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Matthias Muntwiler :: Beamline Scientist :: Paul Scherrer Institut

PEARL – Photo-Emission and Atomic Resolution Laboratory

outline

- current status
- scientific case
- instrumental upgrades
- beamline concept for SLS 2.0
- conclusions

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present status

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PEARL – surface science at the synchrotron

Photo-Emission and Atomic Resolution Laboratory

surface science

nano-structured surfaces
2D materials/ultrathin films
molecular networks
magnetic molecules
on-surface chemistry
surfaces of novel materials (topological, multiferroic, …)
…

soft x-ray photoelectron spectroscopy & diffraction

high-resolution XPS
angle scanned (XPD)
photon energy-scanned (PhD)
resonant excitation
x-ray spectroscopy (XAS/NEXAFS/XMCD)

scanning tunnelling microscopy

topography
atomic resolution
dI/dV spectroscopy

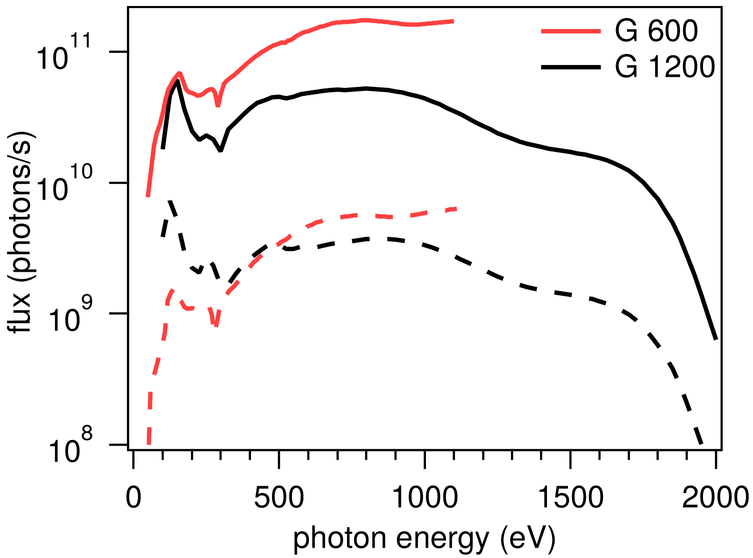
unique combination worldwide

synchrotron radiation

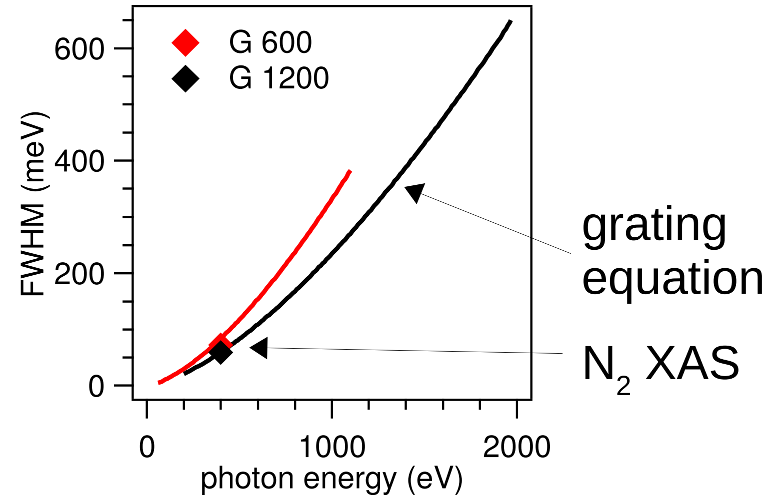
bending magnet
soft x-rays (60-2000 eV)
flux ≤ 10^{12} ph/s on sample
resolution E/ΔE ≤ 7000
polarization linear/elliptical
spot size 100 µm / 1 mm

photon beam characteristics

photon flux



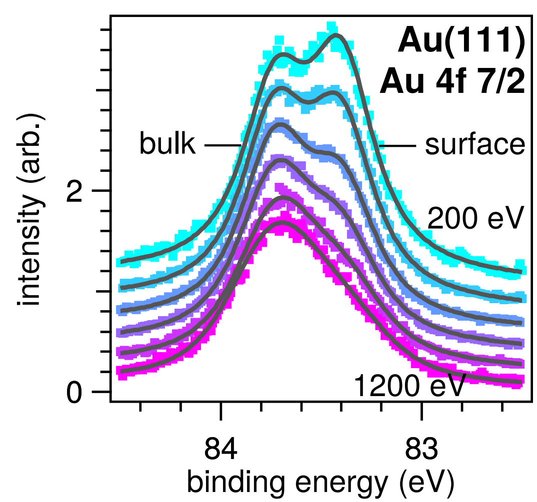
energy resolution



photon energy	60 – 1100, 200 – 2000 eV
ultimate energy resolution	< 0.1 eV (E < 1000 eV)
polarization	linear horizontal circular +/- (< 70%)
spot size	200 µm x 70 µm (H x V, FWHM) 1000 µm x 1000 µm

