

Status of the *h*RIXS Project

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on behalf of the *h*RIXS consortium

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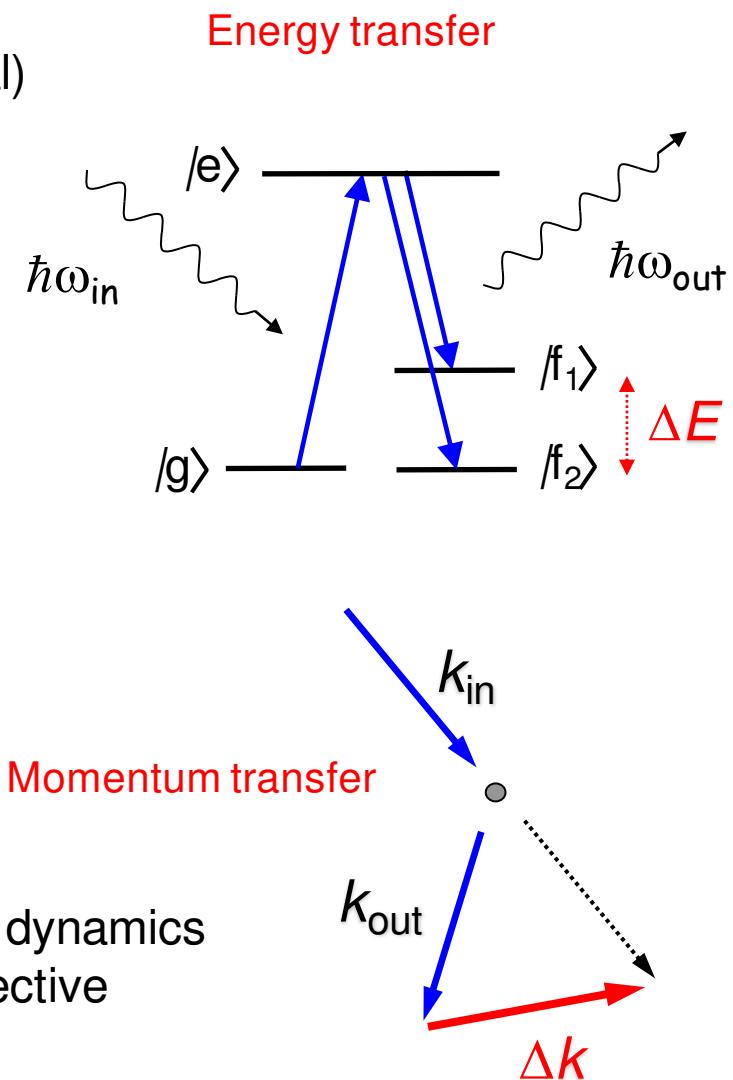
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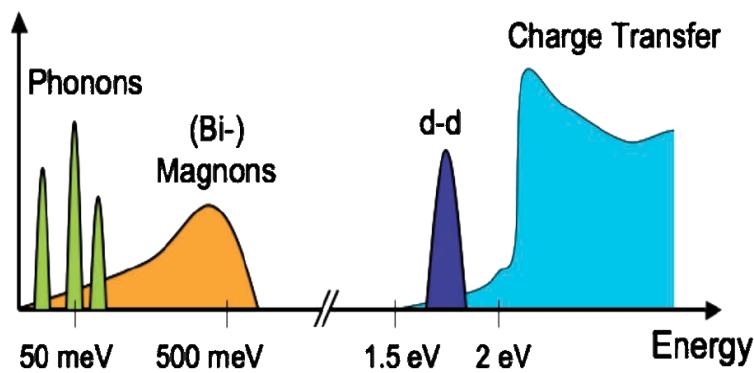
Spokesperson & Scientific Coordinator: Prof. Alexander Föhlisch

Goal: Implementation of a High-Resolution X-ray Spectrometer for Time- & Momentum-Resolved Resonant Inelastic X-ray Scattering (RIXS) Experiments at the SCS Instrument

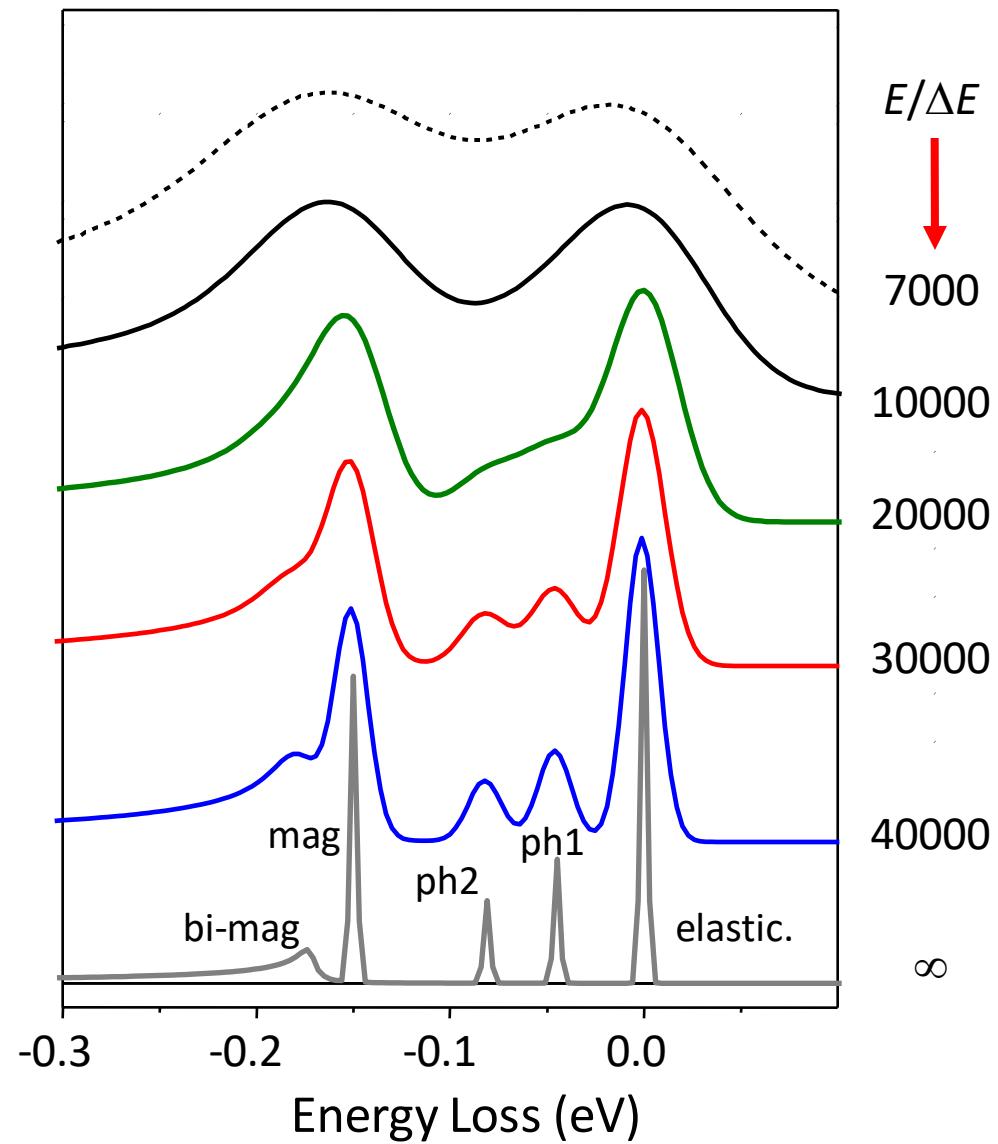
- Element and symmetry selective probe: chemical state, electronic (spin, charge, orbital) and nuclear degrees of freedom
- Photon-in/photon-out → bulk-sensitive, insulating samples, external fields
- Probes low-energy valence excitations: phonons, spin-excitation...
- Direct probe of energy and momentum of elementary excitations
- Optically forbidden transitions accessible (e.g. d-d transitions)

→ Monitoring phase transitions and chemical dynamics in complex systems from an atomic perspective



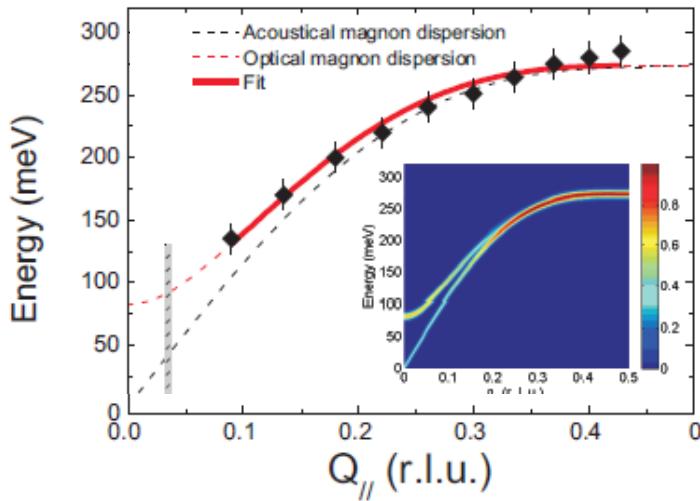
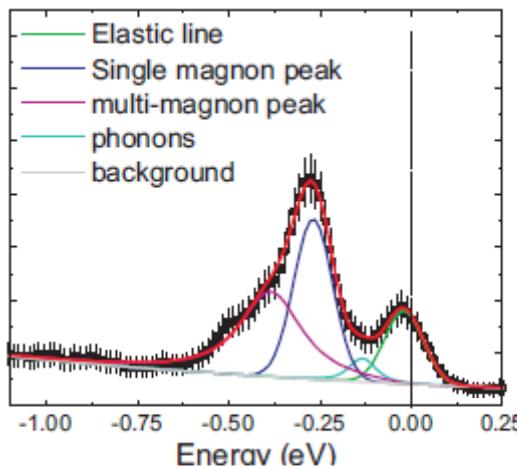
High-Resolution RIXS – Static Case

