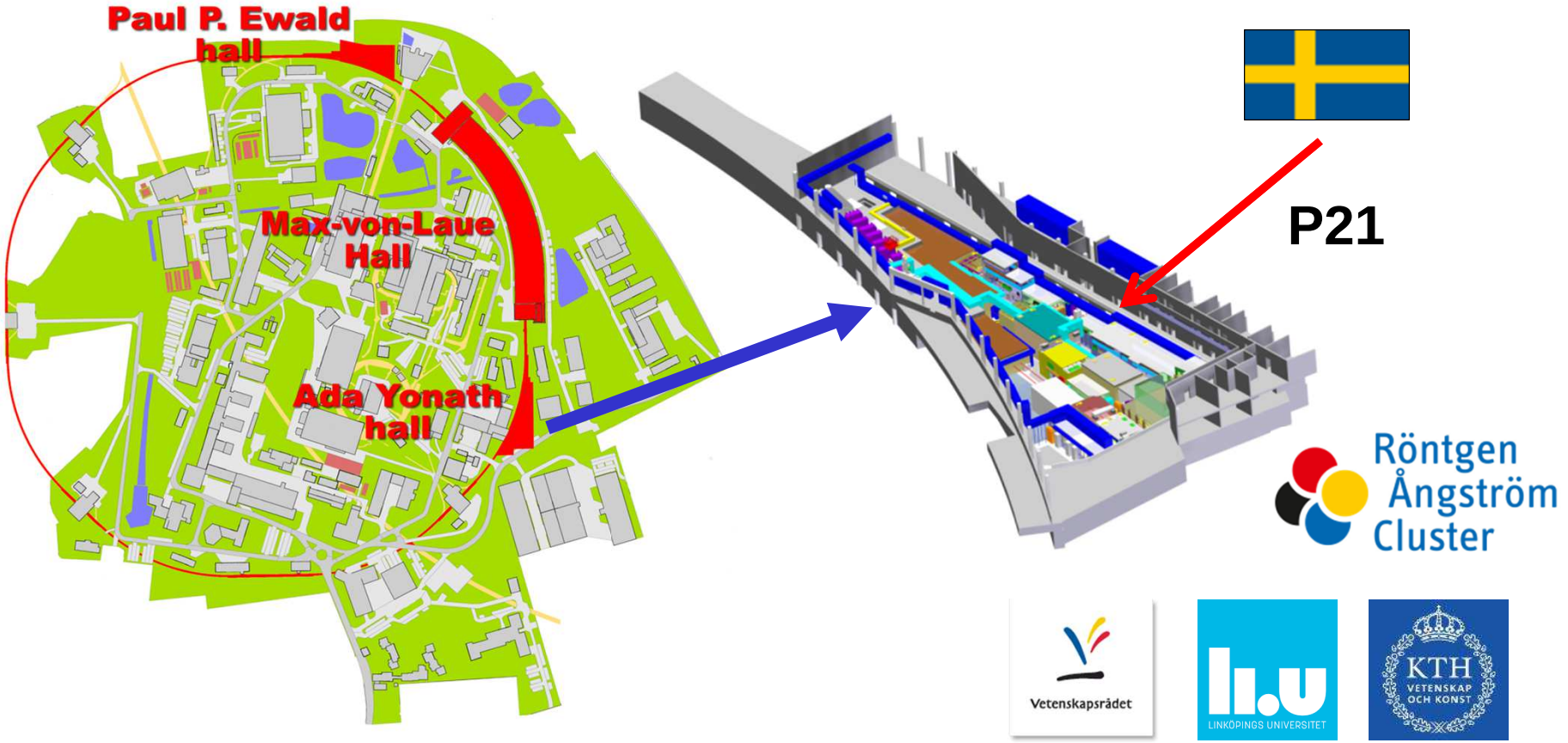
The Swedish beamline at PETRA III



Röntgen Ångström Cluster

Vetenskapsrådet

LINKÖPINGS UNIVERSITET

KTH VETENSKAP OCH KONST

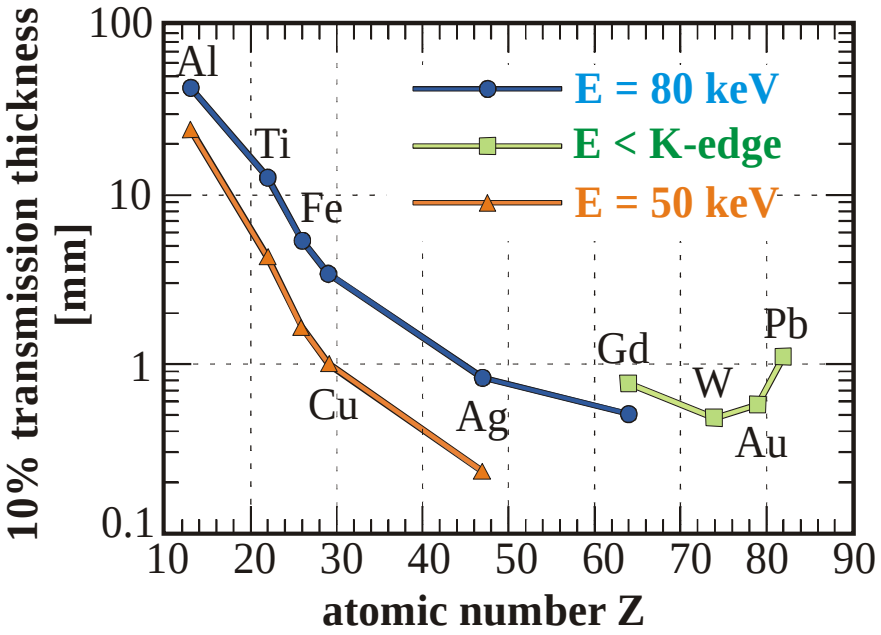
Wolfgang Drube

HELMHOLTZ GEMEINSCHAFT

RÅC workshop
DESY June 9, 2017

DESY

PETRA III: Brilliant source of high energy X-rays (~50-150 keV)



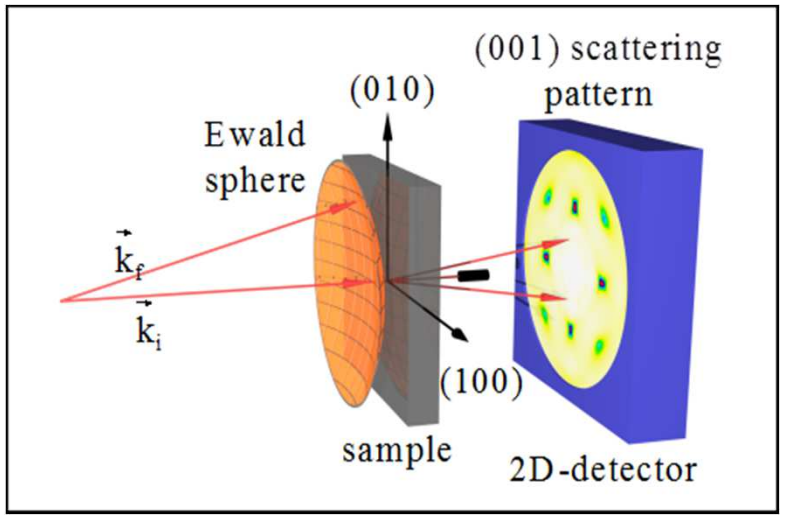
- o large penetration depth ($\mu \sim E^{-3}$, $I \sim e^{-\mu t}$)
- o large momentum transfer
- o large scattering volume
- o small scattering angles
- o large reciprocal space coverage
- o kinematical diffraction ($I \sim E^{-2}$)
- o heavy element K-edges
- o flux ~10^{11} photons/s at 100 keV

