Diamond II – I21-RIXS upgrade

Ke-Jin Zhou

Diamond Light Source

Acknowledgement – I21-RIXS upgrade UWG

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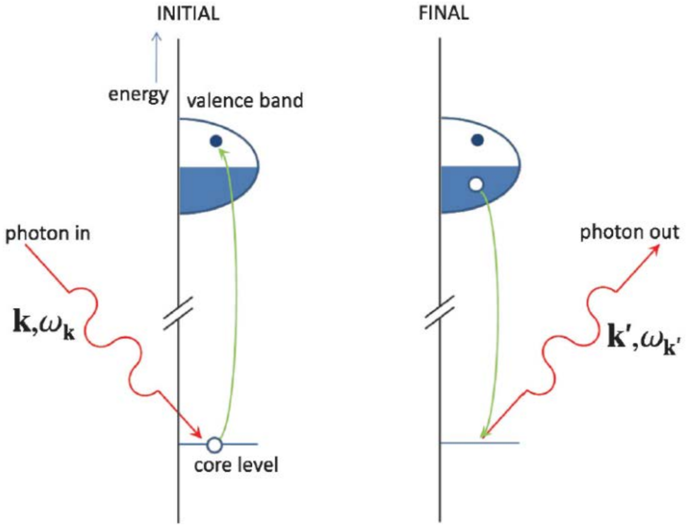
- Stefano Agrestini, DLS
- Hongchang Wang, DLS
- George Howell, DLS
- Sarnjeet Dhesi, DLS

What can we learn from RIXS?

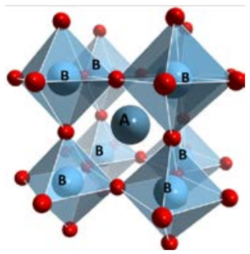


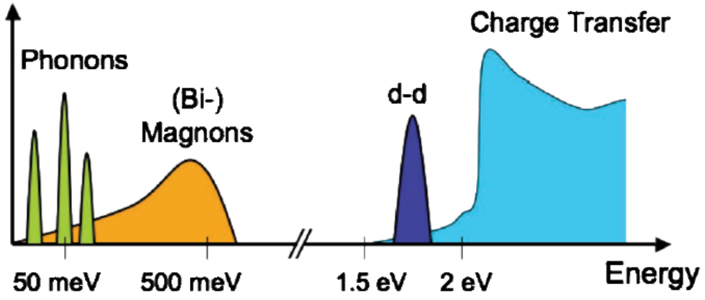
Luuk J.P. Ament et al.
Rev. Mod. Phys. (2011)

$$h\boldsymbol{q} = h\boldsymbol{k}' - h\boldsymbol{k}$$

$$h\omega = h\omega_{k'} - h\omega_k$$

Solid state materials



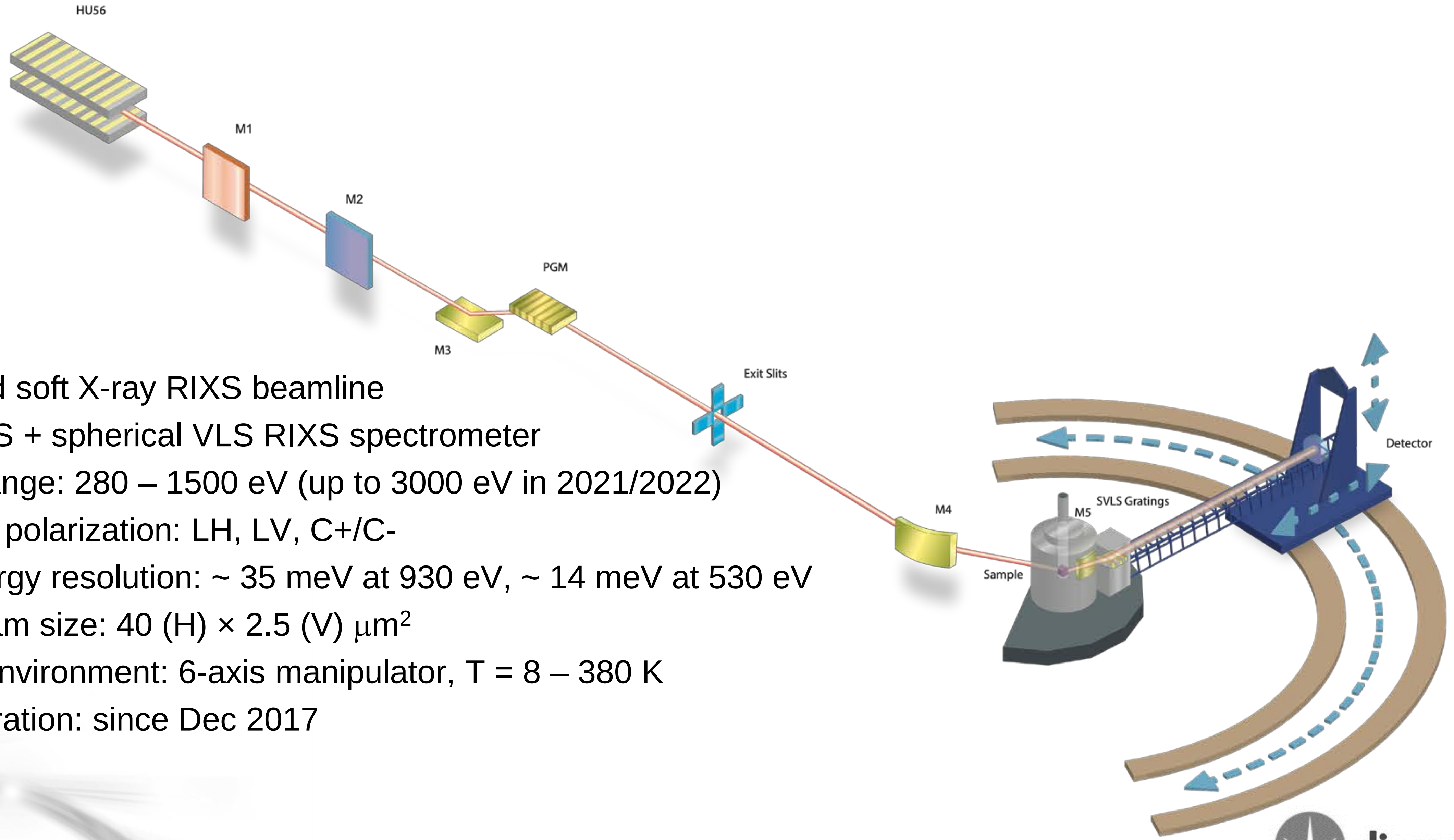


- Superconductors (Cuprates, Nickelates, Iron-based)
- Large spin-orbital coupling systems
- Heavy fermions and actinides
- Quantum spin liquid
- Itinerant/band magnetism
- Molecular magnetism
- 1D quantum spin-chain systems
- Orbital physics (Orbital ordering)
- Van der Waals magnetism, spintronics
- Battery materials

Electron (orbital)-phonon coupling	Charge-charge correlation Charge order, charge excitations	Spin-spin correlation magnons, Spin order	*dd* orbital excitation (crystal field splitting)	Ligand-cation charge transfer excitation
Γ (e-phonon coupling)	$\chi(\boldsymbol{q},\omega)$	$S(\boldsymbol{q},\omega)$	$10Dq$, U_{dd}	Δ, T_{pd}, T_{dd}