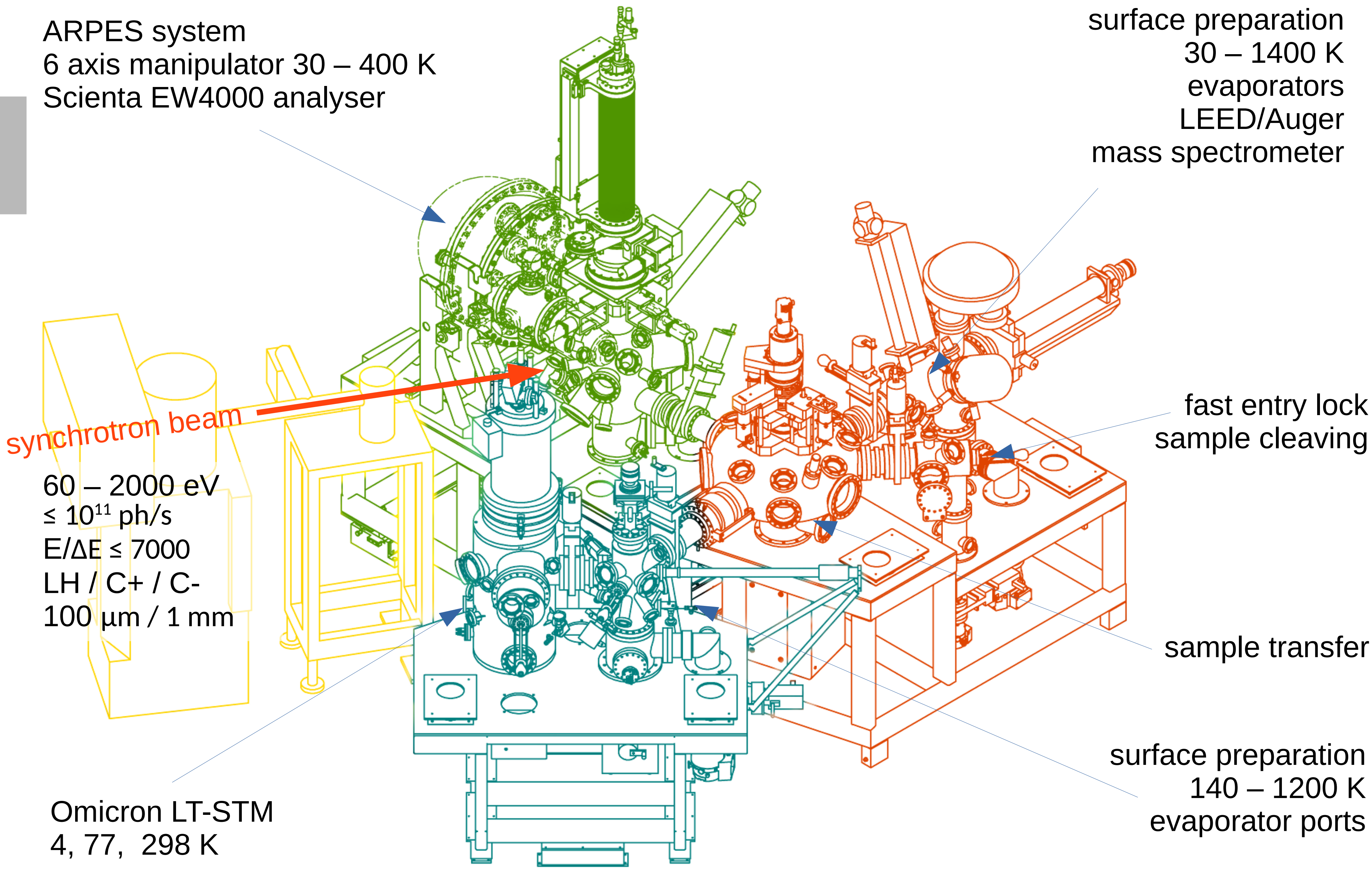
XPS

surface core level shift



[Muntwiler et al, J Synchrotron Rad 24, 354 (2017)]

PEARL beamline (SLS)

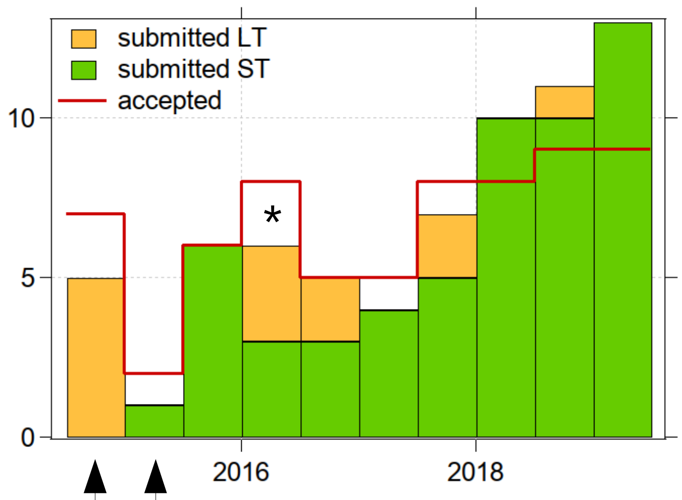


PEARL = Photo-Emission and Atomic Resolution Laboratory

[www.psi.ch/sls/pearl]

performance figures

proposals (long term/short term)

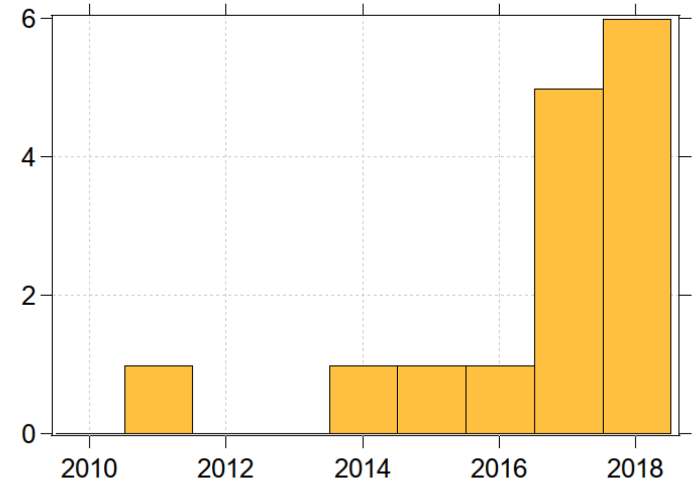


begin of user operation

pilot experiments

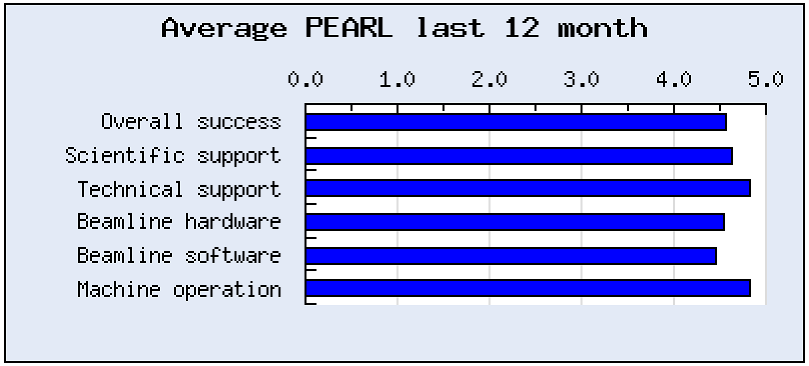
** transferred from other beamlines*

publications



begin of user operation

user feedback
(10/2018)



PEARL team

Matthias
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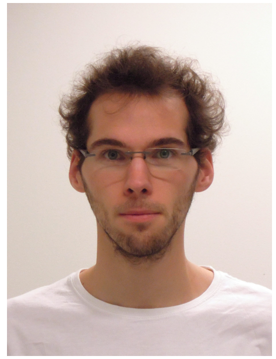
beamline
scientist



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(10/2018)

scientific case

user workshop

- joint user workshop of the ADRESS/SX-ARPES, PEARL and SIS beamlines
  «photoelectron spectroscopy at the SLS 2.0»
  10.-11.9.2018
- topics
  - scientific focus
  - instrumental development
  - complementary methods
- strategy for three beamlines
  - SIS
  - ADRESS/SX-ARPES
  - PEARL
- support from the community

results from the workshop

inorganic surfaces	**nanostructured surfaces**	**molecular nanoscience**
chalcogenides	patterned surfaces	molecular networks
transition-metal oxides	2D materials, graphene etc.	magnetic molecules
spin-orbit coupling	ultrathin films	coupled quantum systems
topological insulators	on-surface chemistry	
heavy fermions		
interfaces		

bulk systems/physics
non-local probes
radiation resistant

surface systems/physics
local probes
radiation sensitive samples

ARPES (SIS/ADRESS)	**complementary surface science methods**
high resolution ARPES	in-situ preparation
low temperature	ARPES
high flux	XPS, XPD
nano-focus	resonant ARPES
spin resolved	STM/STS
	XAS/NEXAFS/XMCD

