Atomic-like Quantum System End-Station

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Scientific Instrument SQS
Instrument Scientist

SQS Early User Workshop
Schenefeld, 12th February 2018
**SQS: Small Quantum Systems**

**SASE3 – SQS beam parameters on the sample, day 1**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$h\nu$</td>
<td>1000 eV</td>
</tr>
<tr>
<td>$\Delta h\nu$</td>
<td>0.5% (but monochr. is also available)</td>
</tr>
<tr>
<td>Pulse duration</td>
<td>50 - 100 fs</td>
</tr>
<tr>
<td>Pulse energy</td>
<td>$\leq$ 3 mJ</td>
</tr>
<tr>
<td>Beam size</td>
<td>$\sim$ 1.5 – 2.5 $\mu$m</td>
</tr>
<tr>
<td>Rep. rate</td>
<td>1 MHz</td>
</tr>
</tbody>
</table>

**Science:**
- Non-linear X-ray physics on small samples
- Time-resolved fs molecular dynamics: isomerization, fragmentation, ...
The AQS instrument

Techniques:
- Angle resolved electron spectroscopy
- Ion spectroscopy
- Multi-particle coincidence:
  - UHV, $10^{-10}$ mbar
  - electr.-electr., ions-ions, electr.-ions
- XUV fluorescence

Samples:
- Gas-phase: atoms, molecules
Geometry of the SQS-AQS instrument
during 1\textsuperscript{st} users beam, with interim focus solution

KB focusing mirrors, interim solution

Focus position

2D imager
Laser incoupling
Diff. pumping

HFM 3.300 m VFM 1.800 m
European XFEL Focus position
## Spectrometers of the SQS-AQS instrument

<table>
<thead>
<tr>
<th></th>
<th>Electron Energy Resolution</th>
<th>Angle Acceptance % of $4\pi$</th>
<th>Electrons</th>
<th>Detection</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Kinetic Energy</td>
<td>Rep. rate</td>
</tr>
<tr>
<td>eTOF, x3</td>
<td>10,000</td>
<td>~0.14%</td>
<td>Yes</td>
<td>0-3000 eV</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>≤4.5 MHz</td>
</tr>
<tr>
<td>VMI</td>
<td>100</td>
<td>100%</td>
<td>Yes</td>
<td>0-1200 eV</td>
</tr>
<tr>
<td>Magnetic bottle, MBES</td>
<td>100</td>
<td>≥50%</td>
<td>Yes</td>
<td>0-3000 eV</td>
</tr>
<tr>
<td>XUV spectrometer</td>
<td>-</td>
<td>-</td>
<td>No</td>
<td>-</td>
</tr>
</tbody>
</table>

They can also run together, or even in coincidence.

### When to use each spectrometer?

<table>
<thead>
<tr>
<th>Spectrometer</th>
<th>Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>eTOF</td>
<td>Best electron energy resolution $\Delta E$</td>
</tr>
<tr>
<td></td>
<td>Full energy range 10 – 3000 eV</td>
</tr>
<tr>
<td>VMI</td>
<td>100% of $4\pi$</td>
</tr>
<tr>
<td></td>
<td>Angle resolved</td>
</tr>
<tr>
<td>Magnetic bottle, MBES</td>
<td>Full energy range 10 – 3000 eV</td>
</tr>
<tr>
<td></td>
<td>100% of $4\pi$</td>
</tr>
<tr>
<td></td>
<td>Electrons-ions coincidence</td>
</tr>
</tbody>
</table>
Spectrometers of the SQS-AQS instrument

VMI, 3x eToF coexisting, no need to break vacuum

XUV, MBES spectrometers interchangeable
Geometry of the SQS-AQS instrument

Air-pads to exchange/move chambers

AQS station turned 180deg to switch from VMI/eTOF to MBES
**Electron time-of-flight spectrometer(s)**

- Commissioned at DESY
- Confirmed world record resolution
  - $\Delta E = 70\text{meV} @ 811\text{ eV}$,
  - $E/\Delta E > 10000$
- Full energy range: 0 - 3000 eV
- All 3x tof are installed!

