Christian Bressler, *Femtosecond X-ray Experiments (FXE) Instrument*  
European XFEL  

**XFEL User Meeting, Hamburg, Jan 28, 2015**
Experiment Hall Integration

FXE
Solvation dynamics using the FXE instrument

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Monochromatic</th>
<th>Pink beam</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy range</td>
<td>5-20(25) keV</td>
<td>5-20(25) keV</td>
</tr>
<tr>
<td>Beam position</td>
<td>Sample (fixed)</td>
<td>Sample (fixed)</td>
</tr>
<tr>
<td>Energy bandwidth</td>
<td>$1.4 \times 10^{-4}$ Si(111) $3 \times 10^{-5}$ Si(311)</td>
<td>0.3-1 %</td>
</tr>
<tr>
<td>Bunch charge</td>
<td>$\leq 250$ pC</td>
<td>$\leq 250$ pC</td>
</tr>
<tr>
<td>X-ray pulse duration</td>
<td>$&lt; 25$ fs</td>
<td>$&lt; 25$ fs</td>
</tr>
<tr>
<td>Optical pulse duration</td>
<td>15 fs</td>
<td>15 fs</td>
</tr>
<tr>
<td>Sample delivery: Liquid flat-sheet jets</td>
<td>Up to 15 m/s (sapphire nozzles) Up to 100 m/s (colliding $\mu$jets)</td>
<td>Up to 15 m/s (sapphire nozzles) Up to 100 m/s (colliding $\mu$jets)</td>
</tr>
<tr>
<td>X-ray beam spot</td>
<td>1-10 $\mu$m in focus Up to 0.1 mm out of focus</td>
<td>1-10 $\mu$m in focus Up to 0.1 mm out of focus</td>
</tr>
<tr>
<td>Energy resolution</td>
<td>ca. 1 eV (cylindrical) 0.3 - &lt;1 eV (spherical)</td>
<td>ca. 1 eV (cylindrical) 0.3 - &lt;1 eV (spherical)</td>
</tr>
<tr>
<td>Q range (XDS)</td>
<td>0.7 – 13 Å$^{-1}$</td>
<td>0.7 – 13 Å$^{-1}$</td>
</tr>
</tbody>
</table>

FXE Overview Specifications

- **FXE will offer world-wide unique and versatile end station for dynamical studies of guest-host interactions.**
- It will exploit the high repetition rate, x-ray photon flux and ultrashort pulse duration of the European XFEL.
- FXE will offer a flexible sample environment optimized for liquid-phase photochemistry using a suite of complementary x-ray spectroscopic and scattering techniques in pump-probe arrangement.
- Simultaneous measurements of several observables deliver a more complete picture of the dynamics both of the solute (guest) and solvent molecules (host).

Coupled electronic, spin and nuclear changes of solute and solvent molecules can be resolved in “real-time”
What are the fundamental timescales?

Femtochemistry, Photosynthesis and Catalysis
Solid State Dynamics
Vision
Molecular Vibrations
Protein Folding
Molecular Rotations

Strings, Cosmology
Particle Collisions

Electron dynamics

Time / seconds

- harpo $10^{-27}$
- yacto $10^{-24}$
- zepto $10^{-21}$
- atto $10^{-18}$
- femto $10^{-15}$
- pico $10^{-12}$
- nano $10^{-9}$
- micro $10^{-6}$
- milli $10^{-3}$
See Afternoon Talk in this Auditorium:

- Wojciech Gawelda, 17:00

“Tracking Chemical Reactions with Ultrafast X-Ray Spectroscopies and Scattering”

Visit our posters on Friday:
Posters # 90 and #219
**FXE**: Make use of all incident x-ray photons

- Absorption
- Scattering

Combine Femtosecond
- XRD
- XAFS (XANES)
- XES, RIXS, …
Strategy: Combine Complementary Structural Tools
Simultaneous Techniques at the FXE instrument

- **X-Ray Absorption Spectroscopy**
  - XANES: oxidation state changes, valence orbitals, DOS…
  - EXAFS: coordination shells (geometric)

- **X-Ray Emission Spectroscopy**
  - spin momentum of the absorber, charge state, molecular orbitals,…

- **Resonant Inelastic X-Ray Scattering (RIXS)**
  - Low energy excitations (d-d, charge transfer, even phonons), tunable to different final states, i.e. 3d orbitals (dipole-forbidden for 1s→nd excitation)

- **X-Ray Raman Spectroscopy**
  - Access K-edges of light elements (N, O, C…) constituting solvent molecules

- **X-Ray Diffuse Scattering**
  - Short- and medium-range geometric environment, solute + solvent (cage) contributions to the structural factor
Emphasis for „on-axis“ configuration (pink, mono, 5-20 keV)

- single OM position/angle (5 – 20 keV)
- Si(111) 4-bounce for startup (upgrade possible)
FXE Instrument: Overall Design

Top view of FXE hutches (SASE1)