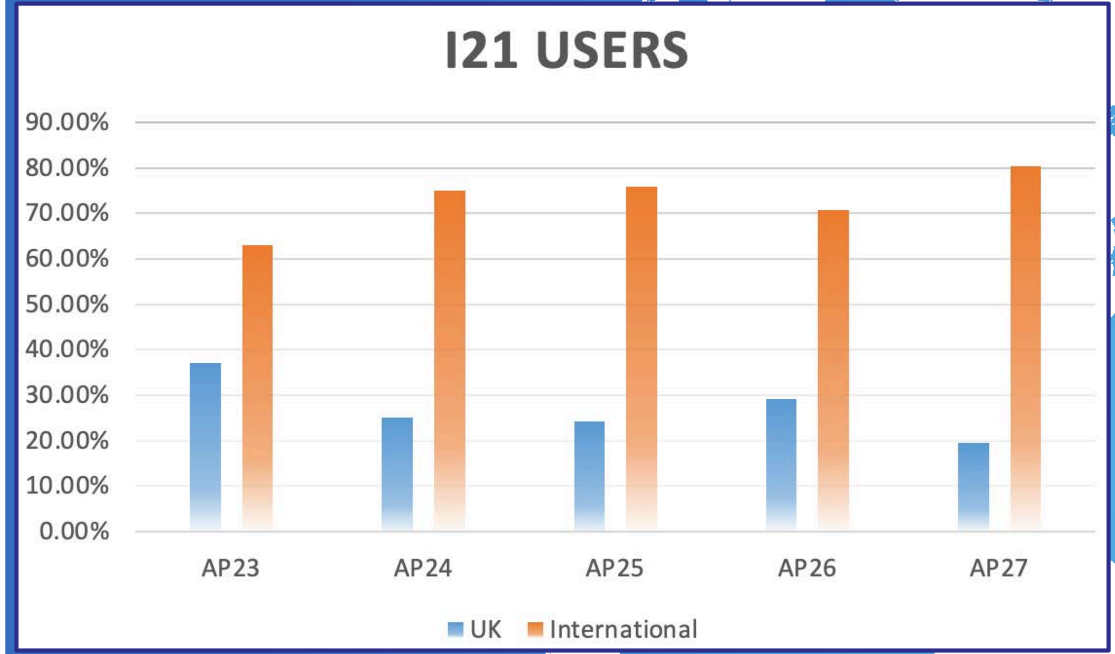
diamond

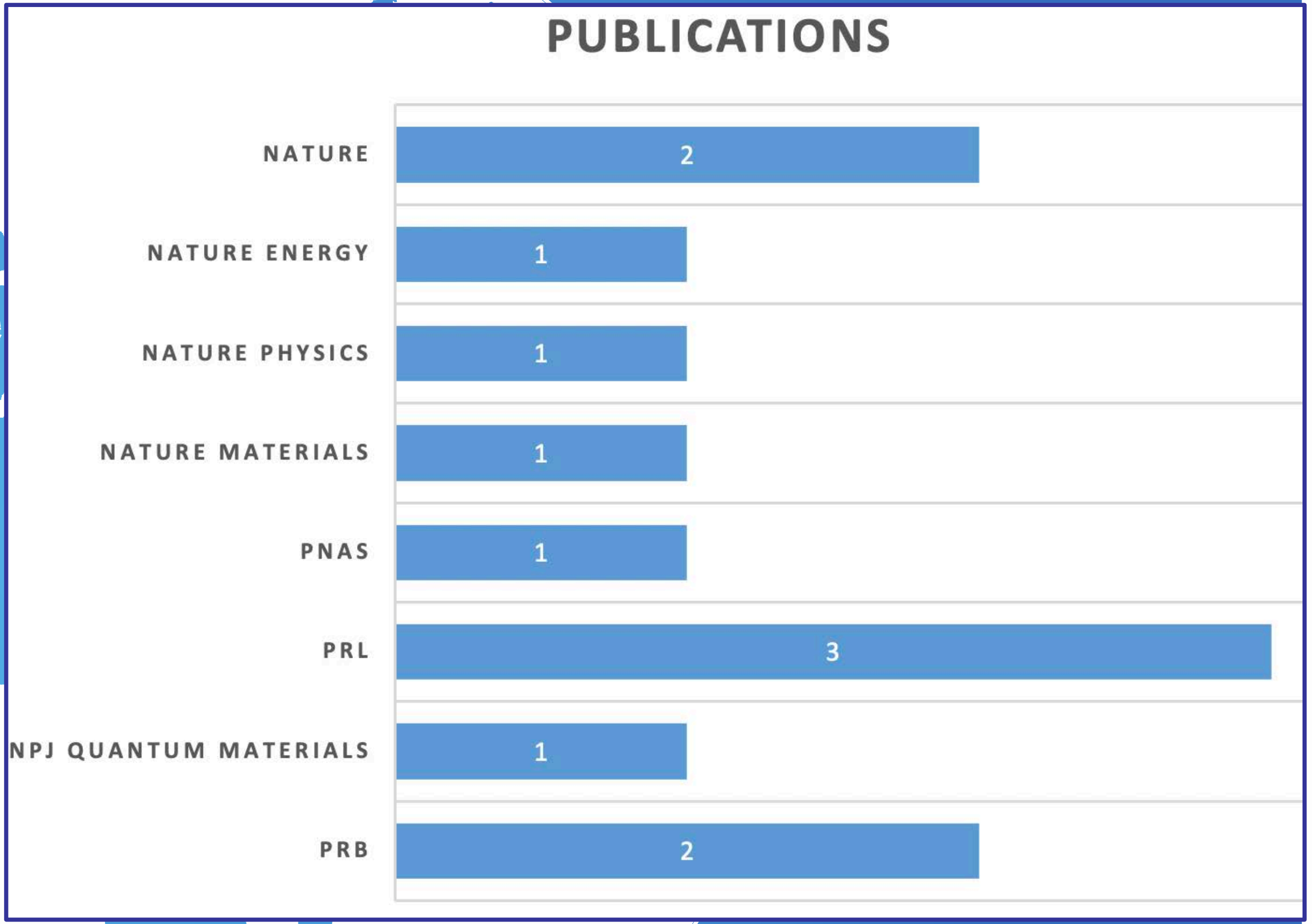
I21-RIXS beamline



- Dedicated soft X-ray RIXS beamline
- Plane VLS + spherical VLS RIXS spectrometer
- Energy range: 280 – 1500 eV (up to 3000 eV in 2021/2022)
- Beamline polarization: LH, LV, C+/C-
- Total energy resolution: ~ 35 meV at 930 eV, ~ 14 meV at 530 eV
- Focal beam size: 40 (H) × 2.5 (V) μm^2
- Sample environment: 6-axis manipulator, T = 8 – 380 K
- User operation: since Dec 2017

diamond


I21 USERS
90.00%
80.00%
70.00%
60.00%
50.00%
40.00%
30.00%
20.00%
10.00%
0.00%
AP23
AP24
AP25
AP26
AP27
UK
International


