# Workshop on the Soft X-Ray Spectroscopy and Coherent Scattering Endstation

PSI, Villigen, Jun. 2-4, 2009

Serguei L. Molodtsov
*European XFEL Project Team*

European XFEL

# Scope of the Workshop



This Meeting forms part of a series of workshops aiming at discussion of scientific cases and designs of the European XFEL instruments.

This Workshop brings together potential users of the SCS instrument with purposes:

- to review the areas of application of the instrument

- to identify beam parameters and requirements to the experimental station(s) from the side of different experimental techniques

- to constitute user community and set user groups for close interaction with the European XFEL in developing equipment and facilities related to spectroscopies and coherent scattering experiments in the soft X-ray range of radiation

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# Conference Photo



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## Statistics


European XFEL SCS Workshop

86 participants

Speakers or Participants from

14 countries

Students, PhD Students and Junior Scientists

14 bursaries

Number of Participants from

Germany - 27
Switzerland - 22
Russia - 12

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# Program: Introduction Session



**Introduction Session, Auditorium**

Chair: R. Abela

14:00 – 14:05 Welcome by Organizers (R. Abela, PSI Villigen)

14:05 – 14:25 Status of the European XFEL Project (M. Altarelli, European XFEL Hamburg)

14:25 – 14:40 Start-up Boundary Conditions for the SCS Instrument (S. Molodtsov, European XFEL Hamburg)

14:40 – 14:55 Detectors Developments (H. Graafsma, European XFEL Hamburg)

14:55 – 15:10 Expected Properties of Radiation from SASE3 Undulator (M. Yurkov, DESY Hamburg)

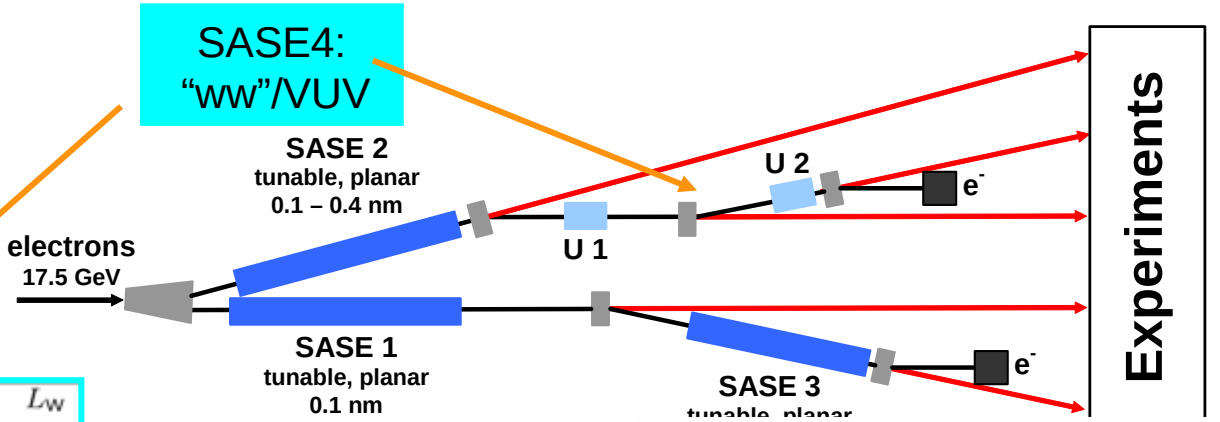
15:10 – 15:25 Circular Polarisation at SASE3 (Y. Li, European XFEL Hamburg)

15:25 – 15:40 Light Monochromatization Options at the SASE3 beamline (J. Gaudin, European XFEL Hamburg)

# Introduction Session, „Expected Properties of Radiation from SASE3 Undulator“, E. Saldin, E. Schneidmiller, M. Yurkov

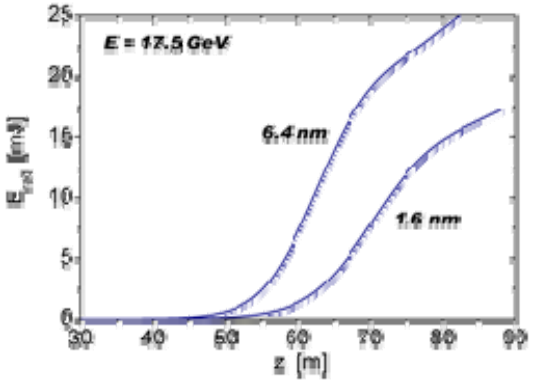


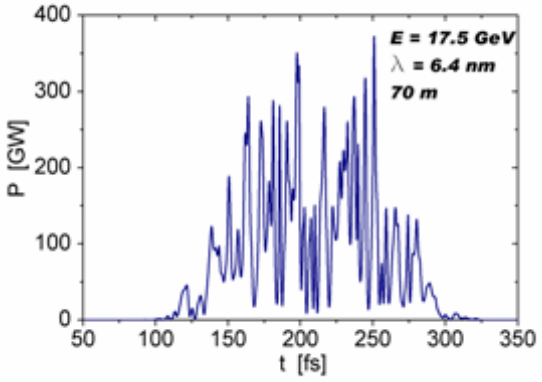
| Location | Tunnel length | Undulator |
|---|---|---|
| XS1-XS3 | 620 m | SASE1 |
| XS3-XHDU1 | 310 m | SASE3 |
| XS1-XS2 | 550 m | SASE2 |
| XS2-XS4 | 190 m | Spont. |
| XS4-XHDU2 | 250 m | Spont. |




| $\lambda_r$ nm | $\lambda_u$ mm | gap mm | $B_w$ T | $K_{rms}$ | $\beta_f$ m | $L_w$ m |
|---|---|---|---|---|---|---|
| 1.6-6.4 | 110 | 19-37 | 0.7-1.6 | 5.7-12 | 10-20 | 80 |

| | Units | Value |
|---|---|---|
| Wavelength range | nm | 1.6/6.4 |
| Peak power | GW | up to 150 GW |
| Average power | W | up to 800 W |
| Ph. beam size | $\mu$m | 60/90 |
| Ph. beam divergence | $\mu$rad | 11/27 |
| Saturation length | m | 70/80 |



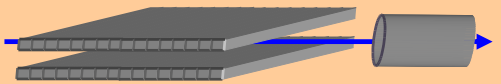
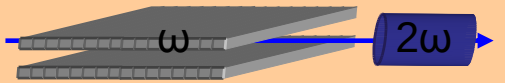
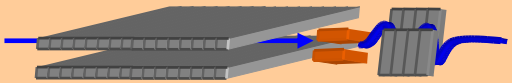
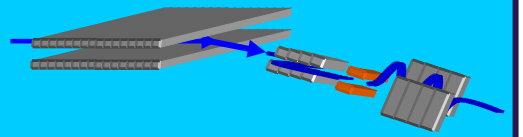
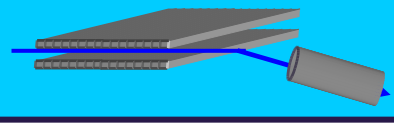

- Can be placed in one of the tunnels for spontaneous undulators U1 or U2.
- Can use spent beam after SASE2.
- Attractive feature: extremely high energy in the radiation pulse, about two orders of magnitude above project value of FLASH (500 uJ).