Hypothetical Cu-L₃ RIXS spectrum →

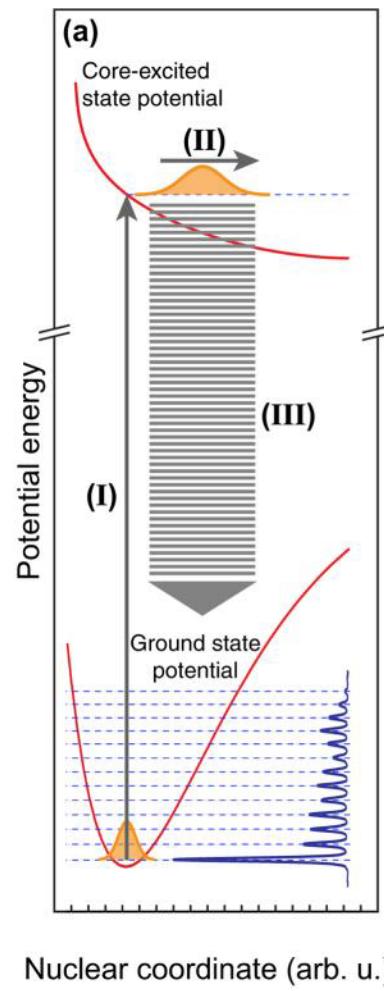


RIXS Spectrometer Benchmarks

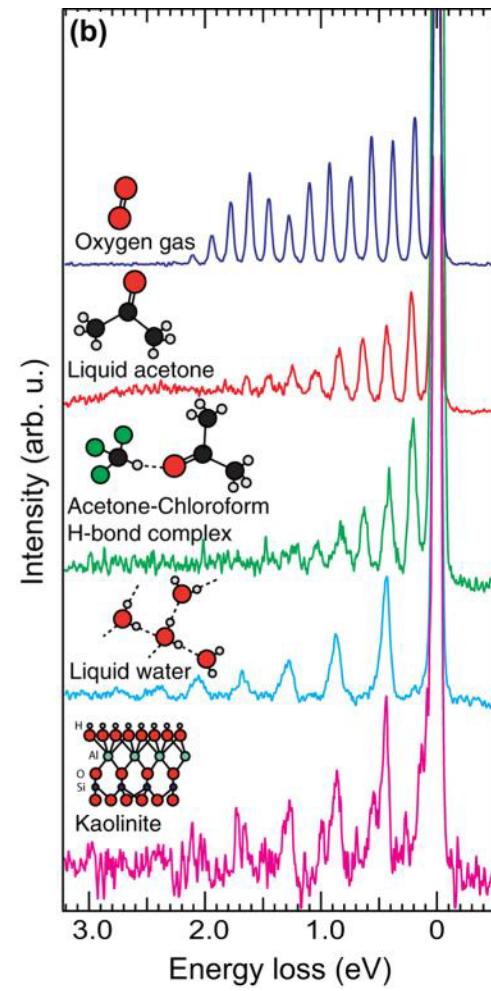
Start of operation	Name	Light Source	Total Length [m]	Combined resolving power @900eV
2011	SAXES	SLS	5	11.000
2015	€RIXS	ESRF	12	25.000
2016	PEAXIS	BESSY-II	5	12.000
2017	SIX	NSLS-II	15	70.000
2017	VERITAS	MAX-IV	10	40.000
2017	IXS	DIAMOND	14	40.000

High Resolution RIXS – Static CaseMagnon dispersion in cuprates

M. Le Tacon, et al., *Nature Phys.* **7**, 725 (2011)

Ground state PES via vibrational resolution

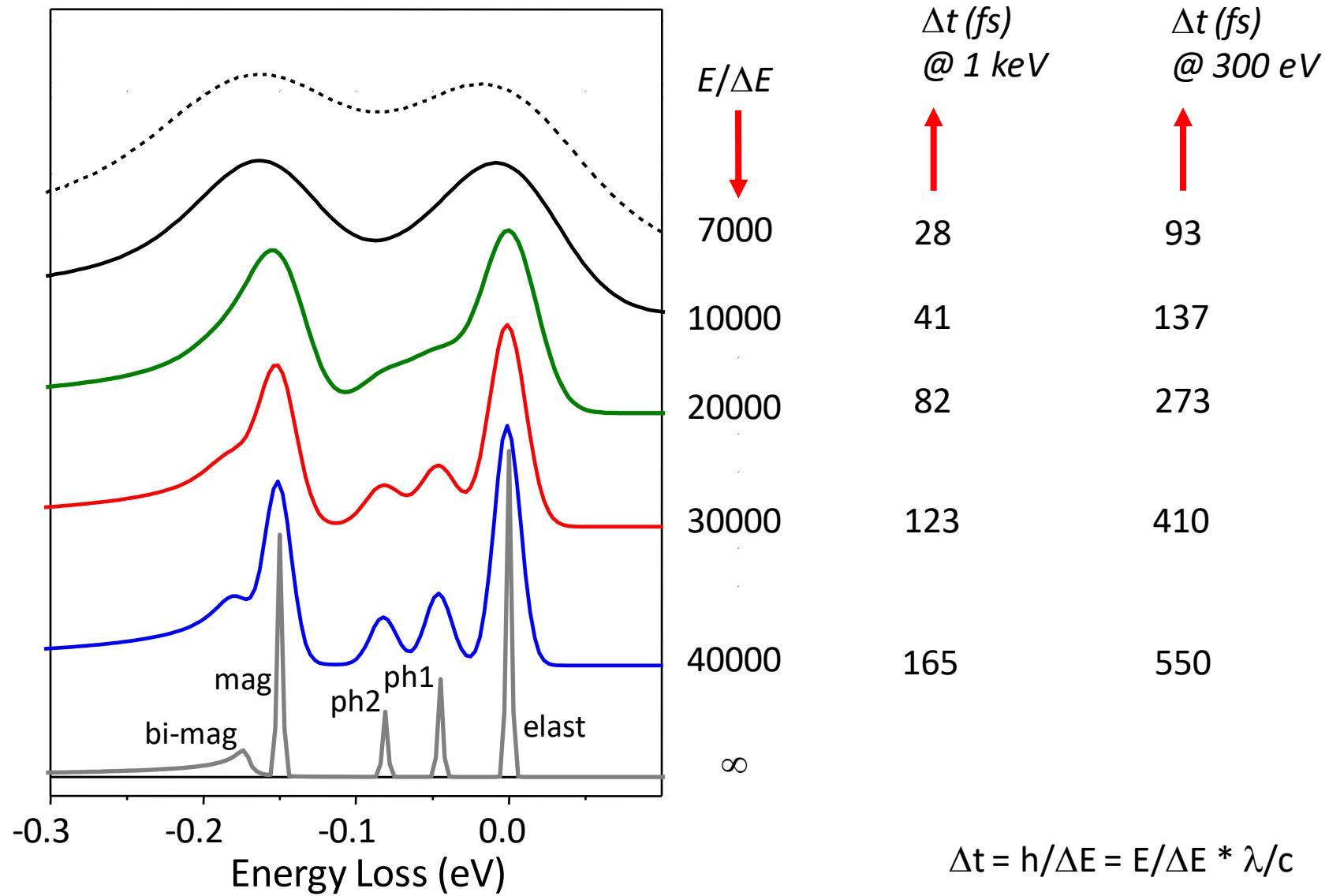
Nuclear coordinate (arb. u.)



S. Schreck et al., *Sci. Rep.* **7**, 20054 (2016)

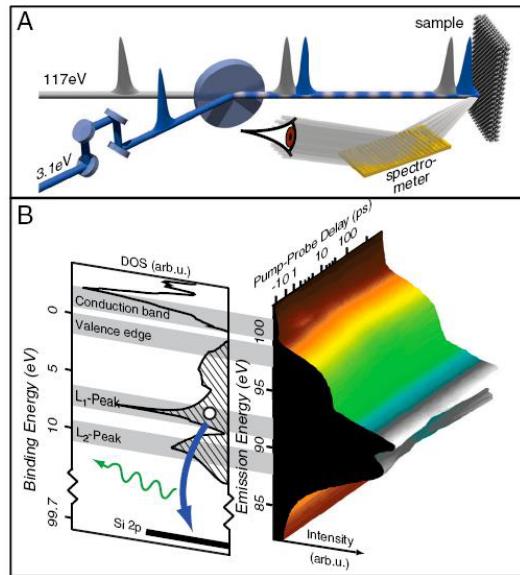
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2017	IXS	DIAMOND	14	40.000
2018	hRIXS	XFEL	5	25.000

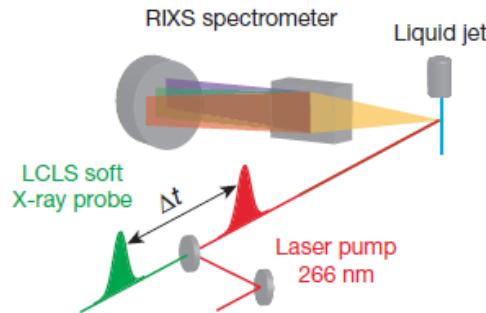


Time Resolved RIXS/XES

Liquid-liquid phase transition in silicon

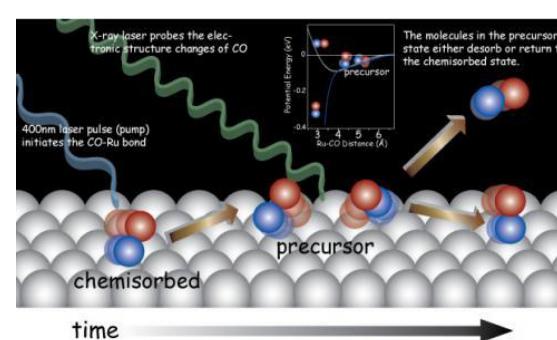


M. Beye et al. PNAS 2010 **107** 16776



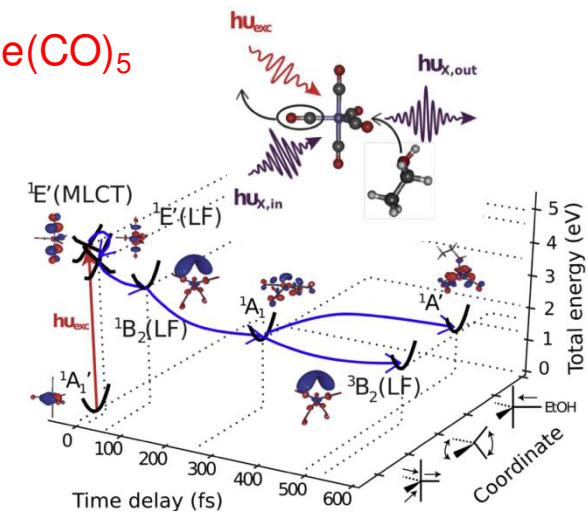
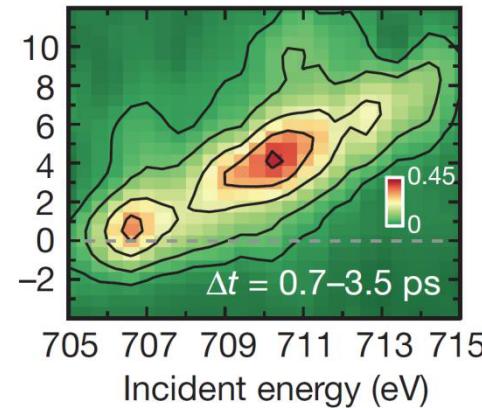
Ph. Wernert et al. Nature 2015 **520** 78