PUBLICATIONS
NATURE
2
NATURE ENERGY
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NATURE PHYSICS
1
NATURE MATERIALS
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PNAS
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PRL
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NPJ QUANTUM MATERIALS
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PRB
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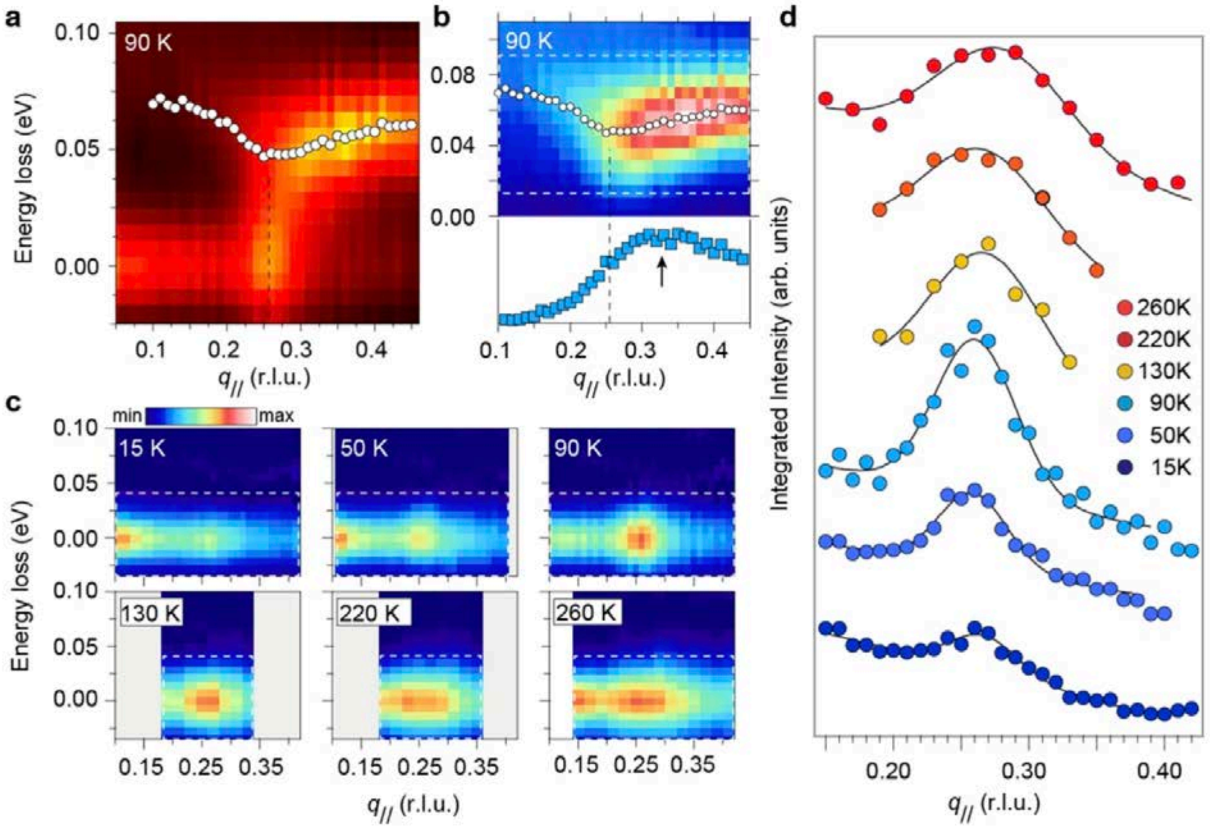
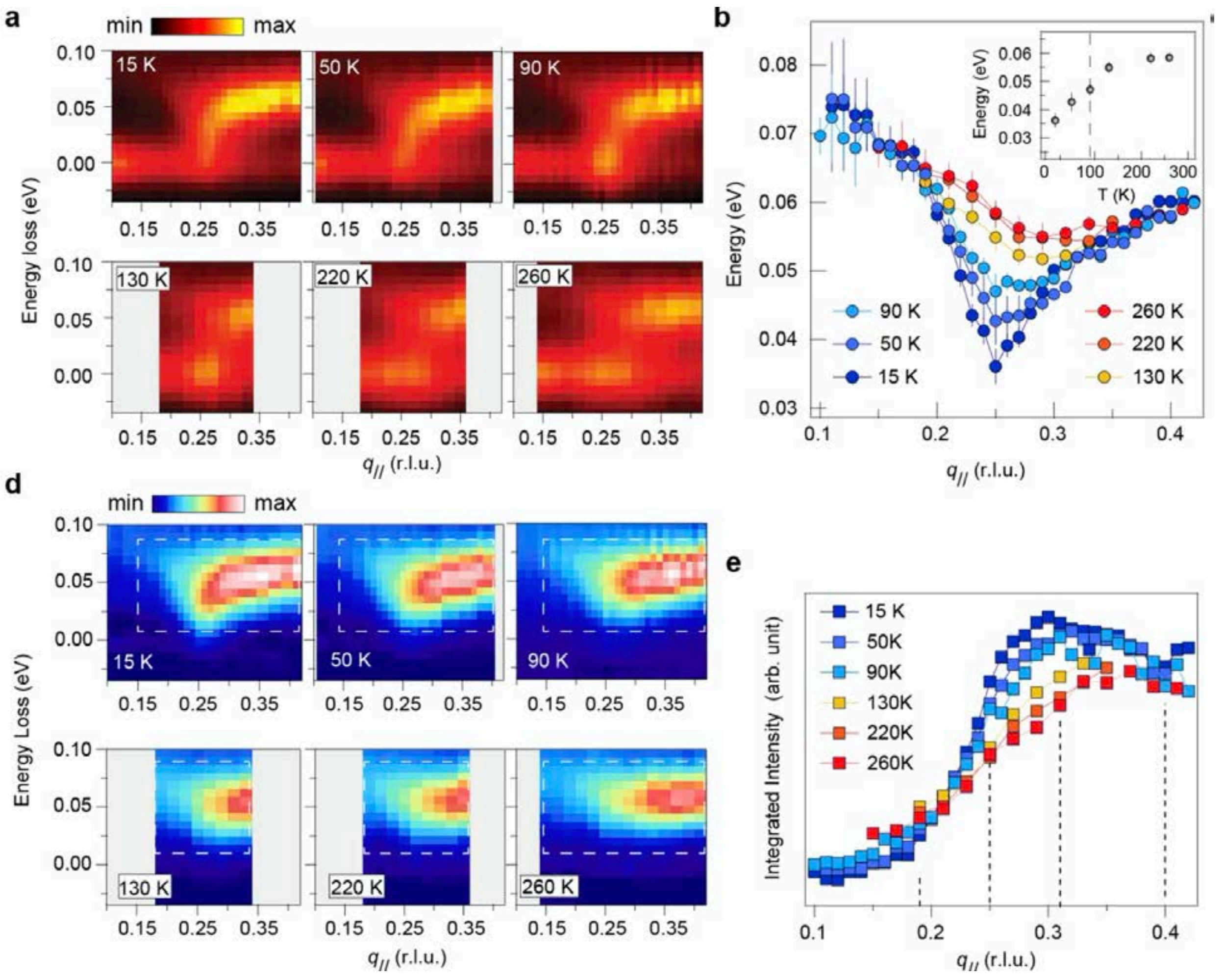
I21- Science cases

Superconductivity

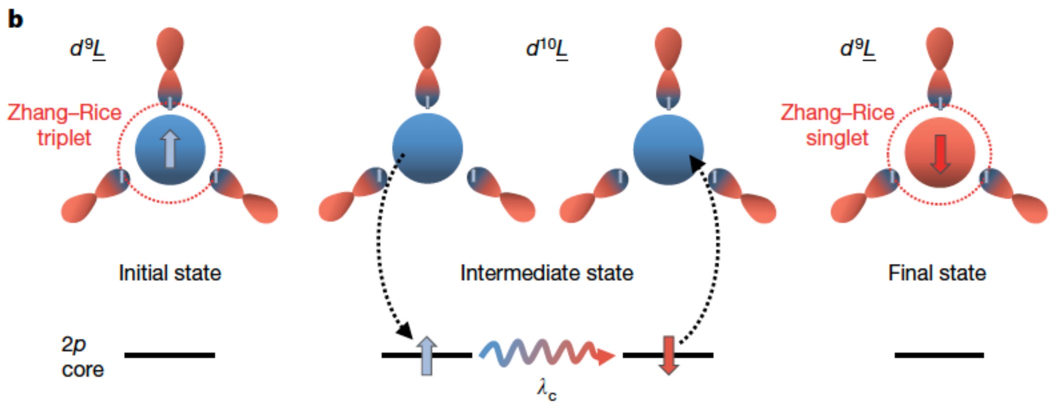
Charge order and quantum fluctuation in Bi2212 cuprate superconductors