SSY, TESLA FEL 2004-02

# Introduction Session, „Options for Circular Polarization at SASE3“, Yuhui Li



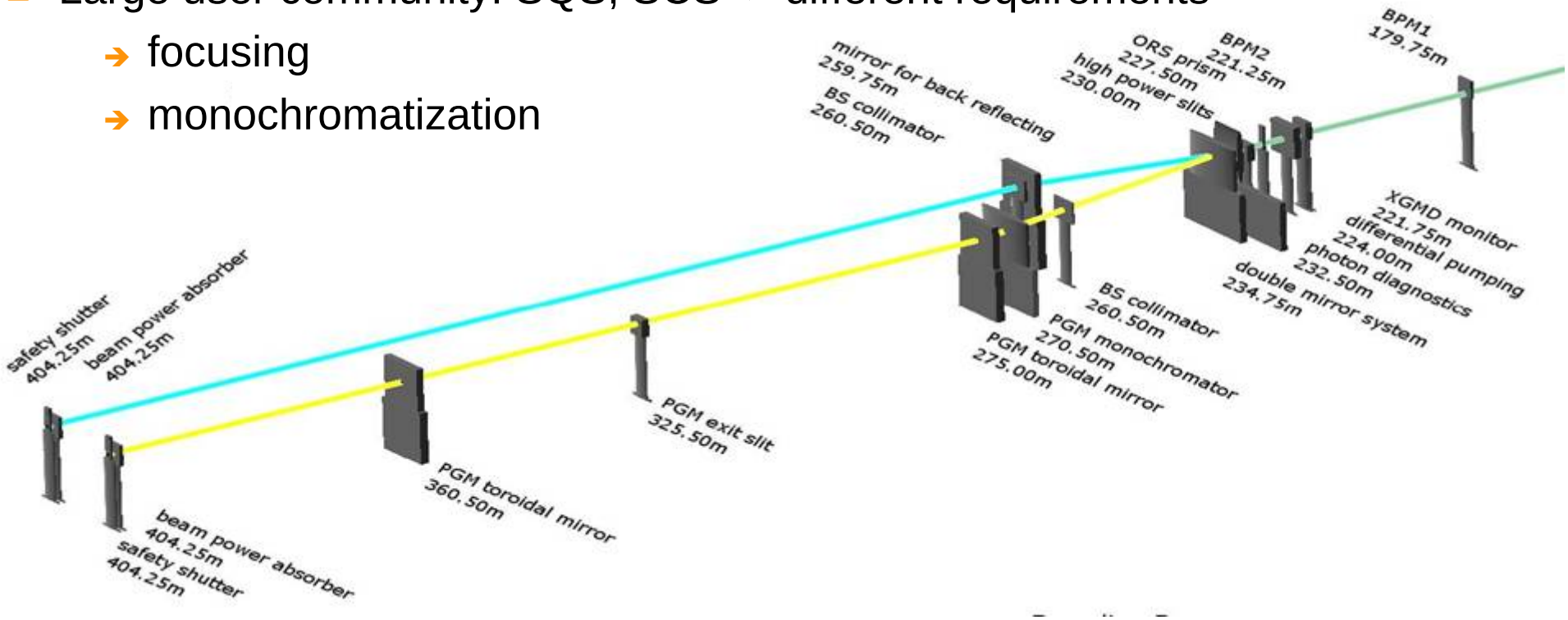
- Based on the SASE3 start up scenario, there are several helical polarization solutions:

| Scheme | Power | $S_3/S_0$ | Polarization Fluctuation | Helical Und. Length | Planar Und. Length | Beam line |
|---|---|---|---|---|---|---|
| **Planar Und. (start-up)** | **50~100 GW 100%** | | | | **~100 m** | |
| **Full helical** | **~100%** | **1** | **0** | **~80 m** | | |
| **Planar + Helical** | **~100%** | **≠ 1** | **≠ 0** | **~30 m** | |  |
| **8 Å Planar + 4 Å Helical** | **~100%** | **?** | **?** | **~40 m** | |   |
| **Planar + Crossed Planar** | **~10%** | **≠ 1** | **≠ 0** | **0 m** | **+ ~3 m** |  |
| **Crossed Planar** | **~10%** | **~ 0.95** | **>2%** | **0 m** | **+ ~ 6 m** |  |
| **Helical** | **>10%** | **1** | **0** | **~10 m** | |  |

# Introduction Session, „Light Monochromatization Options at the SASE3 Beamline“, J. Gaudin



- energy range: 0.2 to 3.1 keV
- high flux 1e14 ph/pulse @ at 200 eV
- possible circular polarization
- 2 branches: pink beam + monochromatized
- Large user community: SQS, SCS=> different requirements
  - focusing
  - monochromatization



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# Program: Session I



**Session I, Auditorium**

Chair: M. Kiskinova

***Photon-in/Photon-out & Electron-out Spectroscopic Experiments***

16:00 – 16:30 Soft X-Ray Spectroscopies at FLASH (A. Föhlisch, Uni Hamburg)

16:30 – 17:00 RIXS from 3rd to 4th Generation Experiments (Th. Schmitt, PSI Villigen)

17:00 – 17:30 Time-Resolved Photoemission of Solids (M. Wolf, FHI Berlin)