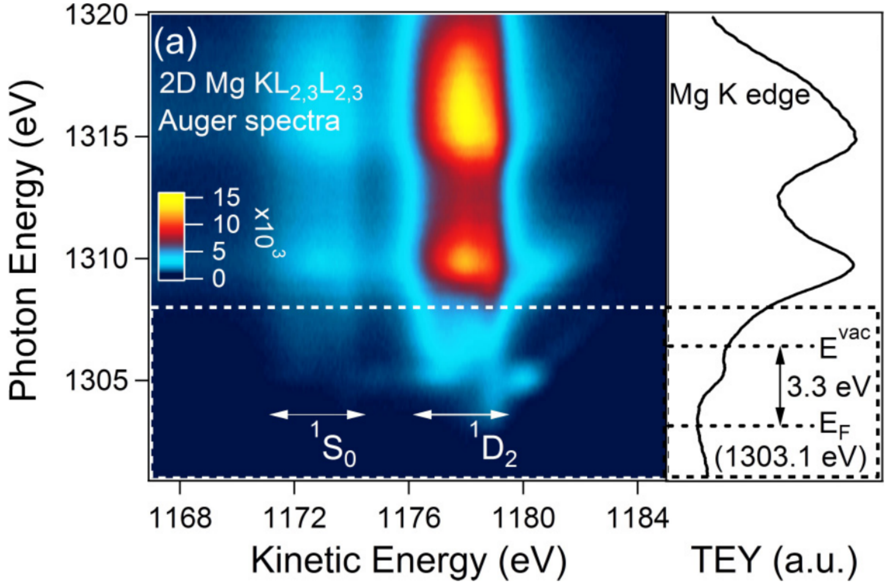
PEARL

method portfolio of PEARL

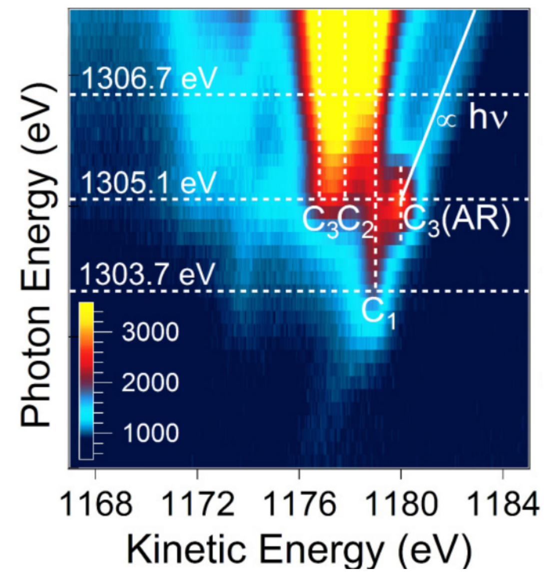
- XPS/ARPES – photoelectron spectroscopy
  - core levels, chemical analysis
  - on-surface reactions *(→ temperature control)*
  - molecular electronic states
  - *band mapping, Fermi surface mapping (→ energy range, angle resolution)*
- resonant XPS/AES
  - excited states *(→ lower harmonic contamination)*
  - orbital momentum *(→ circular polarization)*
  - core-hole clock
- XPD – photoelectron diffraction (angle scanned, photon energy scanned)
  - «fingerprinting» of surface and crystal structure
  - detailed structural parameters
  - *orbital tomography (→ energy range)*
- STM – scanning tunnelling microscopy and spectroscopy
  - real space surface structure
  - local density of states (occupied and unoccupied) ↔ ARPES

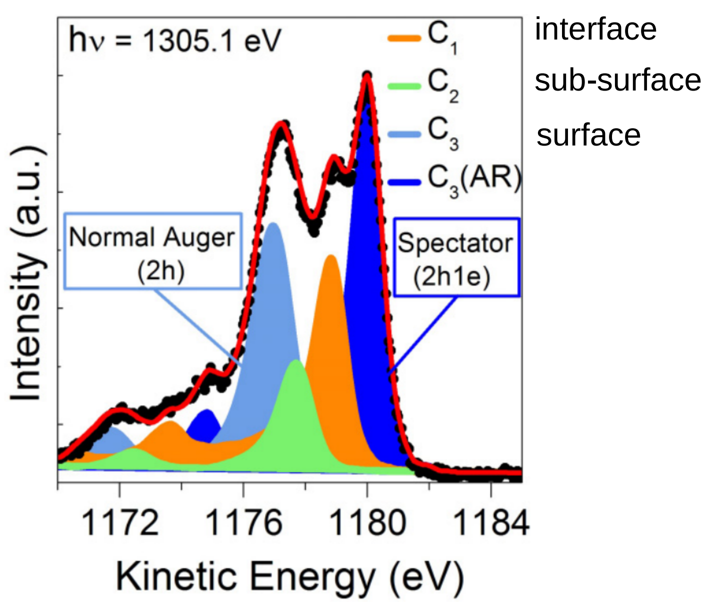
red = new or improved feature

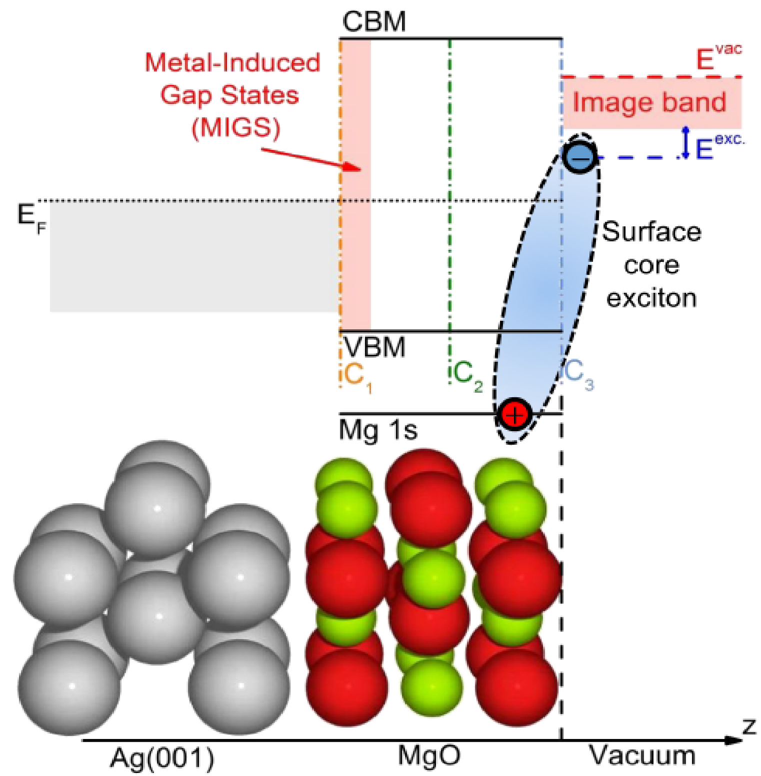
resonant spectroscopy: MgO/Ag(001)



pre-edge

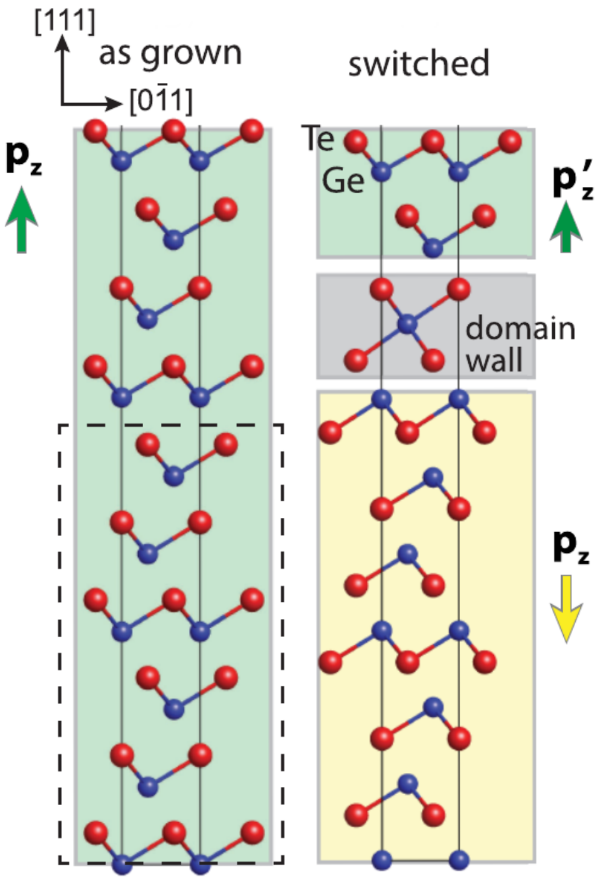




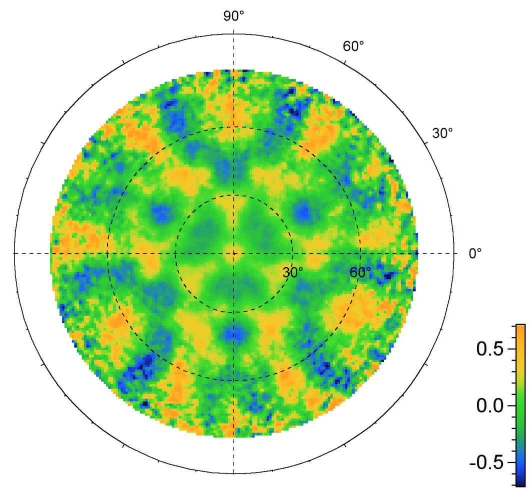


[Jaouen et al, PRB 91, 161410(R) (2015)]

