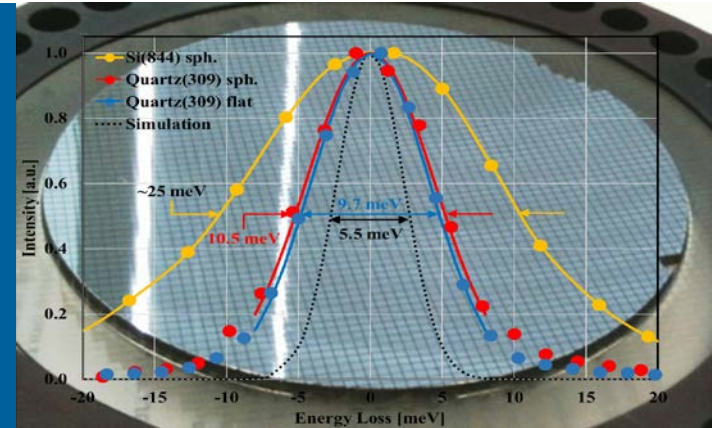


# New Developments in Inelastic X-ray Scattering at the Advanced Photon Source

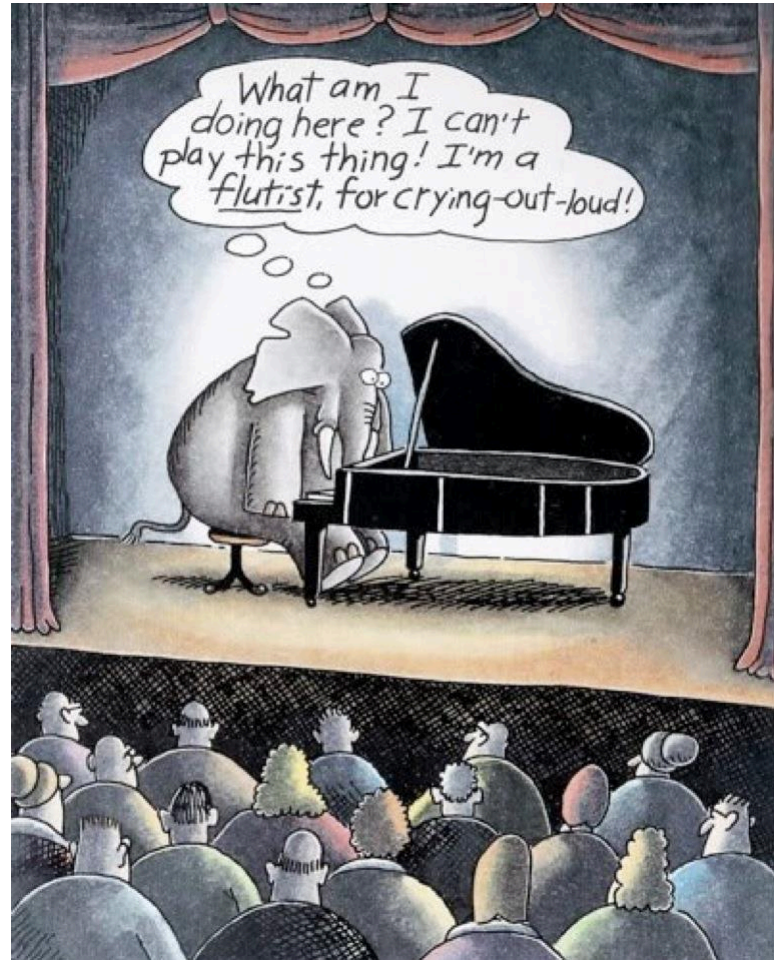
**THOMAS GOG**

On behalf of the Inelastic X-ray and  
Nuclear Resonant Scattering Group  
@ APS @ Argonne Nat'l Laboratory



IXS 2019  
June 28<sup>th</sup>, 2019

## The Elephant's Nightmare (Garry Larson)



## Progress in IXS Instrumentation, Theory, ...

(Spectrometers, Analyzer Systems, Detectors, Sample Environments, ...)



## Upgrade of Synchrotron Radiation Sources

(Conversion to Low-Emittance MBA Machines)

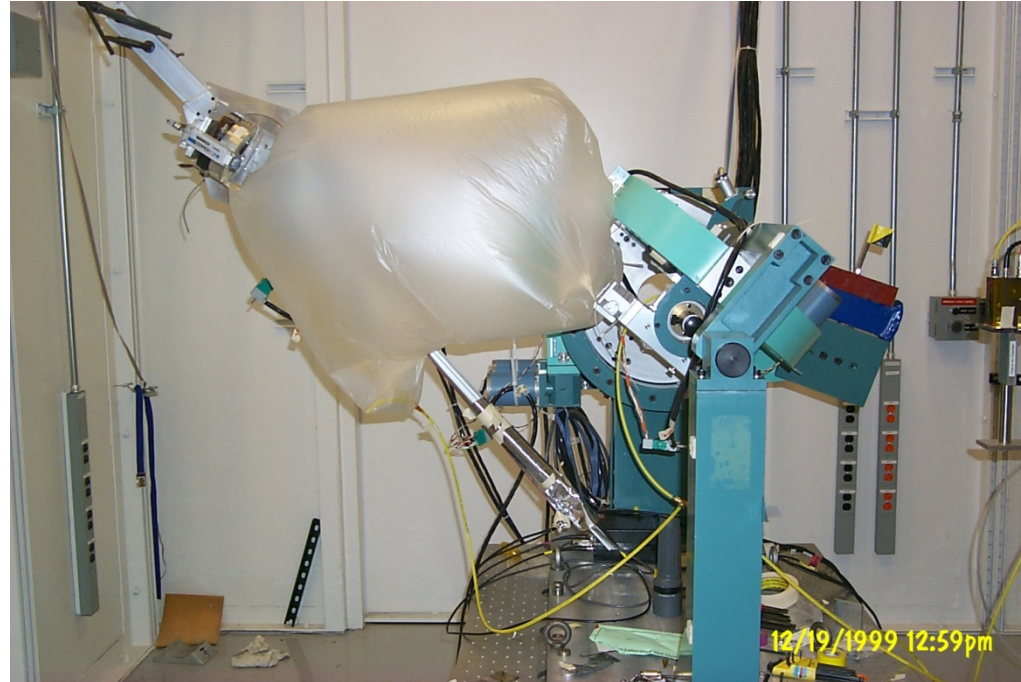


**New Opportunities for IXS Experimentation, Science at Synchrotrons**

# RIXS at the APS

**9-ID**

**1999**



# RIXS at the APS

**9-ID**

**2004**

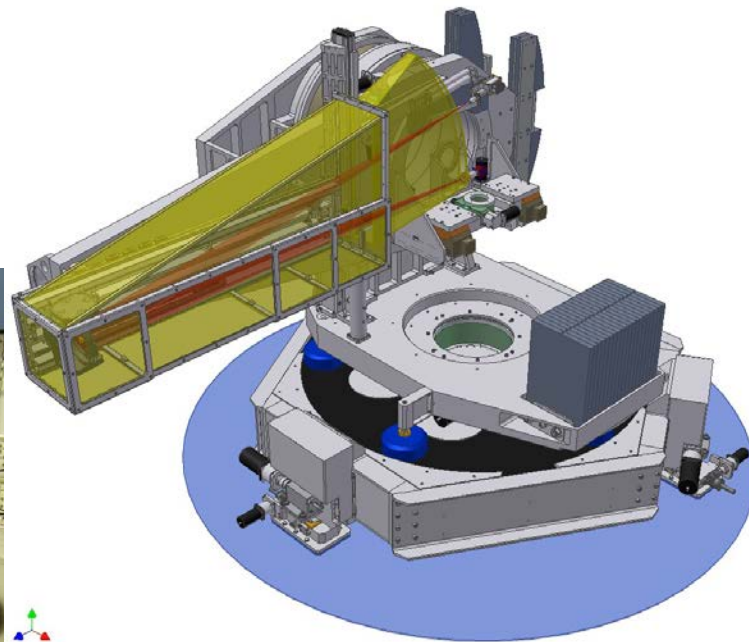
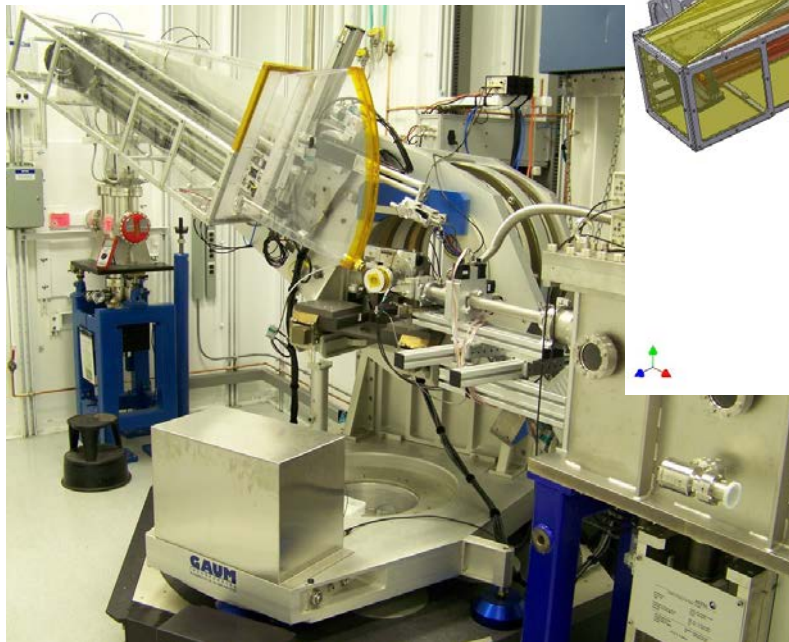




# RIXS at the APS

30-ID

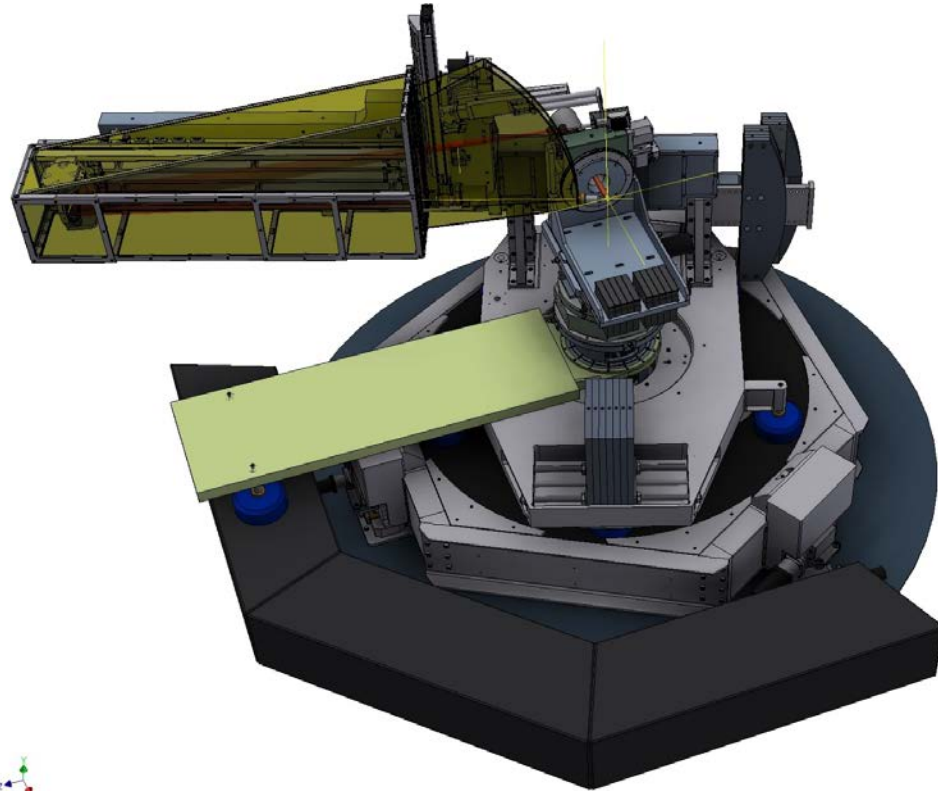
2007  
“MERIX”



# RIXS at the APS

27-ID

2020



## Progress in IXS Instrumentation, Theory, ...

(Spectrometers, Analyzer Systems, Detectors, Sample Environments, ...)



## Upgrade of Synchrotron Radiation Sources

(Conversion to Low-Emittance MBA Machines)



**New Opportunities for IXS Experimentation, Science at Synchrotrons**



# New Opportunities for IXS

- Polarization Analysis
- Imaging (of heterogeneous materials)
- Time-Resolved Measurements
- Improved Energy Resolution (in Resonant Techniques)
- Novel In situ Sample Environments
- ...

Progress in IXS Instrumentation, Theory, ...

(Spectrometers, Analyzer Systems, Detectors, Sample Environments, ...)