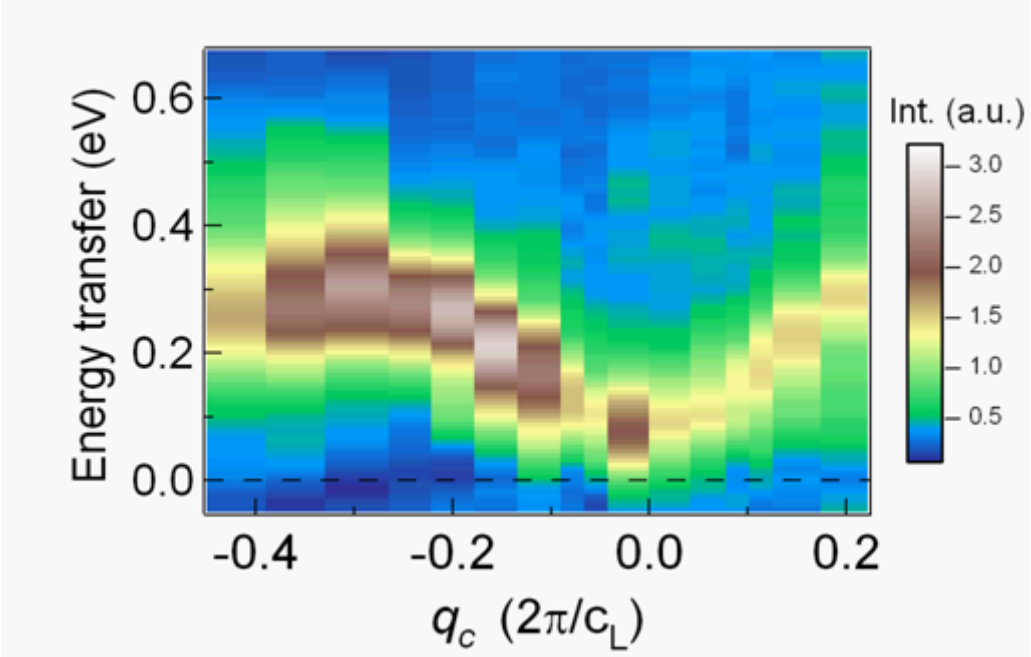
17:30 – 18:00 Spectroscopic Studies of Complex Materials with Soft X-Rays (Z. Hussain, ALS Berkeley)

18:00 – 18:30 X-Ray Spectra, Electronic Structure and Correlation Effects in FeAs-Superconductors (E. Kurmaev, IMP RAS Yekaterinburg)

# Photon-in/Photon-out & Electron-out Spectroscopies, „RIXS from 3rd to 4th Generation Experiments“, Th. Schmitt, PSI



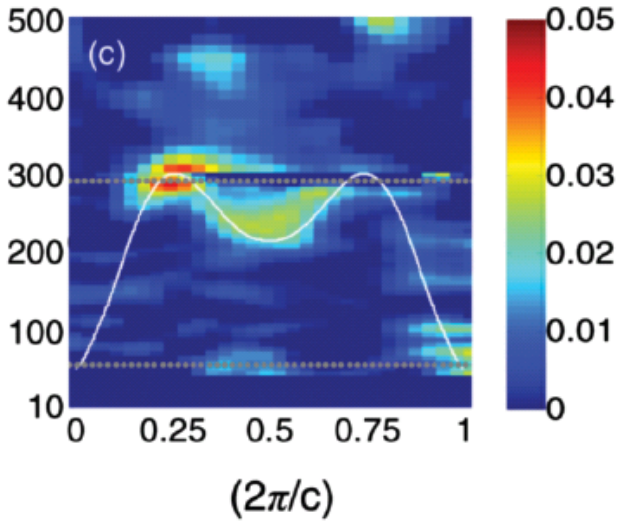
## RIXS from $Sr_{14}Cu_{24}O_{41}$




J. Schlappa et al. submitted to PRL arXiv:0901.1331

homogeneous cross-section over the full Brillouin zone !