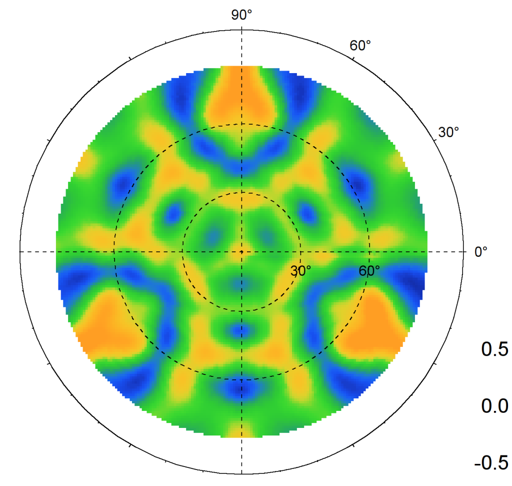
surface relaxation in multiferroic GeTe



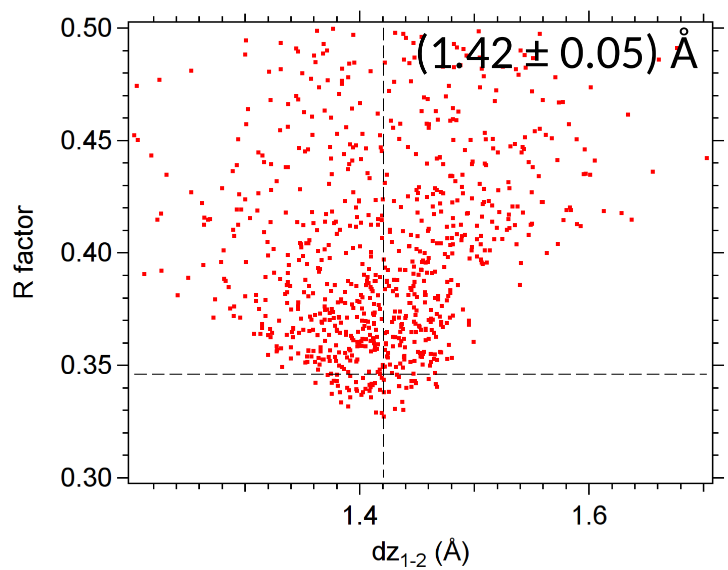
Ge 3s photoelectron diffraction



measurement



scattering calculation



variation of parameters

[Muntwiler, Krempasky, unpublished]

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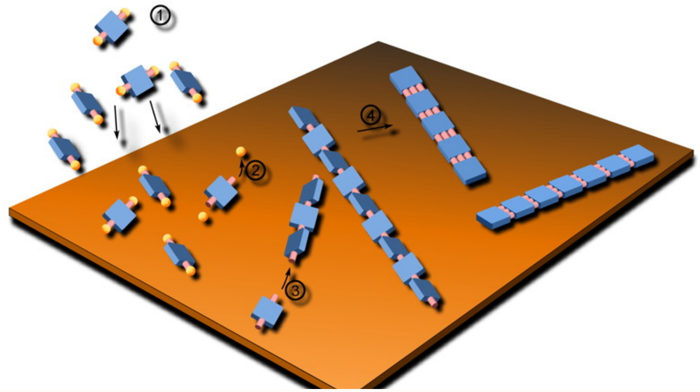
Empa
Materials Science and Technology

on-surface reactions: chemistry in 2D

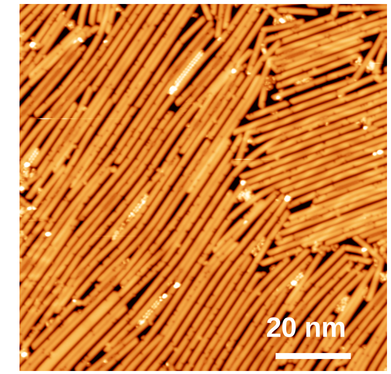
bottom-up fabrication of atomically precise carbon nanomaterials

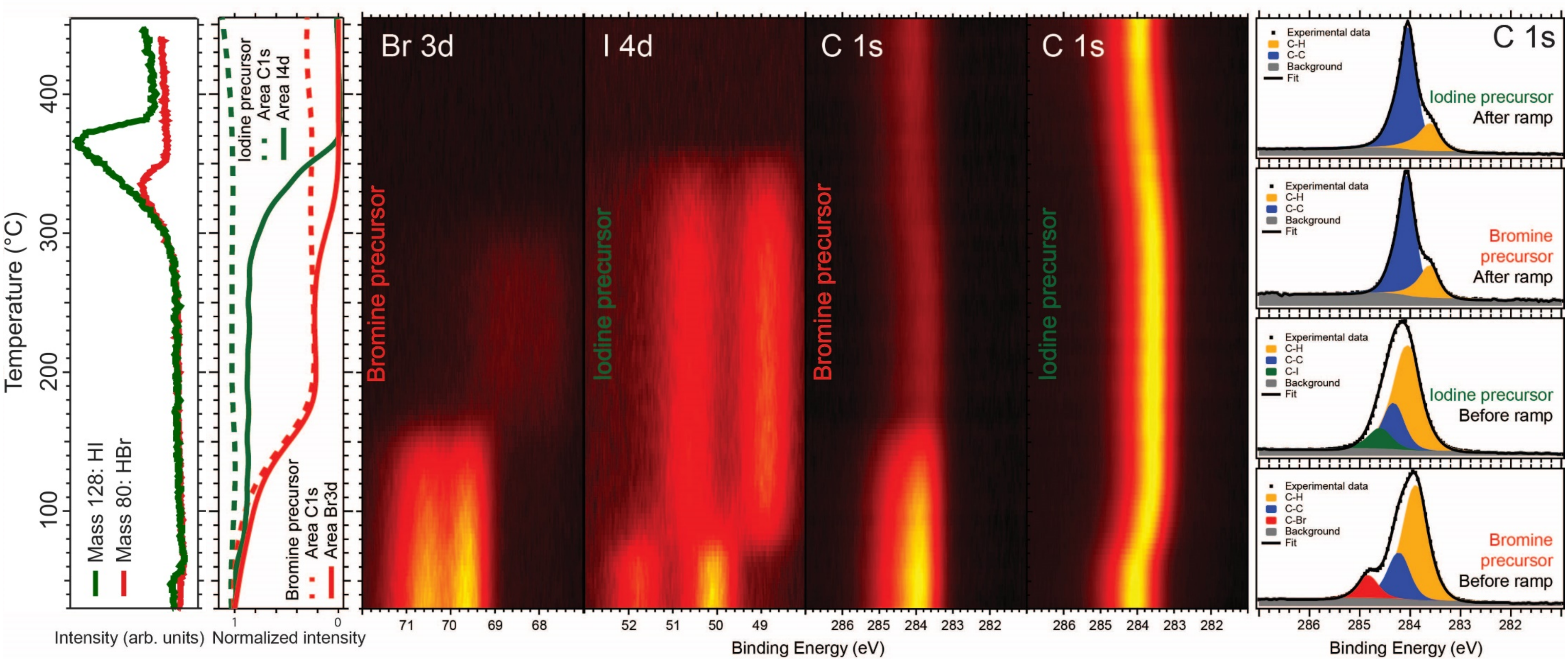


metal surface as template (and catalyst)
here: mostly Au(111)