**Upgrade of Synchrotron Radiation Sources**

(Conversion to Low-Emittance MBA Machines)



New Opportunities for IXS Experimentation, Science at Synchrotrons

# World-wide MBA Low-Emittance Synchrotron Sources

**HEPS (China)** – Greenfield accelerator facility to be built near Beijing; planned completion in early 2020s

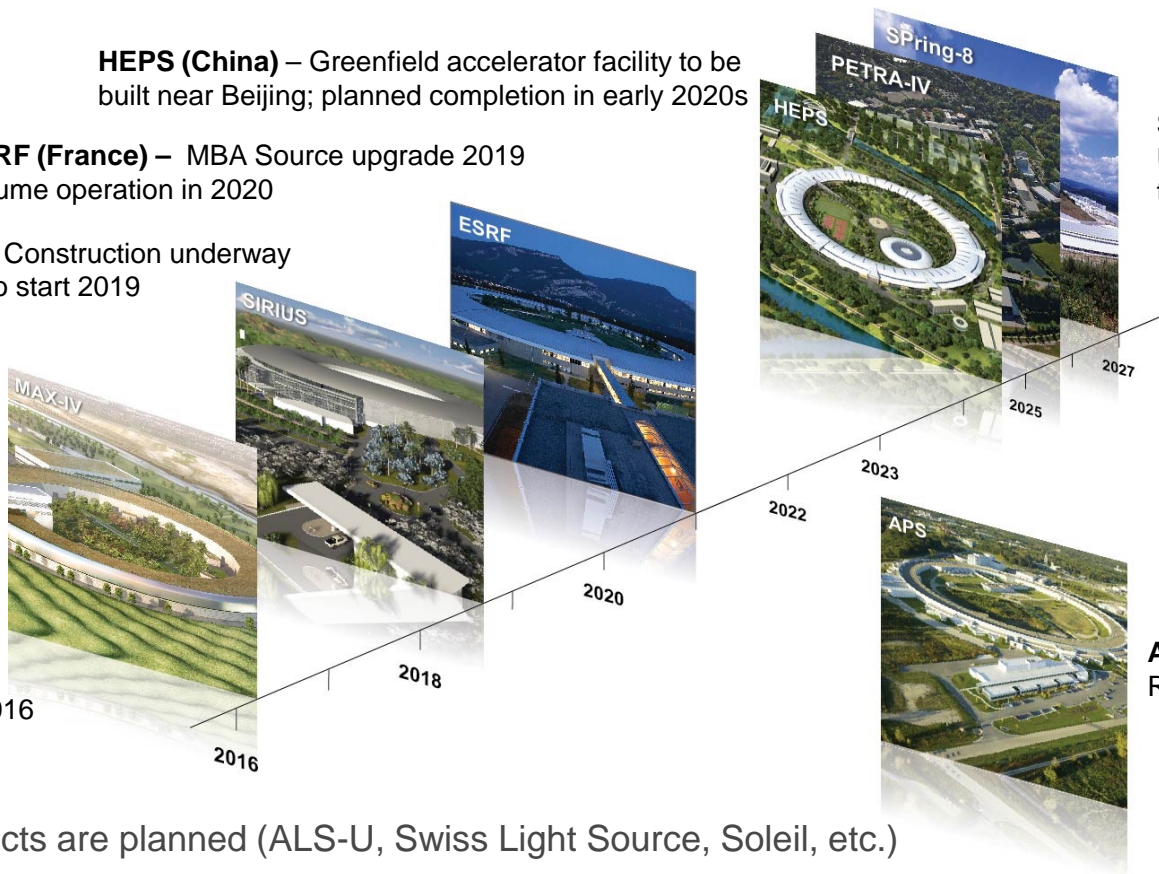
**ESRF (France)** – MBA Source upgrade 2019  
resume operation in 2020

**SIRIUS (Brazil)** – Construction underway  
Commissioning to start 2019

**MAX-IV (Sweden)**  
Inauguration June 2016  
in operation

**SPring-8 (Japan)** –  
Upgrading in 2027  
timeframe

**APS-U** – Upgrade 2022  
Resume operation in 2023

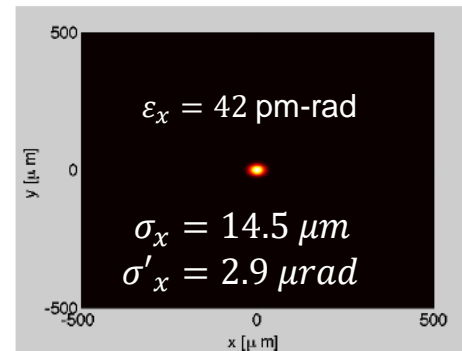
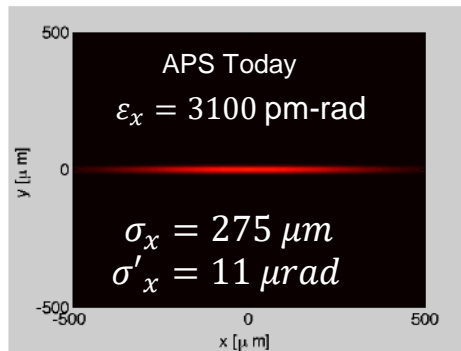


Many other projects are planned (ALS-U, Swiss Light Source, Soleil, etc.)

# APS - Upgrade

- Dramatically improved Brilliance (Flux / (Area  $\times$  Solid Angle) )  
(... mostly through reduction of horizontal emittance)

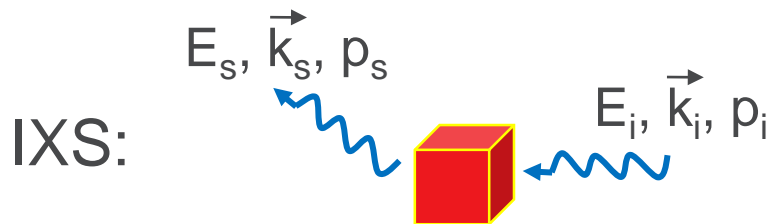
## Electron Beam at APS



- Double the Ring Current to 200 mA
- Improved Focusing, Smaller (sub- $\mu\text{m}$ -, nm-) beams
- Improved Coherence (IXS?)

# New Opportunities for IXS

- Polarization Analysis
- Imaging (of
- Time-Resolved Me
- Improved Energy
- Novel In situ



polarization largely ignored in the past  
(... hard to do experimentally)

## Sources of (variable) Polarization

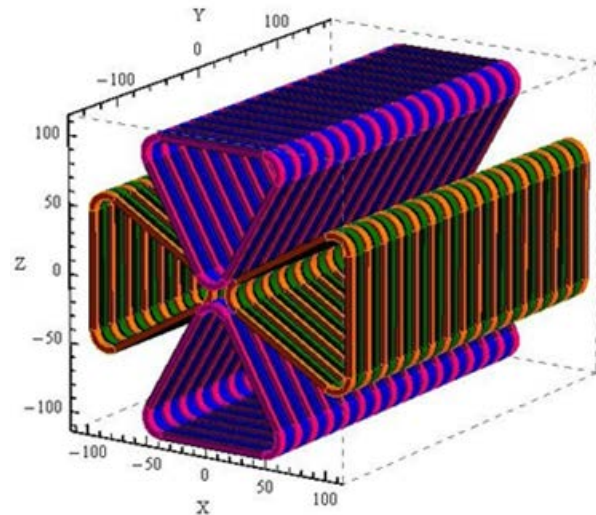
- Phase Plates (low efficiency, low polarization purity)
- Special Insertion Devices (availability)



# New Undulator Concepts: SCAPE (Yuri Ivanyushenkov, APS)

(Superconducting Arbitrarily Polarizing Emitter)

- Would like Undulator capable of generating linear and circular polarized photons
- Electromagnetic, superconducting undulator with four planar, magnetic cores, assembled around a cylindrical beam vacuum chamber
- APS Upgrade MBA-lattice enables cylindrical vacuum chambers with 6 mm ID
- Prototype successfully tested

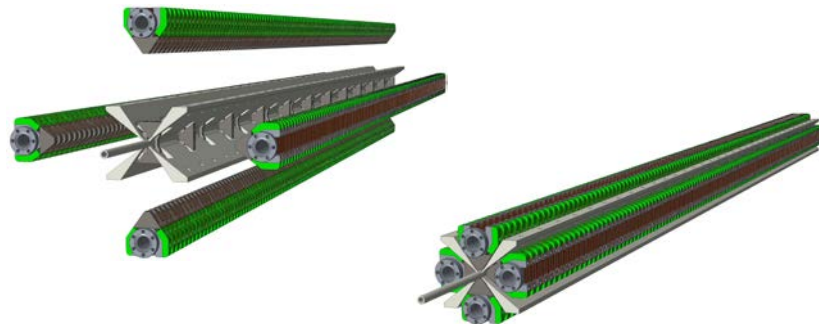


Concept of SCAPE: a universal SCU with four planar superconducting coil structures. A beam chamber is not shown.

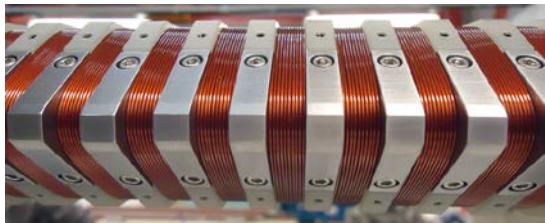
# SCAPE PROTOTYPE TEST

- SCAPE 0.5-m long prototype magnet is built:
  - period length – 30 mm
  - magnetic gap – 10 mm
- The prototype has been successfully tested in a LHe bath cryostat equipped with a movable Hall probe.

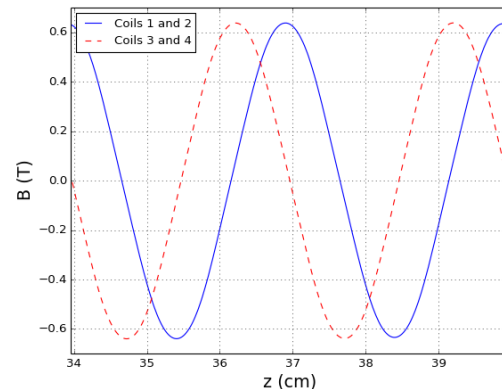
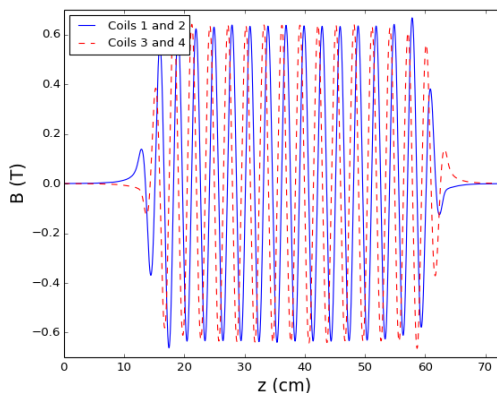
SCAPE design model



SCAPE prototype mechanical structure and a single core



Measured field profiles



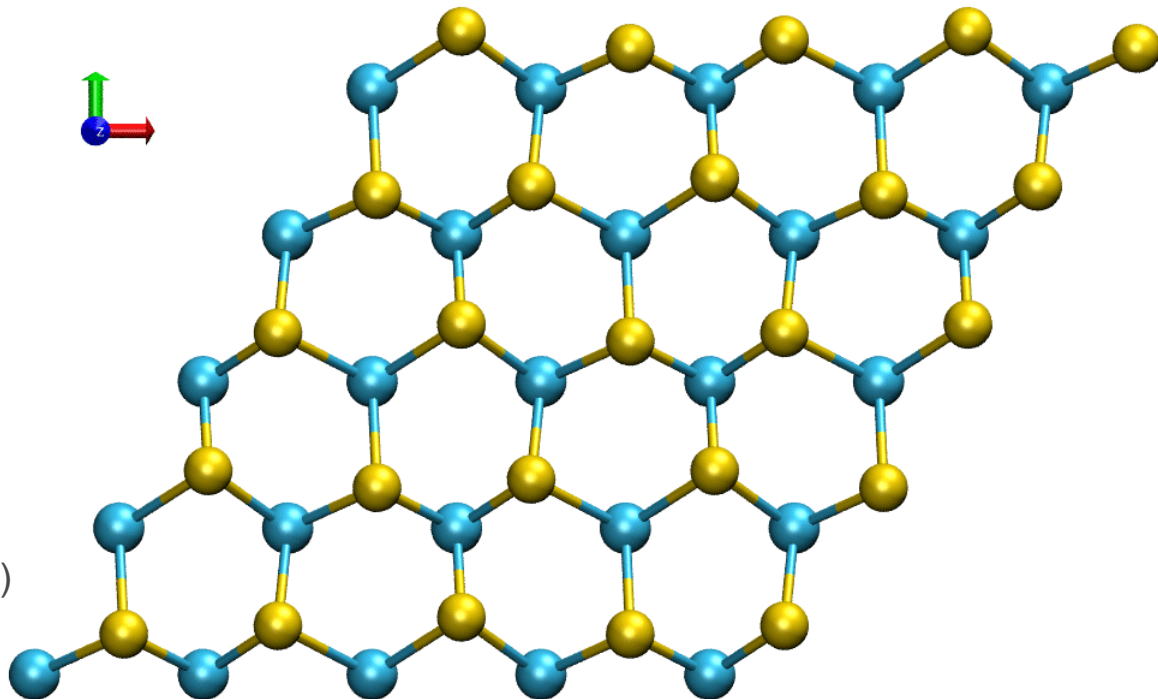
# Why Polarization ?