Transient precursor state in CO/Ru

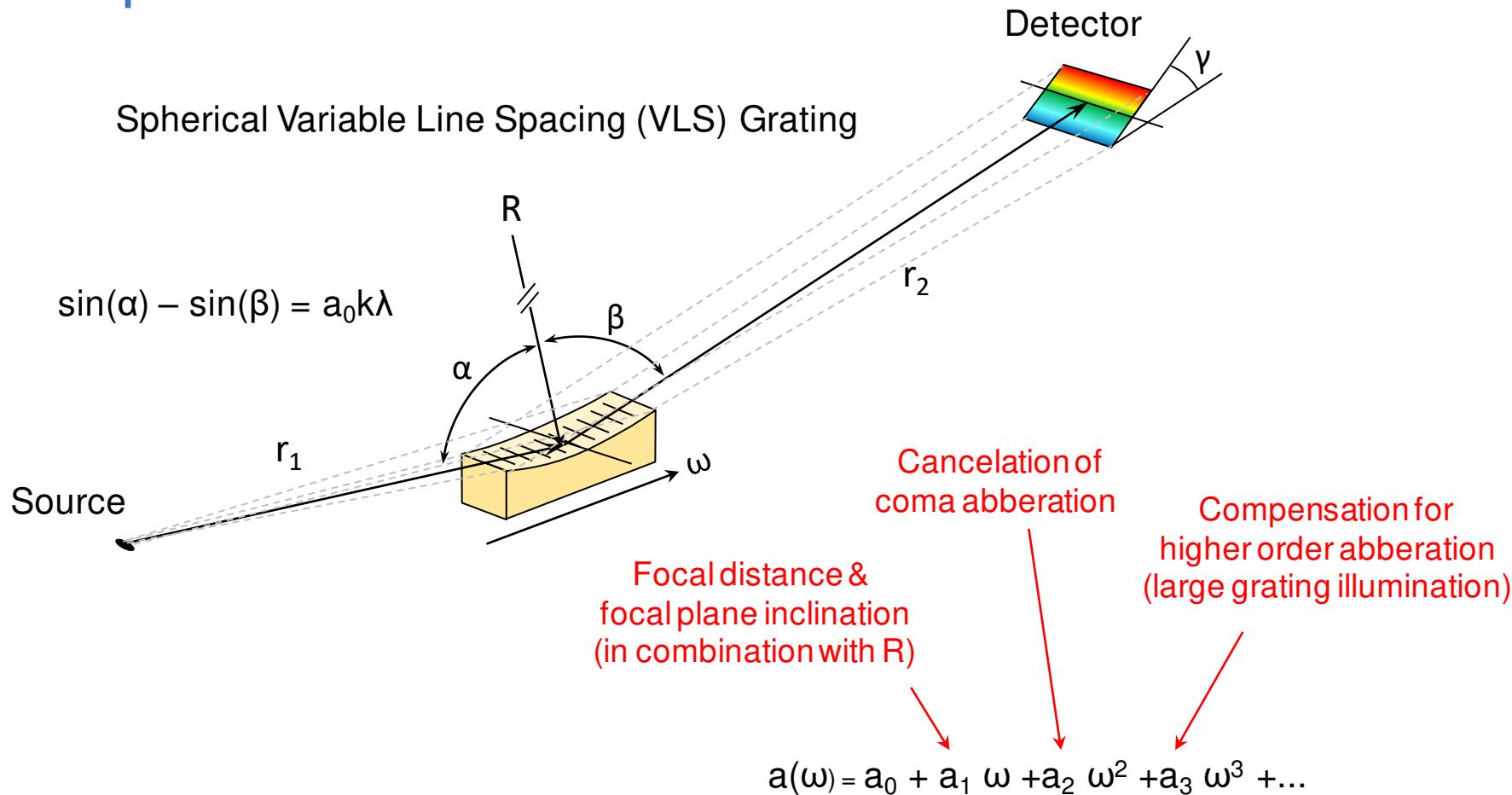


M. Dell'Angela et al. Science 2013 **339** 1302

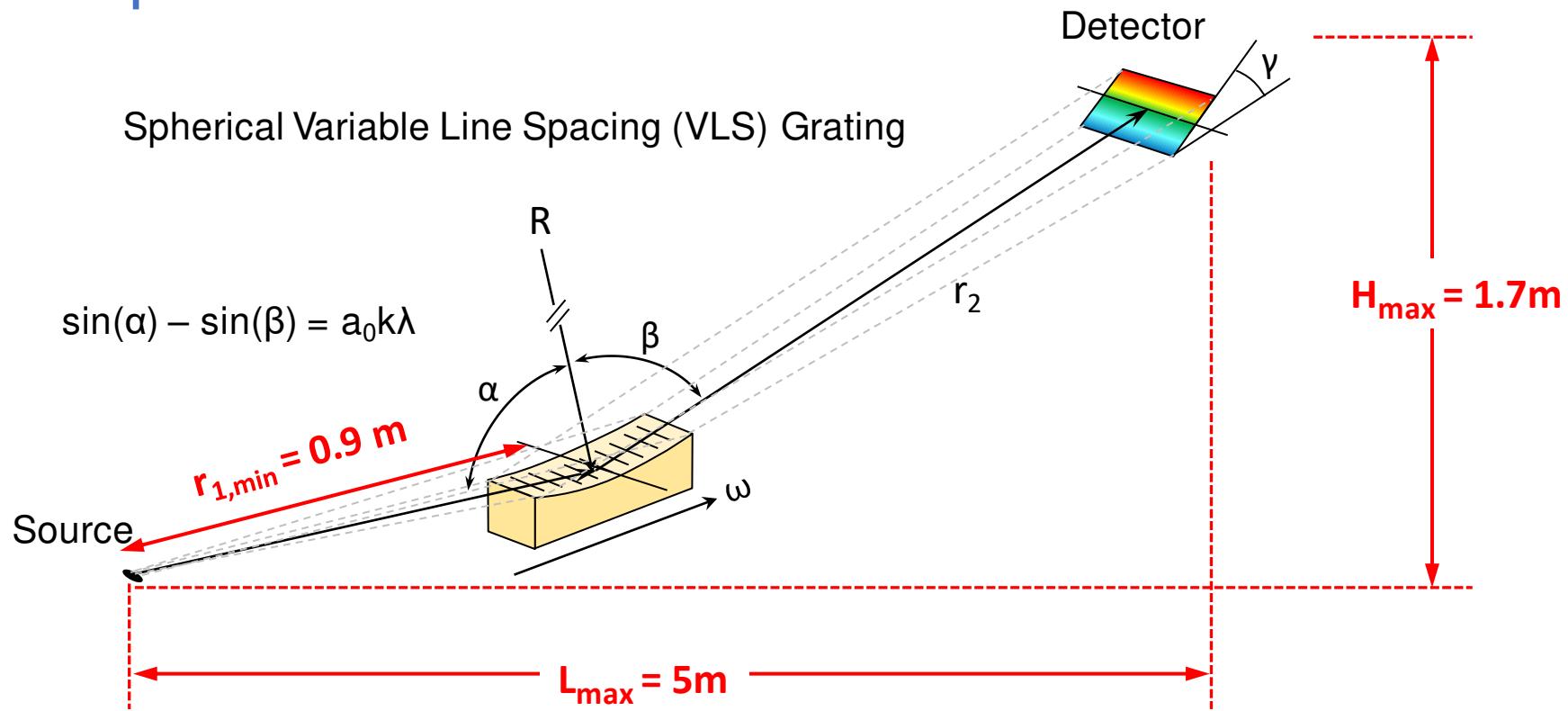
Ligand-exchange dynamics in Fe(CO)₅



K.Kunnus et al. NJP 2016 **18** 103011



- Single optical element
- Ease of operation & alignment
- Constrained VLS parameters optimization



- Single optical element
- Ease of operation & alignment
- Constrained VLS parameters optimization

Gratings for the *h*RIXS Spectrometer

3000 l/mm high resolution grating

Optimized parameters @ $E_0 = 900\text{eV}$	
$a_0 [\text{mm}^{-1}]$	3000
$a_1 [\text{mm}^{-2}]$	1.23162
$a_2 [\text{mm}^{-3}]$	5.35663×10^{-4}
$a_3 [\text{mm}^{-4}]$	3.5524×10^{-7}
$R [\text{mm}]$	64647.3
α	$88^\circ - 89^\circ$
$r_1 [\text{mm}]$	1970.41
$r_2 [\text{mm}]$	3029.59

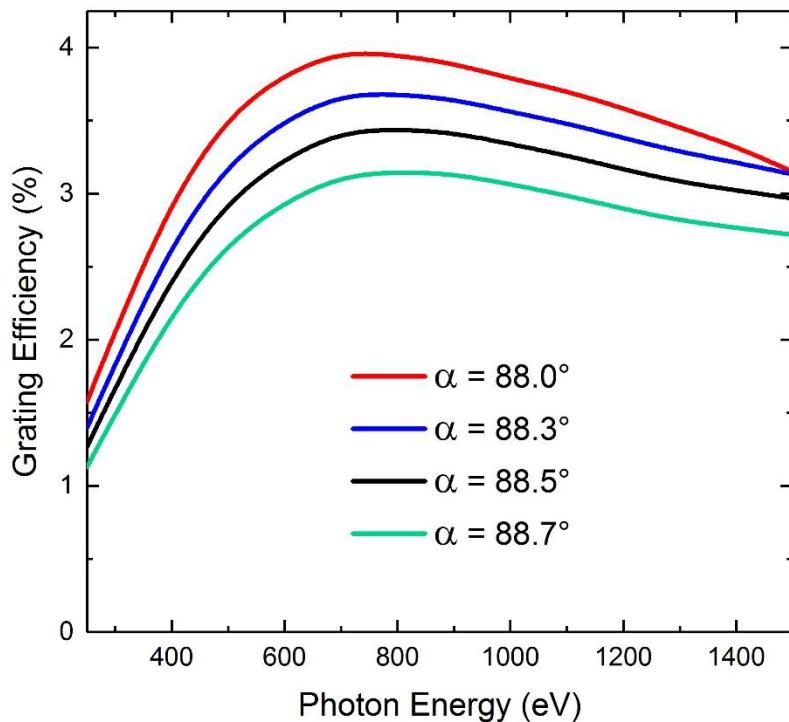
1000 l/mm high efficiency grating

Optimized parameters @ $E_0 = 600\text{eV}$	
$a_0 [\text{mm}^{-1}]$	1000
$a_1 [\text{mm}^{-2}]$	0.446456
$a_2 [\text{mm}^{-3}]$	2.06068×10^{-4}
$a_3 [\text{mm}^{-4}]$	1.5749×10^{-7}
$R [\text{mm}]$	70114.1
α	$88^\circ - 89^\circ$
$r_1 [\text{mm}]$	2201.72
$r_2 [\text{mm}]$	2798.28