Instrumentation

(sub) micron focusing
efficient large area detectors
sample environment

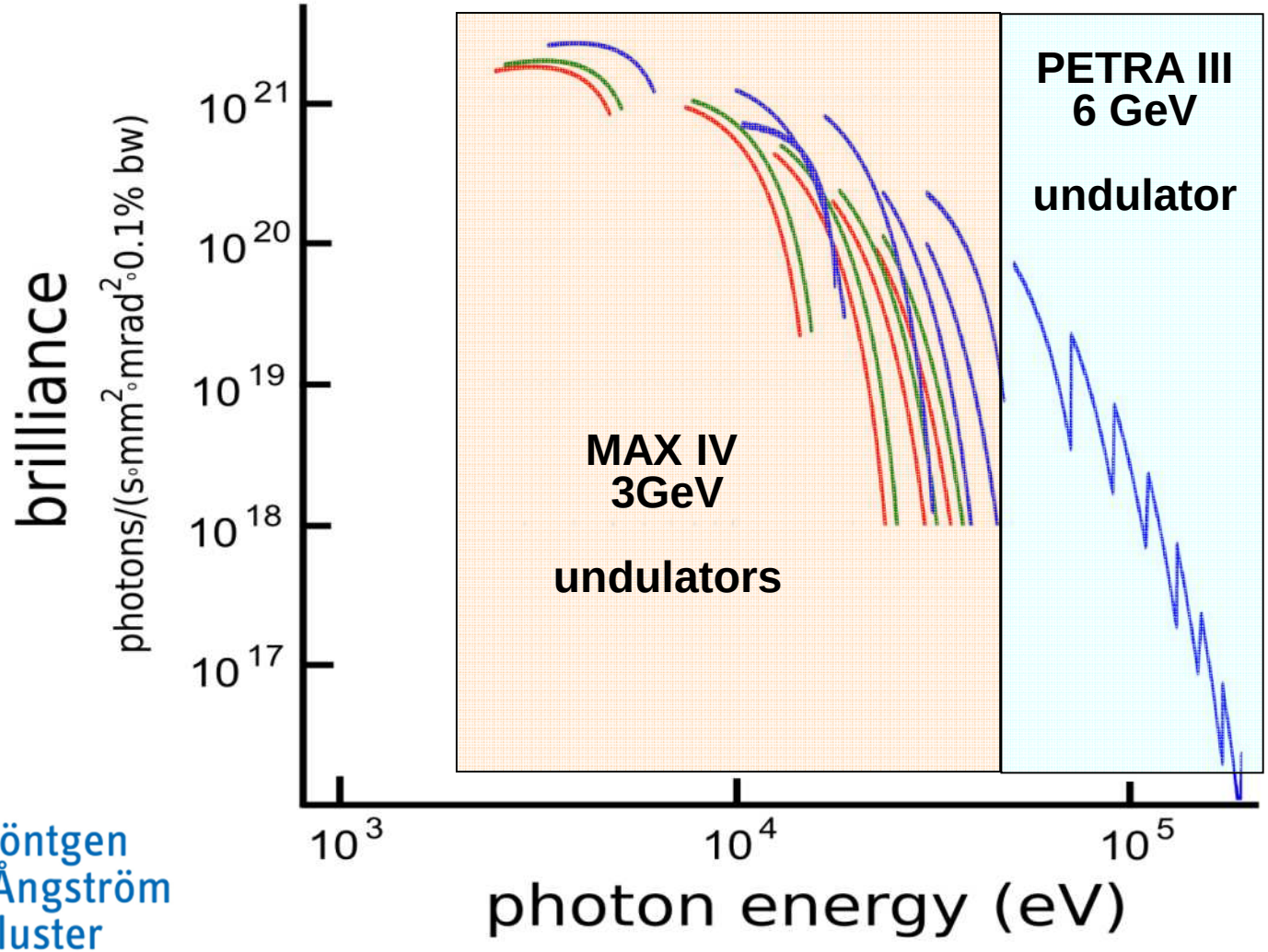
Applications

bulk probe
(buried) interfaces
weak scattering



Swedish Materials Science Beamline at PETRA III

complements MAX IV spectral range at energies >40keV
very attractive for Swedish mat. sci. user community



Röntgen Ångström Cluster

DESY

The launch: MoU with Swedish Research Council

Swedish beamline at PETRA III
Signing ceremony at DESY on 25. February 2011

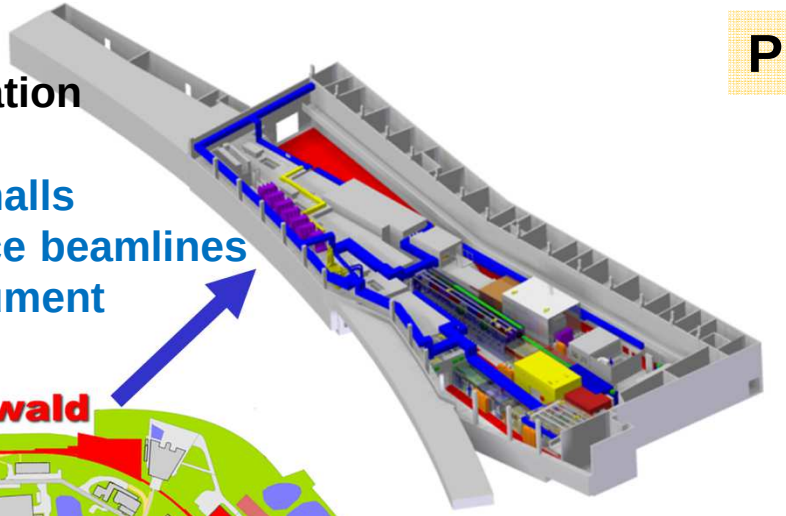
Röntgen Ångström Cluster

Ulf Karlsson, KTH
Peter Honeth, Swedish State Secretary
Leif Erikson, Swedish RC

Georg Schütte, German State Secretary (BMBF)
Helmut Dosch, DG DESY
Edgar Weckert, DESY

PETRA III extension: up to 11 new beamlines

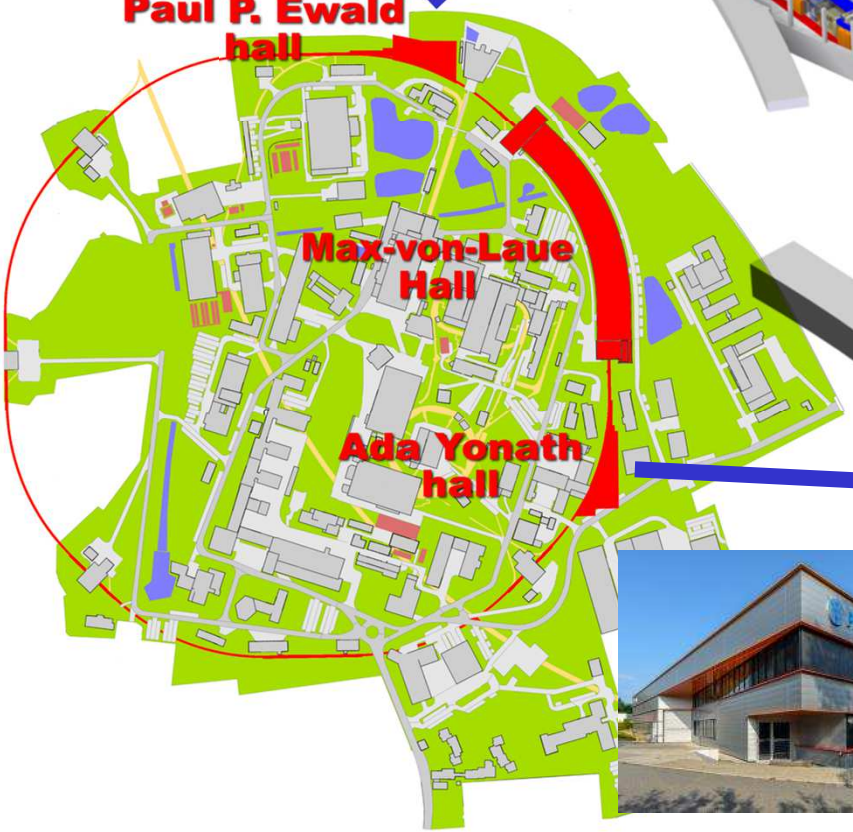
Facilities in operation
(June 2017):
3 experimental halls
18 insertion device beamlines
40 different instrument