Phonons can carry angular momentum:

## CHIRAL PHONONS

(in materials with  
broken inversion  
Symmetry)

Chiral Phonon in  
Mono-layer of  $\text{WSe}_2$   
From: Hanyu Zhu et al.,  
Science **359**, 579 (2018)



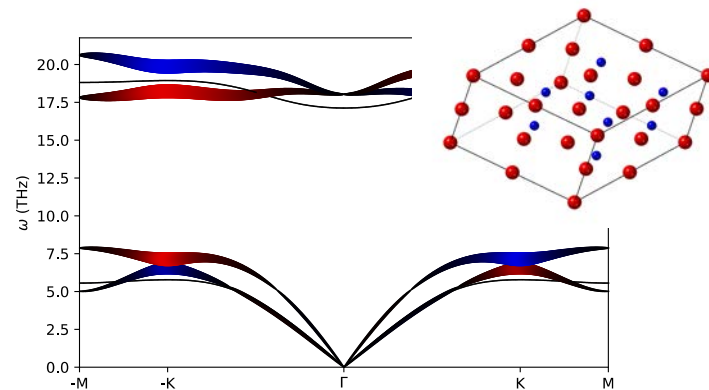
# PROBING PHONONS WITH ANGULAR MOMENTUM BY IXS (HERIX@30-ID, Chen Li, UCR)

- WC lacks space inversion symmetry

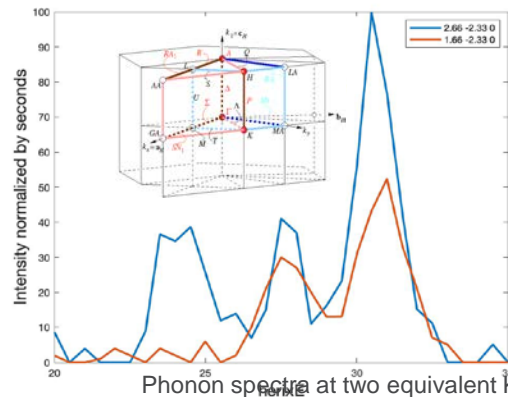
➡ may exhibit chiral phonons

Scientific questions:

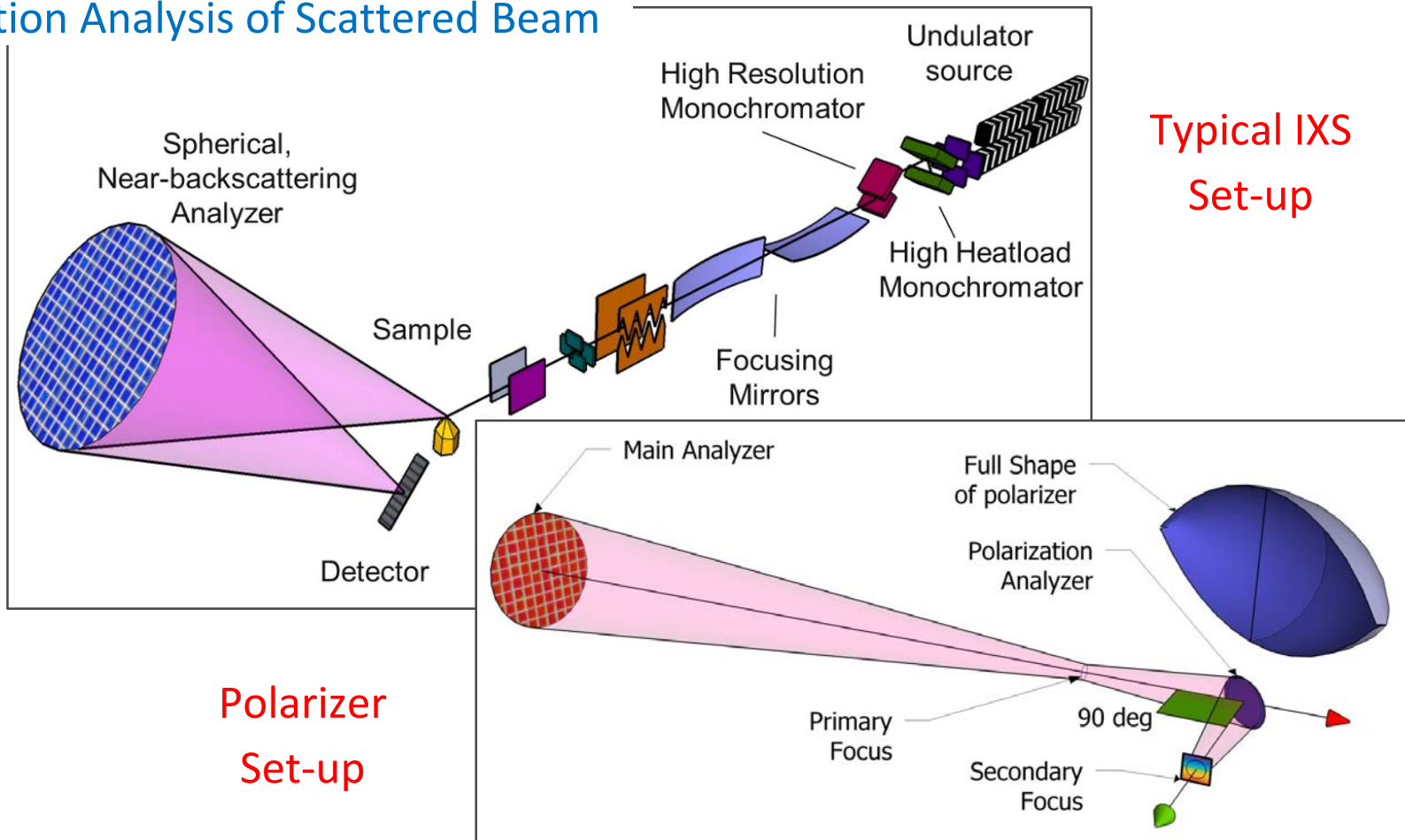
- Is it possible to identify chiral phonons by meV-IXS, using circular- or linear-polarized X-ray?
- Are the rules governing the scattering different?
- How do such chiral phonons contribute to the thermal and transport properties in materials with broken inversion symmetry?
  - Phonon-phonon scattering and phonon lifetime
  - Spin-phonon and electron-phonon interactions



First-principle phonon dispersion calculation of WC (structure in insert). The linewidth indicates the angular momentum of phonons. Blue: right-handed; red: left-handed.



# Polarization Analysis of Scattered Beam





# Polarization Analysis of Scattered Beam

PHYSICAL REVIEW B 83, 241101(R) (2011)



## Polarization-analyzed resonant inelastic x-ray scattering of the orbital excitations in $\text{KCuF}_3$

K. Ishii,<sup>1</sup> S. Ishihara,<sup>2,3</sup> Y. Murakami,<sup>1,2,4</sup> K. Ikeuchi,<sup>1,4</sup> K. Kuzushita,<sup>1</sup> T. Inami,<sup>1</sup> K. Ohwada,<sup>1</sup> M. Yoshida,<sup>1</sup> I. Jarrige,<sup>1</sup> N. Tatami,<sup>2</sup> S. Niioka,<sup>2</sup> D. Bizen,<sup>2</sup> Y. Ando,<sup>2</sup> J. Mizuki,<sup>1</sup> S. Maekawa,<sup>3,5</sup> and Y. Endoh<sup>1,6</sup>

<sup>1</sup>Spring-8, Japan Atomic Energy Agency, Hyogo 679-5148, Japan

<sup>2</sup>Department of Physics, Tohoku University, Sendai 980-8578, Japan

<sup>3</sup>CREST, Japan Science and Technology Agency (JST), Tokyo 102-0075, Japan

<sup>4</sup>Photon Factory / Condensed Matter Research Center, Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), Tsukuba 305-0801, Japan

<sup>5</sup>Advanced Science Research Center, Japan Atomic Energy Agency, Tokai 319-1195, Japan

<sup>6</sup>International Institute for Advanced Studies, Kizu, Kyoto 619-0025, Japan

(Received 18 May 2011; published 16 June 2011)

Spherical Analyzer + Flat HOPG crystal

HOPG reflectivity  $\sim 2\%$

Energy Resolution: 400...600 meV

Could distinguish orbital excitations between

$$e_g \Rightarrow e_g \text{ and } t_{2g} \Rightarrow e_g$$

Spherical Analyzer + Sculptured HOPG crystal

HOPG reflectivity  $\sim 6\%$

Energy Resolution:  $\sim 200$  meV

Preliminary measurements on  $\text{CuGeO}_3$

## Development of a graphite polarization analyzer for resonant inelastic x-ray scattering

Cite as: Rev. Sci. Instrum. **82**, 113108 (2011); <https://doi.org/10.1063/1.3662472>

Submitted: 07 September 2011 . Accepted: 30 October 2011 . Published Online: 23 November 2011

Xuan Gao, Clement Burns, Diego Casa, Mary Upton, Thomas Gog, Jungho Kim, and Chengyang Li







# Polarization Analysis of Scattered Beam (soft x-ray)

## The simultaneous measurement of energy and linear polarization of the scattered radiation in resonant inelastic soft x-ray scattering

Cite as: Rev. Sci. Instrum. **85**, 115104 (2014); <https://doi.org/10.1063/1.4900959>

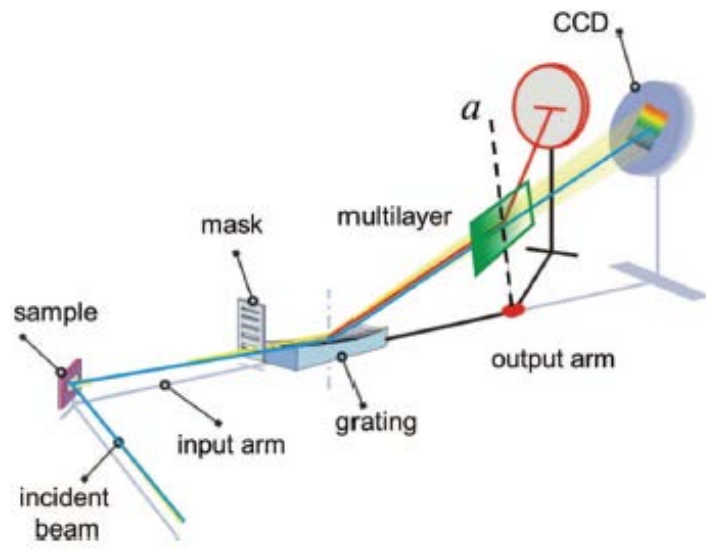
Submitted: 09 September 2014 . Accepted: 22 October 2014 . Published Online: 11 November 2014

L. Braicovich, M. Minola, G. Dellea , M. Le Tacon, M. Moretti Sala, C. Morawe, J.-Ch. Peffen, R. Supruangnet , F. Yakhou, G. Chiringhelli , and N. B. Brookes 

Graded, parabolic W/B<sub>4</sub>C multilayer mirror as polarizer

underdoped YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6.6</sub>

Energy Resolution: ~200 meV



## Interlude: Flat Crystal Optics

- Striving for greatly improved energy resolution ( $\approx < 5\text{meV}$ )
- Flat crystal optics:
  - Additional variable: crystal asymmetry, no figure errors
  - Opportunity for polarization analysis

**BUT: Very little** Solid-Angle Acceptance

Ø25mm Sph. Analyzer at 2m:  $\Omega \approx 100 \mu\text{sr}$

Flat X-tal  $20 \times 100 \mu\text{rad}^2$ :  $\Omega \approx 0.002 \mu\text{sr}$

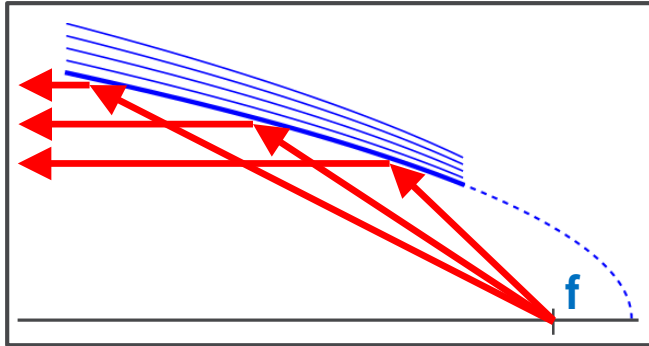


**Need Collimator to bridge the gap**

## Interlude: Flat Crystal Optics

Honnicke et al., J. Synchr. Rad.  
**18**, 862 (2011)  
Mundboth et al., J. Synchr. Rad.  
**21**, 16 (2014)