UHV conditions

surface-science approach





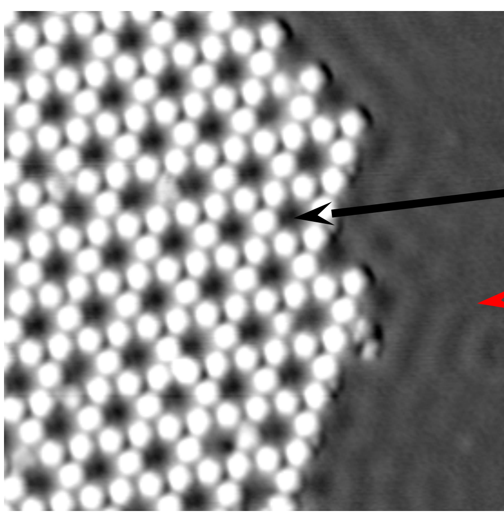
[Di Giovannantonio et al, ACS Nano 12 (2018), 74]

slide courtesy of R. Widmer

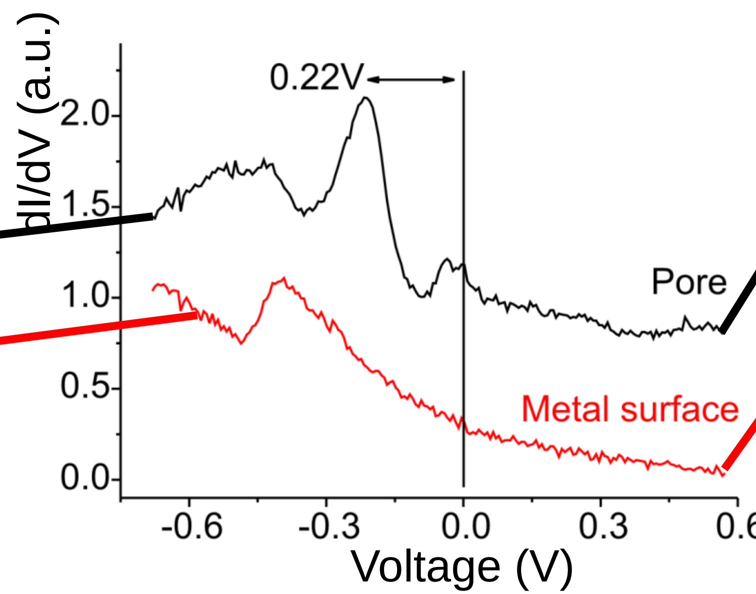
“electronic metamaterials” from coupled quantum wells at surfaces

- porous molecular network @ Cu(111):
- confinement of surface states to quantum well
- periodicity of quantum wells
  → new electronic band structure in 2D
- tunability
  → metamaterial

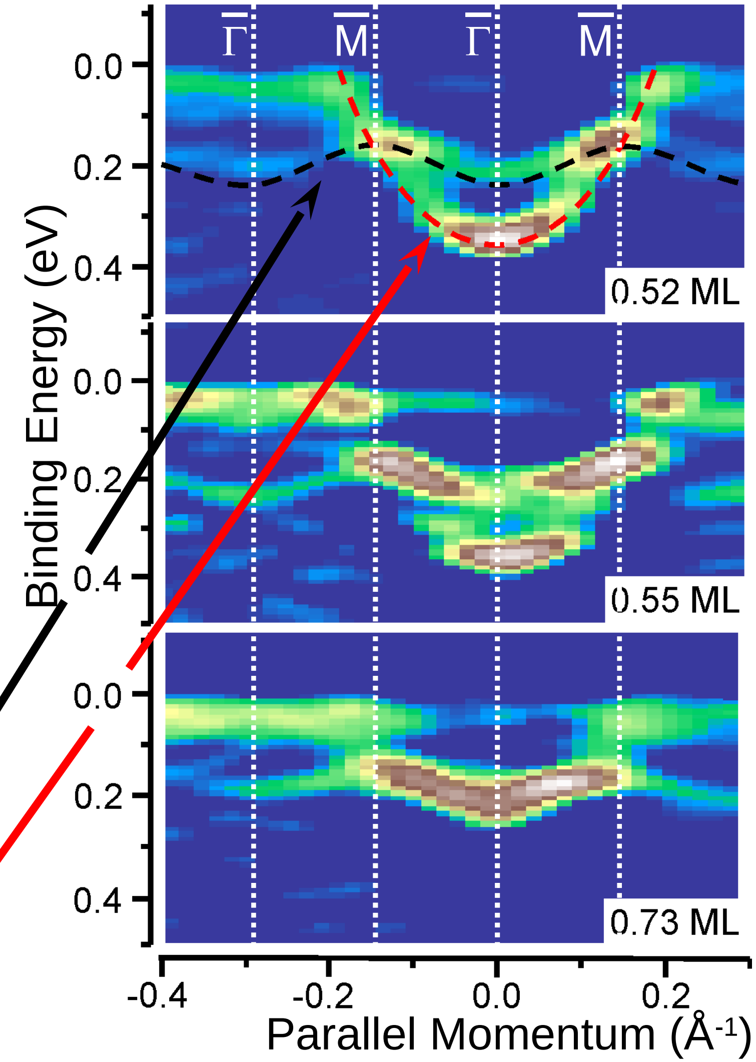
STM micrograph



21nm x 21nm



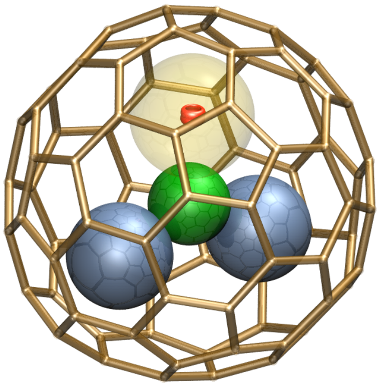
ARPES Results

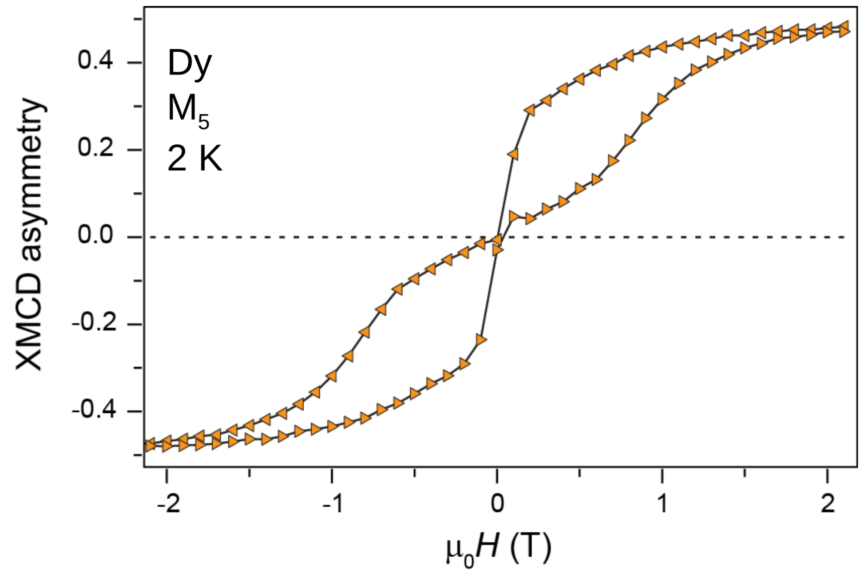


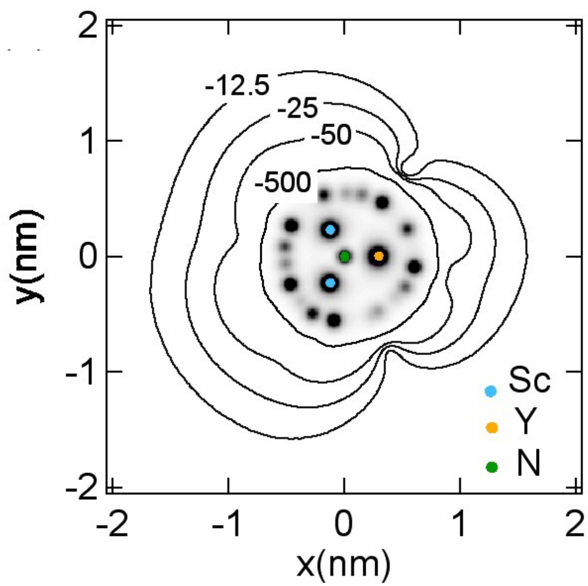
J. Lobo-Checa et al., Science 325, 300 (2009)