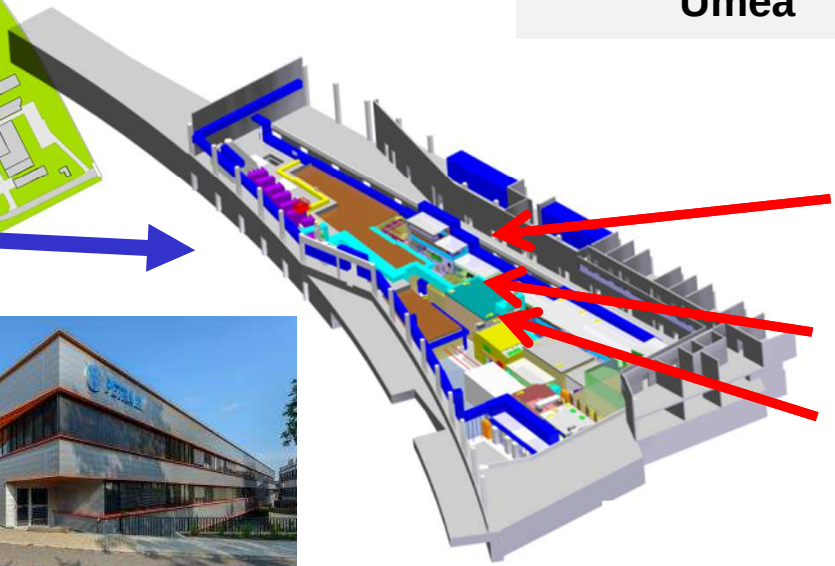


PETRA & FLASH 2012 -16

Users	189
Visits	442
Institutes	46

Universities:
Chalmers Göteborg
Karolinska KTH
Linköping Lund
Malmö Stockholm
Umeå Uppsala





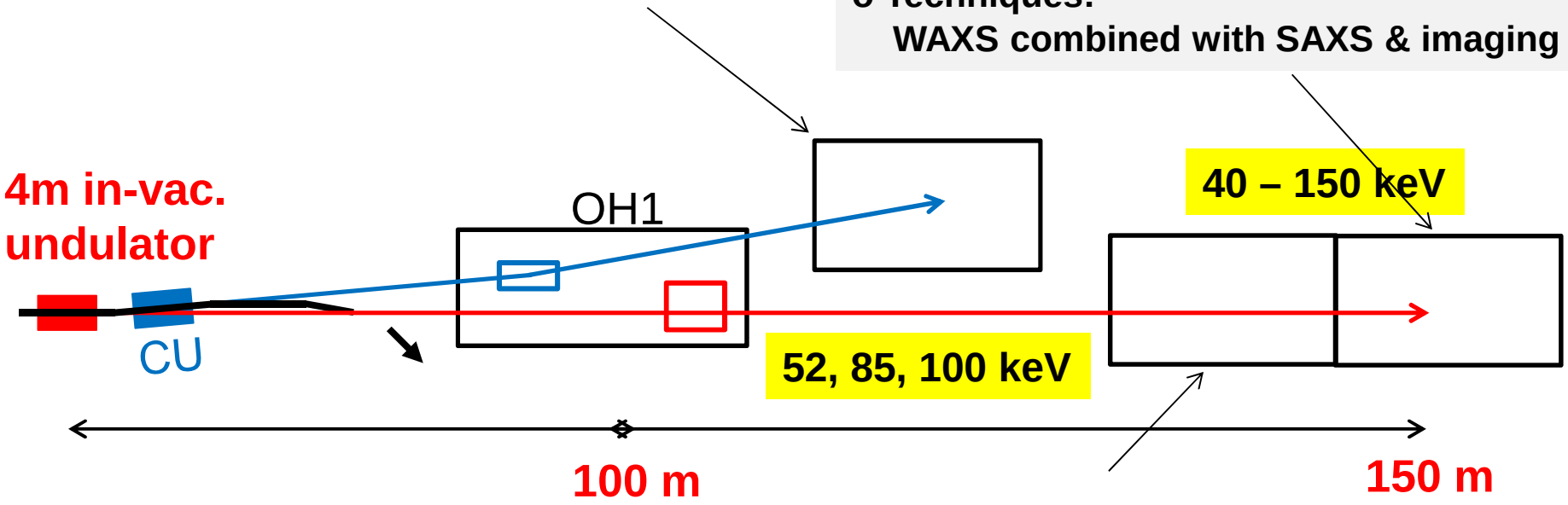
Swedish Materials Science Beamline (P21)

Hutch 1:
Side station (broad band diffraction)

- o Beamsize: 0.05 mm … 2 mm
- o Energy bandwidth: $2x10^{-3}$ … 10^{-2}
- o Techniques: WAXS & PDF

Hutch 3:
Diffraction station

- o Beamsize: 0.2 μm … 6 mm
- o Energy bandwidth: 10^{-4} … $2x10^{-3}$
- o Time resolution down to milli-seconds
- o Techniques:
  WAXS combined with SAXS & imaging



Hutch 2: **“roll-in” station (“empty”)**

- o Beamsize: 0.05 mm … 6 mm
- o Bulky sample environments

longest beamline at PETRA III: 160m

Swedish Materials Science Beamline (P21)

Inline station

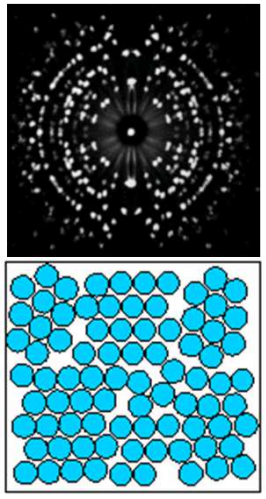
Ulrich Lienert
Sylvio Haas
Sven Gutschmidt
Thomas Bäcker

Grain mapping

3D-XRD

Small angle x-ray scattering

Surface diffraction

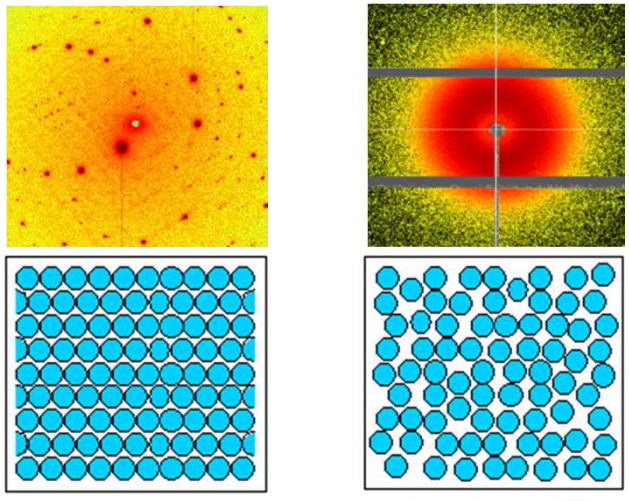


Side station

Martin v. Zimmermann
Rüdiger Nowak
Stefan Sonntag

Single crystal diffraction
– diffuse scattering

Pair distribution function (PDF)



Swedish Materials Science Beamline (P21)