## INS: two-triplon from $La_4Sr_{10}Cu_{24}O_{41}$



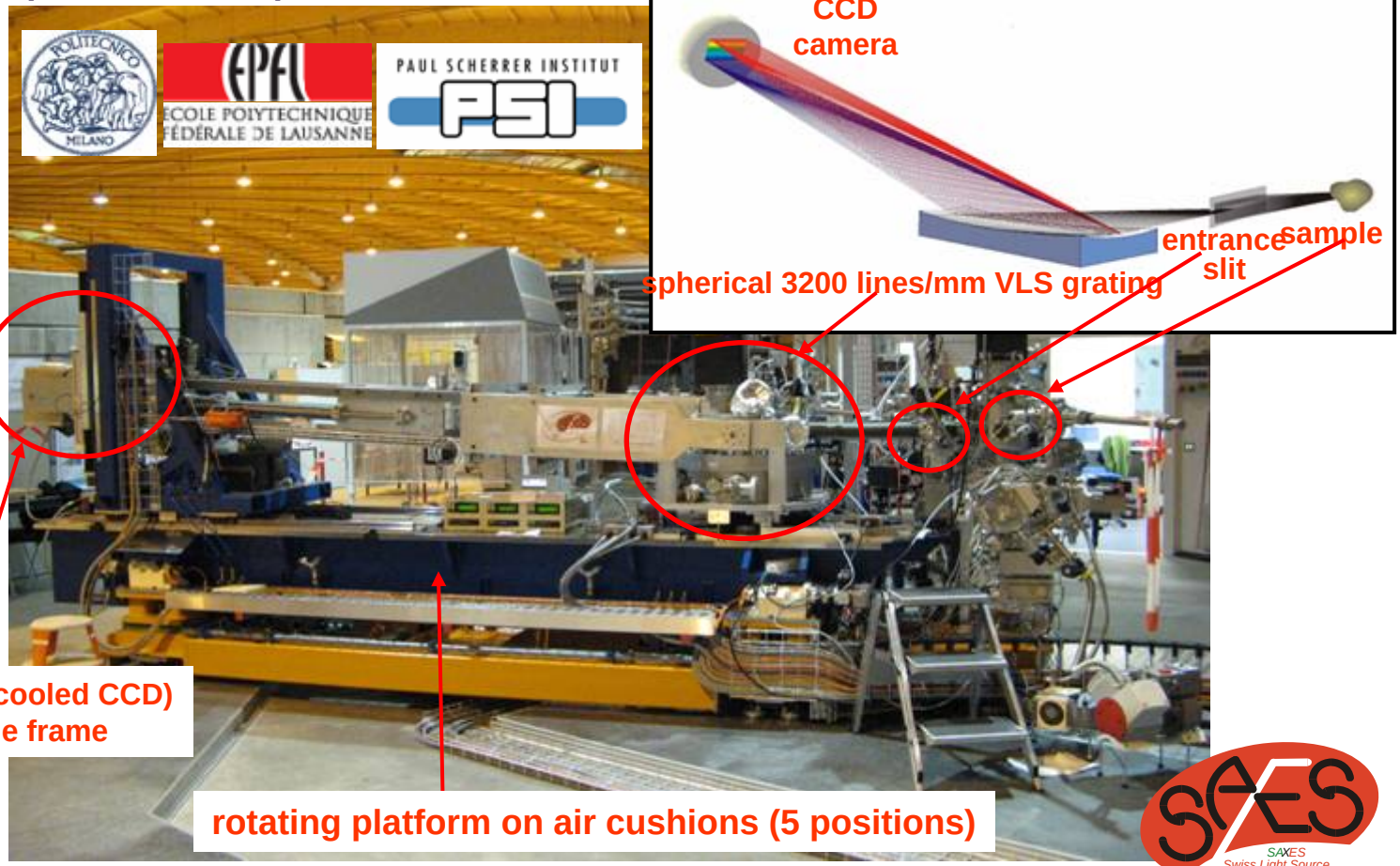

S. Notbohm *et al.*, PRL **98**, 027403 (2007).

low sensitivity for small q-transfer

# Photon-in/Photon-out & Electron-out Spectroscopies, „RIXS from 3rd to 4th Generation Experiments“, Th. Schmitt, PSI



**Super Advanced X-ray Emission Spectrometer (SAXES) on rotating platform: collaboration of SLS / PSI with *Politecnico di Milano (*L. Braicovich et al.) and *EPFL Lausanne* (M. Grioni et al.)**