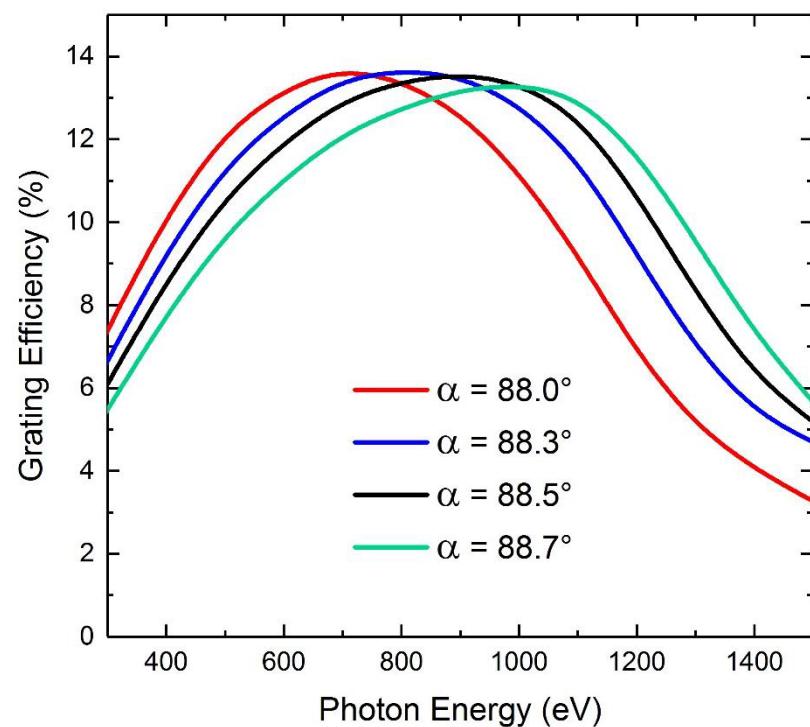
- Large grating surface of $4 \times 20 \text{ cm}^2$ to improve spectrometer acceptance
- For $h\nu \leq E_0$, α and r_1 need to be adjusted: $250 \text{ eV} \leq h\nu \leq 1600 \text{ eV}$
- Additional factors limiting final resolution: Δ_{source} , Δ_{detector} & $\Delta_{\text{slope-error}}$

Grating Efficiencies

3000 l/mm high resolution grating

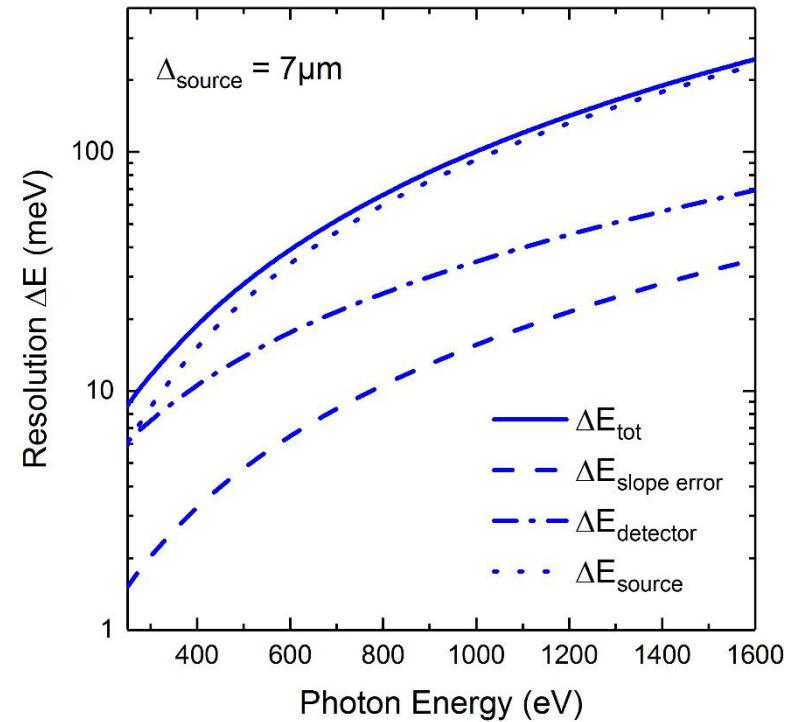
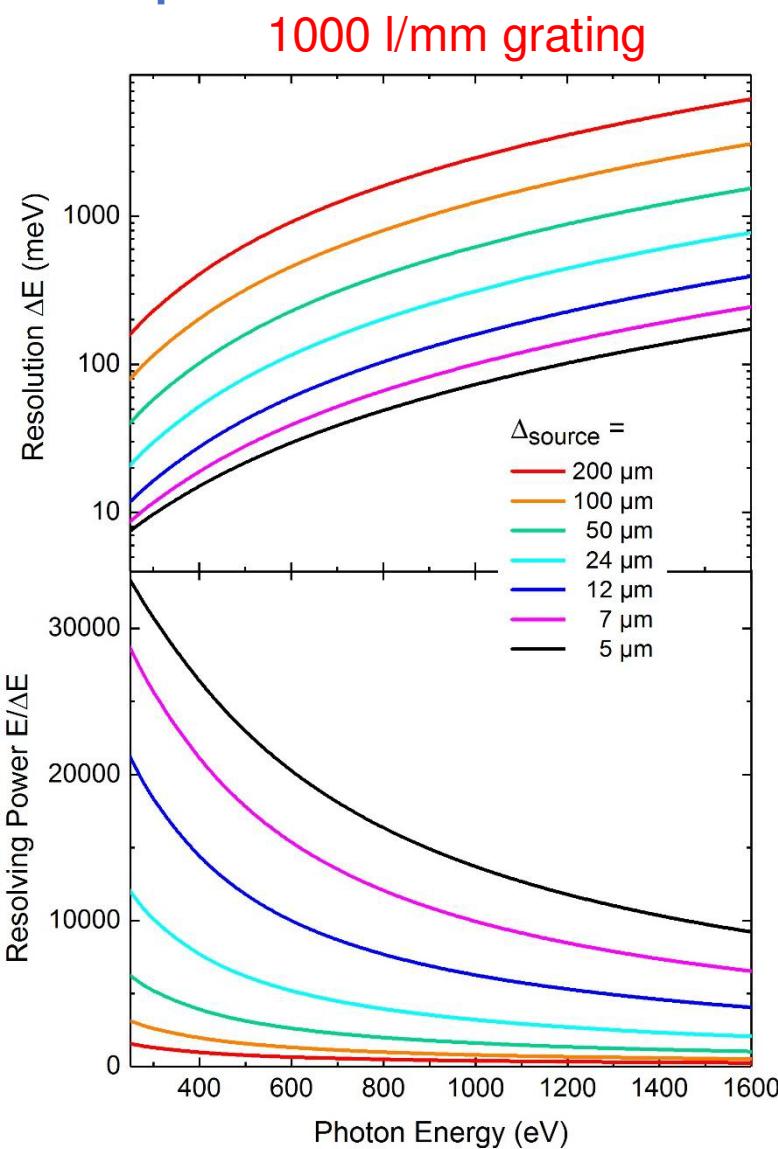


1000 l/mm high efficiency grating



- Laminar grating profile with Au coating

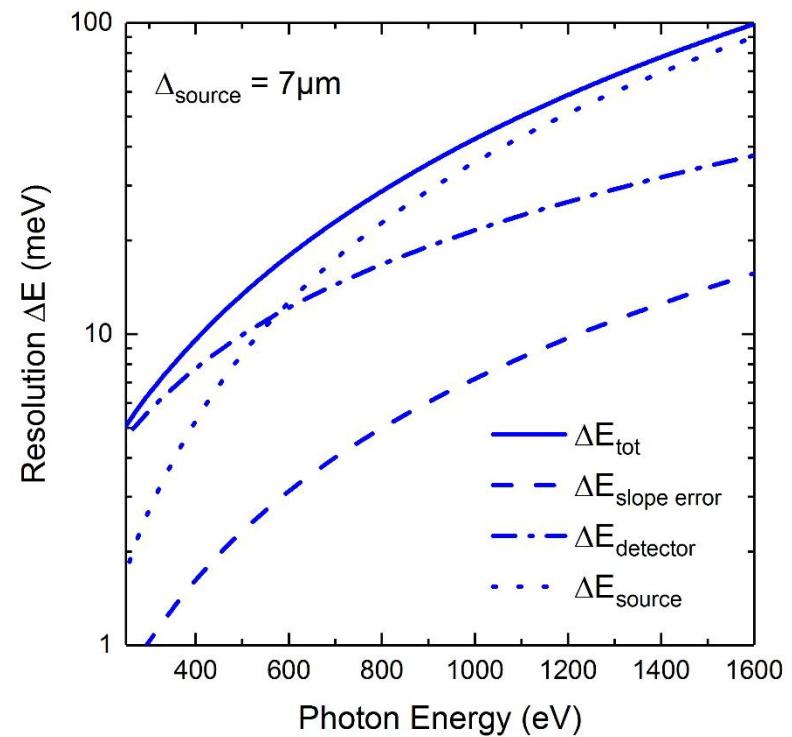
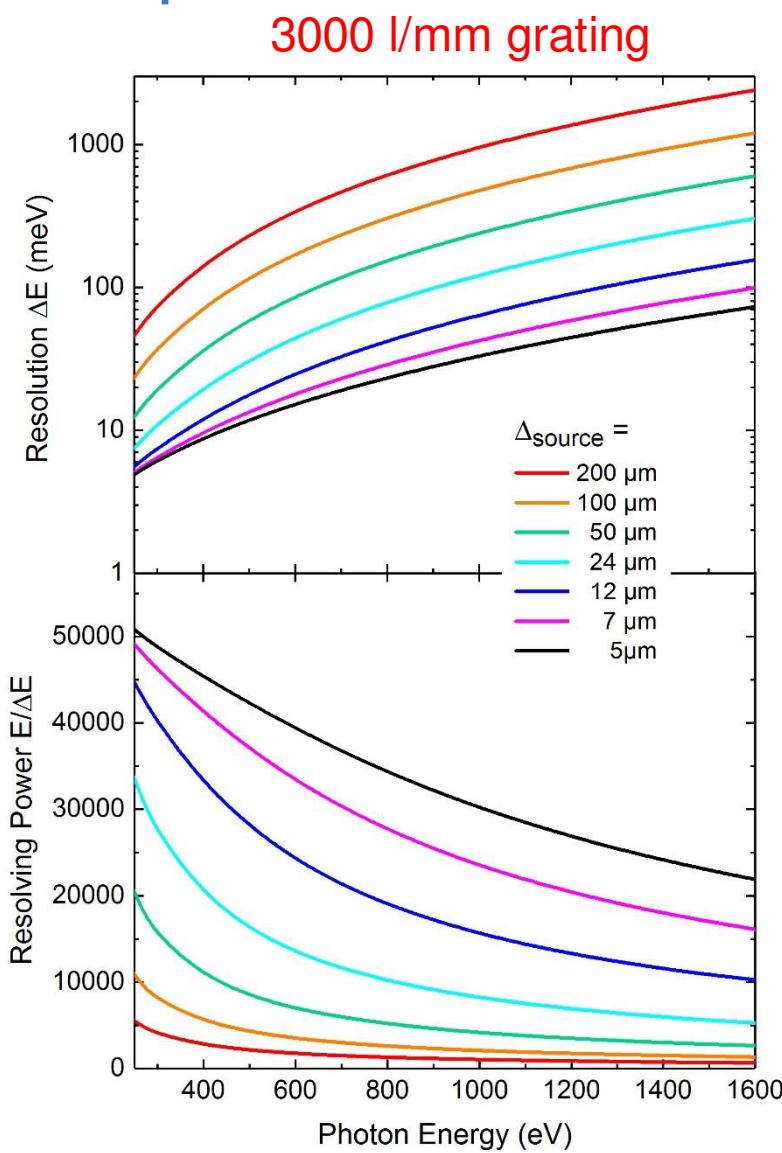
Resolving Power vs. Source Size