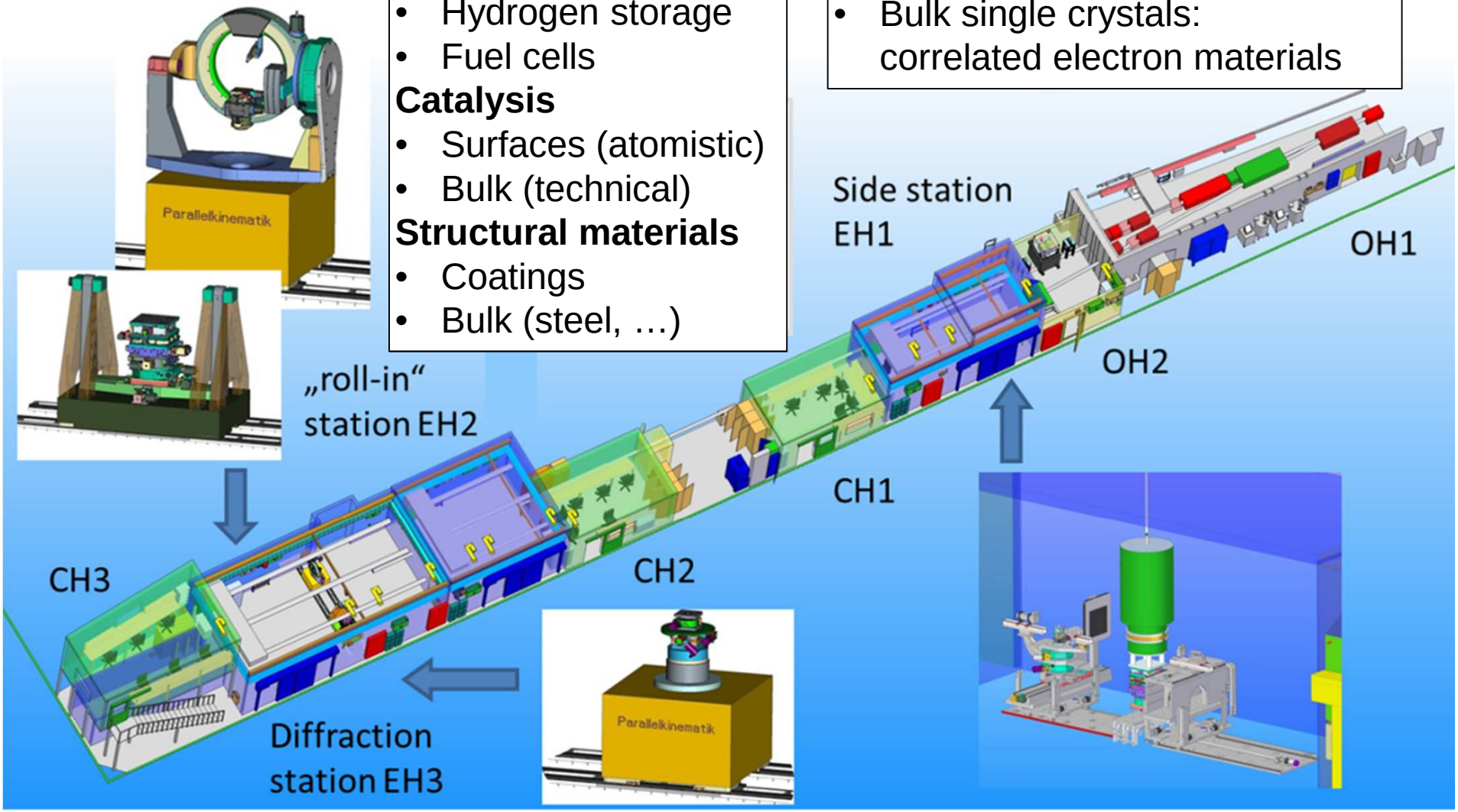
Röntgen Ångström Cluster

Energy materials
- Batteries
- Hydrogen storage
- Fuel cells

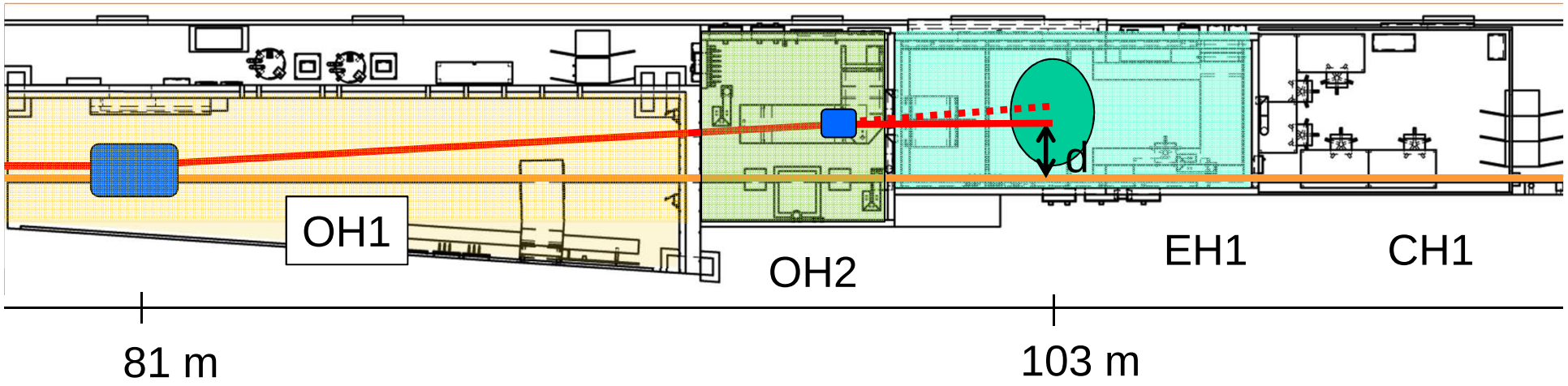
Catalysis
- Surfaces (atomistic)
- Bulk (technical)

Structural materials
- Coatings
- Bulk (steel, …)

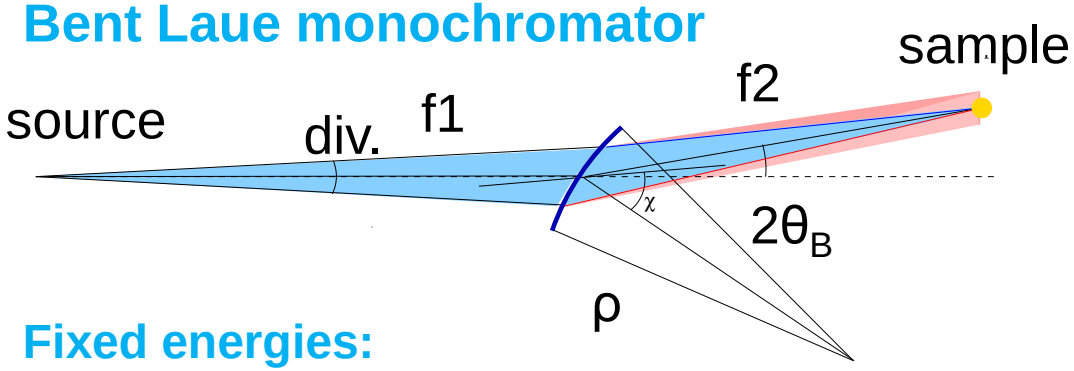
- Metallic glasses, melts, liquids, nano-crystalline matter (PDF)
- Bulk single crystals: correlated electron materials



Side station

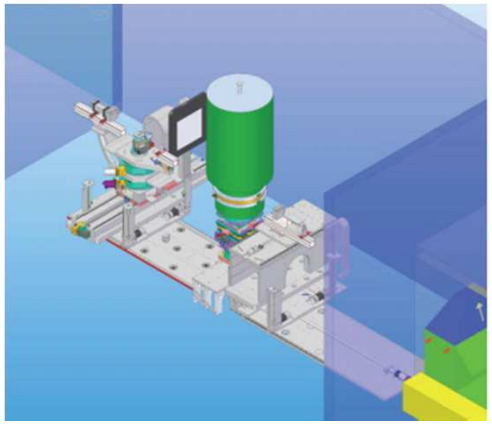


Bent Laue monochromator



Fixed energies:

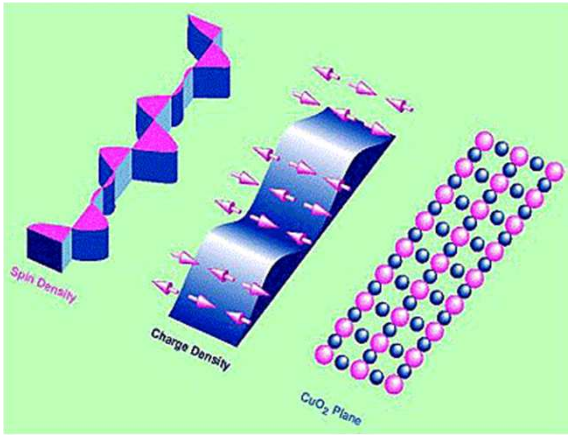
52 keV Si(111)
85 keV Si(220)
100 keV Si(311)