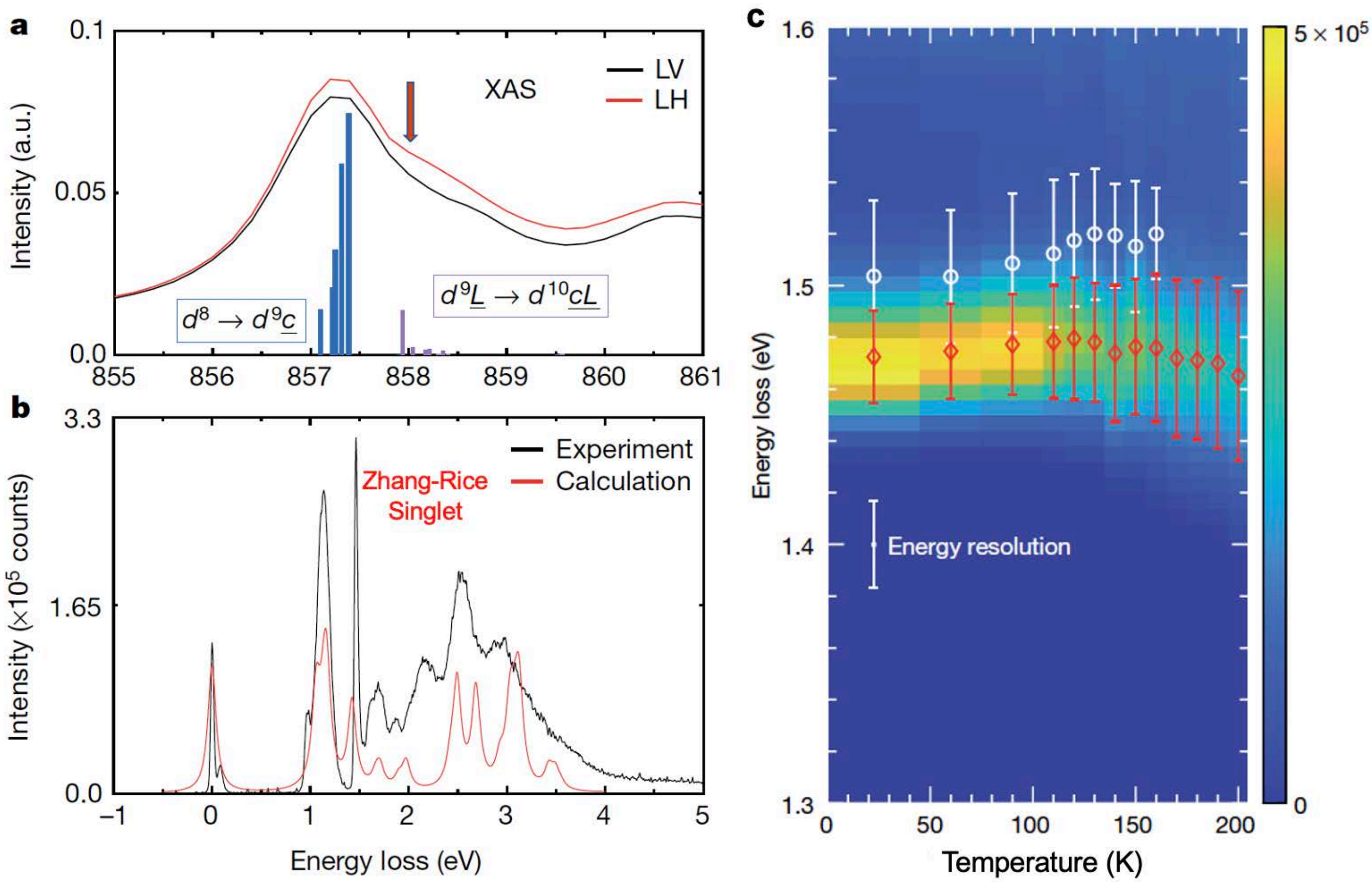




W. S. Lee *et al.* Nature Physics (2020)

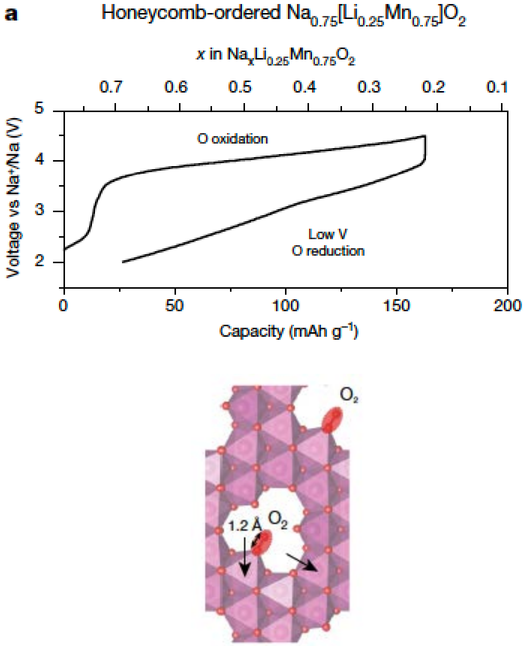
van der Waals antiferromagnet $NiPS_3$

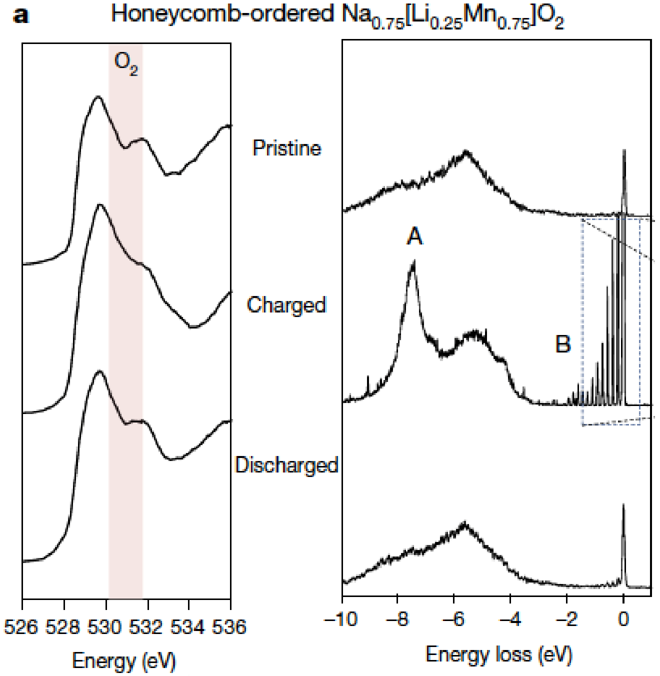


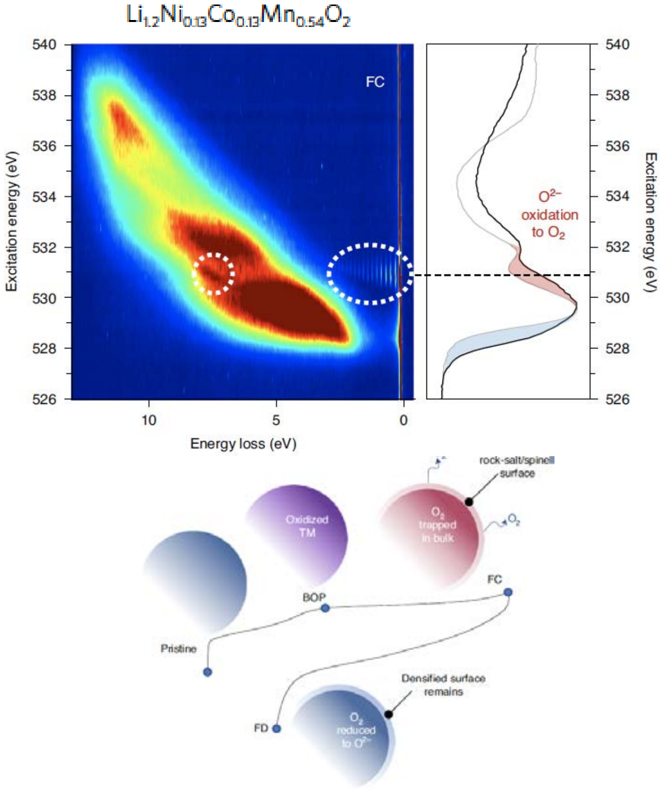


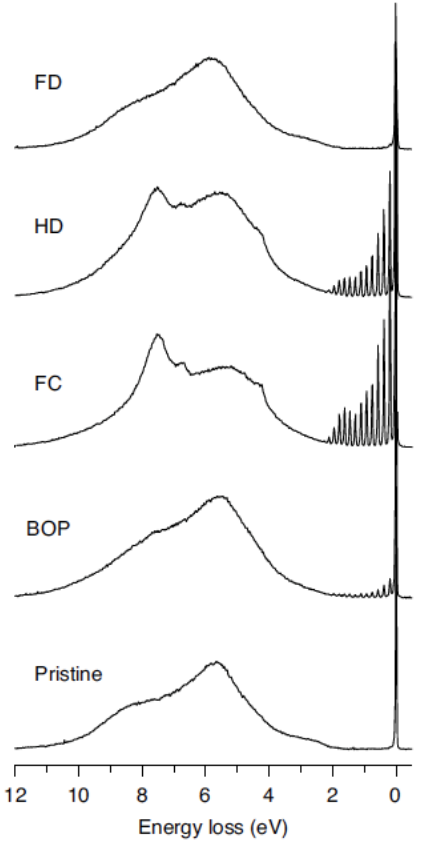
Soonmin Kang *et al.* Nature **583**, 785 (2020)