### Parabolic, laterally graded multi-layer mirror

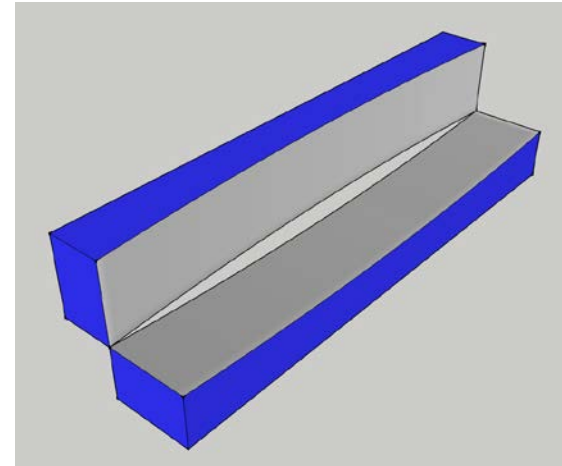


Angular Acceptance:  $10 \times 10 \text{ mrad}^2$

$$\Rightarrow W \approx 100 \text{ } \mu\text{rad}$$

Angular Emittance:  $100 \times 100 \text{ } \mu\text{rad}^2$

Manufacturer: Incoatec GmbH



Multi-layer: Ruthenium / Carbon

Substrate: Si(100)

Dimension  $150 \times 7 \times 7 \text{ mm}^3$

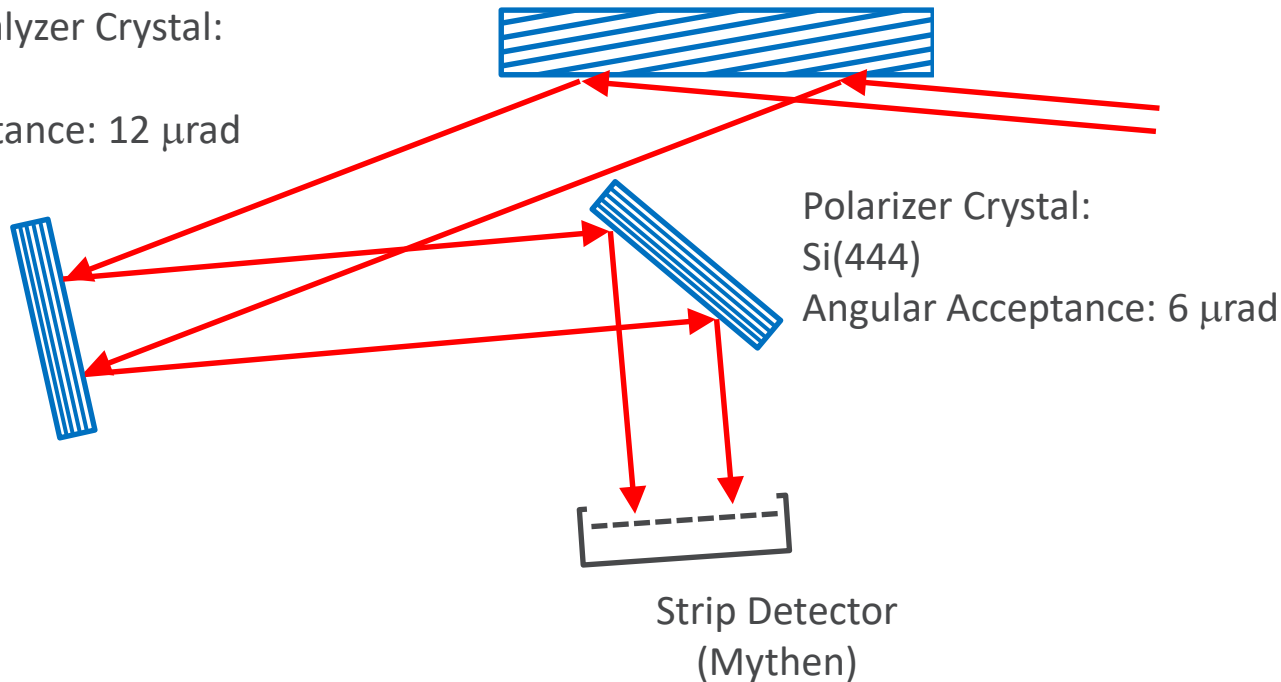
Focal distance: 200 mm

Reflectivity:  $> 80 \%$

# Flat Crystal Analyzer with Polarizer

Asymmetric Collimator Crystal:  
Si(111),  $b=-0.064$   
Angular Acceptance:  $95\text{ }\mu\text{rad}$   
Angular Emission:  $6\text{ }\mu\text{rad}$

Symmetric Analyzer Crystal:  
Quartz(309)  
Angular Acceptance:  $12\text{ }\mu\text{rad}$

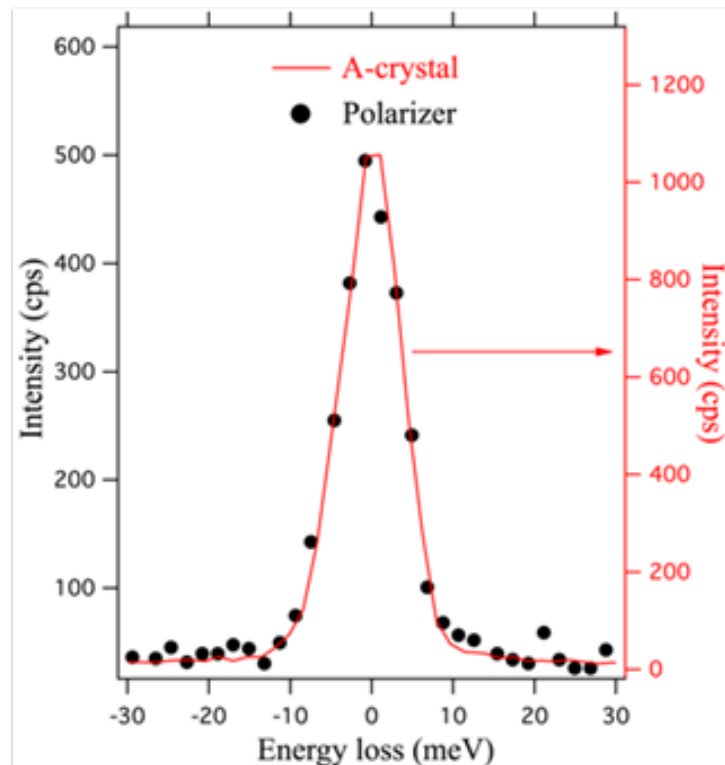




# Flat Crystal Analyzer with Polarizer

Elastic spectra w/ and w/o polarizer:

- No loss in resolution
- ~50 % throughput
- ~80 % w/ asymmetric polarizer crystal



## Resonant Inelastic X-Ray Scattering Response of the Kitaev Honeycomb Model

Gábor B. Halász,<sup>1</sup> Natalia B. Perkins,<sup>2</sup> and Jeroen van den Brink<sup>3,4</sup>

<sup>1</sup>Kayli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA

<sup>2</sup>School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55116, USA

<sup>3</sup>IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany

<sup>4</sup>Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

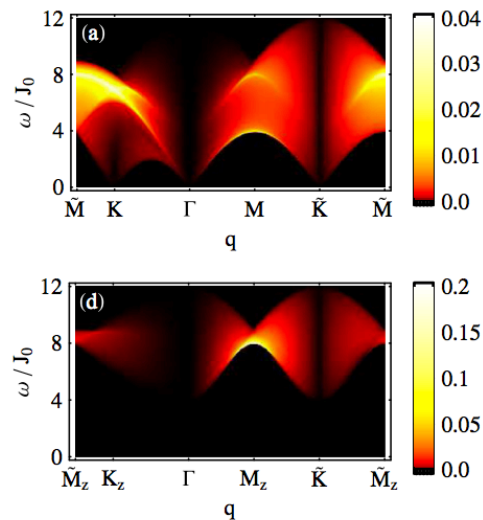
(Received 10 May 2016; published 16 September 2016)

We calculate the resonant inelastic x-ray scattering (RIXS) response of the **Kitaev honeycomb model**, an exactly solvable quantum-spin-liquid model with fractionalized Majorana and flux excitations. We find that the fundamental RIXS channels, **the spin-conserving (SC)** and the **non-spin-conserving (NSC)** ones, do not interfere and give completely different responses. SC RIXS picks up exclusively the Majorana sector with a pronounced momentum dispersion, whereas NSC RIXS also creates immobile fluxes, thereby rendering the response only weakly momentum dependent, as in the spin structure factor measured by inelastic neutron scattering. RIXS can, therefore, pick up the fractionalized excitations of the Kitaev spin liquid separately, making it a sensitive probe to detect spin-liquid character in potential material incarnations of the Kitaev honeycomb model.

DOI: 10.1103/PhysRevLett.117.127203

## Probing the elusive fractionalized Majorana excitations

→ Polarization analysis is required to distinguish the SC from the NSC (magnon).



# New Opportunities for IXS

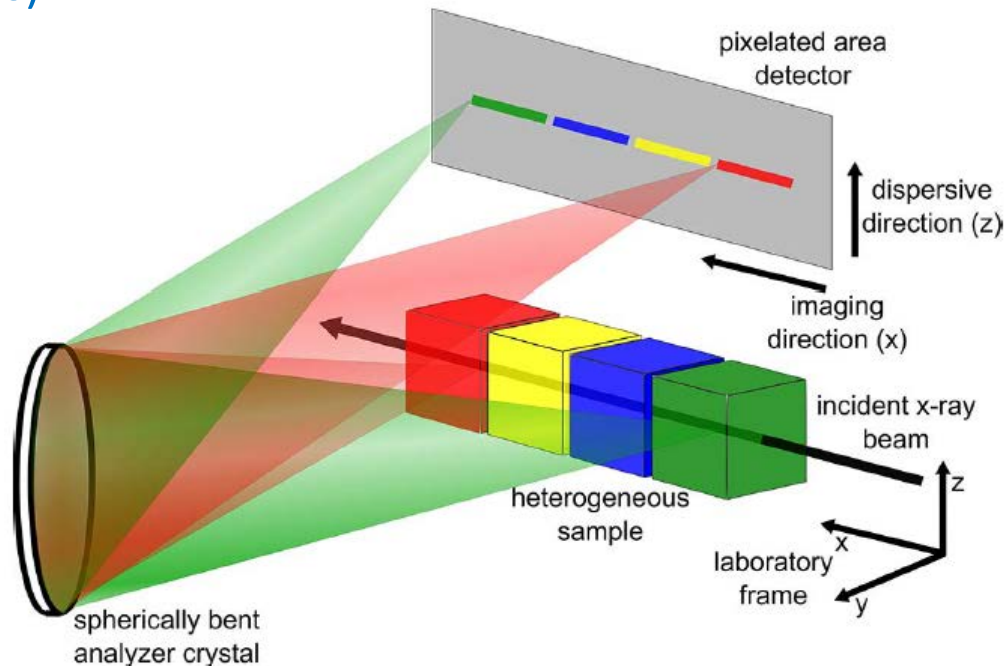
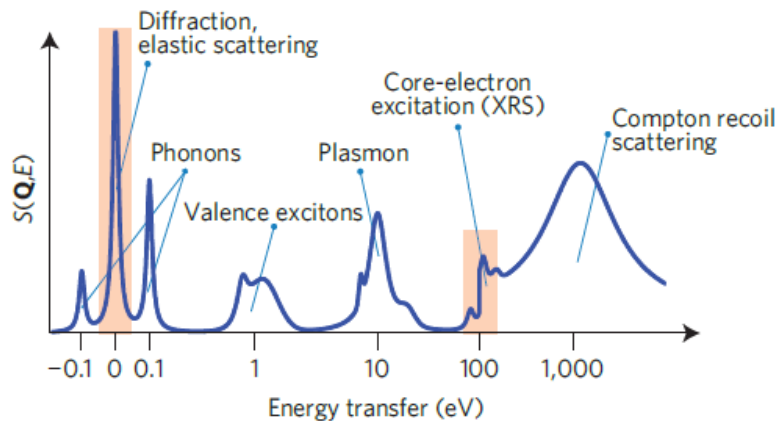
- Polarization Analysis
- Imaging (of heterogeneous materials)
- Time-Resolved
  - ... for hard x-rays, now possible
- Improved Efficiency
  - efficiently and without loss of resolution, using
- Novel In situ
  - new insertion devices
  - flat crystal optics
- ...

# New Opportunities for IXS

- Polarization Analysis
- Imaging (of heterogeneous materials)
- Time-Resolved Measurements
- Improved Energy Resolution (in Resonant Techniques)
- Novel In situ Sample Environments
- ...