- Heavy load sample tower
- Flexible detector stage

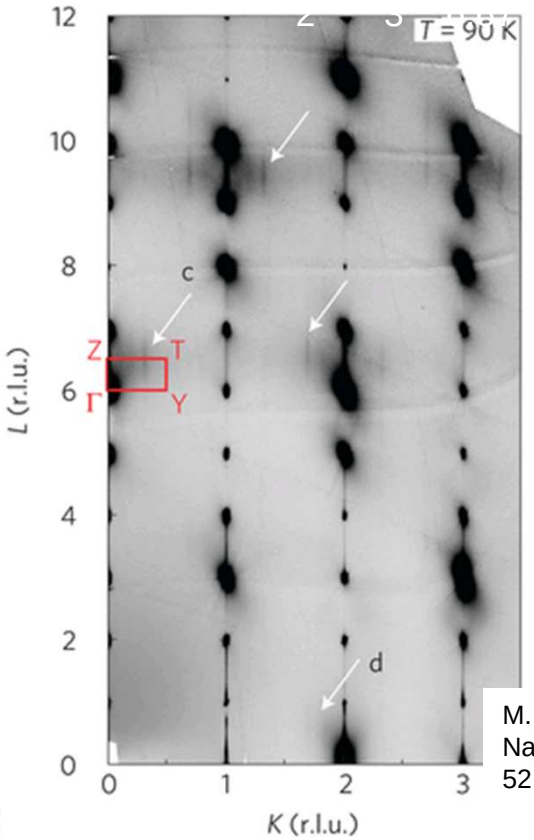
Side station: single crystal diffraction

- Correlated electron materials: breakdown of Fermi liquid model
- Properties largely determined by Spin, Charge, Orbital and Lattice degrees of freedom
- Ordering phenomena on the nano scale → diffuse scattering



Materials:

- High Tc superconductors
- Colossal magneto-resistance (CMR) materials
- Multiferroics



M. Le Tacon et al. Nature Physics 10, 52 (2014)

Wol

Side station: PDF analysis

Local structure materials

High resolution data due to large momentum transfer

materials

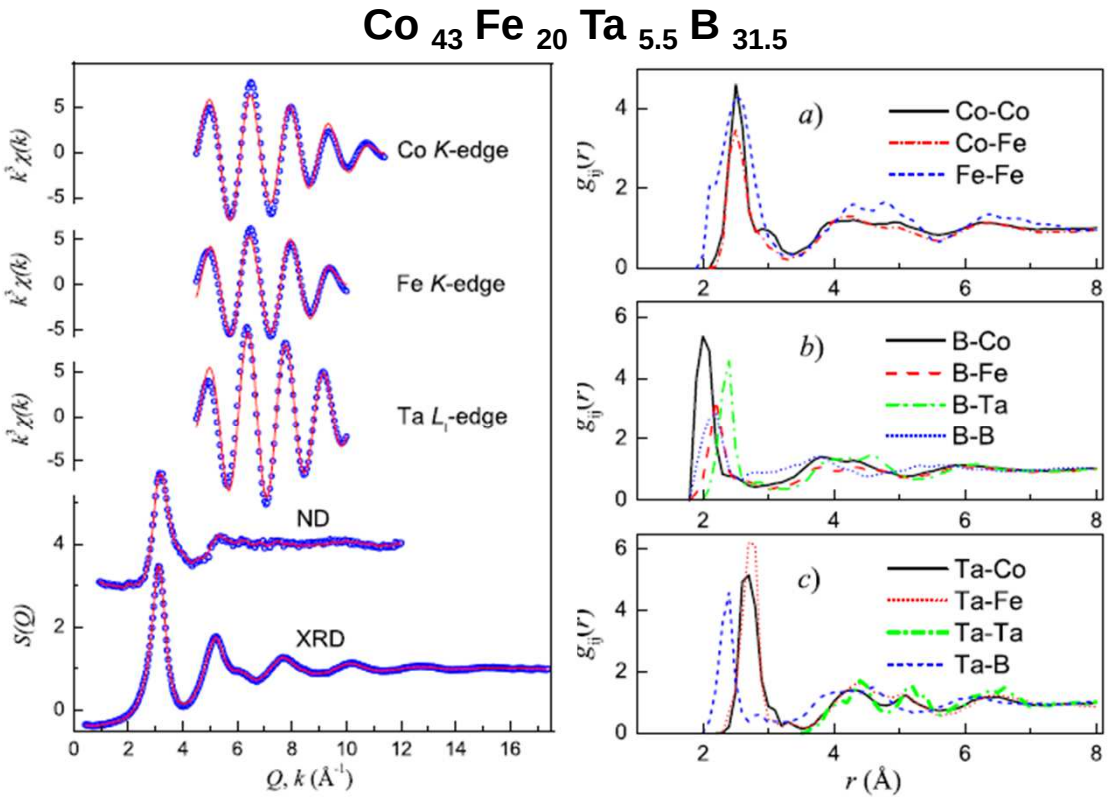
- Bulk metallic glasses
- Melts, liquids
- Nano-crystalline matter