Oxygen-redox cathodes – Na^+ and Li^+ ion batteries





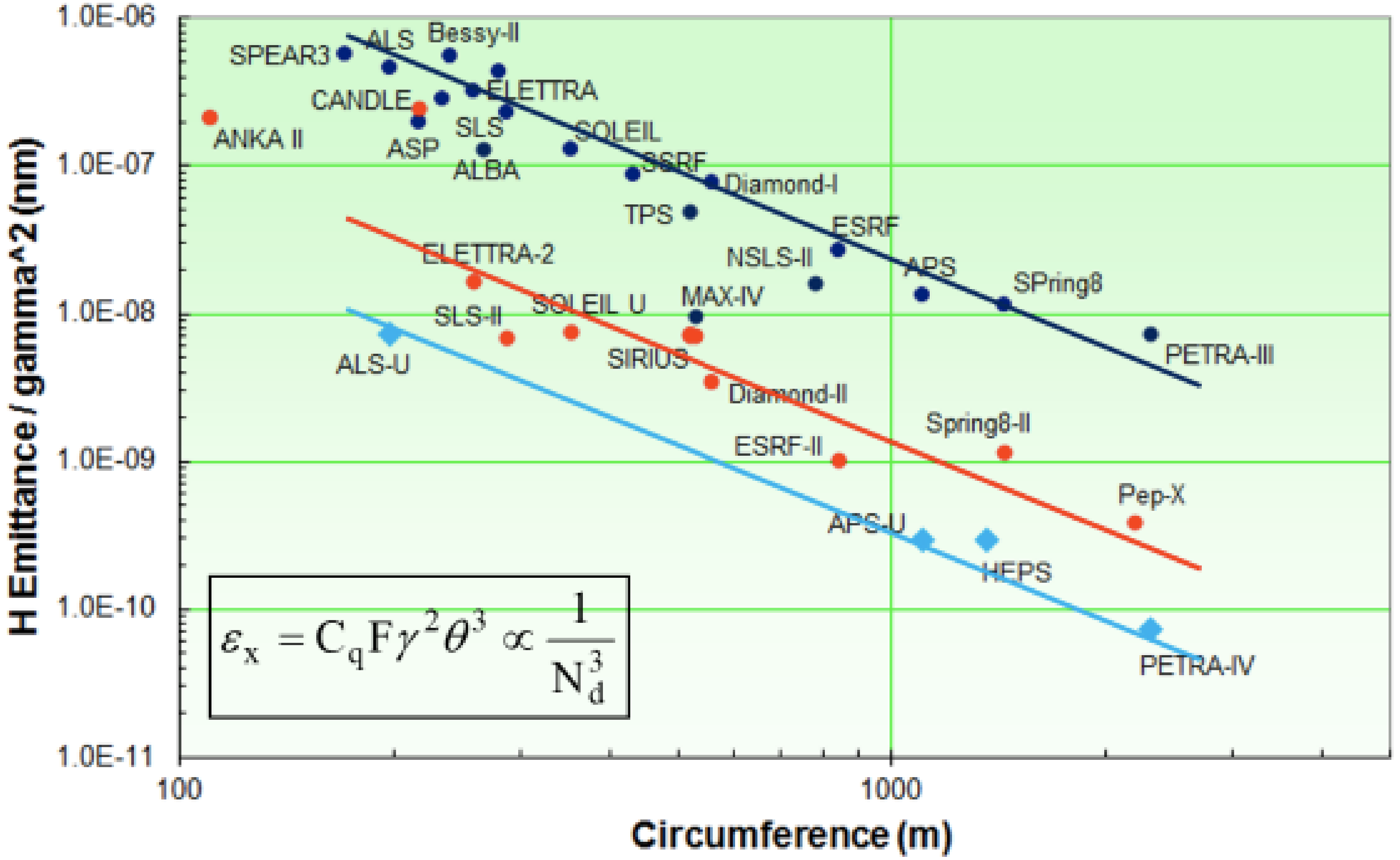




Robert A. House *et al.* Nature **577**, 502 (2020)

Robert A. House *et al.* Nature Energy (2020)

Diamond II upgrade



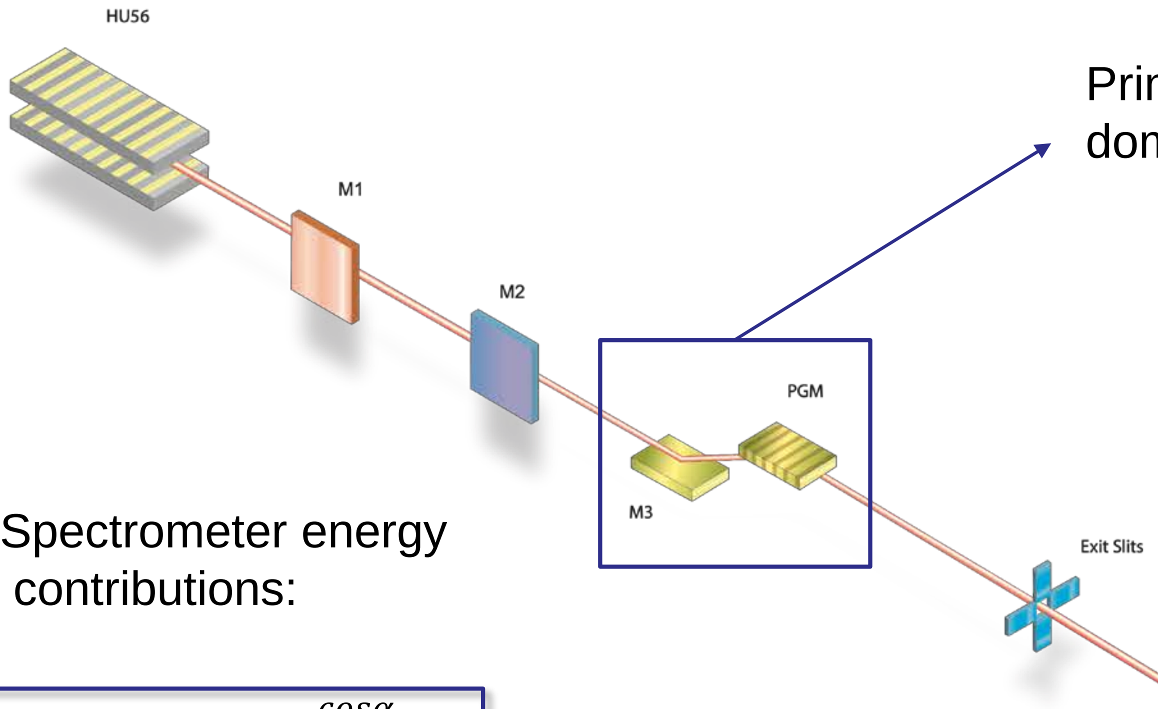
Energy: 3 → 3.5 GeV

Horizontal emittance: 2.7 nm rad → 146 (270) pm rad

I21- What needs to be improved?

