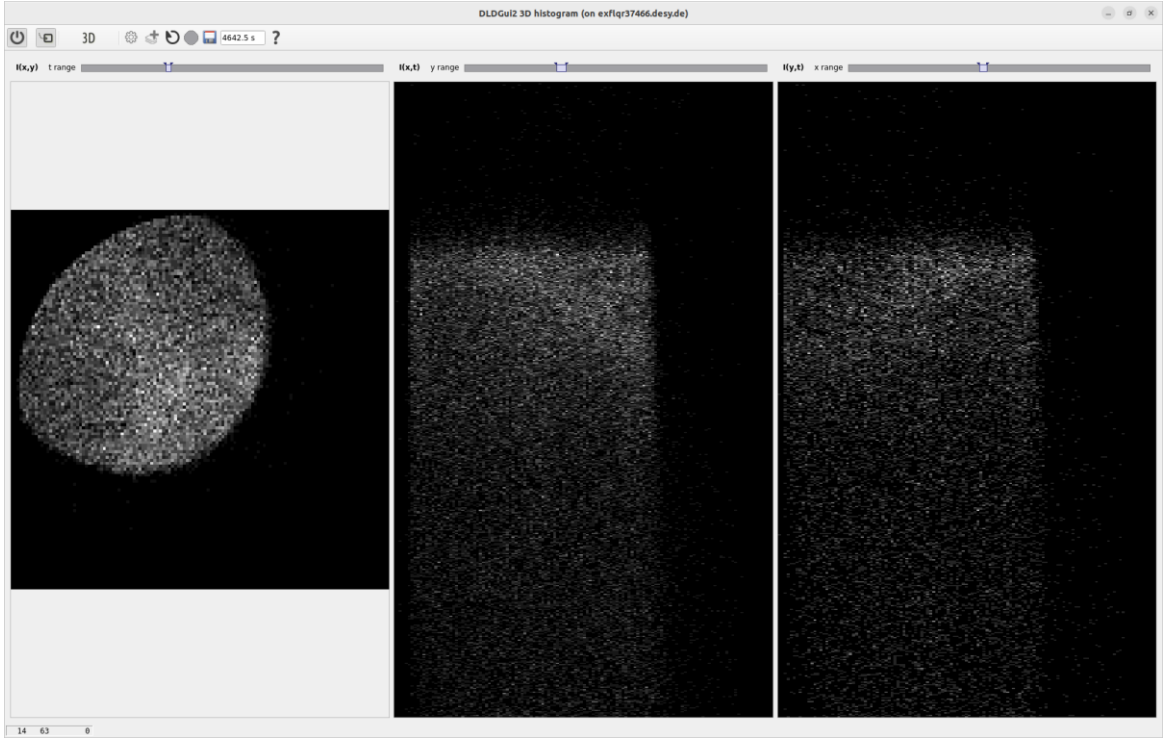


Graphene/Ir(111)