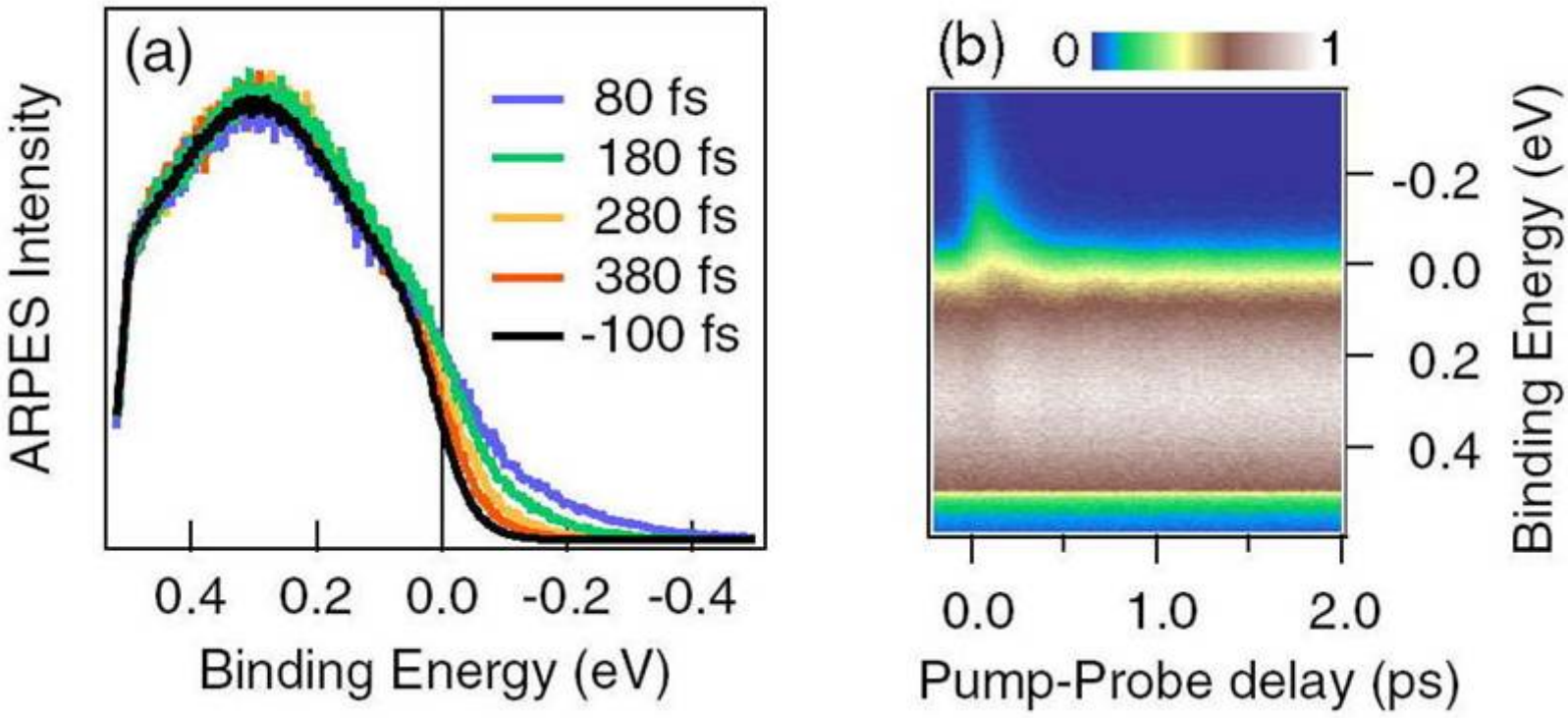



**G. Ghiringhelli et al., Rev. Sci. Instrum. 77, 113108 (2006).**

# Photon-in/Photon-out & Electron-out Spectroscopies, „Time-Resolved Photoemission of Solids“, M. Wolf, FHI



Electronic structure of 1*T*-$TaS_2$ at a temperature above MI transition



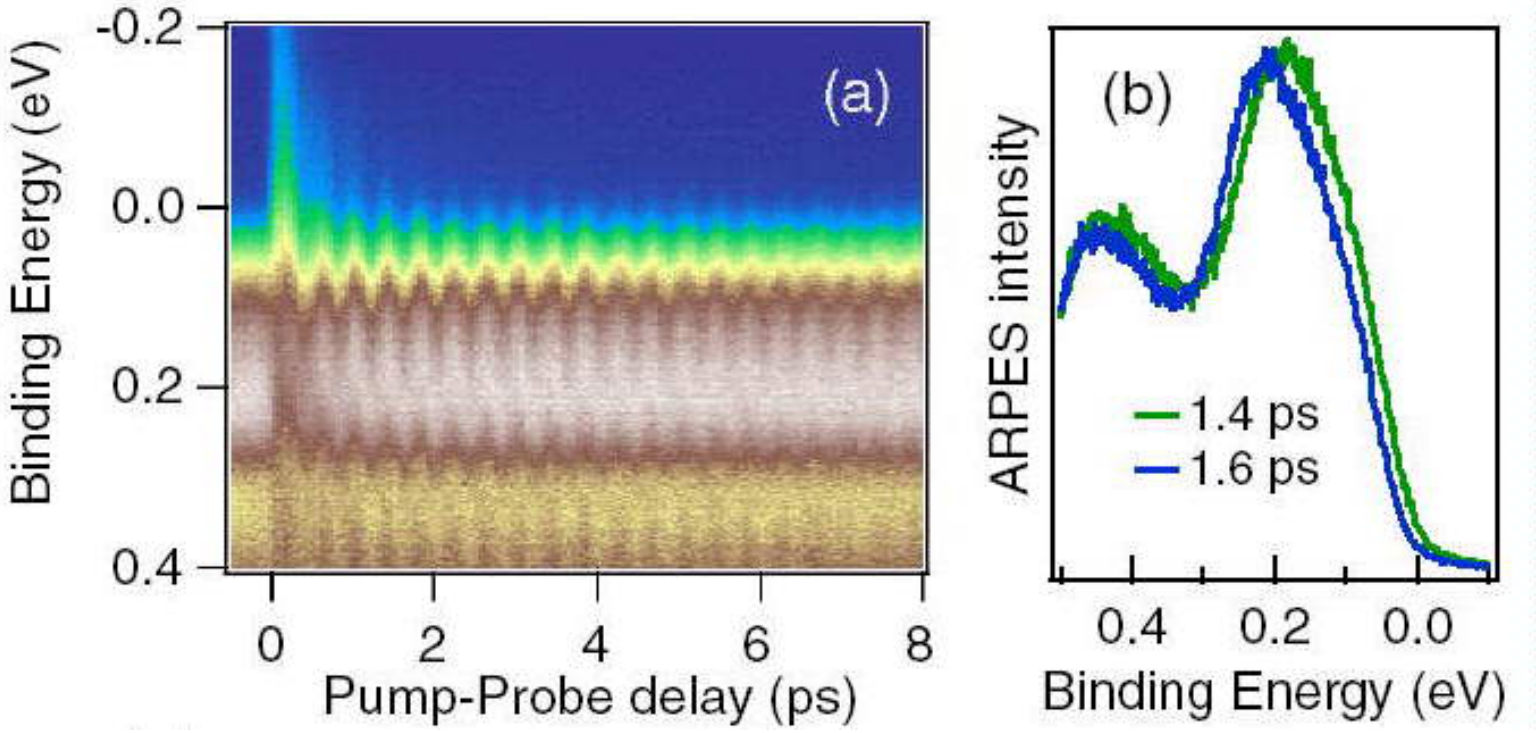

**pump-probe experiments, relaxation of “hot” electrons**

Perfetti *et al.*, PRL **97** (2006) 067402

# Photon-in/Photon-out & Electron-out Spectroscopies, „Time-Resolved Photoemission of Solids“, M. Wolf, FHI



Electronic structure of 1*T*-$TaS_2$ at a temperature below MI transition




**pump-probe experiments, electron-system oscillations**

Perfetti *et al.*, PRL **97** (2006) 067402

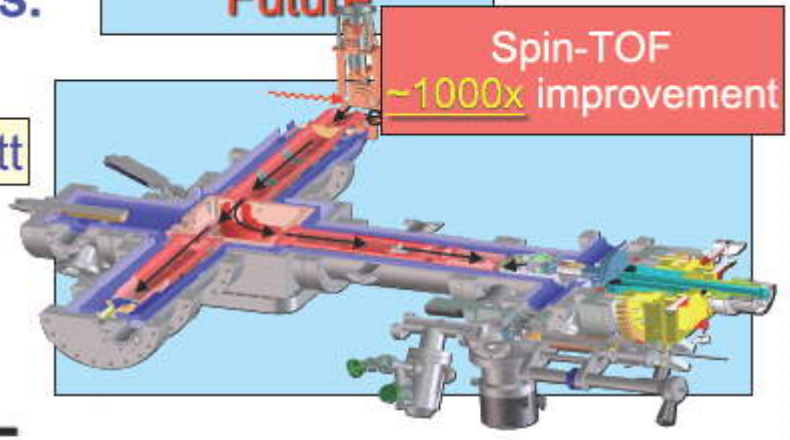
# Photon-in/Photon-out & Electron-out Spectroscopies, „Spectroscopis Studies of Complex Materials … “, Z. Hussain, ALS



## Spin-ARPES w/ spin-TOF analyzer

BERKELEY LAB

| Present | vs. | Future |
|---|---|---|
| Hemisphere + Mott<br>Low Efficiency | | Spin-TOF<br>~1000x improvement |



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**Spin Analysis**

| Spin-Orbit Scattering (Mott detector) | Exchange Scattering |
|---|---|

+

**Energy Analysis**

| Hemispherical Analyzer | Time-of-Flight Analyzer |
|---|---|

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# Program: Session II



**Session II, Auditorium**

Chair: G. Faigel

***Imaging, Dynamics & Photon Correlation Spectroscopy I***

09:00 – 09:30 Imaging of Non-Reproducible Cells with Single Pulses (H. Chapman, CFEL Hamburg)