- **Energy resolution**
- **Imaging RIXS**
- RIXS throughput
- User friendliness

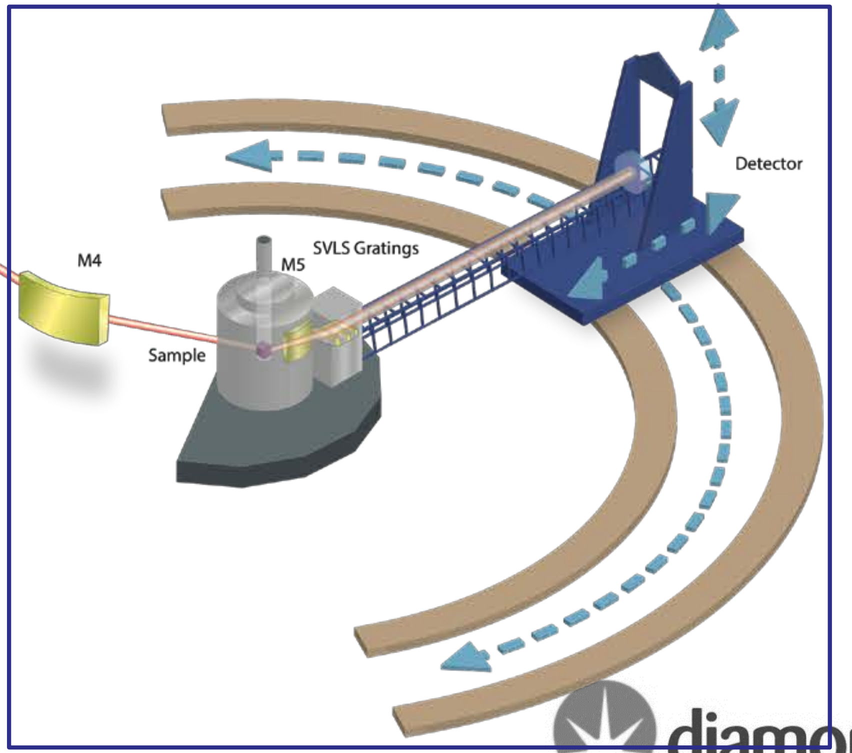
I21-RIXS beamline



Primary Beamline energy resolution:
dominated by PGM optics (effective) slope error

Secondary Spectrometer energy resolution's contributions:

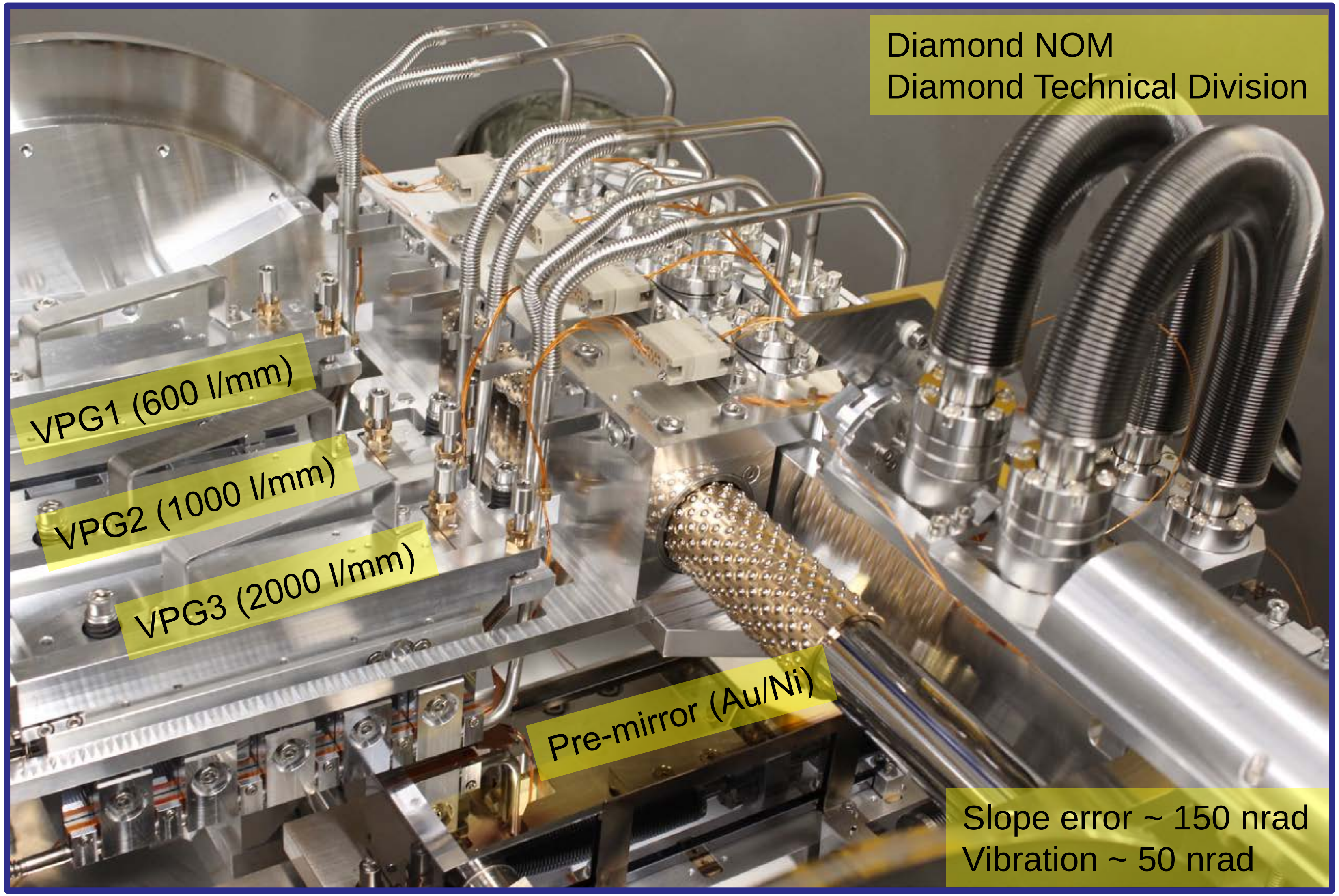
- Source size $\Delta E_s = \Delta_{vs} \frac{cos\alpha}{r_1 a_0 k\lambda} E$
- Grating slope error $\Delta E_{SE} = \Delta_{SE} \frac{cos\alpha + cos\beta}{a_0 k\lambda} E$
- Detector spatial resolution $\Delta E_D = \Delta_D sin\gamma \frac{cos\beta}{r_2 a_0 k\lambda} E$



I21-RIXS Primary Beamline energy resolution

- BL PGM optics slope error

(1) Replacement of VPG gratings
(2) Improvement of grating clamping
(3) Replacement of M3 mirror
(4) Improvement of PGM mechanics

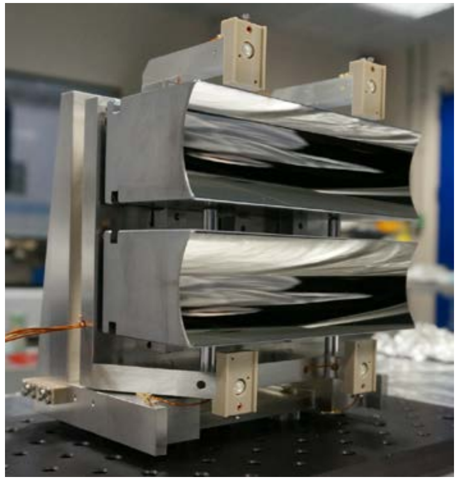


I21-RIXS Secondary Spectrometer energy resolution

- Source size $\Delta E_s = \Delta_{vs} \frac{\cos\alpha}{r_1 a_0 k\lambda} E$

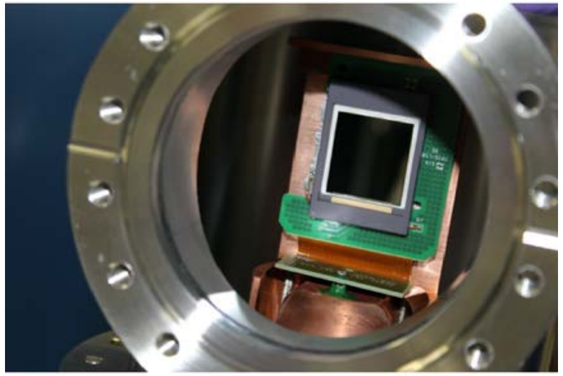
Improvement of the refocusing –
(1) replacement of M4 mirror