## Imaging (of heterogeneous materials)

- XRS-based Direct Tomography
- Energy / Spatial Resolution:  
1 to 3 eV / 50 to 150  $\mu\text{m}$



Direct Tomography with Chemical-bond Contrast  
Simo Houtari et al., *Nature Mat* **10**, 489 (2011)  
Sahle et al., *J. Synchrotron Rad* **24**, 476 (2017)

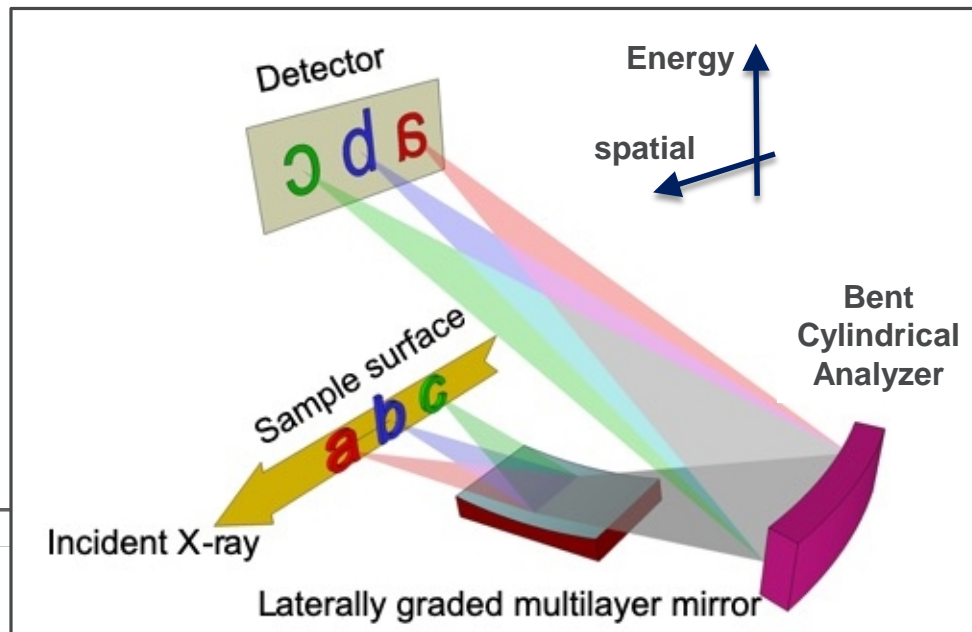
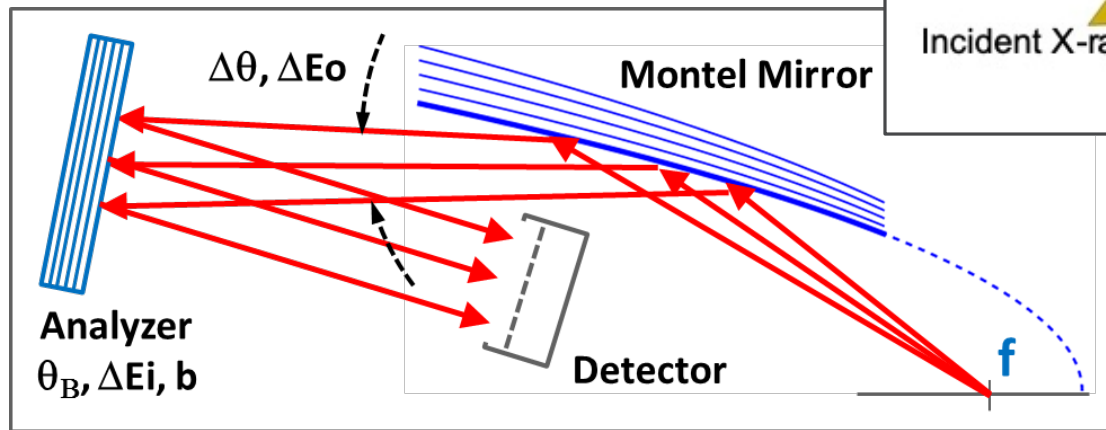


# Imaging (of heterogeneous materials)

- RIXS
- Improved Energy Resolution using multi-layer collimator

$$\Delta E \approx \sqrt{\Delta E_o^2 + \Delta E_i^2 + (E_o \cot(\theta_B) \Delta \theta)^2}$$

$$E_o = 11.215 \text{ keV, Si(844): } \Delta E \approx 125 \text{ meV}$$

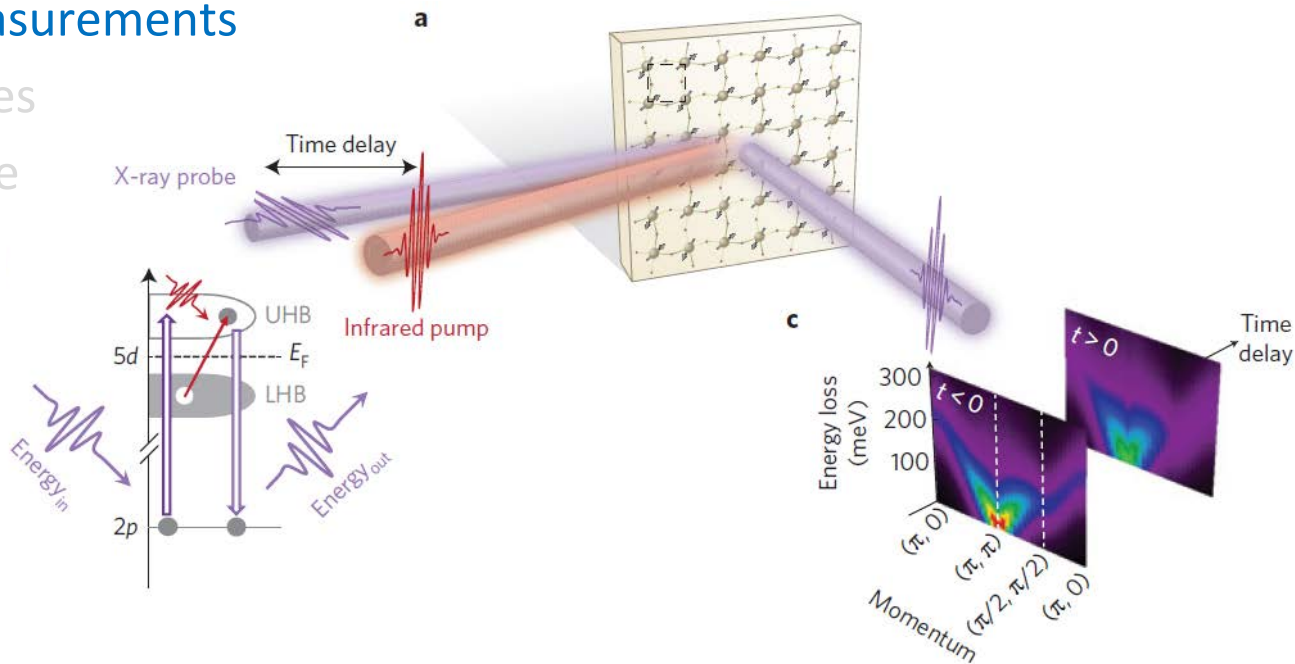


- Mapping electronic / magnetic excitations
- Batteries, Catalysts

# New Opportunities for IXS

- Polarization Analysis
- Imaging (of heterogeneous materials)
- Time-Resolved Measurements
- Improved Energy Res
- Novel In situ Sample

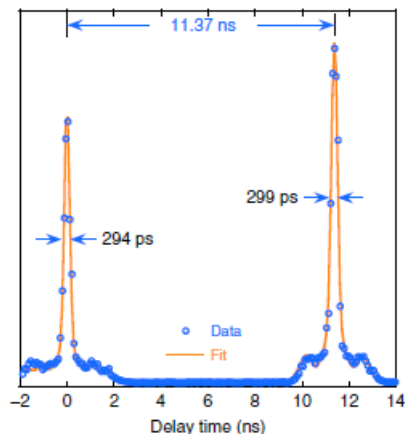
First RIXS study to probe the dynamic response of magnetic and orbital excitations



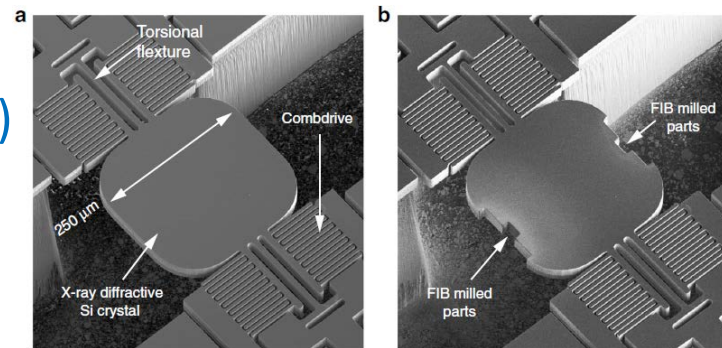
Ultrafast energy- and momentum-resolved dynamics of magnetic correlations in the photo-doped Mott insulator  $\text{Sr}_2\text{IrO}_4$   
Dean et al., Nature Mat **15**, 601 (2016)

# Time-Resolved Measurements

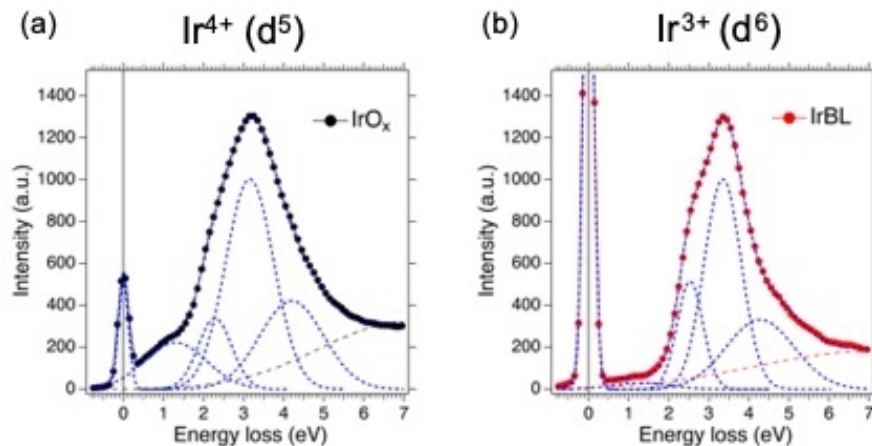
- Exploit unique time structure at APS (152 ns)
- MEMS (micro-electro-mechanical-system)



Study the electron-hole recombination dynamics response of two Iridium oxide catalysts,  $\text{IrO}_x$  and IrBL, by time- and energy resolved RIXS imaging



Chen et al., Nature Comm **10:1158** (2019)

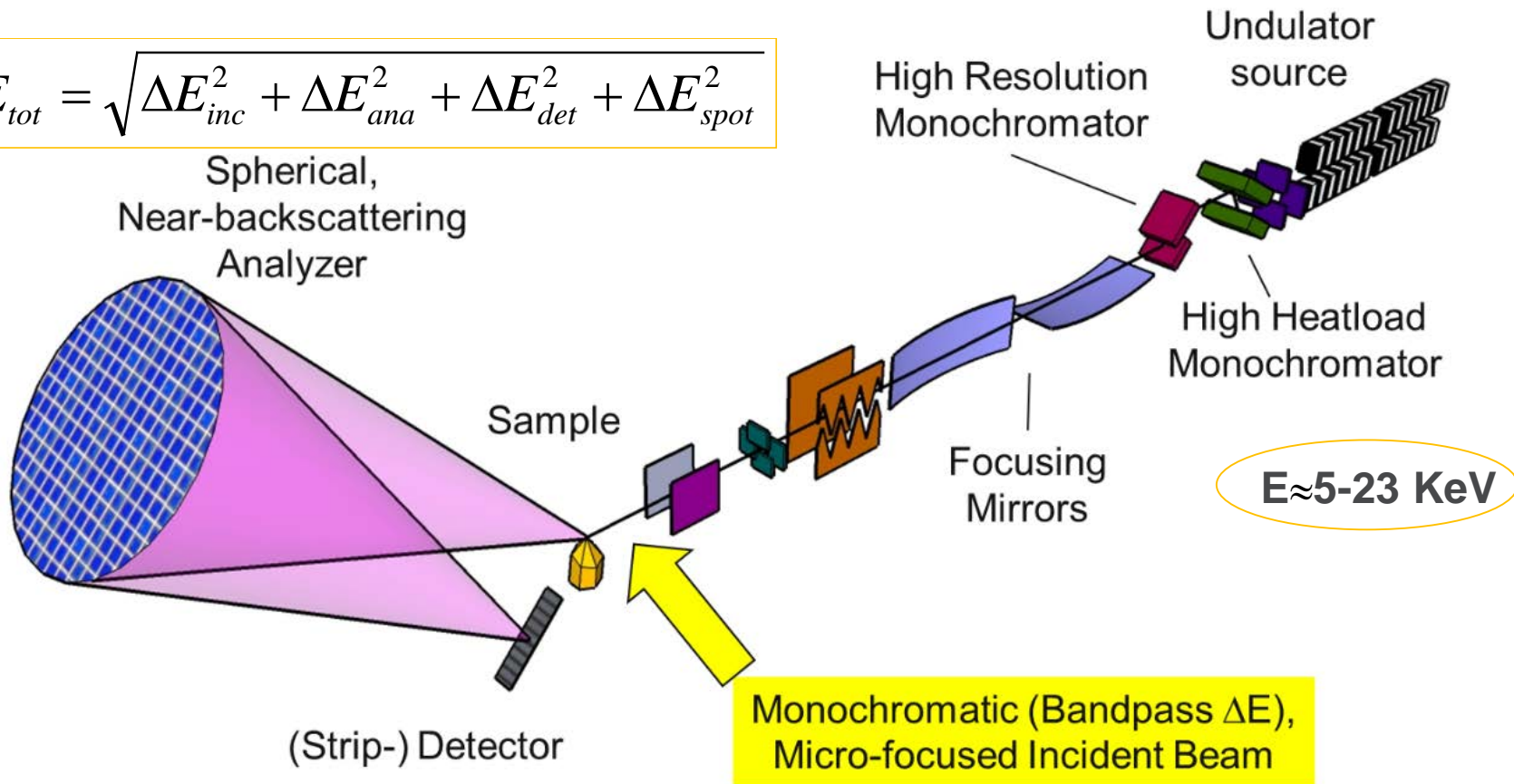


# New Opportunities for IXS

- Polarization Analysis
- Imaging (of heterogeneous materials)
- Time-Resolved Measurements
- Improved Energy Resolution (in Resonant Techniques)
- Novel In situ Sample Environments
- ...