instrumentation

Flux hungry technique

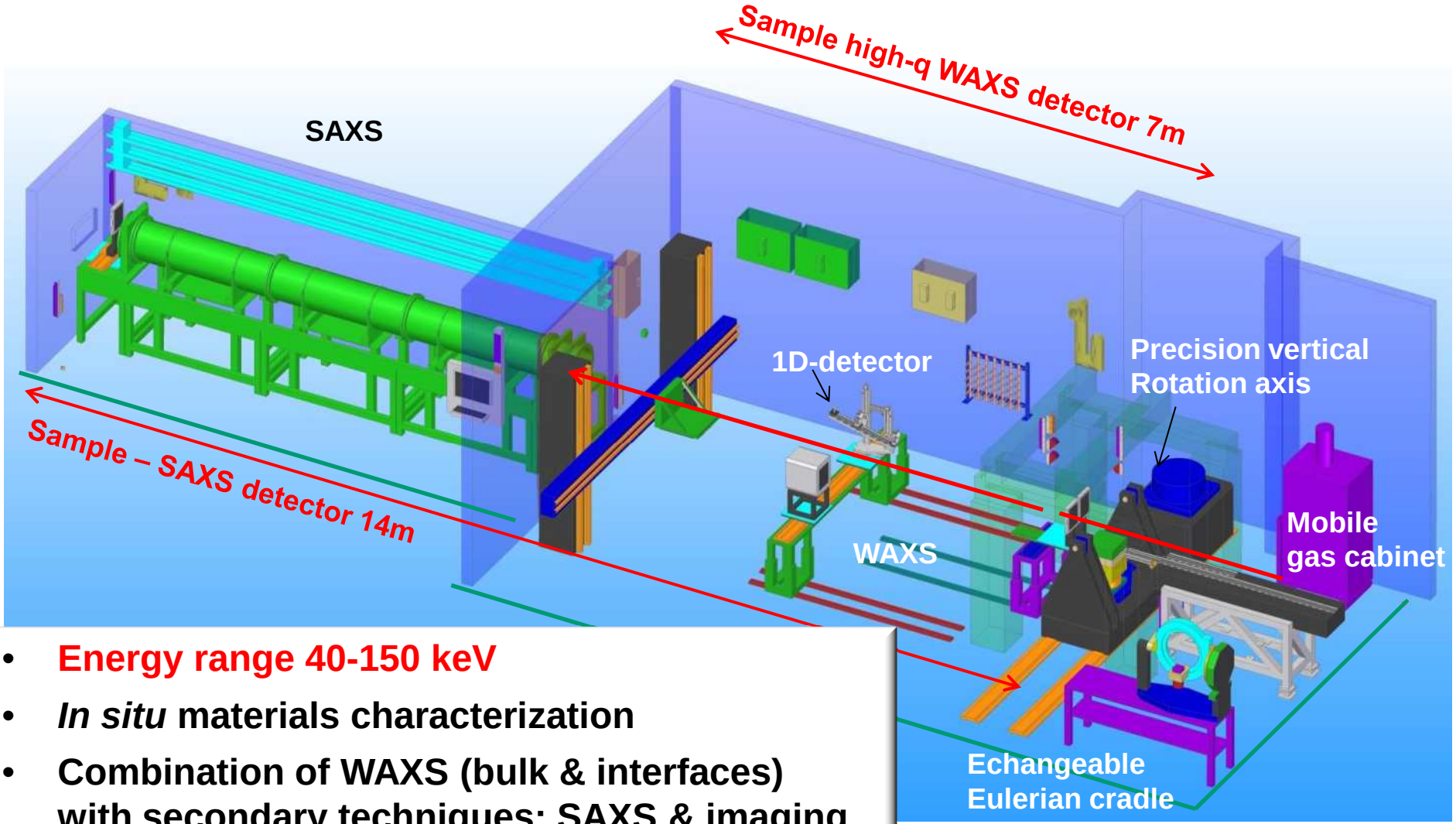
Large bandwidth mono

2d-detector, 2-axis mode



I. Kaban *et al.*
Phys. Rev. B 79, 212201 (2009)

Inline diffraction station



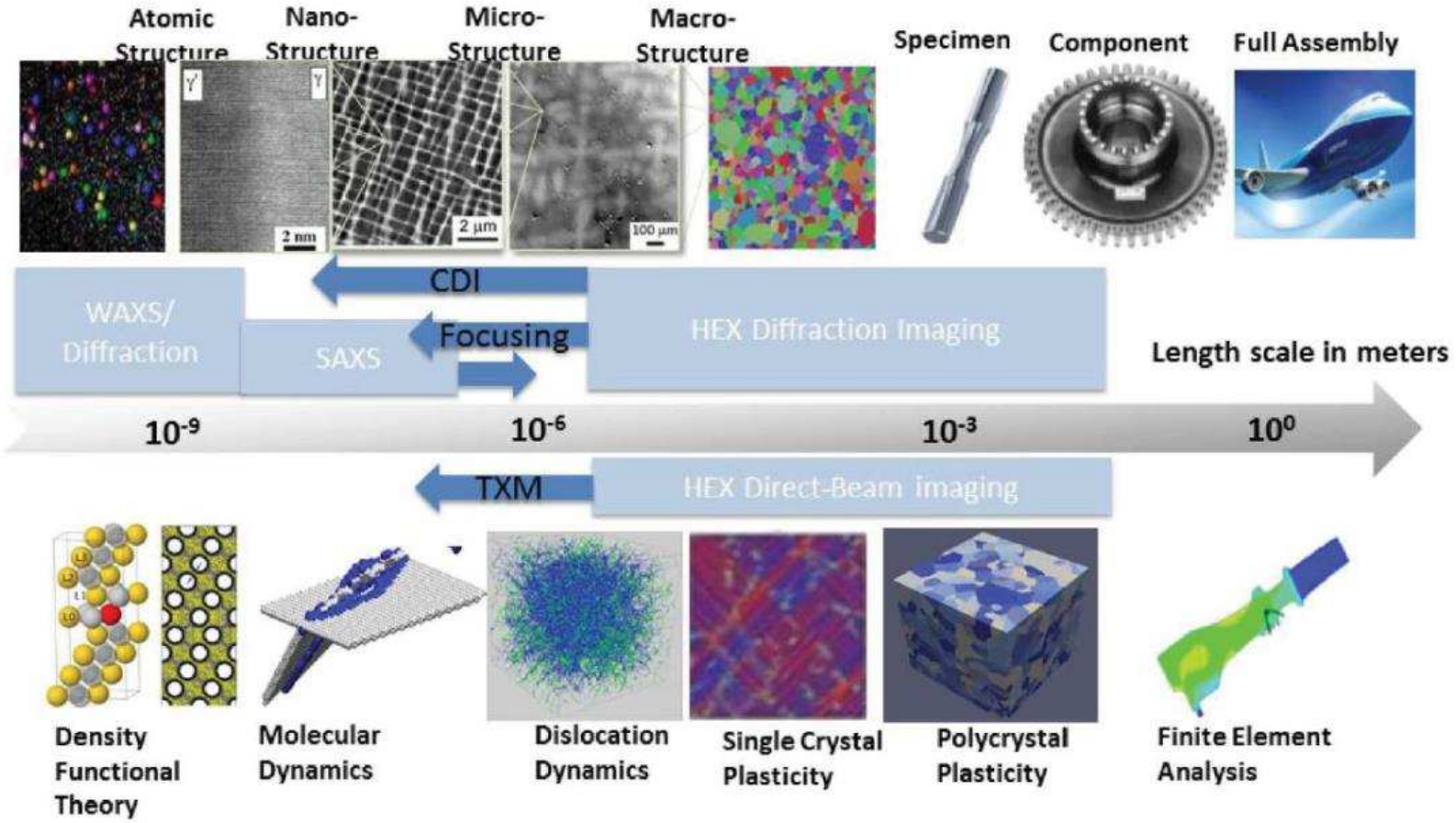
- **Energy range 40-150 keV**
- ***In situ* materials characterization**
- **Combination of WAXS (bulk & interfaces) with secondary techniques: SAXS & imaging**
- **“Zoom-in” data acquisition (beamsize 0.2×4 μm –> 3.6×6 mm, v×h)**

Length scale coverage by WAXS/SAXS/Imaging

courtesy J. Almer

HEXM – Multi-modal to bridge size scales

- Exploit MBA-emittance to advance high-energy x-ray characterization capabilities
- Many mm to sub-Å length-scales through direct- and reciprocal-space methods
- Multi-modal techniques: combinations of spatial zoom-in/out methods
- New techniques — high-energy TXM and BCDI

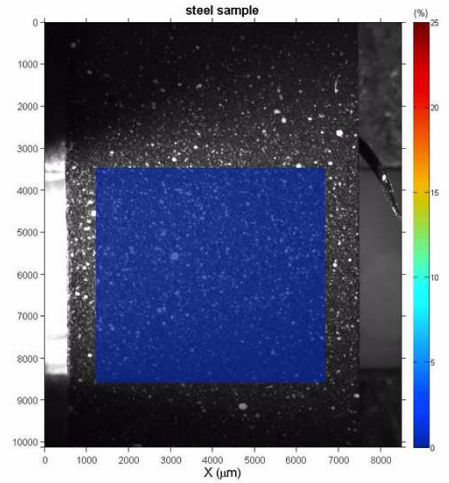


Aerospace is just one example. Others: batteries, SOFCs, nuclear materials, bio-materials

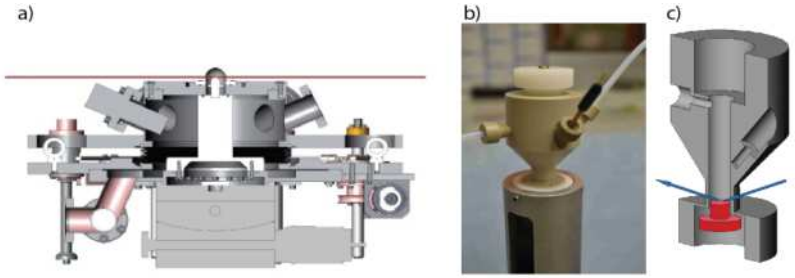
Sample environment & auxiliary probes

- **Compatibility with diffractometers**
- **User driven, will change …**
- **Lab operation?**
- **Auxiliary probes: IR spectroscopy, Digital Image Correlation, …**