(2) Improvement by smaller horizontal emittance in Diamond-II



- Detector spatial resolution $\Delta E_D = \Delta_D \sin\gamma \frac{\cos\beta}{r_2 a_0 k\lambda} E$

(1) New detector with smaller spatial resolution

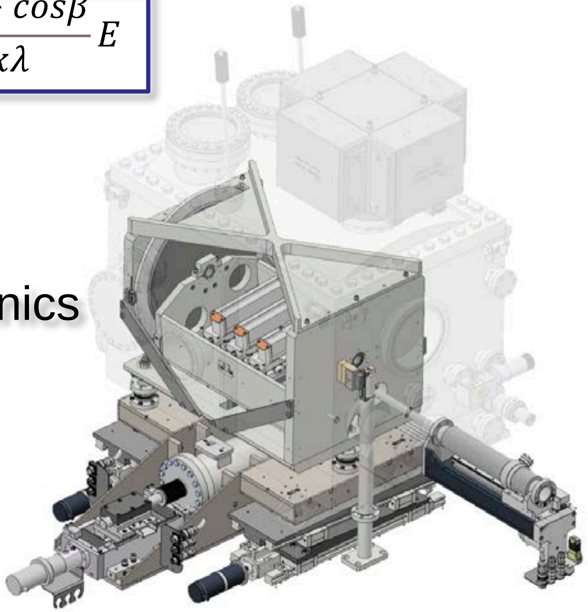


- Grating slope error $\Delta E_{SE} = \Delta_{SE} \frac{\cos\alpha + \cos\beta}{a_0 k\lambda} E$

Improvement of the SGM –

(1) Improvement of gratings / support

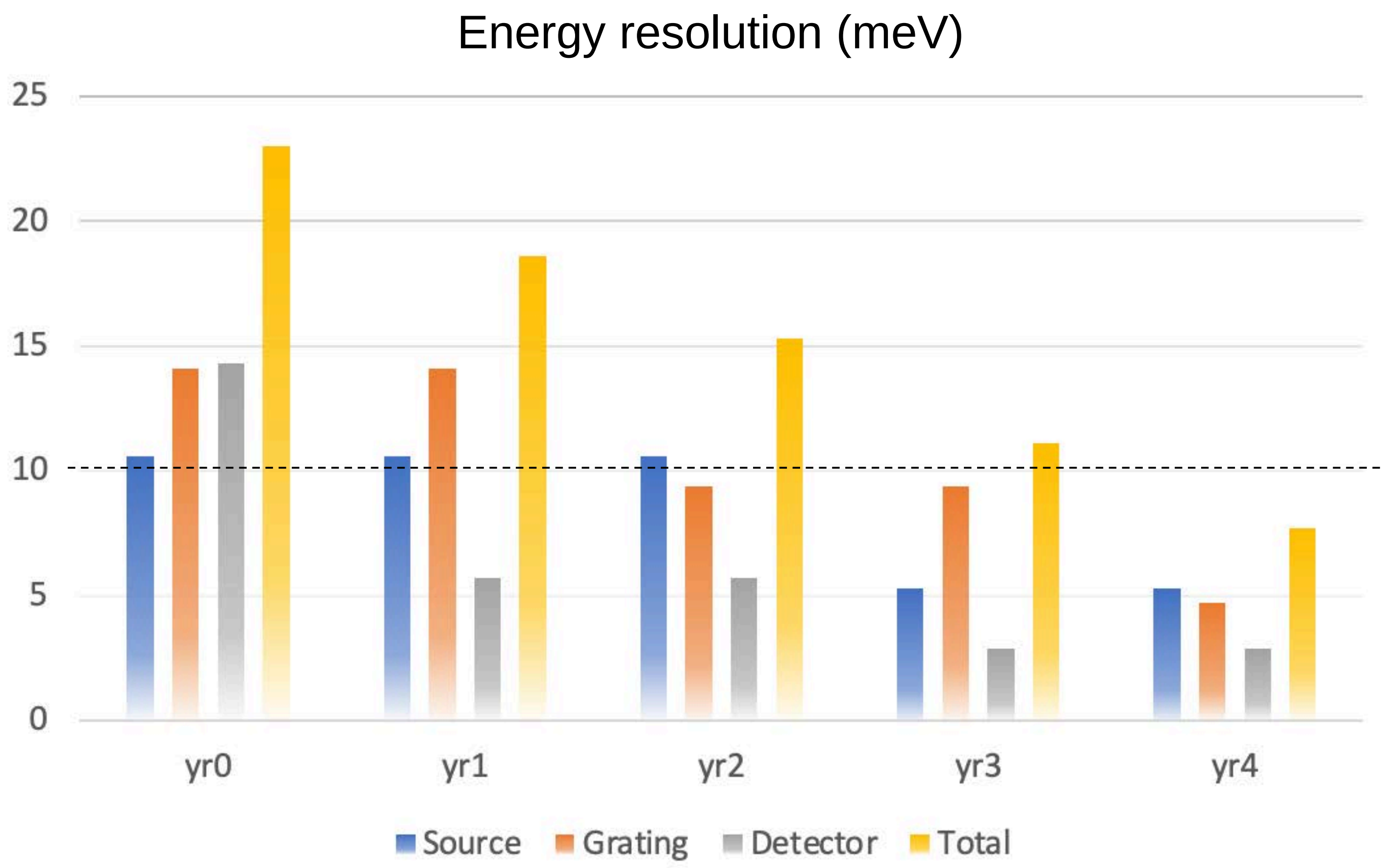
(2) Improvement by new SGM mechanics



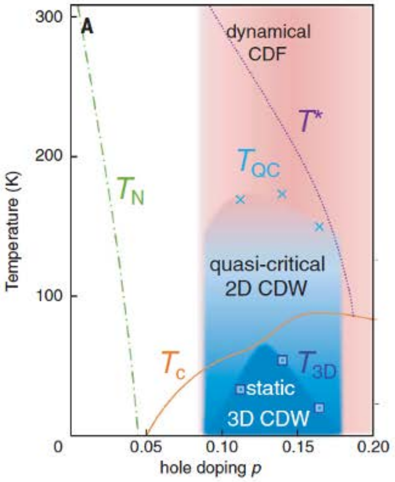
diamond

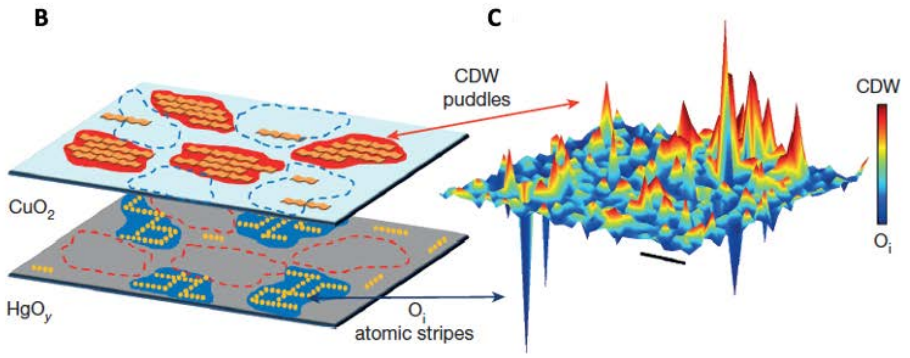
I21-RIXS Secondary Spectrometer energy resolution