# Improved Energy Resolution

$$\Delta E_{tot} = \sqrt{\Delta E_{inc}^2 + \Delta E_{ana}^2 + \Delta E_{det}^2 + \Delta E_{spot}^2}$$



# Improved Energy Resolution

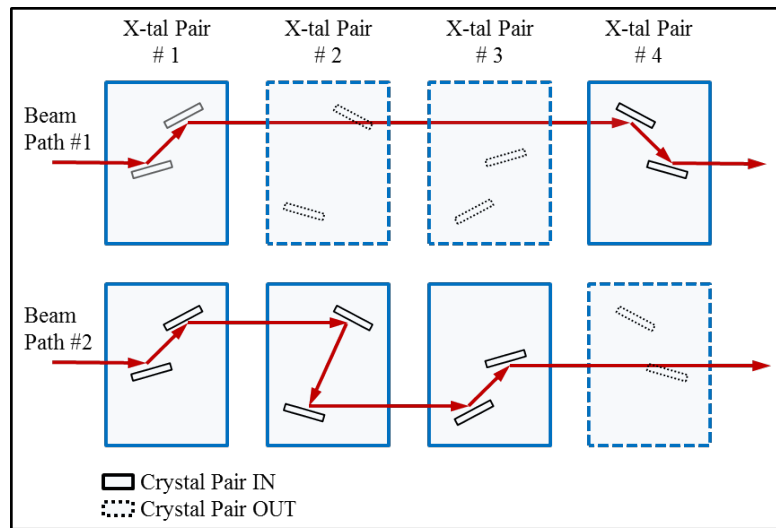
$$\Delta E_{tot} = \sqrt{\Delta E_{inc}^2 + \Delta E_{ana}^2 + \Delta E_{det}^2 + \Delta E_{spot}^2}$$

$\Delta E_{inc}$  : Bandpass determined by High-Resolution Monochromator

suitable  $\Delta E_{inc} < 5$  meV achievable

$\Delta E_{det}$  : Detector Pitch  $< 50$   $\mu\text{m}$

$\Delta E_{spot}$  : Micro-focusing  $< 10$   $\mu\text{m}$

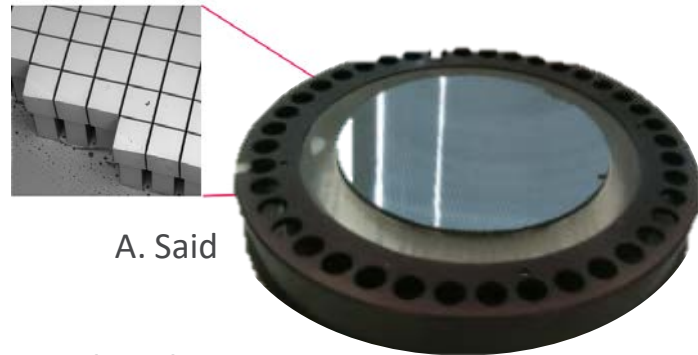


T. Toellner

# Improved Energy Resolution

## $\Delta E_{\text{ana}}$ : Diced, spherical analyzers

- large solid angle coverage
- energy resolution:  $\Delta E = E \cot \theta_B \Delta \theta \Rightarrow$  need near-backscattering
- resonant character of RIXS  $\Rightarrow$  need to find suitable material/reflection for E
- material: typically Si or Ge (large, perfect crystals)
- but: lower symmetry materials offer more choices of reflections
- Quartz, Sapphire, Lithium Niobate, ... available as near perfect crystals
- compiled “Analyzer Atlas” to aid choice of analyzer
- recently, using Q(309)  $\Rightarrow \Delta E_{\text{tot}} = 10.5 \text{ meV}$

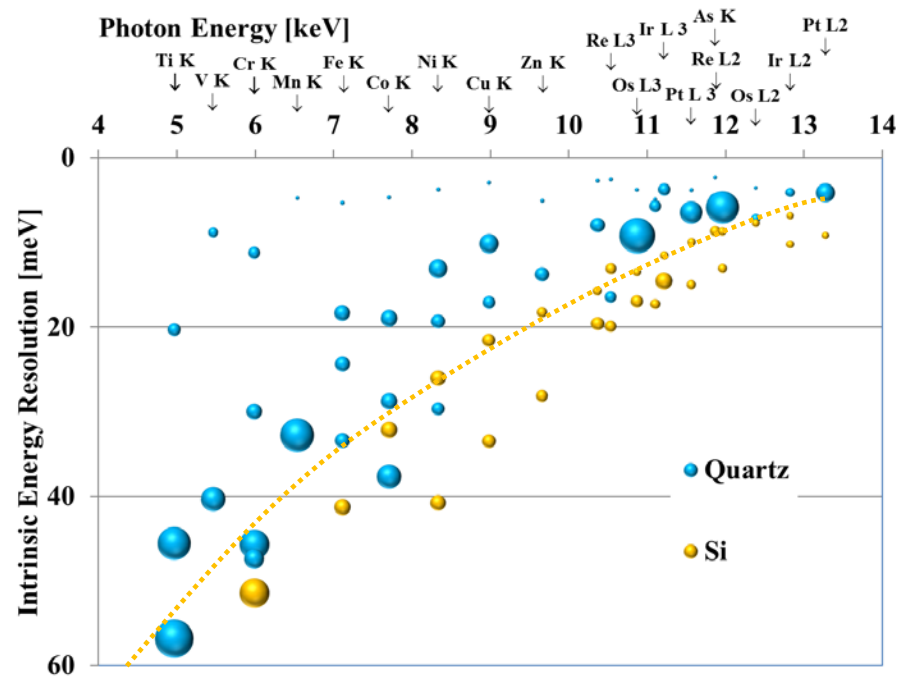
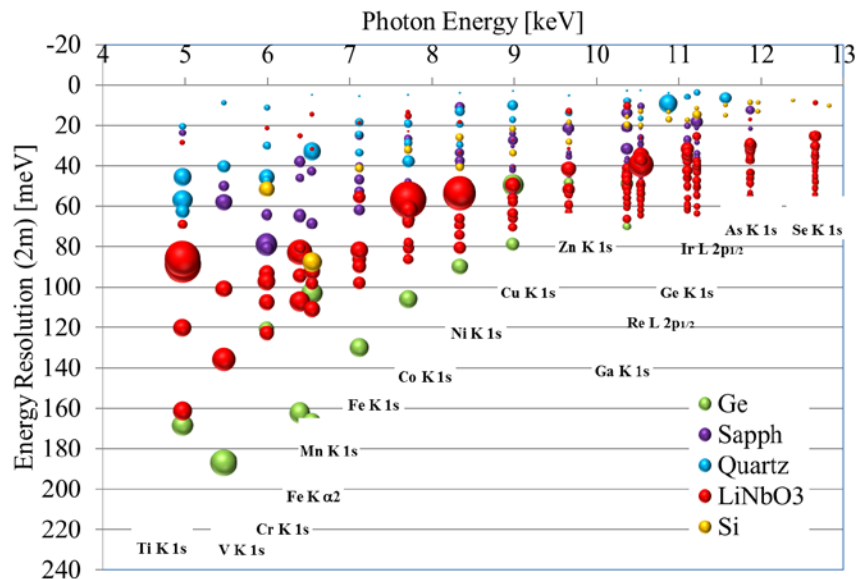


A. Said

**New Record !**

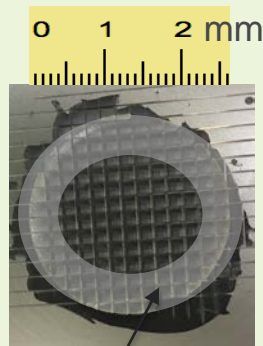


# Improved Energy Resolution

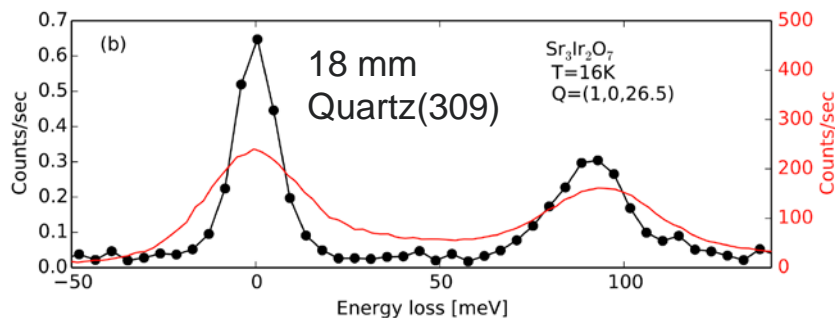
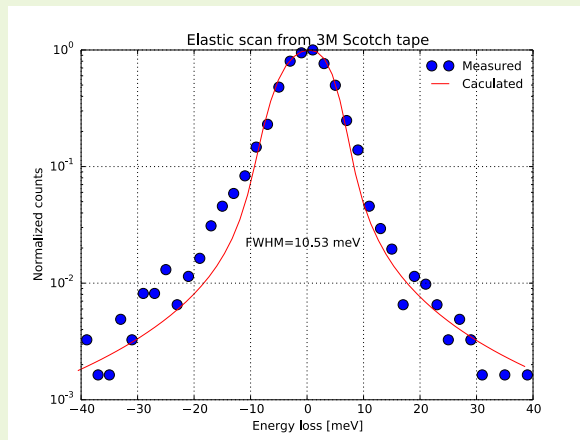


# Spherical Quartz Analyzers

- A prototype spherical quartz (309) analyzer has been made and tested at 27-ID at the APS.
- A record energy resolution was achieved (10.5 meV)
- Joel Bertinshaw talk on  $\text{Sr}_2\text{IrO}_4$  /  $\text{Sr}_3\text{Ir}_2\text{O}_7$  super lattices .



Mask,  
D=18mm

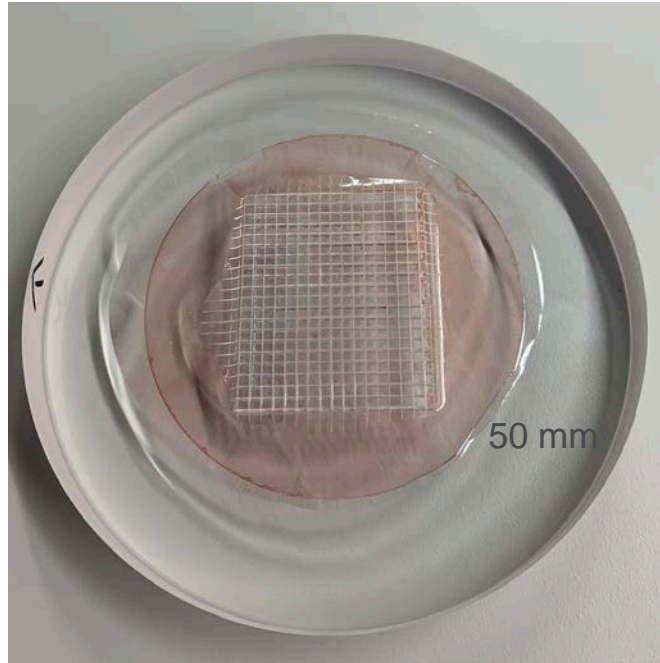


100 mm  
Si(844)

## Issues:

- Small area (lower efficiency)
- We saw degradation of the glue used to hold the quartz pixels.