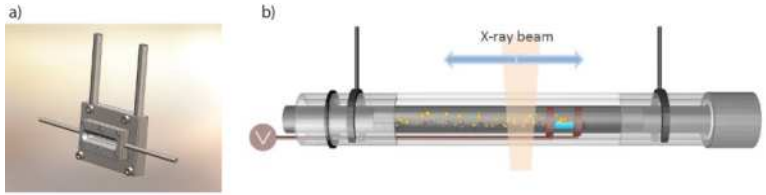
Jerry Lam,
Sen Lin,
KTH 2015

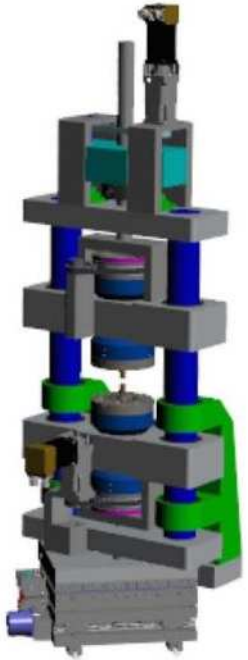


Electrochemical surface environments



Bulk catalysis

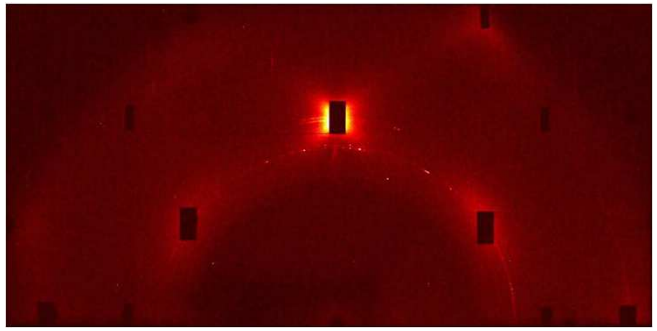




Mechanical testing

Surfaces: Catalytic CO oxidation of Pd vs. gas stoichiometry

PdO (√5x√5) surface oxide



rotational scan

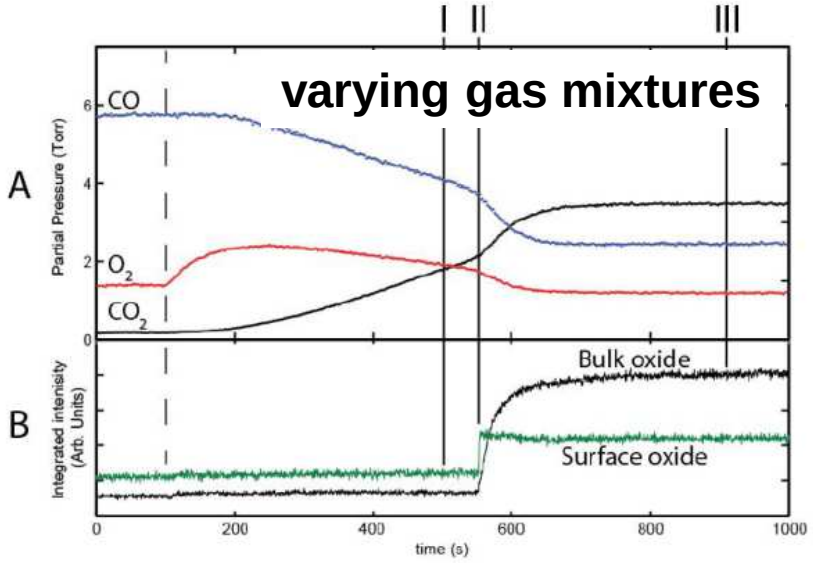
High energy surface x-ray diffraction for in situ surface structure determination - A new view of reciprocal space.

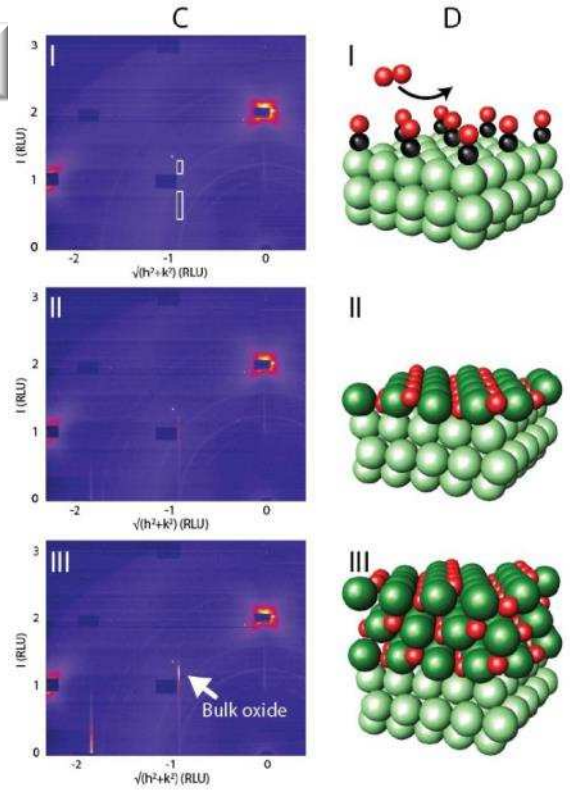
J. Gustafson,[1,*] M. Shipilin,[1] C. Zhang,[1] A. Stierle,[2] U. Hejral,[2] U. Ruett,[2] O. Gutowski,[2] P. A. Carlsson,[3] M. Skoglundh,[3] and E. Lundgren[1]

[1] *Div. of Synchrotron Radiation Research, Lund University, Box 118, SE-221 00 Lund, Sweden*
[2] *Deutsches Elektronen-Synchrotron (DESY), D-22603 Hamburg, Germany*
[3] *Competence Centre for Catalysis, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden*

(J. Gustafson *et al.*, Science 343 (2014), p. 758)

P07 EH2, 85 keV





surface oxide

bulk oxide

- Sample at fixed ω-setting
- Sub-second probe of surface structure & catalytic activity (MS)

P21 Swedish Materials Science Beamline

Construction & operation funded by Vetenskapsrådet
Built and operated by DESY
Hosted by KTH and Linköping Univ.

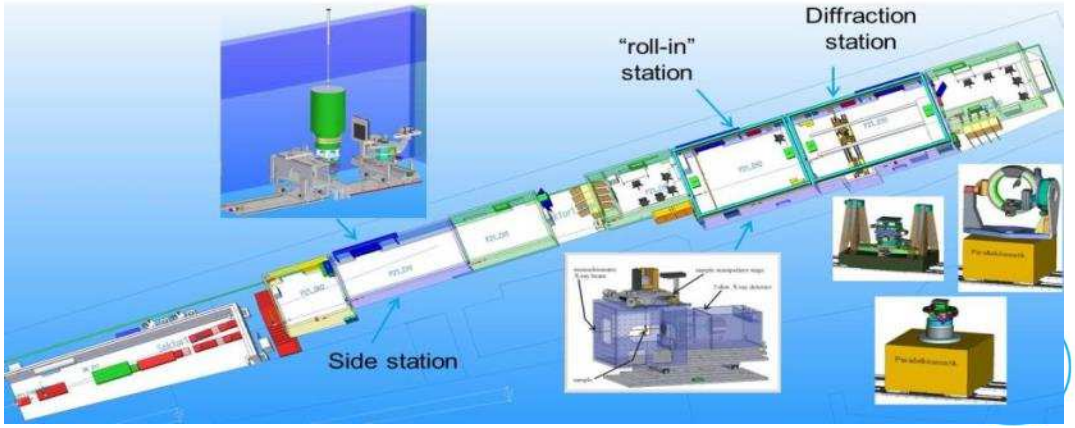
Vetenskapsrådet

KTH VETENSKAP OCH KONST

LINKÖPINGS UNIVERSITET

Official „opening“ Sept. 2016

Röntgen Ångström Cluster



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Vetenskapsrådet

KTH VETENSKAP OCH KONST

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Official „opening“ Sept. 2016

