ChemRIXS Breakout Session

LCLS Run 23 Users Town Hall
January 30th 2024
ChemRIXS Run 23 call

Liquid standard configuration:
Liquid samples, sheet jets.
- Time-resolved XAS with monochromatic beam (scanning)
  - Transmission experiments (sheet jets)
  - Total Fluorescence Yield (TFY) mode
  - Partial Fluorescence Yield (PFY) mode
- Time-resolved RIXS/XES

- Please contact beamline scientist for non-standard configurations.
  - Zero-order operation at high rep-rate (e.g. attosecond XLEAP experiments),
    note: no in-line spectrometer available in run 23
  - Solid samples
ChemRIXS liquid standard configuration

**SCRF operation**
- Repetition rate up to 33 kHz
- Pulse energy up to 100 uJ

**RIX beamline**
- $I_0$ at the IP >$10^{14}$ photons/s
- Photon energy range 250 – 1000 eV and up to 1600 eV
- Mono resolving power 2000
- Spot size 10 – 1000 um (variable)
- $I_0$ detector 5% shot-by-shot noise

**OPCPA laser system**
- Repetition rate 33 kHz
- 800, 400 and 266 nm
- Vis-OPA 480 – 900 nm

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**Transmission XAS**
- Direct detection with downstream X-ray CCD
- 2048x512 Andor CCD read-out 1 Hz (Image), 120 Hz (FVB)

**TFY-XAS**
- APDs mounted close to the jet
- Shot-by-shot readout

**RIXS/XES/PFY-XAS**
- VLS spectrometer mounted at 45 deg backscattering
- 2048x512 Andor CCD read-out 1 Hz (Image), 120 Hz (FVB)
- Resolving power ~2000
- Detection efficiency $4 \cdot 10^{-8}$ (FVB), $1.6 \cdot 10^{-7}$ (Image)
Sample delivery

Liquid sheet jets for Transmission XAS
- Thin gas accelerated sheets (Nat. Commun. 9, 1353)
  - Thickness 0.1 - 1 µm
  - Flow rates 250 µl/min
  - Optimal for bulk liquids measurements
- Converging nozzles (Phys. Rev. Fluids 3, 114202)
  - Thickness 0.2 - 2 µm
  - Flow rates 2 - 4 ml/min
  - Optimal for solutes

Cylindrical jets for FY-XAS and XES
- Gas Dynamic Virtual Nozzle (GDVN)
  - Diameter 1 - 10 µm
  - Flow rates ~20 µl/min
- Rayleigh jet
  - Diameter >20 µm
  - Flow rates ~1 ml/min

Sample recirculation
- Min. sample volume requirement 50-100 ml

Load-lock systems
- Enables fast nozzle exchange
Performance expectations

**Transmission-XAS**

- N K-edge
  - Pyridine, 2 M
  - 120 Hz
  - Noise ~1% (10 mOD) at 120 Hz -> <0.1% (1 mOD) at 33 kHz

**TFY-XAS**

- Fe L3-edge
  - K3[Fe(CN)6] 100 mM
  - 120 Hz
  - x10 SNR improvement at 33 kHz

**RIXS**

- 33 kHz
  - $I_0 = 10^{14}$ photons/s
  - VLS throughput = $10^{-7}$
  - Fl. Yield = 0.005

<table>
<thead>
<tr>
<th>Concentration (mM)</th>
<th>$\mu_{\text{solute}}/\mu_{\text{total}}$</th>
<th>Total count rate (1/s)</th>
<th>Tr-RIXS?</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>1/2</td>
<td>$10^4$</td>
<td>Yes</td>
</tr>
<tr>
<td>100</td>
<td>1/20</td>
<td>$10^3$</td>
<td>Possible</td>
</tr>
<tr>
<td>10</td>
<td>1/200</td>
<td>$10^2$</td>
<td>Hard</td>
</tr>
</tbody>
</table>
# ChemRIXS Run 23 key parameters

## X-ray

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Repetition rate (Hz)</td>
<td>Up to 33 kHz</td>
</tr>
<tr>
<td>Energy Range (eV)</td>
<td>250 - 1600 eV</td>
</tr>
<tr>
<td>Pulse Duration (fs)</td>
<td>20 fs (nominal, 5ASE)</td>
</tr>
<tr>
<td>Energy per pulse at the IP (monochromatic)</td>
<td>&gt;100 nJ (250 - 1000 eV)</td>
</tr>
<tr>
<td></td>
<td>&gt;10 nJ (1000 - 1300 eV)</td>
</tr>
<tr>
<td></td>
<td>&gt;1 nJ (1300 - 1600 eV)</td>
</tr>
<tr>
<td>Beamline Resolving Power</td>
<td>&gt;2000</td>
</tr>
<tr>
<td>Spot Size, FWHM (range)</td>
<td>10 - 1000 (um) diameter</td>
</tr>
<tr>
<td>Polarization</td>
<td>Linear, Horizontal</td>
</tr>
</tbody>
</table>

## Laser

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Repetition rate (Hz)</td>
<td>Synchronized up to 33 kHz</td>
</tr>
<tr>
<td>Wavelength (fs)</td>
<td>800 400 266 480-600 600-900</td>
</tr>
<tr>
<td>Pulse Duration (fs)</td>
<td>20 30 35 &lt;50 &lt;50</td>
</tr>
<tr>
<td>Energy per pulse (µJ) (on target)</td>
<td>500 50 5 &gt;15 &gt;5</td>
</tr>
<tr>
<td>Spot Size, FWHM (800 nm)</td>
<td>50 to 100 µm</td>
</tr>
<tr>
<td>Polarization</td>
<td>Variable: linear, circular</td>
</tr>
<tr>
<td>Angle</td>
<td>~0.5 deg angle with x-ray beam</td>
</tr>
<tr>
<td>Arrival Time Monitor</td>
<td>&lt; 20 fs accuracy in x-ray/laser arrival time tagging should be available. Overall temporal resolution will be dependent on machine and instrument configuration.</td>
</tr>
</tbody>
</table>

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Please contact us for any questions.

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