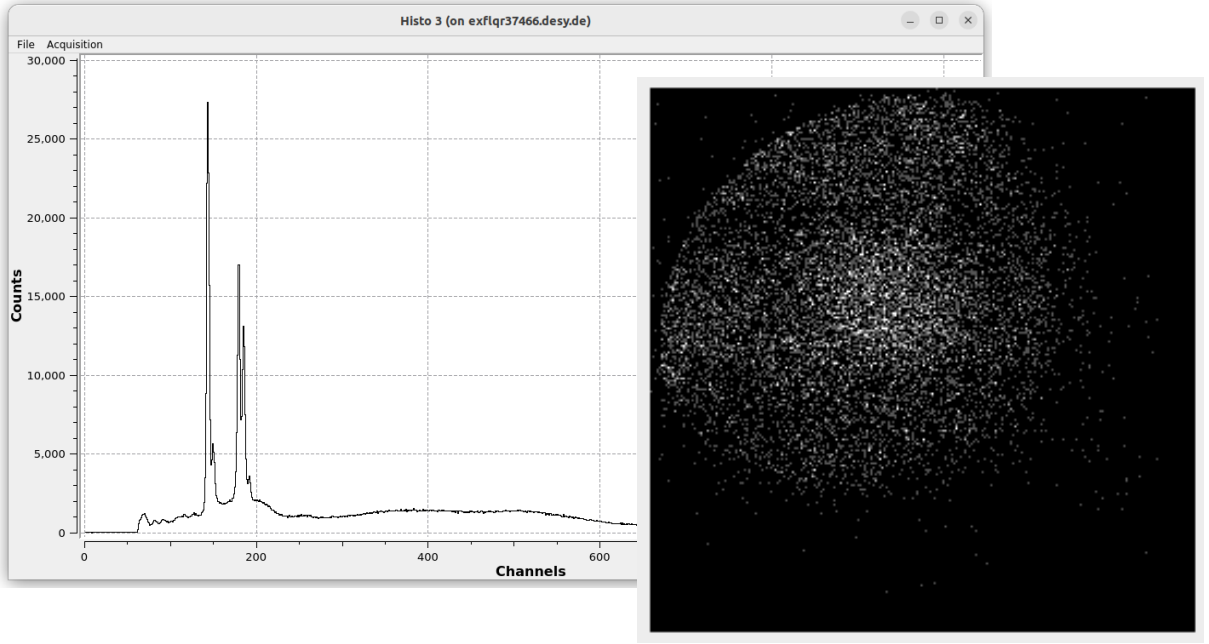


SXP first results: static angular mode

Graphene/Ir(111)
Valence band



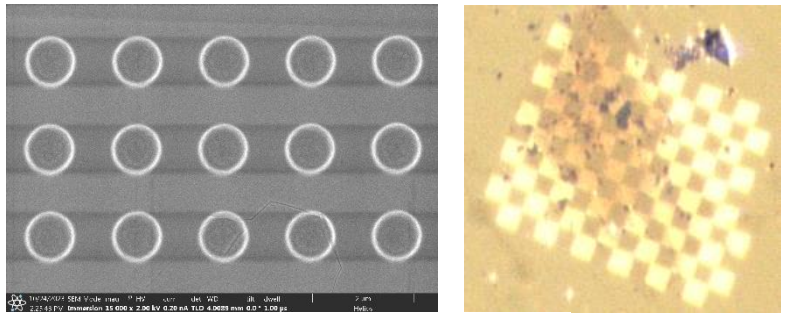
GeTe
Core levels/XPD



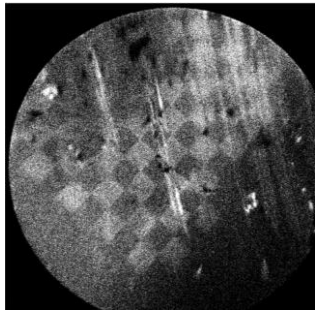
SXP first results: time-resolved experiments

- FEL @ 1 keV, 4.5 MHz, 400 μJ
- PPL @ 760 nm ➔ resonant frequency of the system, 4.5 MHz (first time)