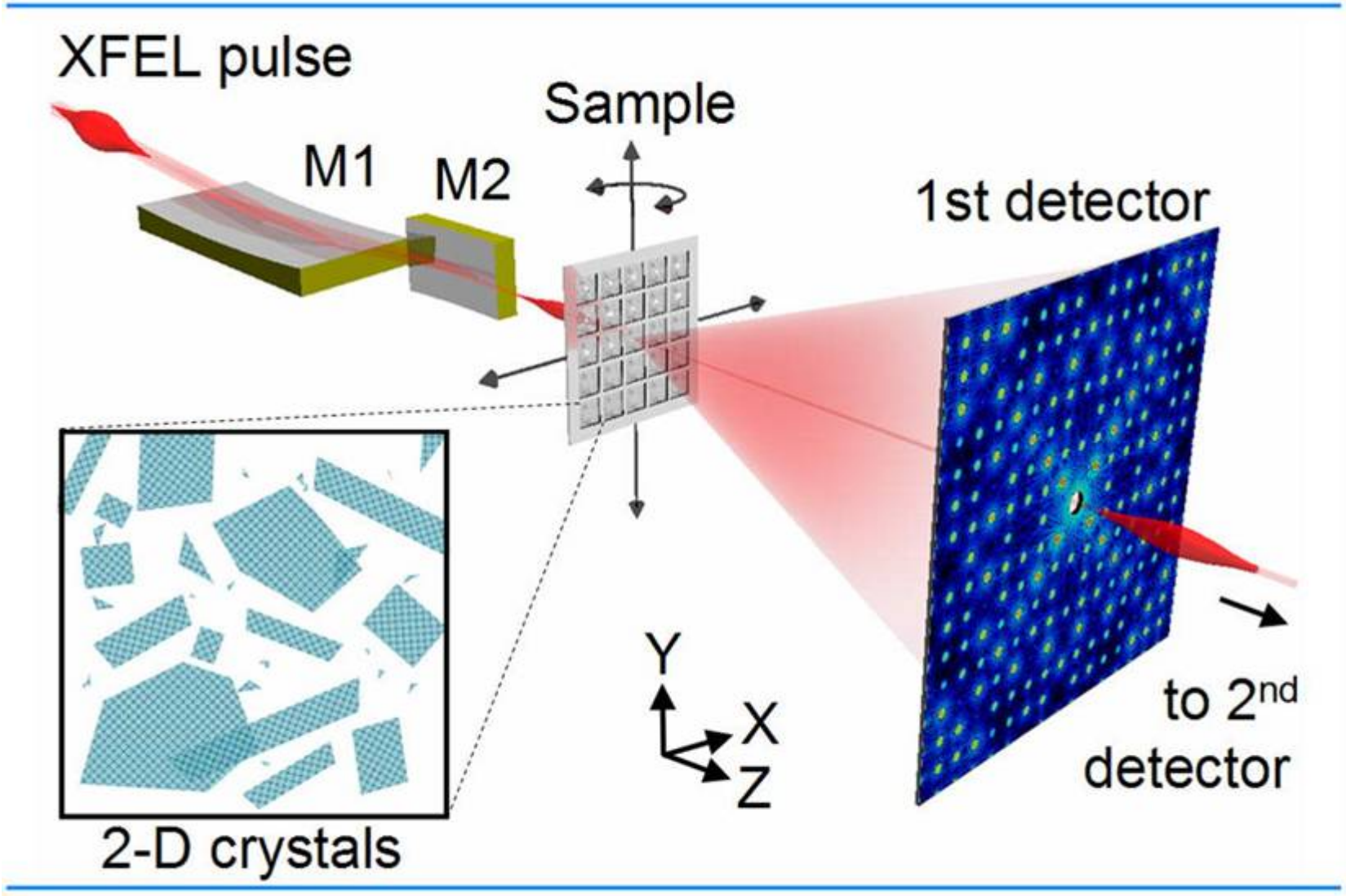
09:30 – 10:00 2D Membrane Flash Crystallography at Future XFEL Sources (C. Kewish, PSI Villigen)

10:00 – 10:30 Time-Resolved Imaging of Magnetic Domains (S. Eisebitt, TU Berlin)

10:30 – 11:00 Magnetic and Orbital Correlations in Space and Time (S. Kevan, Uni of Oregon)

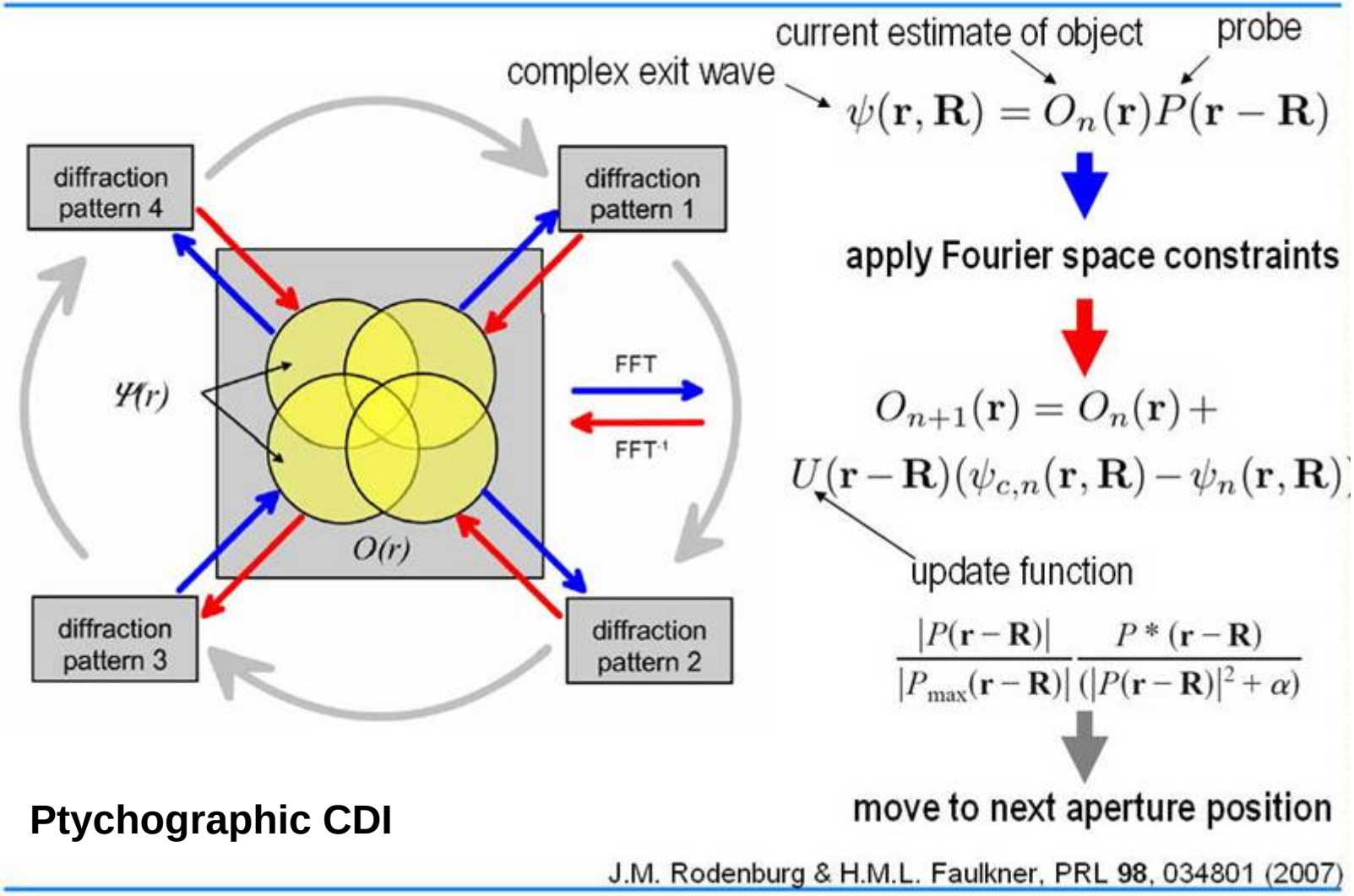
# Imaging, Dynamics & Photon Correlation Spectroscopy, „2D Membrane Flash Crystallography … “, C. Kewish, PSI





# Imaging, Dynamics & Photon Correlation Spectroscopy, „2D Membrane Flash Crystallography … “, C. Kewish, PSI






**Ptychographic CDI**

J.M. Rodenburg & H.M.L. Faulkner, PRL 98, 034801 (2007)