$$\Delta_{\text{detector}} = 10 \mu\text{m}$$

$$\Delta_{\text{slope-error}} = 0.1 \mu\text{rad rms}$$

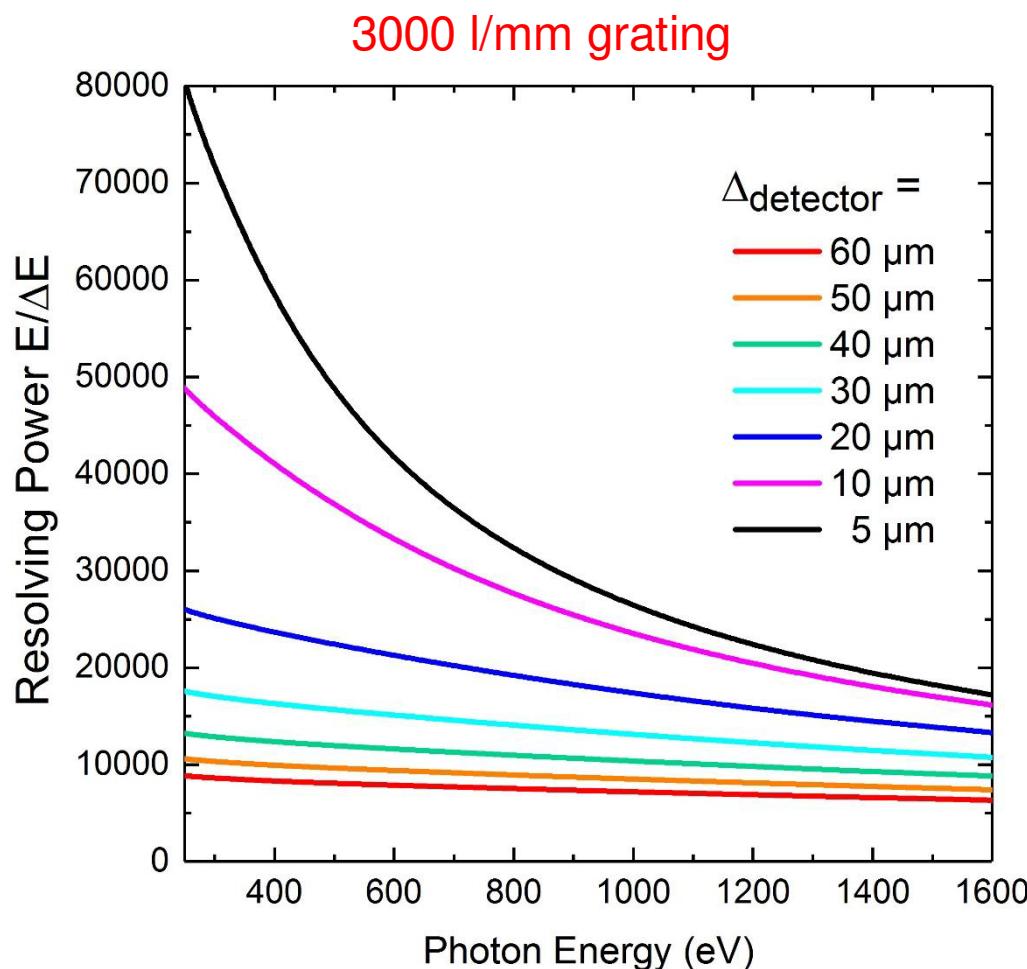
Resolving Power vs. Source Size



$$\Delta_{\text{detector}} = 10 \mu\text{m}$$

$$\Delta_{\text{slope-error}} = 0.1 \mu\text{rad (rms)}$$

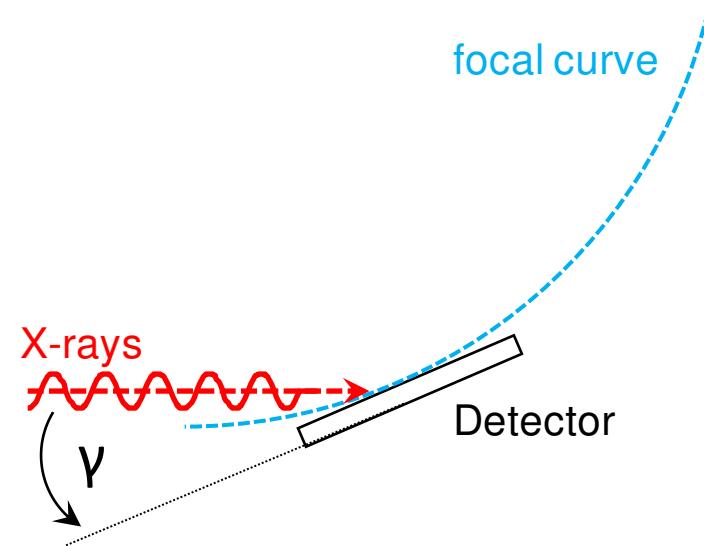
Resolving Power vs. Detector Resolution

 $\Delta_{\text{source}} = 5 \mu\text{m}$
 $\Delta_{\text{slope-error}} = 0.1 \mu\text{rad rms}$

Importance of Variable Detector Angle

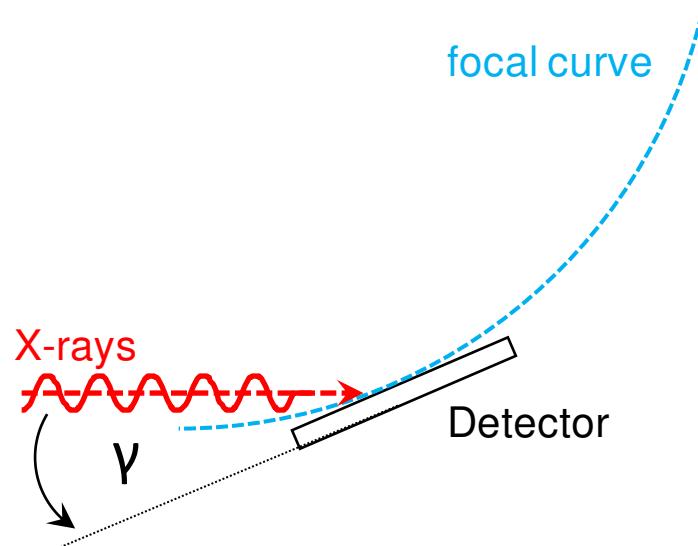
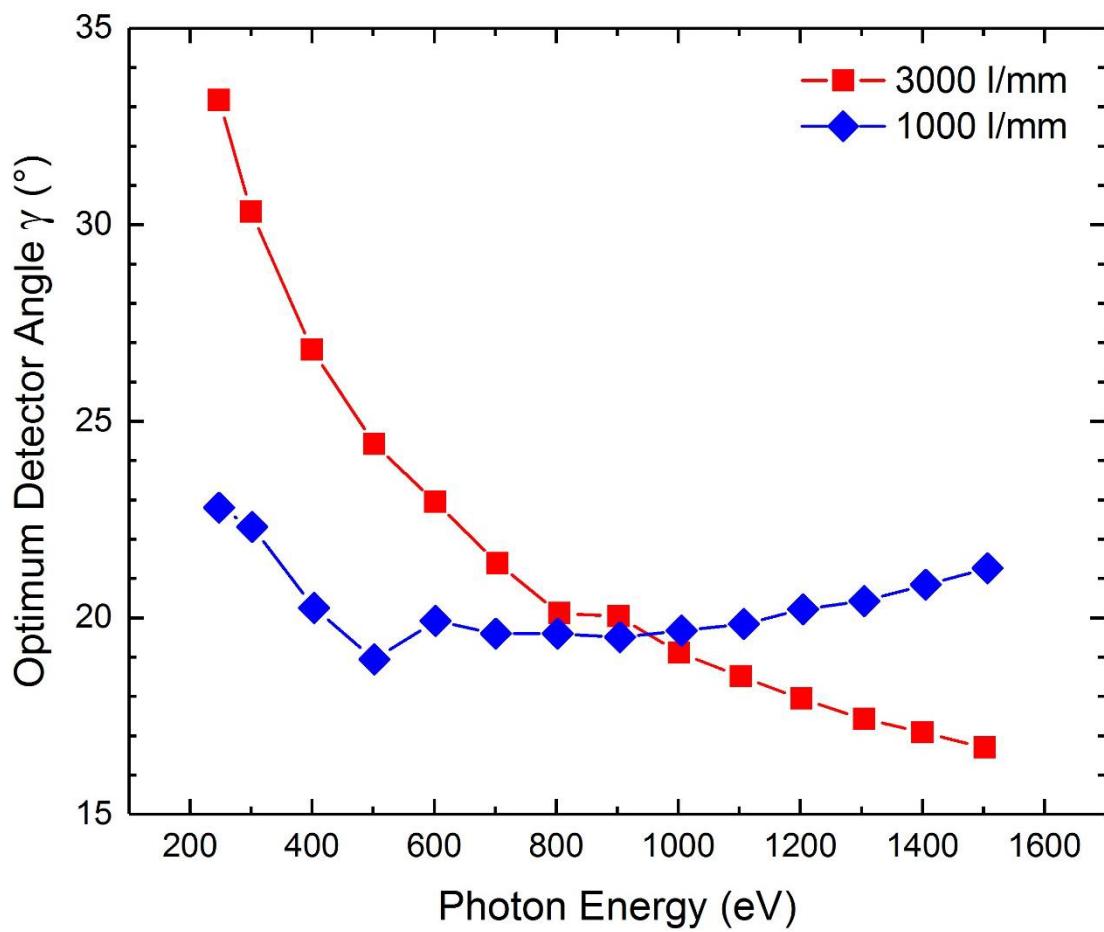
- hRIXS design will allow $15^\circ \leq \gamma \leq 35^\circ$ adjustment
- Extended $h\nu$ range with high resolution on detector