# Spherical Quartz Analyzers

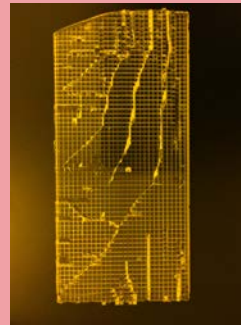


## Current Challenge

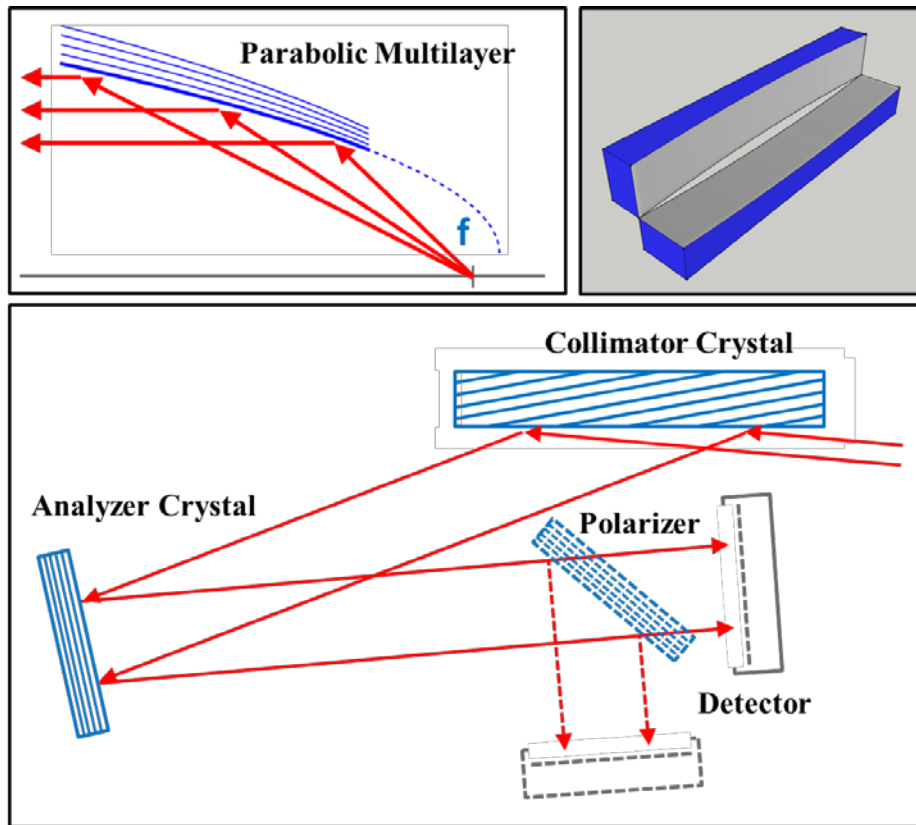
Finding a glue or other bonding method which can survive more than 10 hours of HF etching and keep its integrity over time .

## Overcame Challenge

Dicing (cracking during dicing)

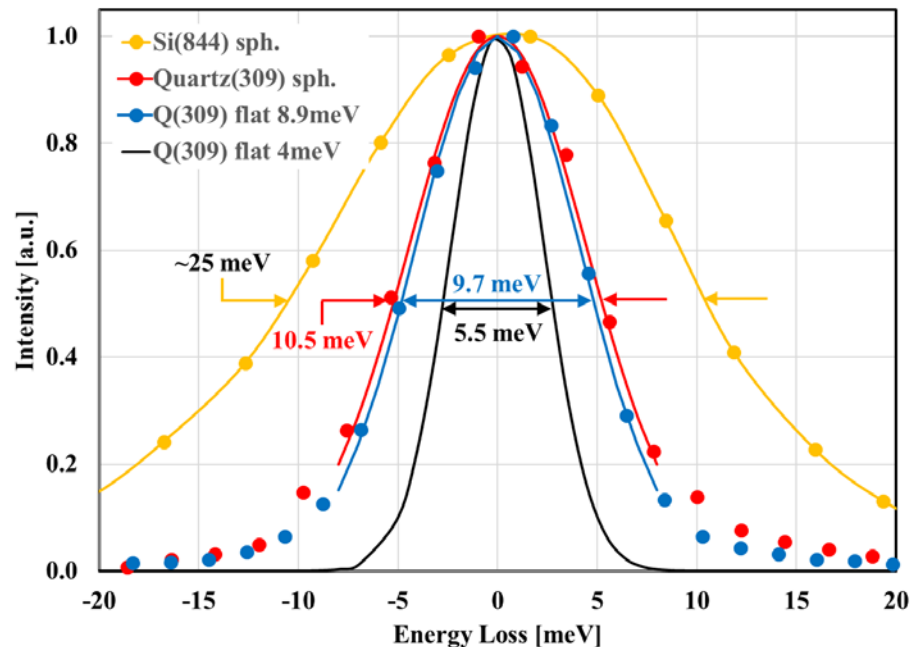


# Improved Energy Resolution



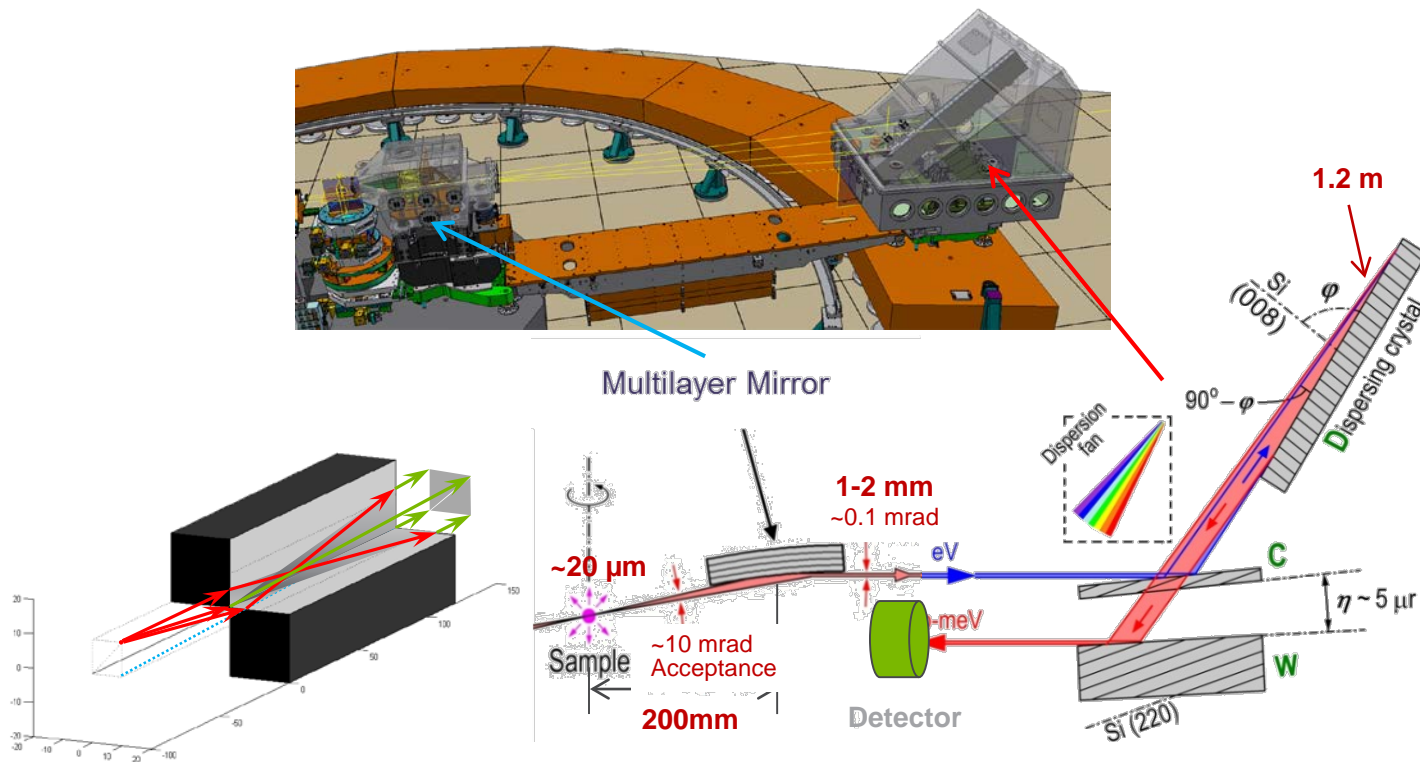
Ang. Acceptance:  $10 \times 10 \text{ mrad}^2 \approx 100 \mu\text{srad}$

Ang. Emittance:  $100 \times 100 \mu\text{rad}^2$



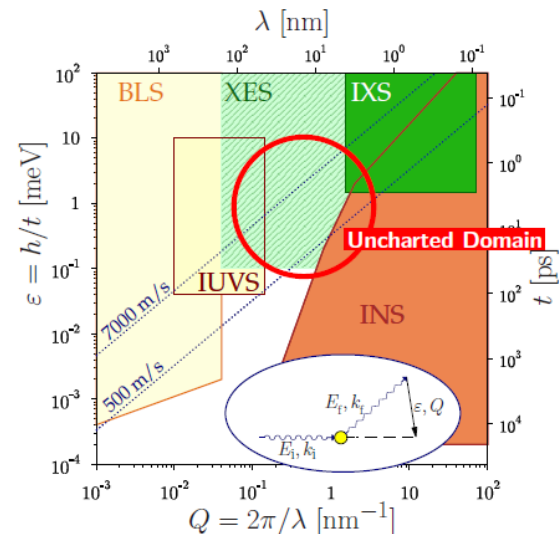
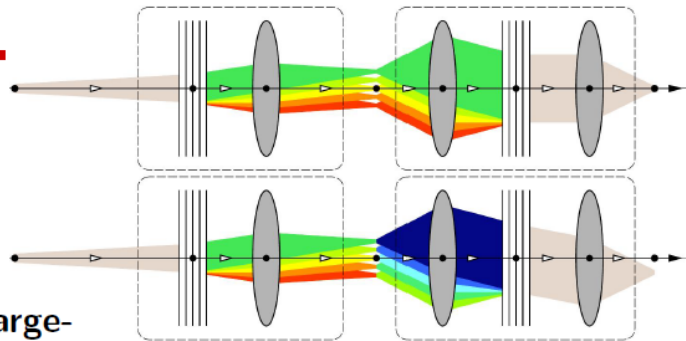
# MONTEL-CDW ANALYZER (FROM: YONG CAI)

10-ID @ NSLS II



## Summary

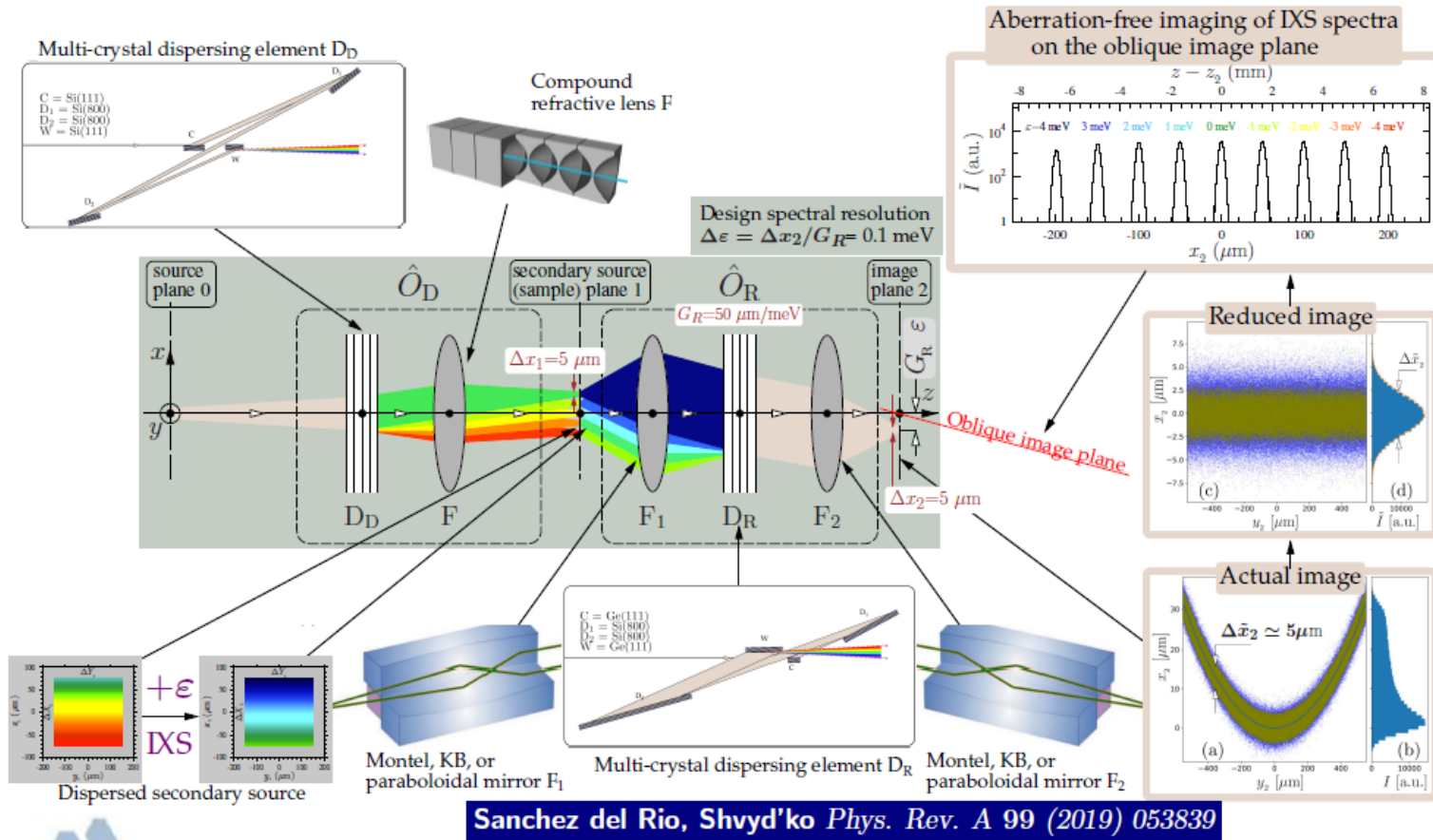
- X-ray echo spectroscopy relies on imaging IXS spectra and does not require x-ray monochromatization, ensuring strong signals along with a very high spectral resolution.
- The hard x-ray optical components (large-dispersion-rate “diffraction gratings”, truly imaging optics, etc.) required for the realization of the x-ray echo spectrometers are feasible.
- X-ray echo spectrometers will either enable up to  $\simeq 1000$ -fold reduction in measurement time for experiments at presently available  $\simeq 1 \text{ meV}/1 \text{ nm}^{-1}$  resolution, or make practical experiments with a  $\simeq 0.1 \text{ meV}/0.1 \text{ nm}^{-1}$  resolution.
- X-ray echo spectrometers (XES) will bridge the gap between the high- and low-frequency inelastic probes and enter the uncharted domain.