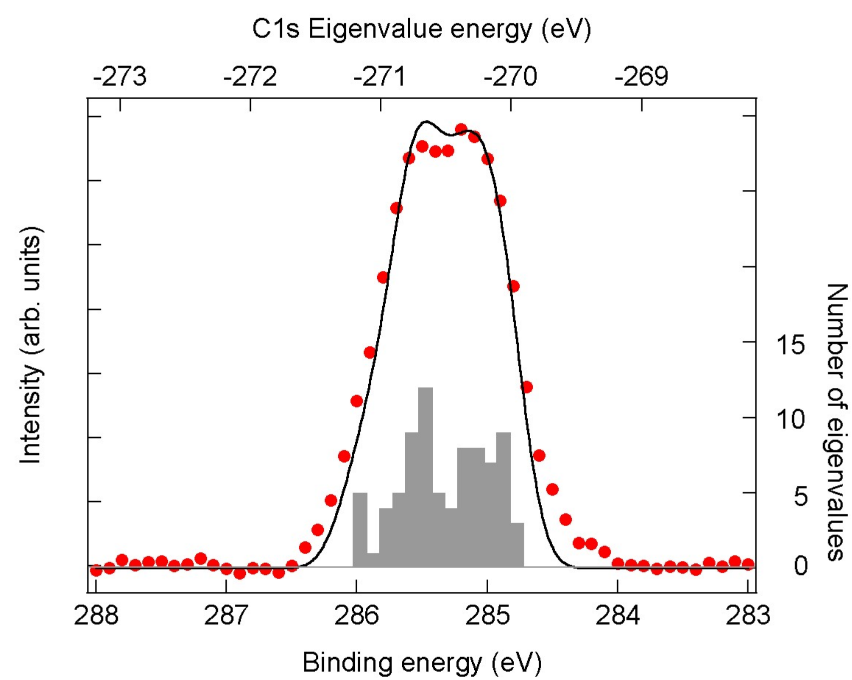
slide courtesy of T. Greber

endohedral fullerenes: from bit to qubit







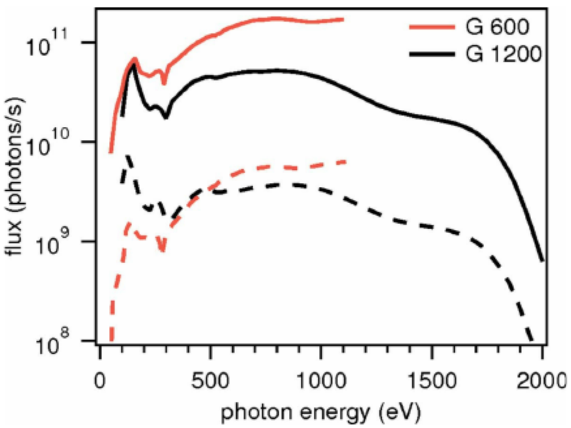


[Westerström, Dreiser et al, JACS 134, 9840 (2012)]
[Stania et al, j phys chem lett 9, 3586 (2018)]

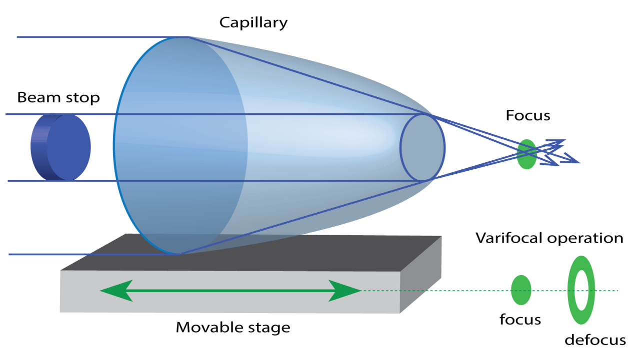
slide courtesy of T. Greber

instrumental upgrades

x-ray optics



(current performance)



- optimize flux (currently 10^{11} photons/s)
  - blazed gratings
- extend photon energy range (currently 70-2000 eV)
  - additional grating for 30-300 eV
- high-order suppression (currently up to 20% harmonic content)
  - 3-mirror system, transmission ~60%
- spot size
  - 100 x 100 μm^2
  - defocusing (1 x 1 mm^2) for radiation sensitive samples
  - 1 x 1 μm^2 (capillary concept → V. Strokov)

end station upgrades

- analyser upgrade
  - improve angle resolution
  - small-spot compatibility (angle-deflecting)
- manipulator
  - heating
  - small-spot compatibility, scanning
- preparation system
  - port for user-supplied growth chamber
  - sample loading in clean/inert atmosphere
- sample environment
  - magnetic/electric field, variable temperature, evaporator sources, gas dosing, …
- STM
  - versatile control system