$h\nu$ [eV]	$\Delta h\nu_{\text{tot}}$ [eV]*
250	18
400	40
900	96
1500	170



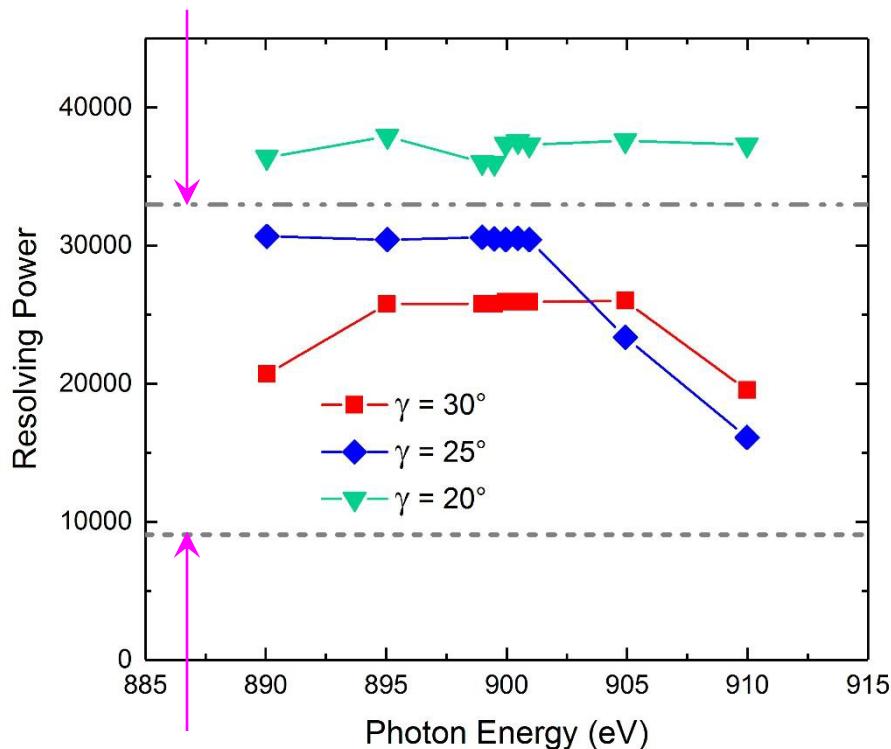
*active sensor surface ($H \times V$) = 160 x 50 mm²