- **FXE Control Hutch**
  - Upstream optics bench

- **FXE Optics**

- **FXE Experiments**

- **FXE Laser Lab**
  - Central Sample Environment Area
    - More flexibility, ambient conditions
    - Compatible with vacuum chamber
    - Secondary spectrometers
    - Pump beam conditioning
  - Downstream area provides space for diagnostics, vacuum chamber option and SAXS.
Our first Component Arrived!
Now cabling it up…
Next Component: Flat Sheet Jet (1-100 um)

- Delivery Feb 2015: thin flat sheet jet (adjustable thickness)
Femtosecond X-Ray Experiments at the European XFEL

FXE Instrument

SPB Transfer Tube (250 mm diameter)
Robot Tower
XES Robot

LPD
SA2
IPM3
BIU4

Johann
Von Hamos
Sample Stack Goniometer

European XFEL Users’ Meeting, Jan 28-30, 2015
Christian Bressler, FXE Instrument, European XFEL
Sample Environment

Optics Branch

- He Environment (ambient conditions, liquid jets)
- Solid State Chamber
FXE Instrument User Workshop
Featuring: Solid State Options
Tomorrow, Jan 29, 13:30
CFEL Seminar Room III

Organizers: F. Boscherini, C. Bressler
Invited speakers:
S. L. Johnson
M. M. Nielsen
...
Patch Panel with Lemo Connectors
Feasibility: solvated molecules (here: H2O)

![Graph showing feasibility of solvated molecules](image)

Photons/s

Photons/s (SR)

Photons (XFEL)
Summary: FXE Instrument

Provide a Suite of Complimentary Tools
→ X-Ray Spectroscopies (XAS, XES, Raman, …)
→ Forward Scattering (1 MPx, WAXS, …)
→ Ambient Conditions (He atmosphere)
→ < 50 fs time resolution
→ Solid State Vacuum Chamber

FXE Instrument well underway…
...and fully on schedule
2015: freeze design, 2016: Install Instrument
Come to the FXE Workshop tomorrow for more details
Acknowledgments

- Wojciech Gawelda (FXE)
- Andreas Galler (FXE)
- Dmitry Khakhulin (FXE)
- Tadesse Assefa (FXE)
- Alexander Britz (FXE)
- Thomas Tschentscher (European XFEL)
- Martin M Nielsen (DTU)
- Christian Mammen et al. (JJ X-Ray)

FXE instrument Workshop: Tomorrow, 13:30-18:00 CFEL SemRoom III (Bldg. 99)
Please visit our posters on Friday: Poster # 90 and #219
The European X-Ray Free-Electron Laser Facility GmbH (European XFEL GmbH) is a multi-national non-profit company. It will make available X-rays of unique quality for studies in physics, chemistry, the life sciences, materials research and other disciplines. Located in the Hamburg area, Germany, it will comprise scientific instruments for a wide range of experimental techniques. Construction of the European XFEL is underway; user operation starts in 2017. For the Femtosecond X-Ray Experiments (FXE) instrument we are looking for a

Scientific Instrument Support Scientist (f/m)

The Position

- participates in planning, installation, commissioning and maintenance of the FXE scientific instrument
- acts as an interface between XFEL internal groups (detector, data management,…), the FXE scientific instrument group and users
- supports and consults instrument users during user operation
- participates in scientific user experiments, but also leads own research efforts at European XFEL

Requirements

- PhD in physics or an equivalent academic degree
- experience in operation of X-ray detectors (1D, 2D)
- beam line experience at a large scale light source facility (SR, FEL)
- knowledge of a programming language like Matlab, C++ or Python is an asset
- good communication skills and ability to work in a multi-lingual, multi-disciplinary team

For additional information, please contact Christian Bressler (christian.bressler@xfel.eu).

General information on working in Germany, Hamburg and the European XFEL can be found under http://www.xfel.eu/careers.

Reference number

S-107

Duration

This appointment is initially limited to 3 years. The conversion into a permanent contract is possible. Salary and benefits are similar to those of public service organizations in Germany. In addition European XFEL provides a non-contributory company pension scheme, as well as broad relocation benefits. The European XFEL GmbH intends to achieve a widely international staff. Non-German candidates hired from abroad receive an international allowance.

Handicapped persons will be given preference to other equally qualified applicants. The European XFEL GmbH is an equal opportunity and affirmative action employer and encourages applications from women. Handicapped persons will be given preference to other equally qualified applicants. The European XFEL GmbH is an equal opportunity and affirmative action employer and encourages applications from women.

Application

Please apply online via www.xfel.eu/careers/job-of ng S-xxx) and provide a motivation letter next to a CV in English, your list of publications, as well as work certificates in one single pdf.

Instrument Engineer (f/m)

The Position

- mechanical integration of FXE instrument components in collaboration with the instrument group and users
- planning and construction of FXE experimental infrastructure
- interface with scientists and other technical groups contributing to the planning and construction of FXE experimental infrastructure
- supports and consults instrument users during user operation
- participates in scientific user experiments, but also leads own research efforts at European XFEL

Requirements

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