### eTOF specifications

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length</td>
<td>400mm</td>
</tr>
<tr>
<td>Detector</td>
<td>Hamamatsu, MCP, diam. 27mm, single anode</td>
</tr>
<tr>
<td>Readout</td>
<td>Digitizer 3GHz 10GS/s 14bit</td>
</tr>
<tr>
<td>Acceptance</td>
<td>0.14% of $4\pi$</td>
</tr>
</tbody>
</table>

- **0 deg**
- **54.7 deg**
- **90 deg**

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**European XFEL**
Electron time-of-flight spectrometer(s)

Keys for resolution and transmission:

► Low magnetic field:
  • 1 µT, 10 mG, 2% of Earth
► Particle optics simulations
► Fast detector and electronics:
  • 450 ps FWHM, 120 ps rise
  • 3 GHz, 10 GS/s
  • 14 bit digitizer -> no need for preamp.

DAQ: see talk of T. Baumann later today
VMI + eTOF for ions spectroscopy

- VMI+eToF spectrometer(s) can work together as an ion spectrometer
  - VMI electrodes push/pull ions into the tof tube
    - Simulations indicate good mass resolution
    - Effective diagnostic of beam power density


Atomic-like Quantum System setup

**Velocity Map Imaging, VMI, spectrometer**

- Energy \( \leq 500 \text{ eV (mode1), } \leq 1200 \text{ eV (mode2)} \)
- Resolution \( \Delta E/E \) confirmed 2%, aiming for 1%
- Detector:
  - 10 Hz: Phosphor-CMOS
  - MHz: PlmMS, Timepix3 (tentative)
- Spectroscopy or coincidence possible
- Can run in parallel with the ToF
- Can do coincidence with the ToF
- Can run in pulsed-mode, for ions

**MHz capability with “tme-stamping” cameras**

<table>
<thead>
<tr>
<th></th>
<th>PlmMS2</th>
<th>TimepixCam</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pixels</td>
<td>324x324</td>
<td>256x256</td>
</tr>
<tr>
<td>Hits/pix</td>
<td>( \leq 4 )</td>
<td>( \leq 1 )</td>
</tr>
<tr>
<td>Dead time</td>
<td>150 ns</td>
<td>1.5 ( \mu \text{s} )</td>
</tr>
<tr>
<td>Rep. rate</td>
<td>10 Hz</td>
<td>Continuous</td>
</tr>
<tr>
<td>Person</td>
<td>Oxford Univ. Brouard and Vallace group</td>
<td>Brookhaven NL A. Nomerotski</td>
</tr>
</tbody>
</table>

Atomic-like Quantum System setup

Prototype commissioned at DESY, 2016

Velocity Map Imaging spectrometer

Ar 2p photoelectrons, ca. 30 eV

VMI-CCD image

VMI inverted

Ar 2p photoelectrons

ΔE/E = 3.5%

ΔE/E = 1.9%
**MBES, magnetic bottle spectrometer**

- XFEL.SQS own-design (S. Deinert)
- Early model existing at DESY
- Resolution aimed at $\Delta E \leq 1$ eV
- Electrons-ions or electrons-electrons coincidence possible
- Electron energy $\leq 3000$ eV, with $\geq 50\%$ acceptance
- Rep. rate $\leq 4.5$ MHz (electrons only)

Innovative MCP “funnel” concept to favor coincidence

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Eland and Feifel *Chemical Physics* 327 85 (2006)
MBES, magnetic bottle spectrometer

Simulation from present model:

Simulated $\Delta M < 2\text{amu}$

at 100amu

Simulated $\Delta E < 0.1\text{ eV}$

at 100eV

Measurements from early model:

N$_2$O N1s XPS

with chemical split

Measured $\Delta E < 1.3\text{ eV}$

at 124eV (DESY.P04)

PLEASE:

Contact us with your specific requests to know what specifications are to be expected (Mass or Energy resolution, transmission, …)
1-D Imaging XUV spectrometer

Not compatible with interim optics: not available on day 1

- In-kind contribution from J.E. Rubensson, Uppsala
  - Spectroscopy in vertical direction
  - Imaging along the beam in horizontal direction
  - Gas or liquid samples
  - Pulse characterization

Expected performance

- Photon energy range 250 – 1000 eV
- Energy resolution $\Delta E/E \sim 10,000$
- Spatial resolution along the beam $10\mu m = 1fs$
- Acceptance $5\times10^{-6}$ of $4\pi$

MCP-stack, 128-fold, DLD multihit detector
## Summary: AQS readiness for 1st users beam

<table>
<thead>
<tr>
<th>Status for 1st users on day-1</th>
<th>Maximum shot resolved rep. rate</th>
<th>Sample of day-1</th>
<th>Detector</th>
<th>Contact person</th>
</tr>
</thead>
<tbody>
<tr>
<td>etof, x3</td>
<td>Ready</td>
<td>Any</td>
<td>Gas</td>
<td>Alberto De Fanis</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>MCP assembly + 3GHz 10GS digitizer</td>
<td></td>
</tr>
<tr>
<td>VMI</td>
<td>Ready</td>
<td>10 Hz with CMOS MHz with Timestamp camera</td>
<td>Gas</td>
<td>Tommaso Mazza Rebecca Boll</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>MCP + Phosphor, with sCMOS or Timestamp camera</td>
<td></td>
</tr>
<tr>
<td>MBES</td>
<td>Ready</td>
<td>Any, electrons ~ 100 kHz, ions</td>
<td>Gas</td>
<td>Sascha Deinert</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>MCP + digitizer + sCMOS imaging</td>
<td></td>
</tr>
</tbody>
</table>
AQS support

- Designed by Y. Ovcharenko with Newport, ready to be installed.
- Stable steel base, Aluminium legs
- Tripod uncoupled system for leveling Z vertical axis motion, a longitudinal X and lateral Y motion, 2 rotation axis Theta (X, Z) and 1 rotation axis Theta Y.

<table>
<thead>
<tr>
<th></th>
<th>Range</th>
<th>Resolution</th>
<th>Repeatability</th>
<th>Speed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Travel X, Y</td>
<td>≤100 mm</td>
<td>≤1 µm</td>
<td>≤5 µm</td>
<td>≤2 mm/s</td>
</tr>
<tr>
<td>Travel Z</td>
<td>≤150 mm</td>
<td>≤1 µm</td>
<td>≤5 µm</td>
<td>≤0.2 mm/s</td>
</tr>
<tr>
<td>Rx Ry</td>
<td>≤2°</td>
<td>≤1 m°</td>
<td>≤5 m°</td>
<td>≤0.01 m°/s</td>
</tr>
<tr>
<td>Rz</td>
<td>≤2°</td>
<td>≤1 m°</td>
<td>≤5 m°</td>
<td>≤0.01 m°/s</td>
</tr>
</tbody>
</table>

ANSYS FEA analysis combined with real hall measurement: extent of vibrations can be tolerated

Support summary:
- Delivered!
- Stable. Simulations shows that vibrations of the floor can be tolerated
- Remotely controlled
- 6-axis adjustable in fine steps and large travel range
Thank you for your attention

The SQS team

- A. Achner
- T.M. Baumann
- R. Boll
- A. De Fanis
- S. Deinert
- P. Grychtol
- M. Ilchen
- T. Mazza
- M. Meyer
- J. Montaño
- Y. Ovcharenko
- N. Rennhack
- R. Wagner
- P. Ziołkowski

In-kind contribution:
- XUV spectrometer
  - J.E. Rubensson, J. Nordgren (Uppsala)

Commissioning of spectrometers with synchrotron beam
- DESY P04
  - J.Viefhaus, J.Buck, G.Hartmann, L.Glaser,
- XFEL Diagnostic group
  - J.Liu

European XFEL