Importance of Variable Detector Angle

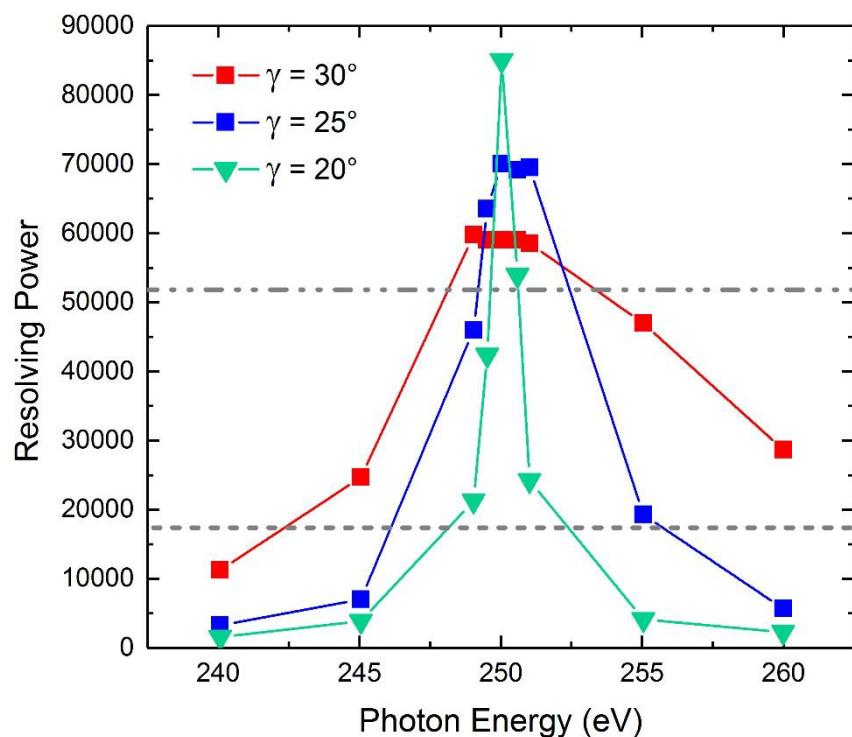


Importance of Variable Detector Angle

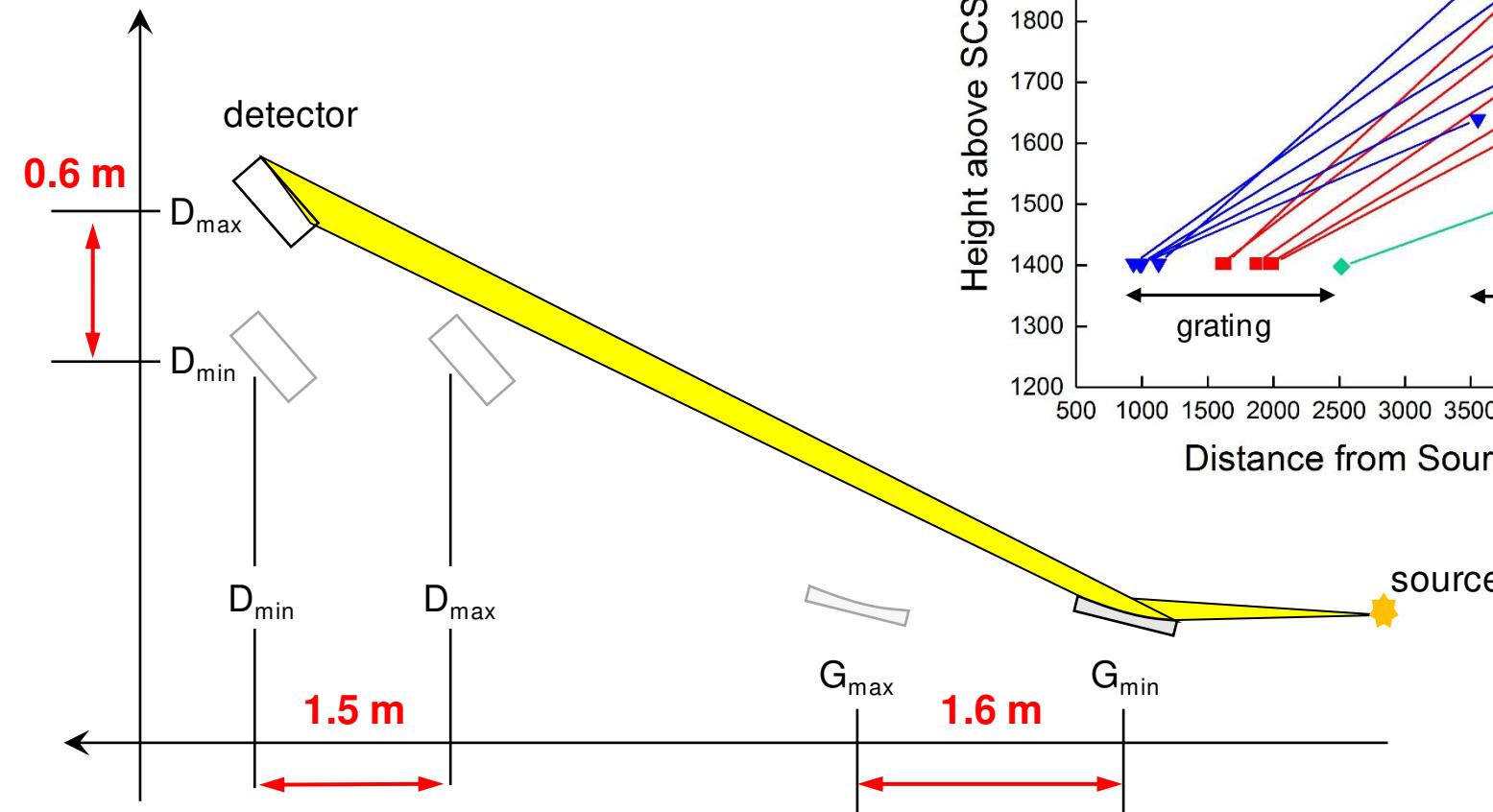
SASE-3 mono 150 l/mm



SASE-3 mono 50 l/mm

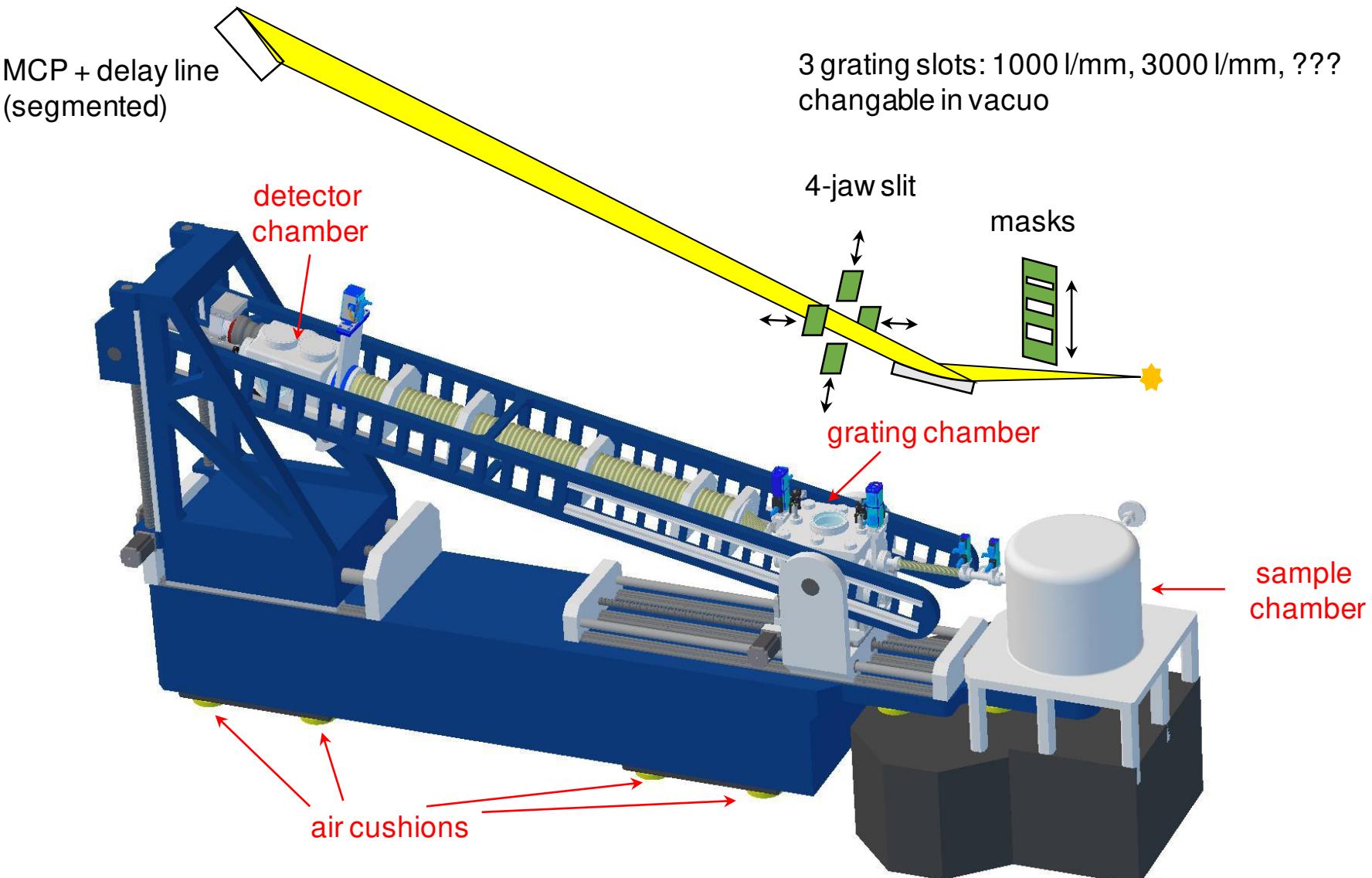


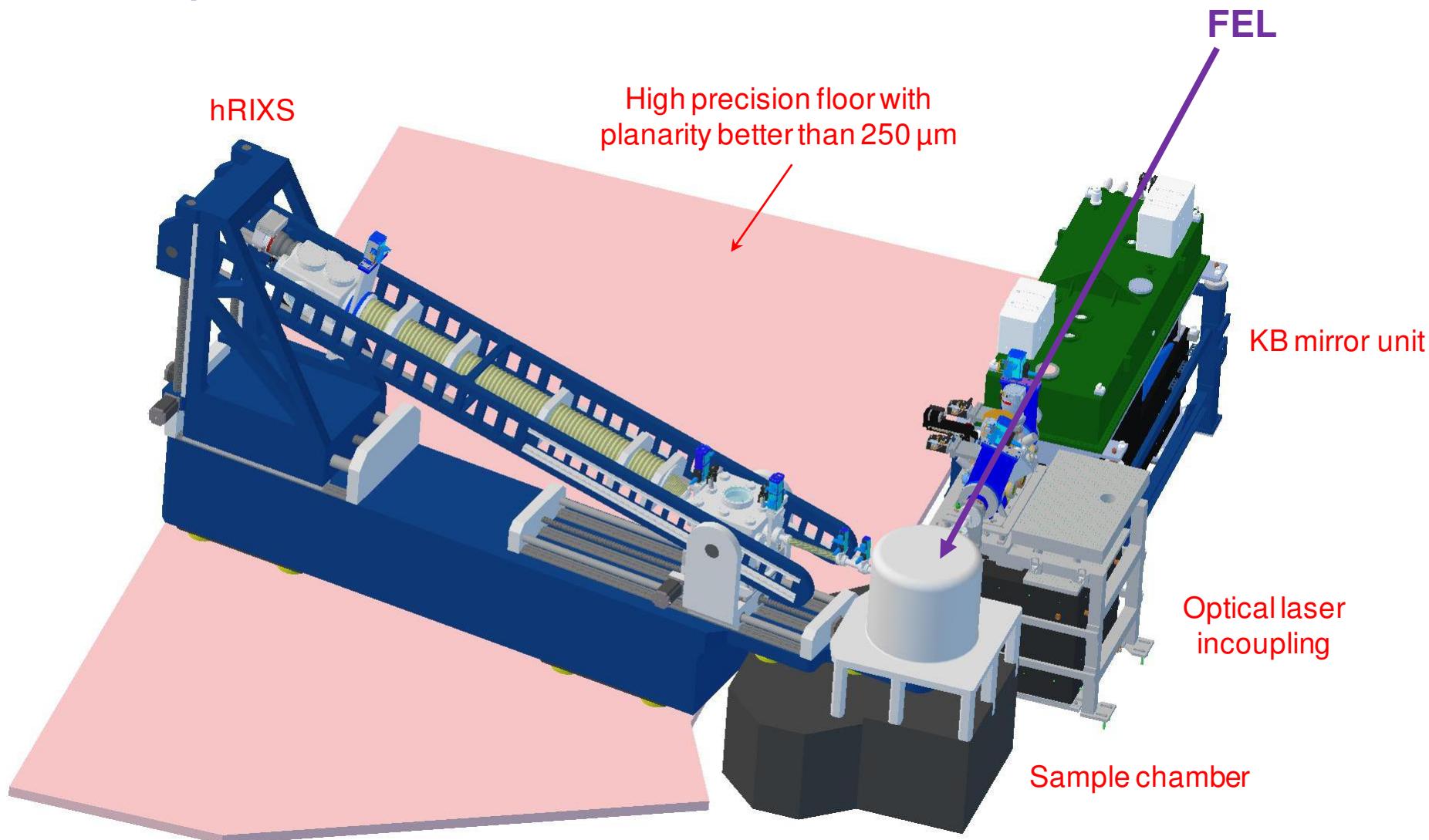
Requirements for Mechanical Design

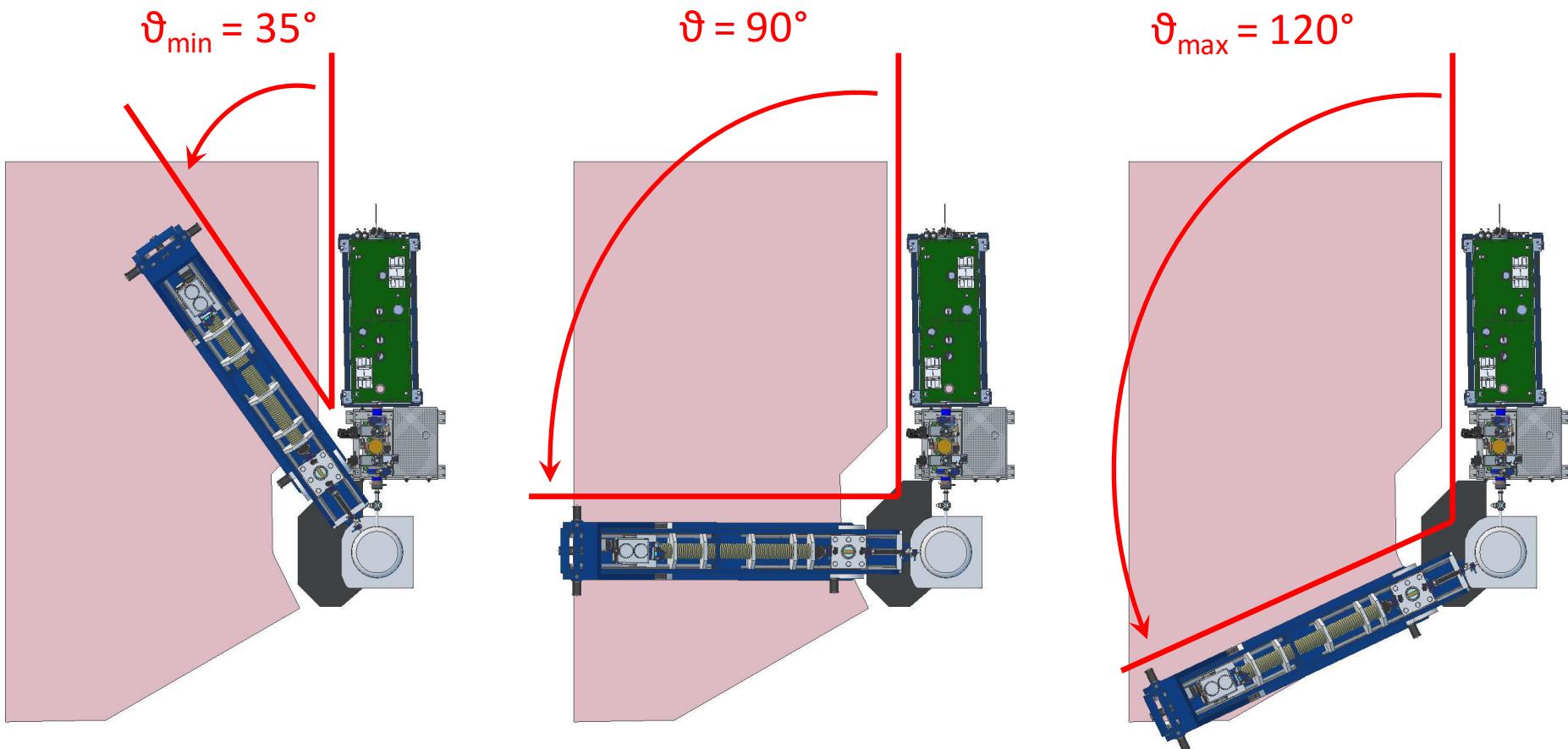


- Extensive motion ranges needed to cover 250 eV – 1600 eV working range

Approximate Mechanical Layout

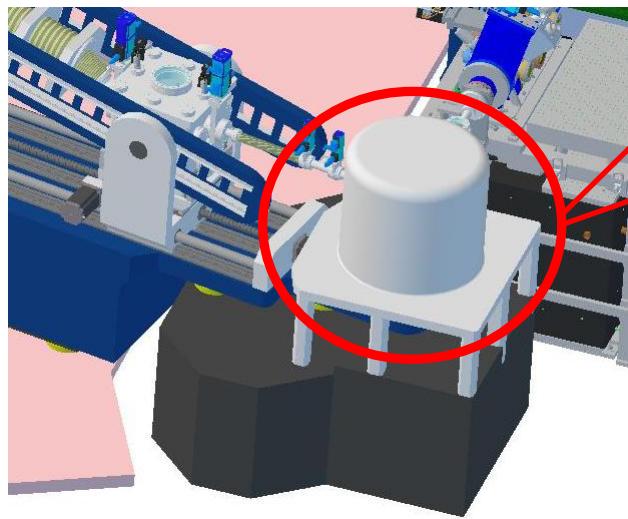






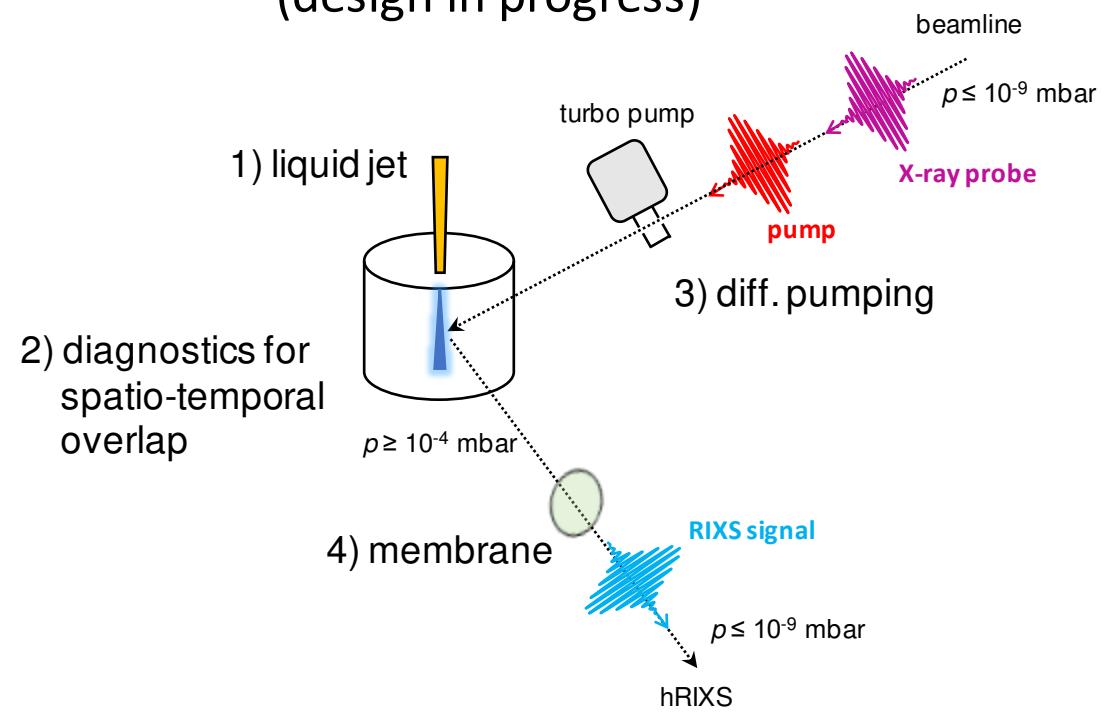
- Momentum-resolved RIXS possible due to rotatable girder structure
- Continuous rotation without braking vacuum