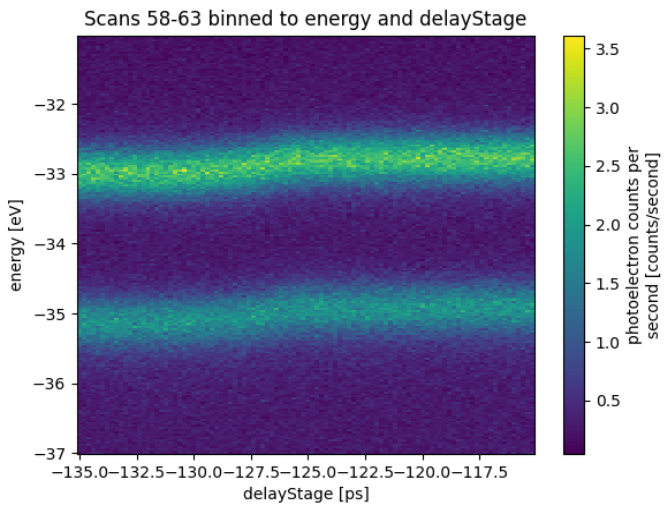
WSe_2 /patterned Au/Mica



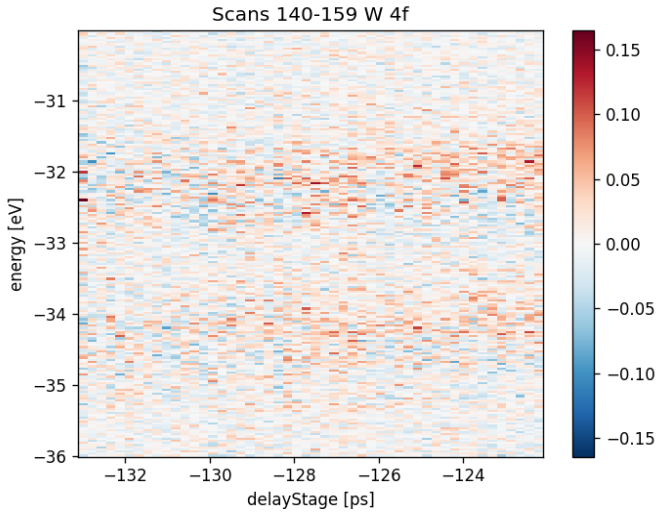
Hg lamp

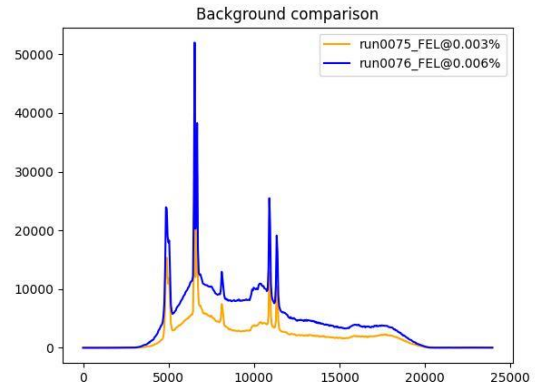


Surface photovoltage



W 4f CL shift ➔ charge transfer?





FEL transmission
~ 0.003 % @ 400 μJ

First completed experiment, beamtime too short !

- Contact:
  - sxp@xfel.eu or manuel.izquierdo@xfel.eu
  - Webpage: https://www.xfel.eu/facility/instruments/sxp/index_eng.html or browse for SXP XFEL

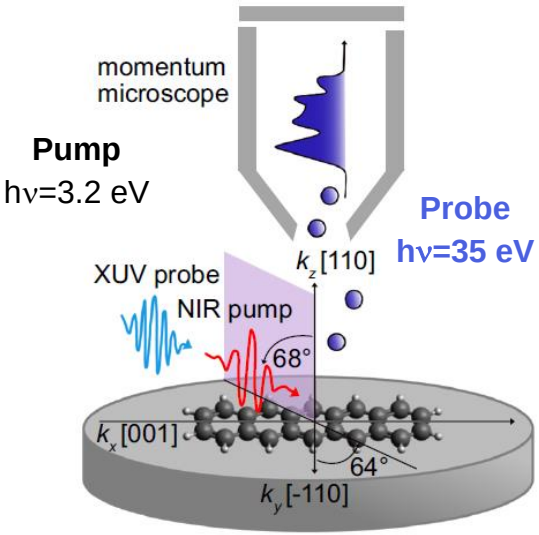
Thank you for your attention!

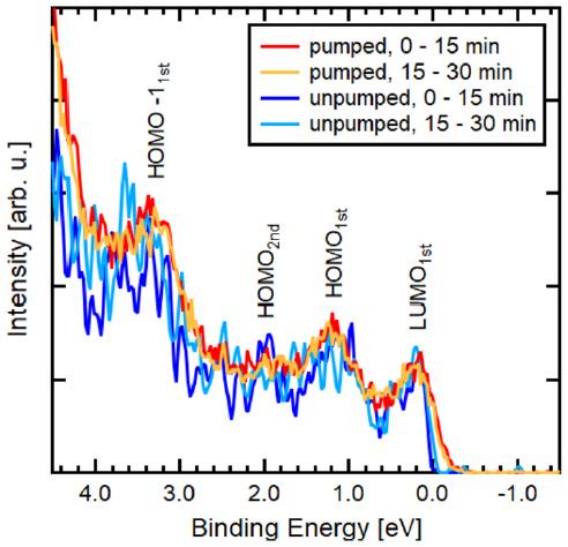
Femtosecond time-resolved experiments at FELs below 100 eV