- E = 1 keV, 2700 l/mm grating



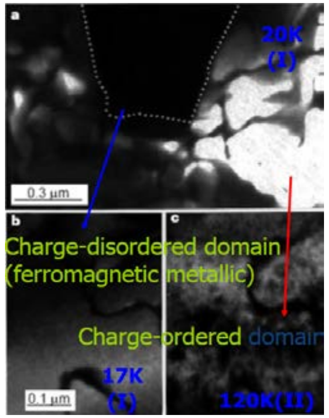
I21- Imaging RIXS



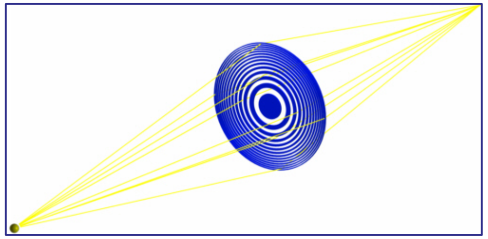


R. Arpaia *et al*., Science 365, 906 (2019)

G. Campi *et al*., Nature 525, 359 (2015)



M. Uehara, et al., Nature 399, 560 (1999)



Zone plate / capillary optics

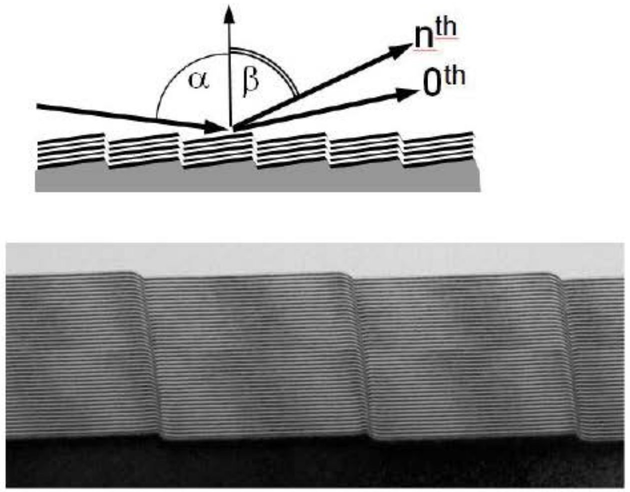
Designed spatial resolution: 0.5 (H) × 0.5 (V) μm^2

New capability/science – phase separation in quantum materials

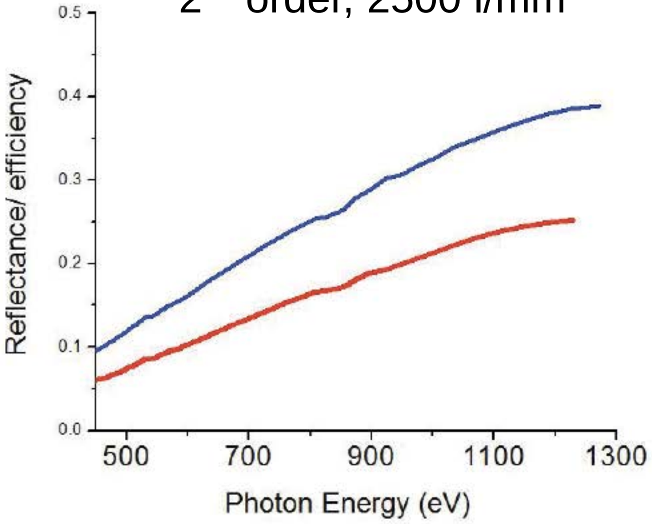
RIXS throughput

Multilayer gratings

Y.D. Chuang *et al*., AIP Conference Proc., 2016



2nd order, 2500 l/mm



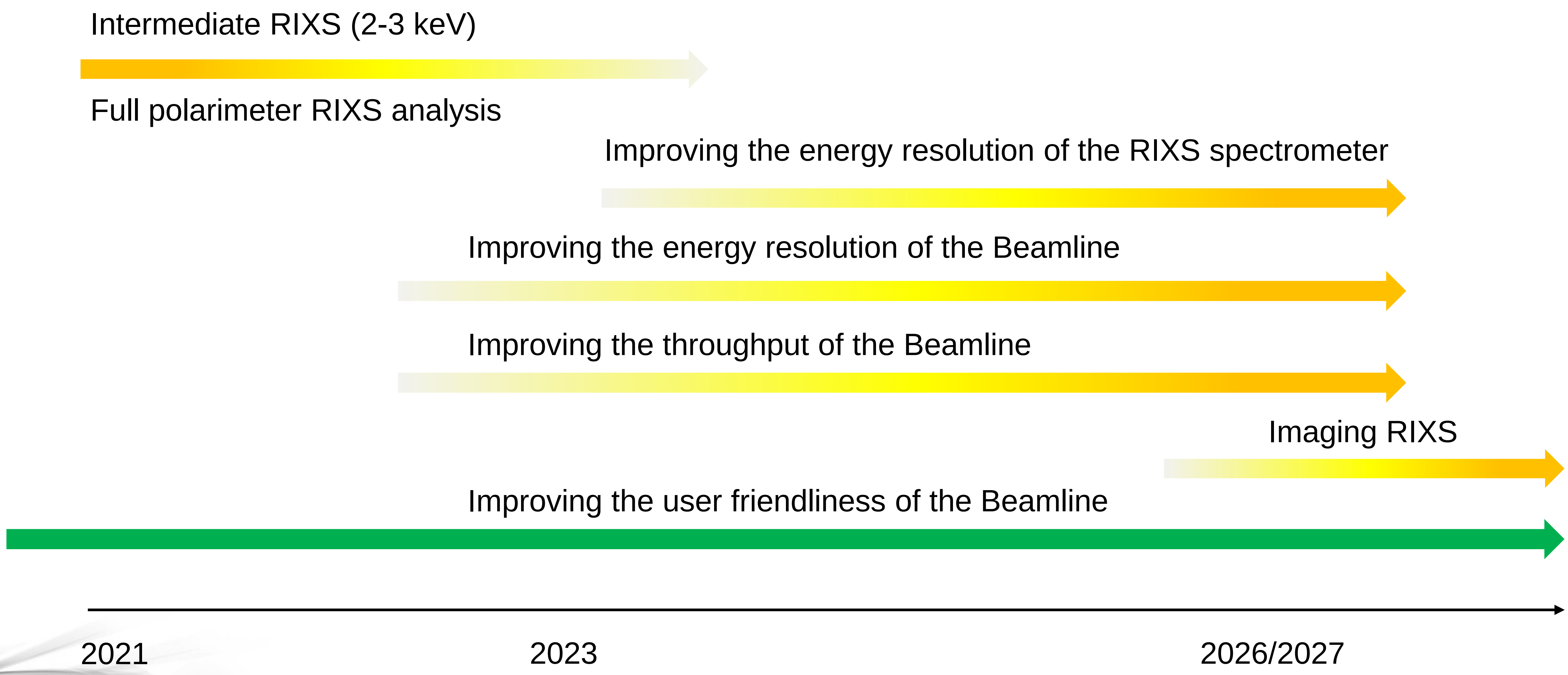
Multilayer grating may attain reflectivity of up to 50% without changing the current mechanics!

I21-RIXS Upgrade Specifications

Outline specification :

• Source:	APPLEII
• Energy range:	280 - 3000 eV;
• Energy resolving power (E/ΔE):	**5×10^4 - 1×10^5 @ 1000 eV**;
• Photon flux:	10^{11} - 10^{13} phs/s;
• Beam-size at sample (FWHM):	35 (H) × 1.0 (V) μm^2 – high-resolution RIXS
• Beam-size at sample (FWHM):	**0.5 (H) × 0.5 (V) μm^2 – Imaging RIXS**
• Sample manipulator:	cryo-cooled six-axes manipulator
• Sample environment:	low temperature, electric/magnetic field
• High-resolution RIXS throughput:	**approx. ×10 compared to the current**

I21-RIXS Upgrade Roadmap



diamond