beamline scenarios

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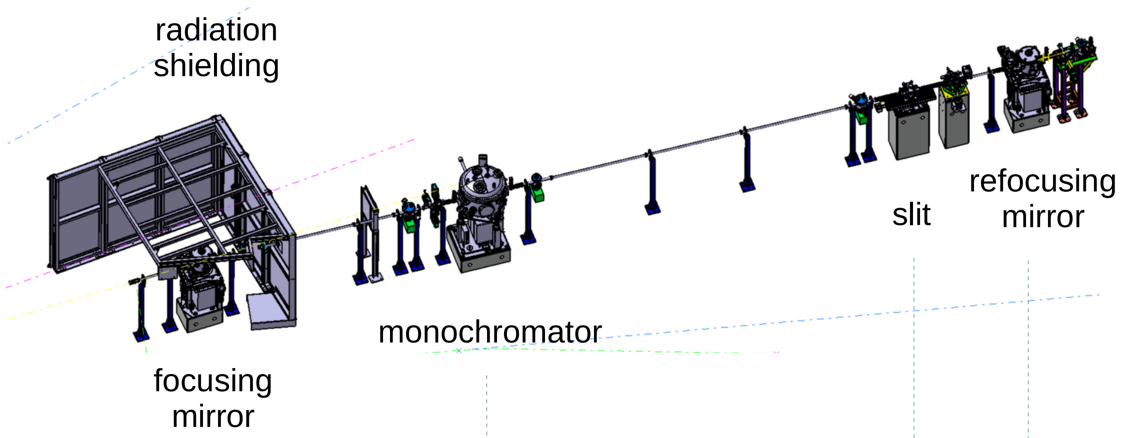
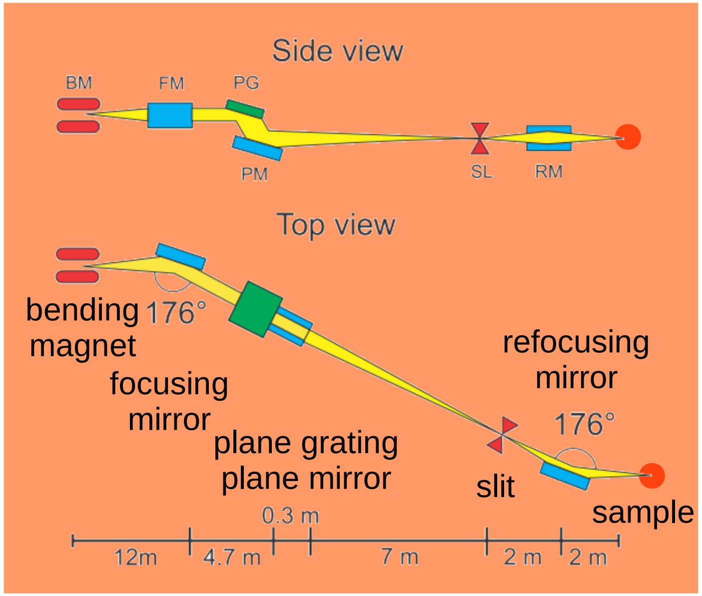
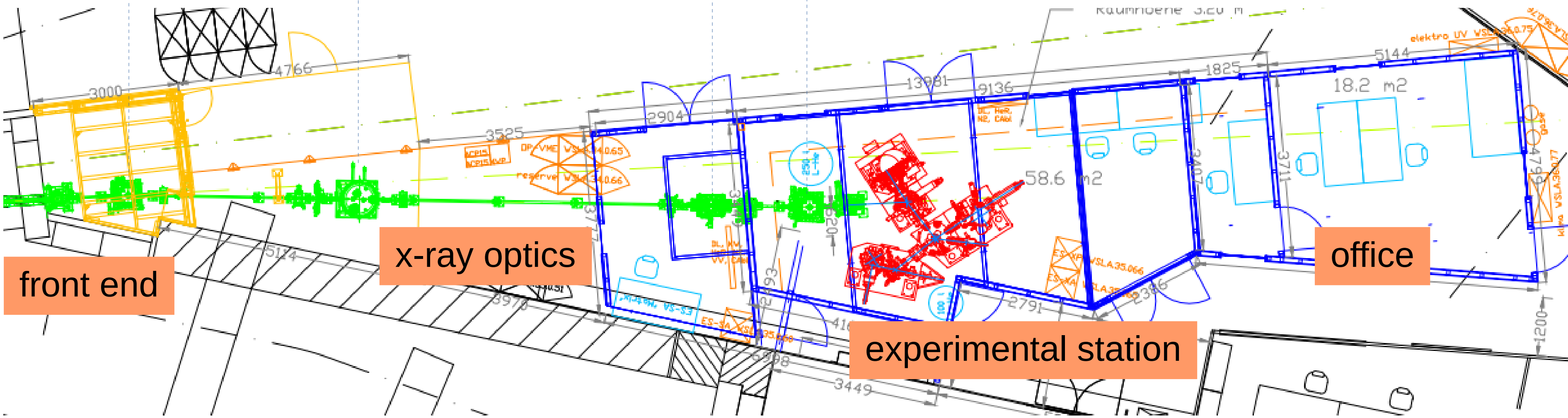
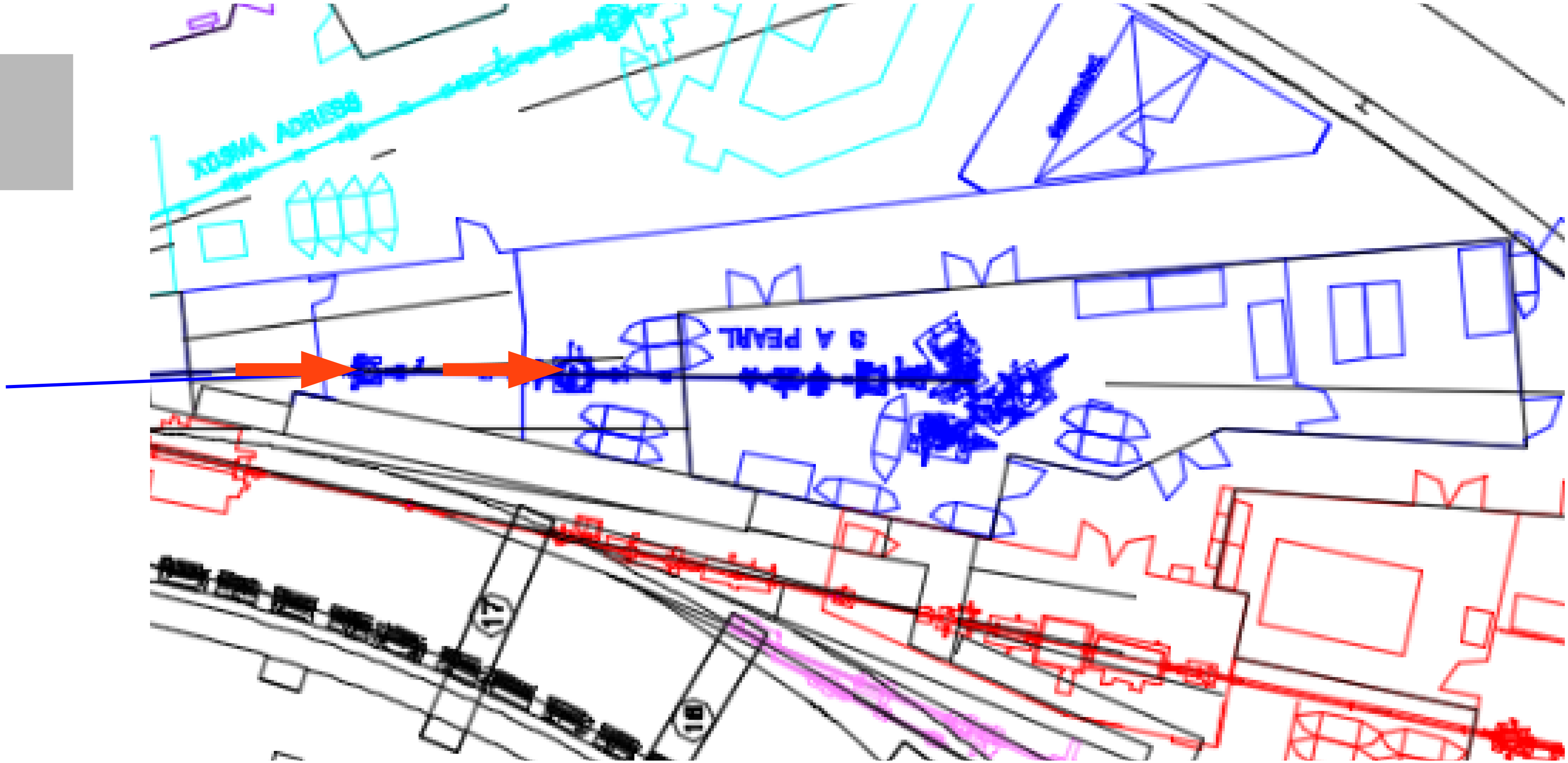
current situation