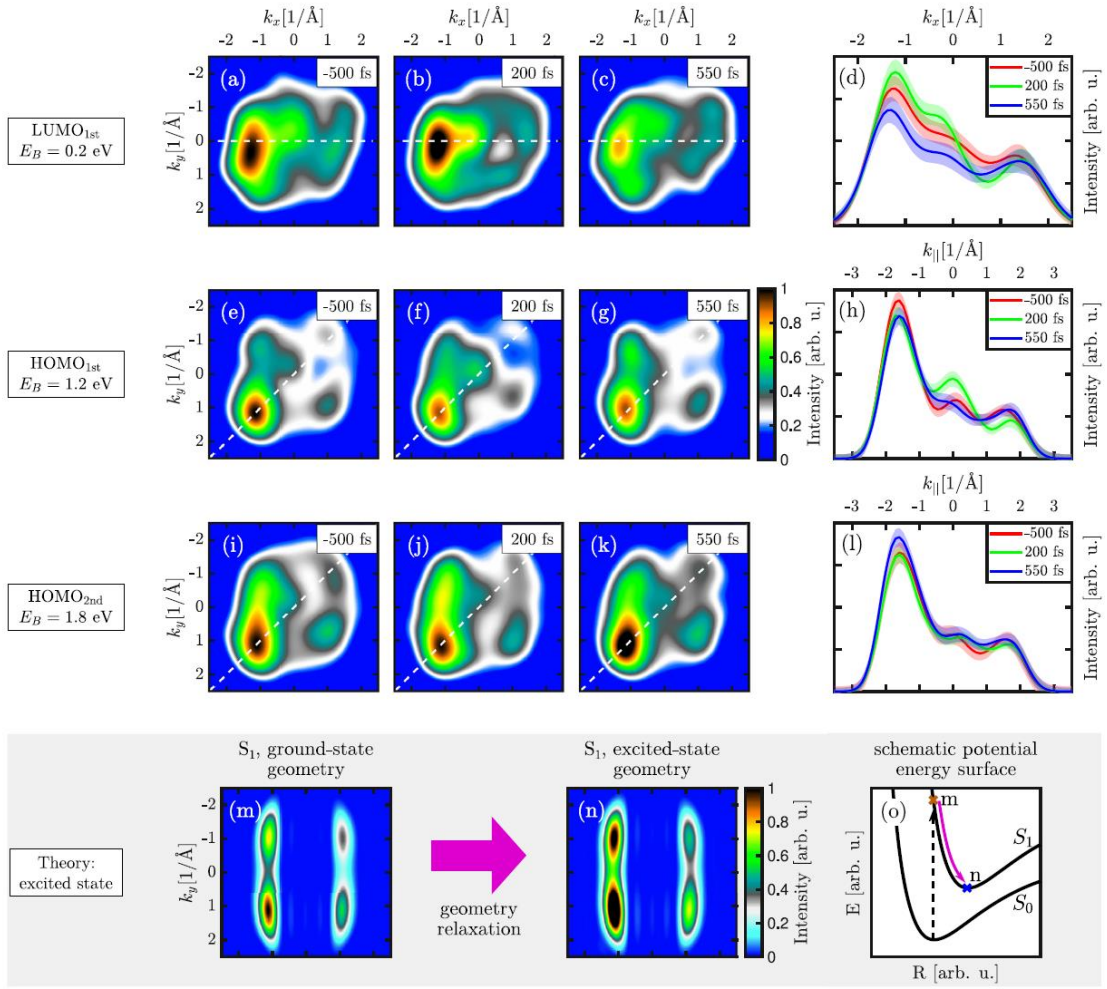
Ultrafast orbital tomography of a pentacene film using time-resolved momentum microscopy at a FEL

Kiana Baumgärtner, Marvin Reuner, Christian Metzger, Dmytro Kutnyakhov, Michael Heber, Federico Pressacco, Chul-Hee Min, Thiago R. F. Peixoto, Mario Reiser, Chan Kim, Wei Lu, Roman Shayduk, Manuel Izquierdo, Günter Brenner, Friedrich Roth, Achim Schöll, Serguei Molodtsov, Wilfried Wurth, Friedrich Reinert, Anders Madsen, Daria Popova-Gorelova & Markus Scholz