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# Program: Session III



**Session III, Auditorium**

Chair: Th. Tschentscher

***Imaging, Dynamics & Photon Correlation Spectroscopy II***

11:15 – 11:45 Ultrafast laser induced magnetization dynamics (A.V. Kimel, Uni Nijmegen)

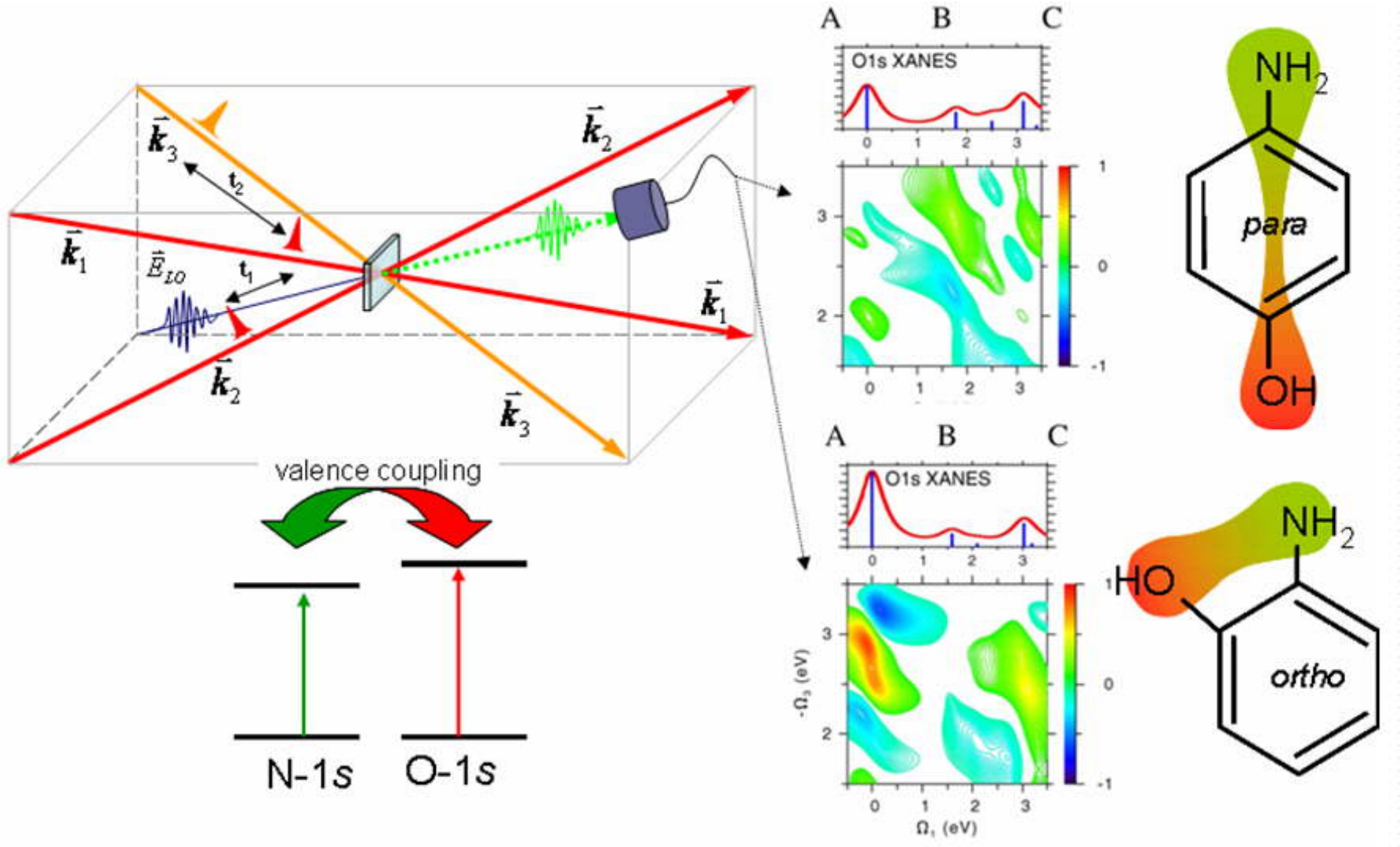
11:45 – 12:15 Nonlinear Multidimensional X-ray Spectroscopy of Molecules (S. Mukamel, Uni of California Irvine)

12:15 – 12:45 Time-Resolved Resonant X-Ray Scattering Experiments (A. Cavalleri, CFEL Hamburg)

12:45 – 13:15 Ultrafast Resonant Magnetic Scattering at the Free Electron Laser FLASH (Ch. Gutt, DESY Hamburg)

# Imaging, Dynamics & Photon Correlation Spectroscopy, „Multidimensional Att. Spectroscopy …“, Sh. Mukamel, PSI





# Imaging, Dynamics & Photon Correlation Spectroscopy, „Correlation, Complexity …“, S. Kevan, Uni. Oregon



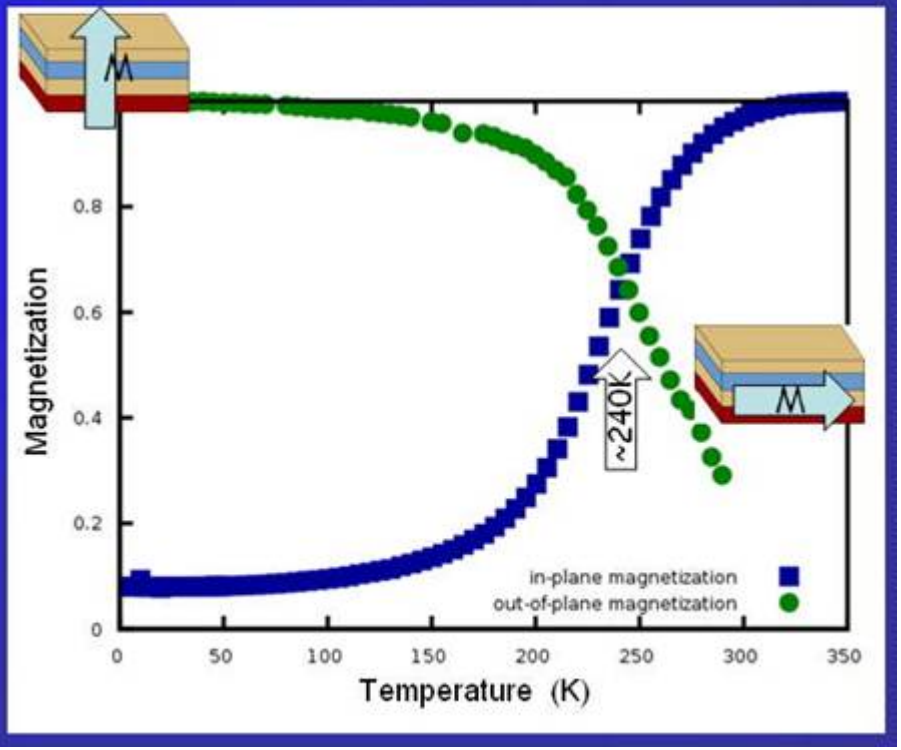
## Spin Reorientation Transition in Au:Co:Au