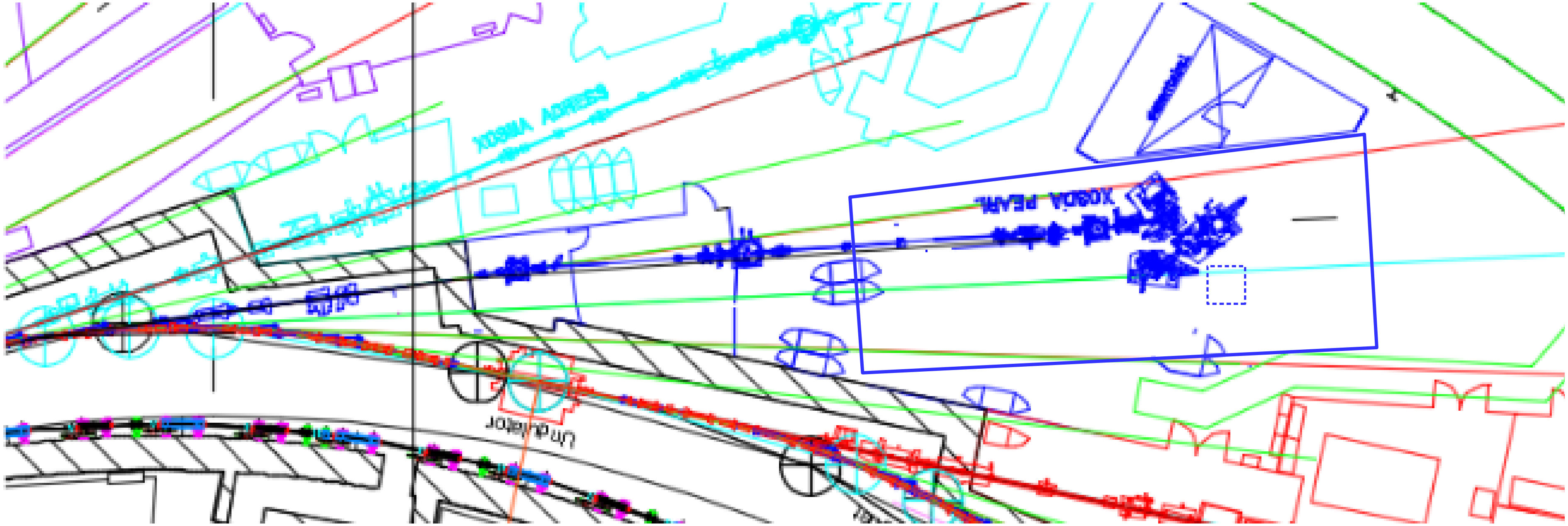
case 1: minimum change



- move focusing mirror unit, replace mirror
- move monochromator
- larger lead hutch
- endstation stays at current position

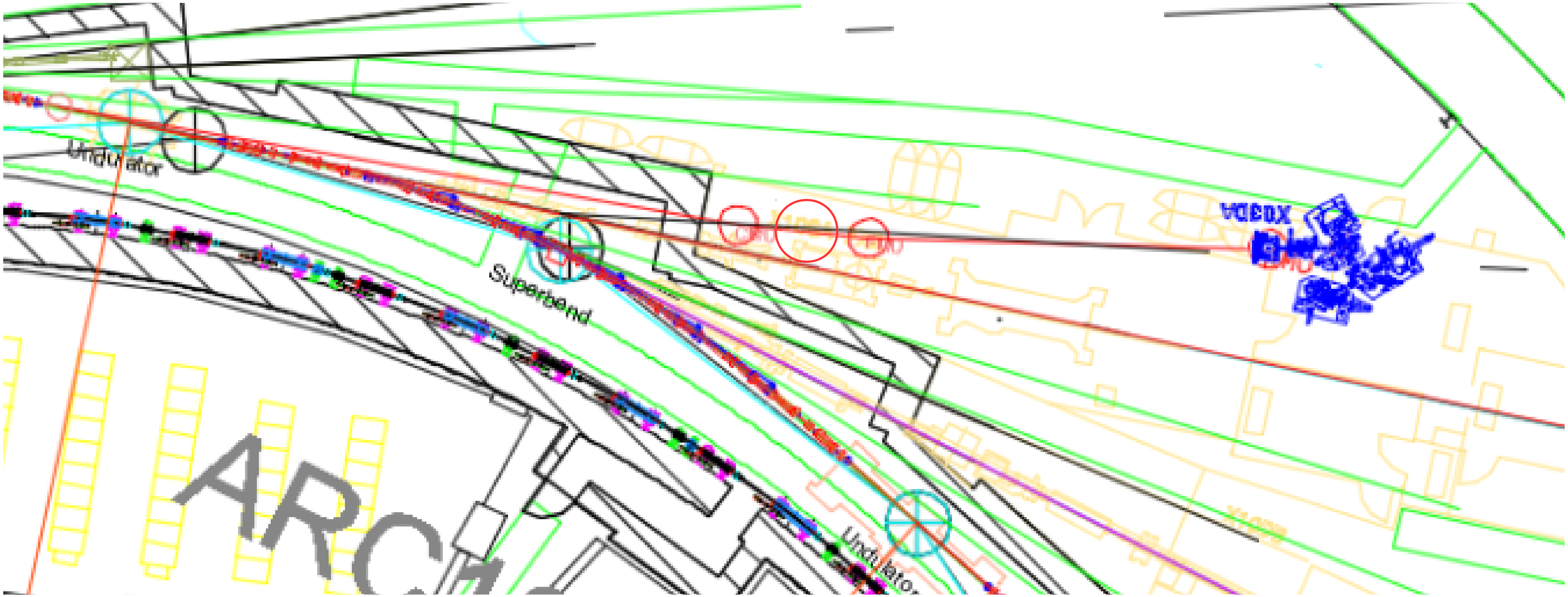
significant performance loss
(transmission, divergence, resolution)
upgrades of optics and endstation difficult
(limited space)

case 2: upstream magnet



- extract beam from upstream LGB
- shift beamline and endstation
- new focusing mirror
- new experiment hutch, re-use existing lead hutch
- sufficient space for optics and endstation upgrades

case 3: undulator



example in straight 10 with hard-x and soft-x undulator (4° extraction angle)

- full PGM optics scheme, 4 x 4° deflection
- limited floor space
- collocation with hard-x branch challenging

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impact on features and performance

feature	SLS 1.0	SLS 2.0	case 1 «minimum»	case 2 «upstream»	case 3 «undulator»
photon energy (eV)	60-2000 (2 gratings)	30-2000 (3 gratings)	😐	🙂	☹️
photon rate on sample (1/s)	10^{11}	10^{12}	☹️ ☹️	🙂 😐	🙂 😐[4]
max. energy resolution (E/ΔE)	7000	10000	☹️ ☹️	🙂 😐	🙂 🙂
spot size (µm²)	 200 x 100 1000 x 1000	1 x 1 100 x 100 1000 x 1000	🙂[1] 🙂 🙂	🙂[1] 🙂 🙂	🙂[1] 🙂 ☹️
polarization	LH C+, C-	LH C+, C-	🙂 😐[2]	🙂 😐[2]	🙂 🙂
harmonic contamination	< 20%	< 2%	☹️	😐[3]	😐
end station		upgrades extensions	🙂 ☹️[5]	🙂 🙂	🙂 ☹️[5]

1. capillary optics
2. dynamic bump
3. high-order suppression unit
4. check for radiation sensitive samples
5. limited space

conclusions

- growing demand
  - complementary local and non-local methods
  - correlate atomic/molecular and electronic structure
- PEARL fulfills many of these demands already today in a unique, versatile setup
  - ARPES performance needs improvement
- concepts for SLS 2.0
  - «minimal changes»
    - lower x-ray performance than at SLS 1.0
  - upstream bending magnet
    - improved (or at least maintained) x-ray performance
    - room for further development
  - undulator
    - highest x-ray quality (flux, resolution, polarization)
    - requires a completely new beamline
    - radiation damage to sensitive samples

acknowledgements

https://www.psi.ch/sls/pearl

recent collaborators

Daria Sostina, PSI
Nicolas Bachellier, PSI
Luis H. de Lima, Zürich
Jun Zhang, PSI
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