Nature Communications **13**, Article number: 2741 (2022) | Cite this article







Soft X-ray femtosecond time-resolved photoemission

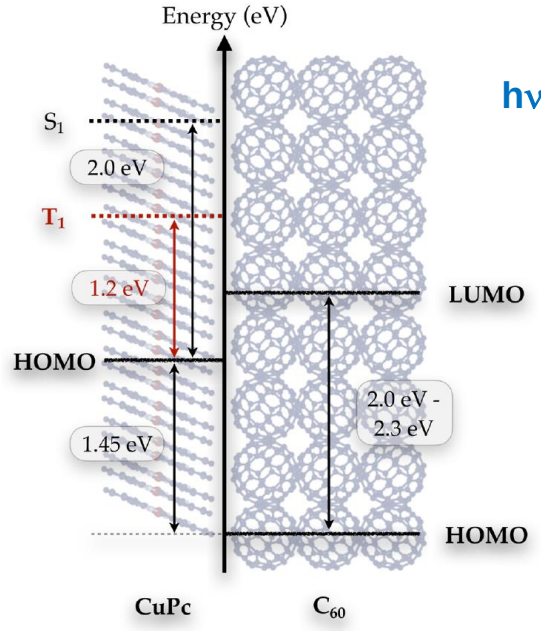
nature COMMUNICATIONS

ARTICLE

https://doi.org/10.1038/s41467-021-21454-3 OPEN

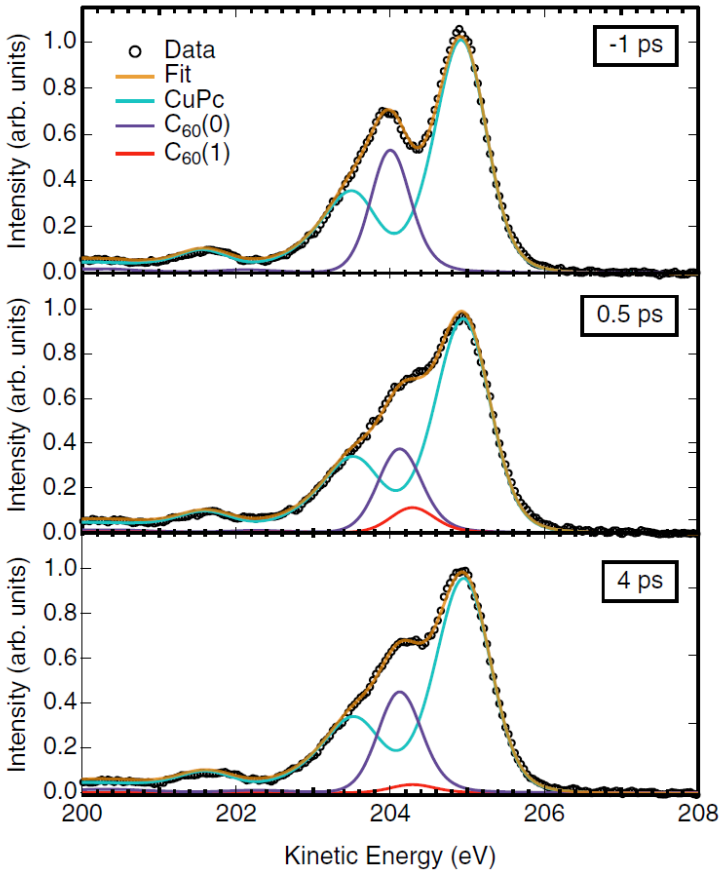
Direct observation of charge separation in an organic light harvesting system by femtosecond time-resolved XPS