Ultrathin Co layers -> spin-reorientation transition. Preferred magnetization direction is determined by competition between shape and crystalline/surface anisotropy (Pescia *et al. PRL* ***65, 2599).***

$$E = \left\{K_2(T) - 2\pi M_s(T)^2\right\}\sin^2(\theta) + K_4(T)\sin^4(\theta)$$

Magnetization rotates from out-of- to in-plane as a function of increasing temperature (Park *et al. APL 86 042504).*

Driving force in SRT is mostly temperature dependent interfacial magnetic anisotropy.



# Definition of Working Groups



WG I: Photon-in/Photon-out & Photon-in/Electron-out Spectroscopic Experiments

*(Chairs W. Wurth & Z. Hussain)* 35 participants

WG II: Imaging, Dynamics & Photon Correlation Spectroscopy: Biological Objects

*(Chairs I. Schlichting & I. Vartaniants)* 12 participants

WG III: Imaging, Dynamics & Photon Correlation Spectroscopy: Magnetic Systems

*(Chairs G. Grübel & J. Luning)* 19 participants

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# Scientific Applications & Experimental Techniques



- Areas of scientific applications:

  studies of atomic, electronic structure and dynamics of nano- and correlated systems as well as of non-reproducible biological objects

  were confirmed.

- As experimental techniques:

  elastic and inelastic, resonant and non-resonant X-ray scattering and diffraction as well as photoelectron and photon correlation spectroscopies in time-resolved and -integrated modes

  were suggested.

- It was underlined that combinations of various suggested experimental techniques should be used to mostly efficiently explore the scientific areas of the SCS application.

Obviously the conclusions should be further reviewed in the light of future results from FLASH, LCLS and SCSS.

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# Photon Beam Parameters



- **Energy range:** for spectroscopic biological and magnetic experiments one needs photon energy range below 800 eV downwards to 400 eV (L edges of transition metals) or even 250 eV (C edge), upwards to 2000 eV (M edges of the rare-earth). For biological imaging up to 3000 eV. One soft X-ray undulator is not enough!

- **High energy resolution:** is of highest important for spectroscopic experiments that do not need naturally monochromatized light.

- **Beam size:** different beam sizes starting from 100 μm downwards to less than 100 nm are highly desirable. A possibility to tune beam size in one experiment was requested.

- **Pulse duration:** from 100 fs to <10 fs (latter to probe dynamics of electron system).

- **Repetition rate:** although 5 MHz are desired to perform time-integrated experiments or measurements of diluted samples, quite a number of experiments can and is willing to be done with ~10 Hz rep. rate. 30 kHz is optimum for study of relaxation of secondary excitations or particles spectroscopic analyses with TOF techniques.

- **Light polarization:** circular light polarization is necessary for studies of magnetic samples and symmetry properties of other samples.

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# Instrumentation Requirements



- Spatial separation of instruments using photon beam with/without monochromatization was confirmed. Space limitations!
- Spectroscopic community is going to use only the branch with monochromator. Two separate endstations, RIXS and PES, are required.
- Separate endstations are necessary for different WGs. Thereby the users are aware that to compliment basic configurations provided by European XFEL they should purchase themselves missing equipment.
- Free ports to mount equipment brought by users should be foreseen.

# Time Schedule SASE 3 Beamline and Instrumentation



**Jun, 09** Workshop in Villigen, rough concept of the SCS instrument, formation of user community.

**end 09** Conceptual design of the SASE 3 beam transport system.

**end 10** Technical design of the SASE 3 beam transport system. Conceptual design of the SCS instrument.

**end 11** Technical design of the SCS instrument.

**end 13** The SASE 3 beam transport system and the SCS instrument are ready for installation.

**2014** Initial beam and pilot experiments.

**2015** Full operation.

# Acknowledgement



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International workshop on the Spectroscopy and Coherent Scattering Endstation and associated instrumentation at the European XFEL

02 – 04 June 2009

Paul Scherrer Institut
Villigen, Switzerland

The Spectroscopy and Coherent Scattering (SCS) instrument is intended for the investigation of atomic and electronic structure as well as of the dynamics of soft and hard matter, biological species and magnetic materials. Areas of application are material sciences, structural and cell biology, nano-materials and dynamics of condensed matter. Experiments utilizing elastic, resonant inelastic and magnetic scattering of soft X-rays as well as photoelectron emission and photon correlation spectroscopy are going to be performed at this instrument.

This meeting forms part of a series of workshops aiming at the discussion of scientific cases and designs of the European XFEL instruments. It will feature a number of invited lectures presenting scientific and technical views, followed by group sessions providing opportunities for extended discussions from broad user communities on the construction of the SCS instrument and its capabilities.

Young scientists bursaries
Deadline 04 May 2009
(for details see website)

The workshop is co-funded by the European Commission through the Pre-XFEL grant. This will allow free of charge access to the workshop.

Hosting the workshop and support by the Paul Scherrer Institut, Villigen, Switzerland, is gratefully acknowledged.

Local organizers

Rafael Abela, Bruce Patterson
Paul Scherrer Institut, Villigen, Switzerland

International programme committee

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Gyula Faigel, Research Institute for Solid State Physics and Optics, Budapest, Hungary
Gerhard Gruebel, DESY, Hamburg, Germany
Zahid Hussain, ALS, Berkeley, USA
Maya Kiskinova, Elettra, Trieste, Italy
Mikhail Kovalchuk, Kurchatov Institute, Moscow, Russia
Jan Luning, University of Paris VI, France
Nils Mårtensson, MAX-Lab, Lund, Sweden
Serguei Molodtsov, European XFEL Project Team, Hamburg, Germany
Wilfried Wurth, University of Hamburg, Germany

www.xfel.eu/scs-workshop-2009
Registration deadline
04 May 2009

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We thank the Organizes:

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Silvia Bacher
H. Schori
*Paul Scherrer Institut, Villigen*

Imke Gembalies
*European XFEL, Hamburg*

Gyula Faigel
*Institute for Solid State Physics and Optics, Budapest*

All participants contributing to the scope of the SCS Workshop

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