Röntgen Ångström Cluster

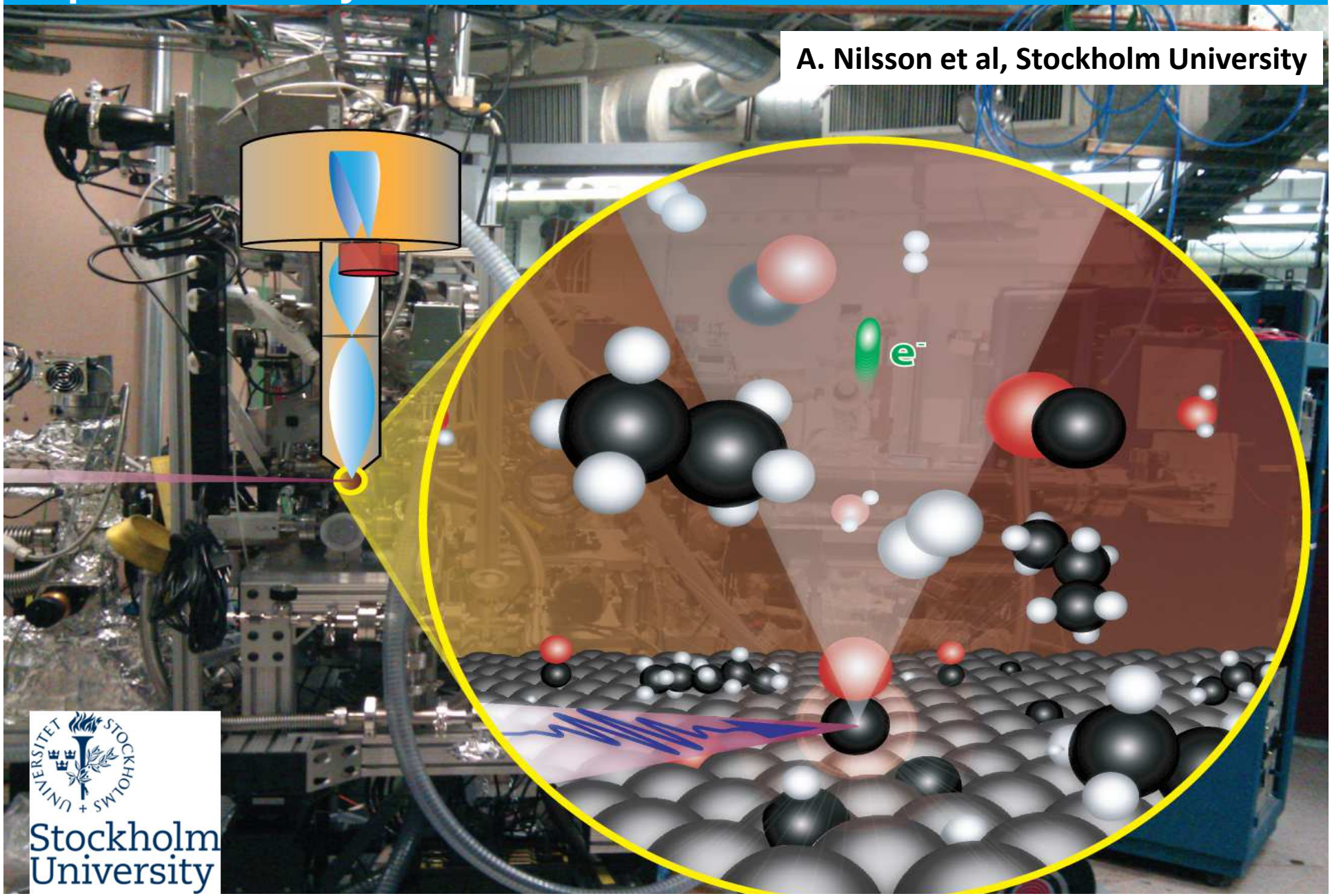
Thanks to our Swedish friends for this wonderful cooperation!

P21 Current status: where are we?

First beam expected Spring 2018

Briefly switching to another upcoming activity at another beamline …

Ambient Pressure XPS for Energy and Catalysis
Operando X-ray Studies at Real Conditions

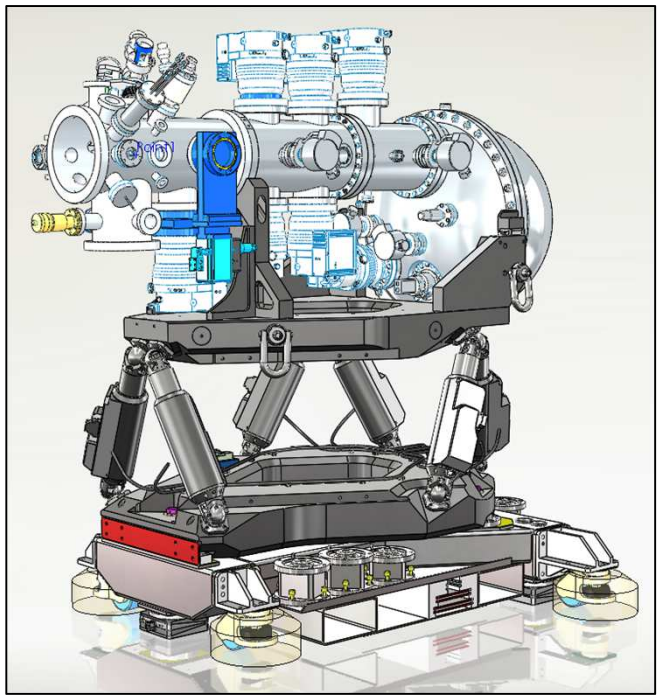


POLARIS - A new instrument for catalysis research

Current status:
Experiments at up to 100 torr at RT

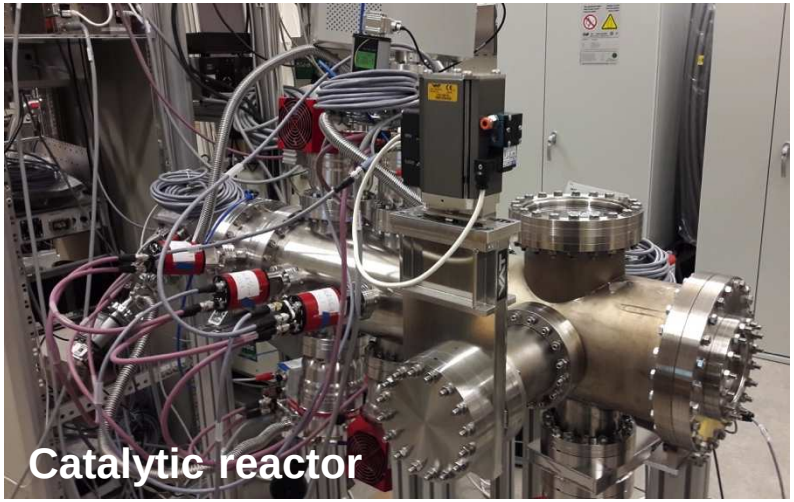
New goal:
Experiments at up to 10 bar and T=400°C

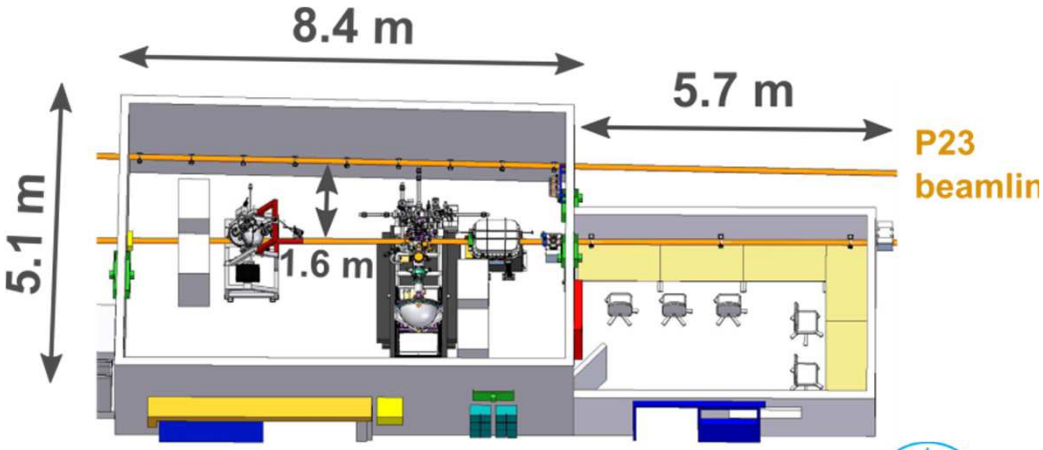
Stockholm University



Instrument will be used at
Hard X-ray Photoemission Beamline P22
Photon energies 4-10 keV @ <10x10 μm²

First tests planned Nov/Dec 2017





DESY

Workshop announcement:

The Swedish High-Energy Materials Science Beamline at PETRA III

Date: **9 - 10 November 2017**

Location: DESY, Hamburg, Germany

Abstract

The mission of the Swedish beamline at PETRA III is to provide access to world class high-energy diffraction, scattering, and imaging techniques to the Swedish materials science community. The beamline is under construction and first beam is anticipated early 2018. The workshop aims at communicating the status of the beamline as well as access to beamtime and mechanisms of collaboration. Case studies and potentially relevant applications will be presented and should stimulate discussion of best use of the beamline and collaborations.

Please note the date, further details will be communicated.

Vetenskapsrådet

LINKÖPINGS UNIVERSITET

KTH VETENSKAP OCH KONST

DESY

Thank you for
your attention