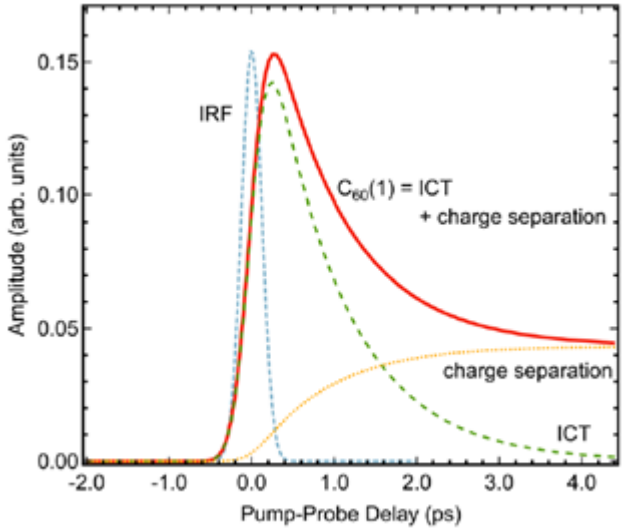
Friedrich Roth[1✉], Mario Borgwardt[2], Lukas Wenthaus[3,4], Johannes Mahl[2], Steffen Palutke[4], Günter Brenner[4], Giuseppe Mercurio[5], Serguei Molodtsov[1,5,6], Wilfried Wurth[3,4,7], Oliver Gessner[2✉] & Wolfgang Eberhardt[3✉]

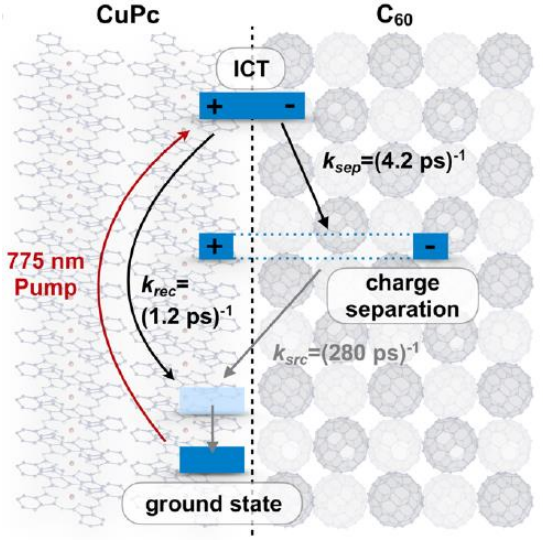


hν= 495.8 eV

Pump
hν=1.6 eV





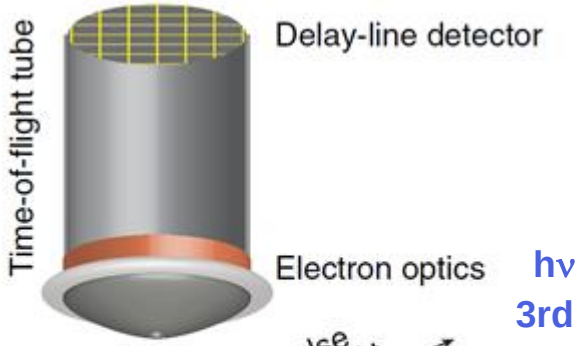


Soft X-ray femtosecond time-resolved photoemission

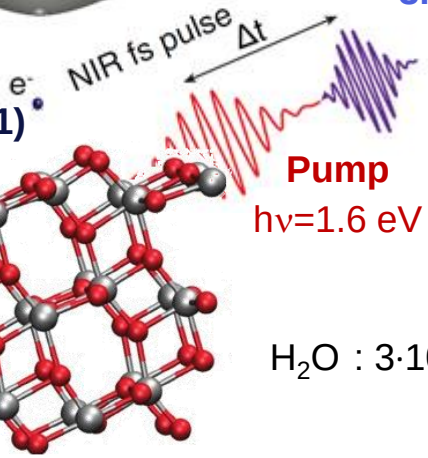
PHYSICAL REVIEW LETTERS 130, 108001 (2023)

Photoinduced Dynamics at the Water/TiO_2(101) Interface

Michael Wagstaffe,[1,*] Adrian Dominguez-Castro,[2] Lukas Wenthaus,[3] Steffen Palutke,[3] Dmytro Kutnyakhov,[3] Michael Heber,[3] Federico Pressacco,[3] Siarhei Dziarzhytski,[3] Helena Gleißner,[1,4,5] Verena Kristin Gupta,[2] Harald Redlin,[3] Adriel Dominguez,[2,6,7,8] Thomas Frauenheim,[2,6,7] Angel Rubio,[9,8,10,11] Andreas Stierle,[1,4,5,†] and Heshmat Noei[1,5]



Probe
hν = 645 eV
3rd harmonic



Pump
hν=1.6 eV

TiO_2: Anatase (101)

H_2O : $3 \cdot 10^{-8}$ mbar