- Compact spectrometer design mandatory for smallest backscattering angle

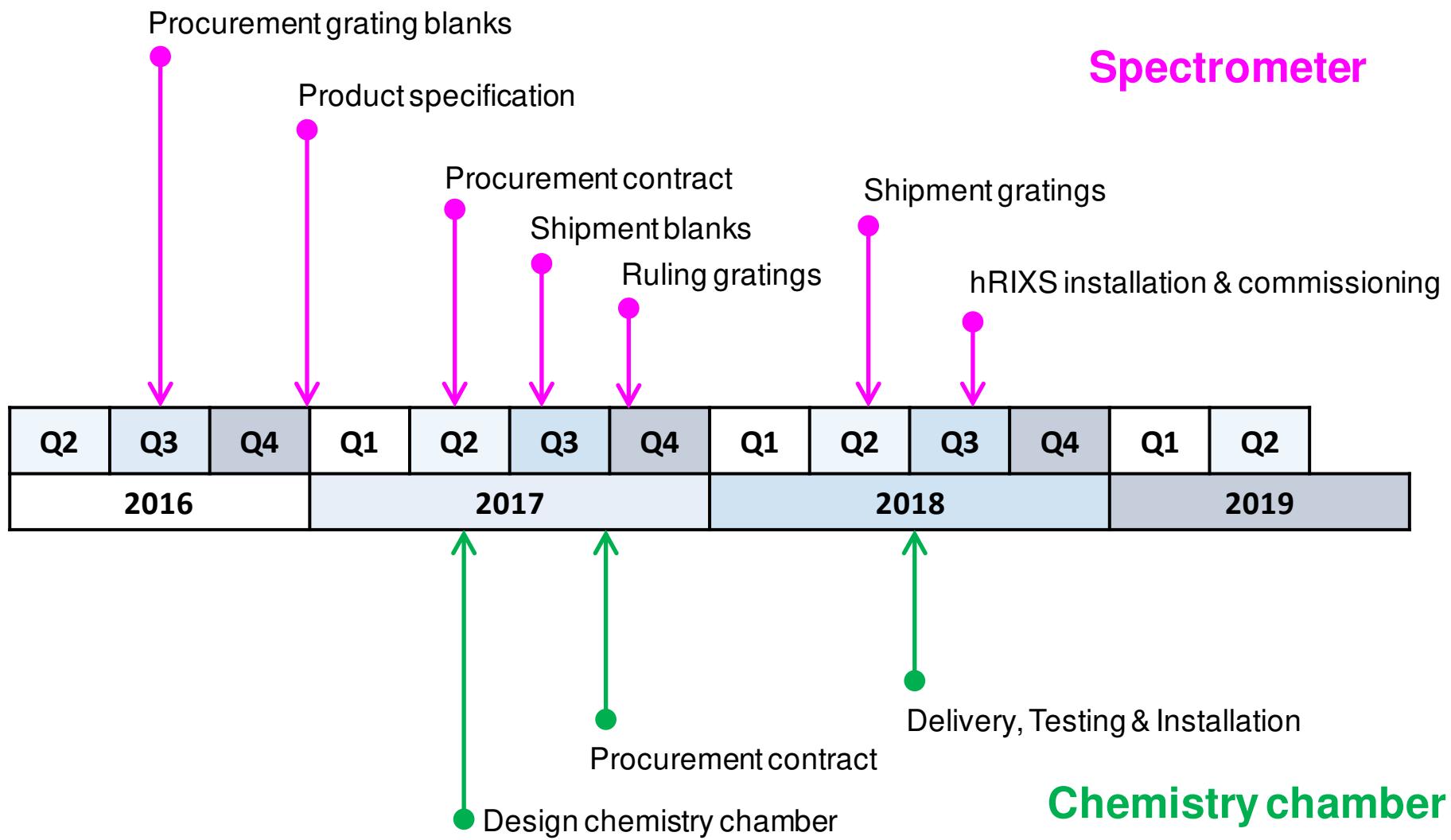
Sample Environments



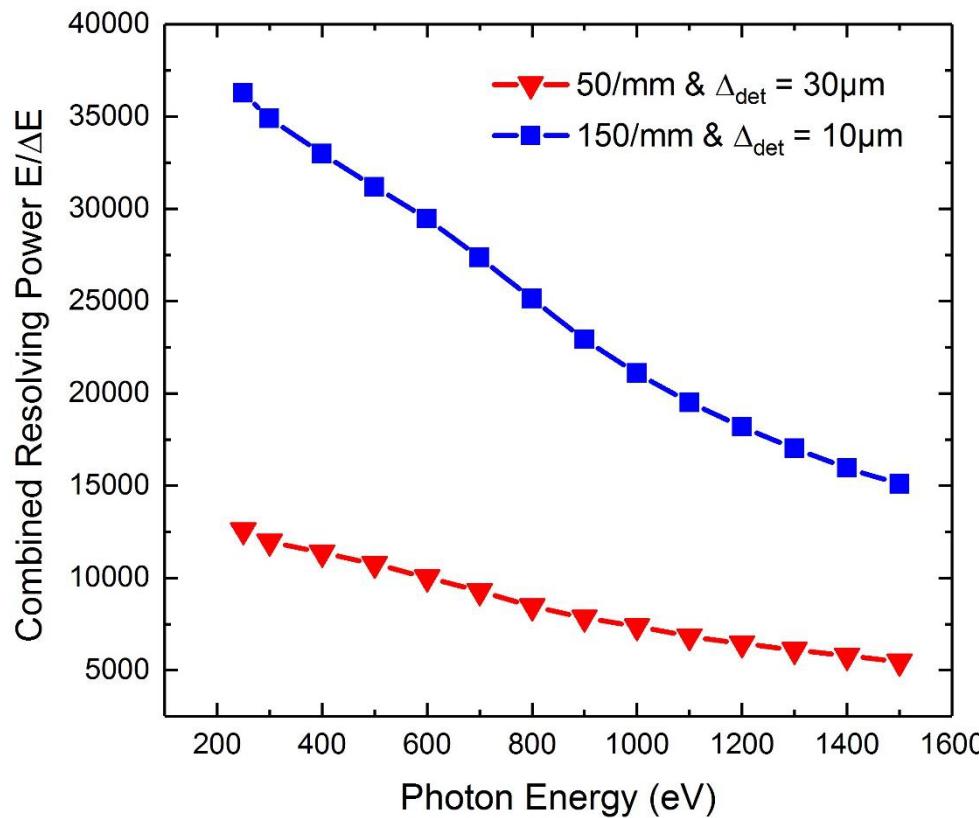
Exchangeable endstations

- For condensed matter systems:
XRD chamber (previous talk)
- Dedicated chamber for solution- and
gas-phase chemistry experiments
(design in progress)





Projected Day-1 Operation



$\Delta_{source} = 5 \mu m$
 $\Delta_{slope-error} = 0.1 \mu rad$
3000 l/mm RIXS grating

- Baseline mono operation: 50 l/mm grating
- MCP/DLD spatial resolution: $\sim 30 \mu m$
- Single pulse discrimination (MCP/DLD) for pump-probe experiments