# X-ray Echo

## Yu. Shvyd'ko





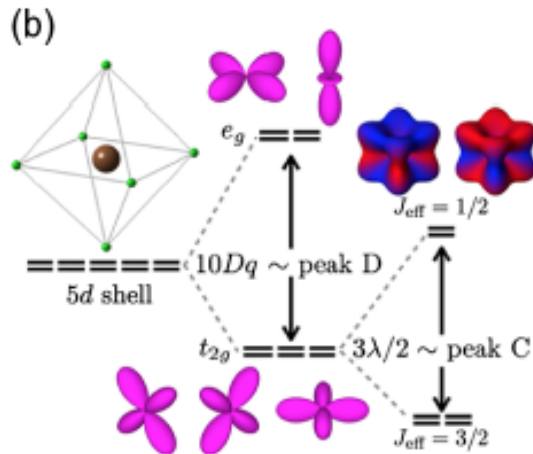
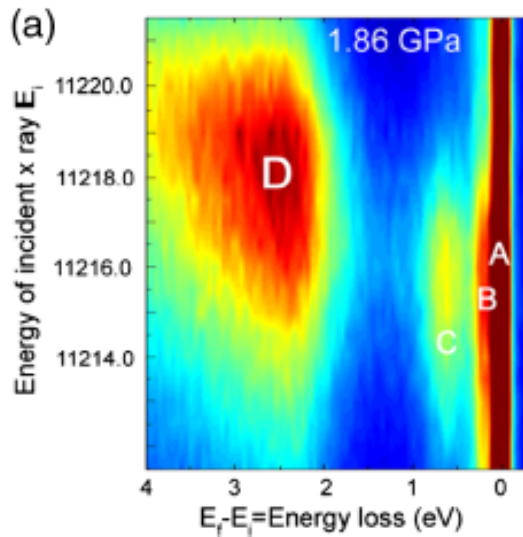
# Improved Energy Resolution

- Polarization Analysis
  - Imaging (of heterogeneous materials)
  - Time-Resolved
  - Improved Energy Resolution
  - Novel In situ
  - ...
- Spherical analyzers:  $\sim 10$  meV might be the limit due to strain and figure errors
  - Flat crystals: everything's possible, but flux will become the limit
  - complexity, stability, ease-of-use will be the issues

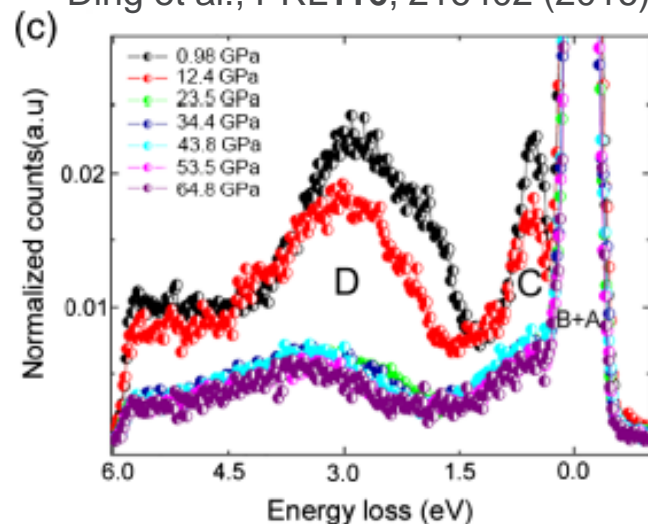
# New Opportunities for IXS

- Polarization Analysis
- Imaging (of heterogeneous materials)
- Time-Resolved Measurements
- Improved Energy Resolution (in Resonant Techniques)
- Meaningful In situ Sample Environments
  - High-Pressure
  - Magnetic Fields
  - Uniaxial Strain

# High Pressure

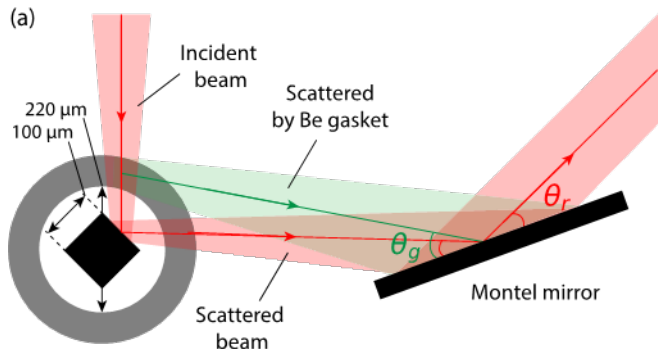


Pressure-Induced Confined Metal from the Mott Insulator  $\text{Sr}_3\text{Ir}_2\text{O}_7$   
Ding et al., PRL116, 216402 (2016)



- Confined metal at 59.5 GPa: metallicity in ab-Plane, insulating along c axis
- No collapse of spin-orbit coupling, rather: first-order structural change
- Intricate interplay between structural and electronic properties in  $\text{Sr}_3\text{Ir}_2\text{O}_7$

# High Pressure



Field of view at focal point of Montel mirror is small enough to see sample but discriminate scattering from surrounding environment

Post sample collimating resonant inelastic x-ray scattering spectrometers for studying low-energy excitation spectrum under high pressure  
Jin-Kwang Kim et al., in preparation



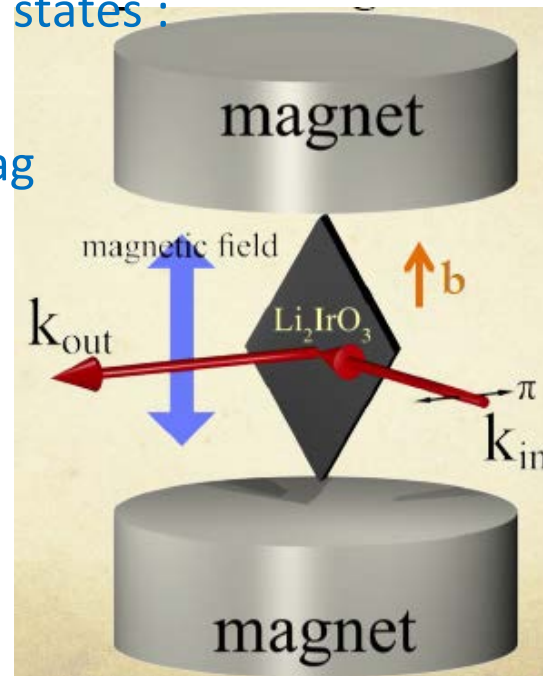
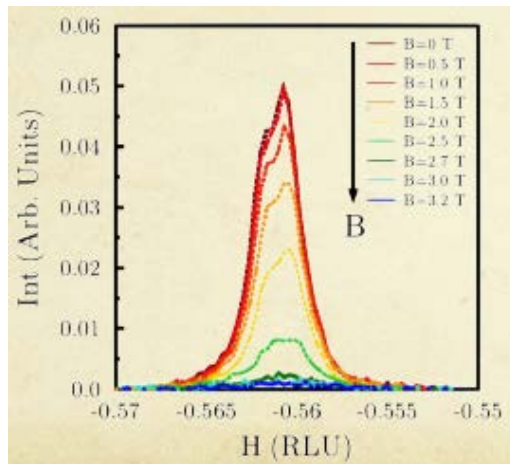
# New Opportunities for IXS

- Polarization Analysis
- Imaging (of heterogeneous materials)
- Time-Resolved Measurements
- Improved Energy Resolution (in Resonant Techniques)
- **Meaningful In situ Sample Environments**
  - High-Pressure
  - **Magnetic Fields**
  - Uniaxial Strain

# Magnetic Fields

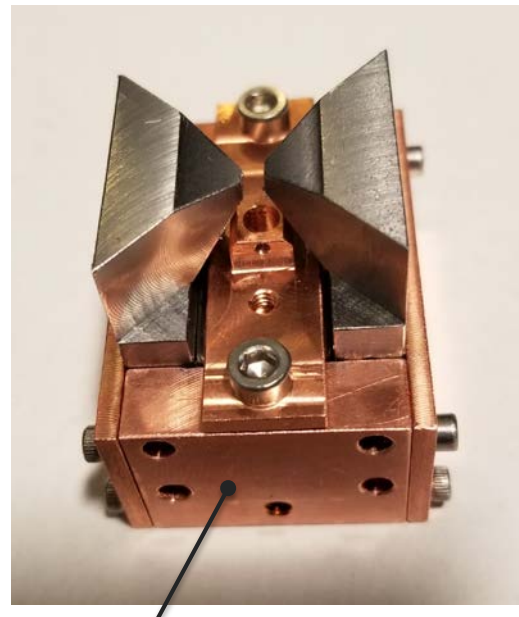
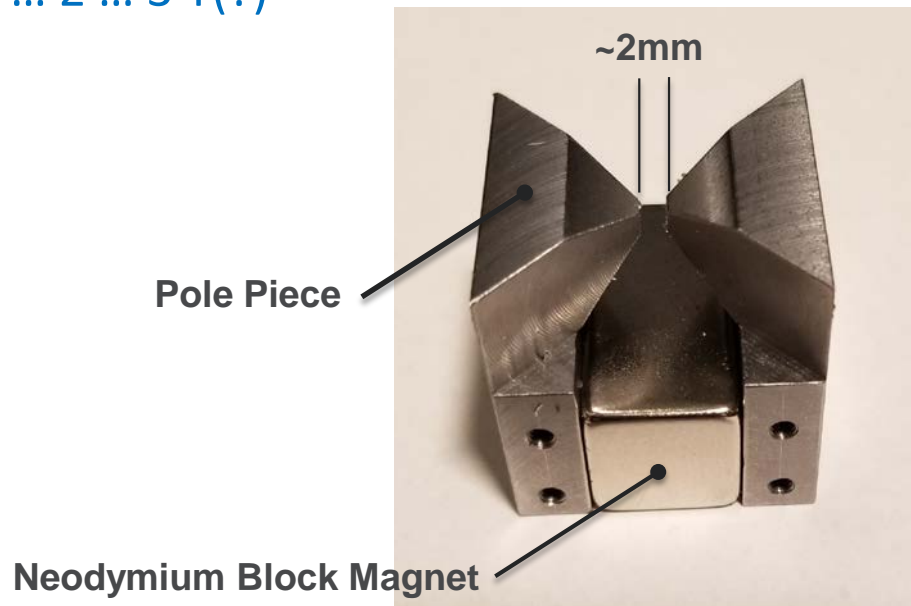
From: Alejandro Ruiz, Alex Frañó, et al., UCSD

- Unconventional magnetism in 5d materials with strong SOC
- Honeycomb- $\text{Li}_2\text{IrO}_3$  promising Kitaev material  $\rightarrow$  QSL ground state (?)
- Ext. magnetic field  $\rightarrow$  degeneracy of magnetic ground states :  
incommensurate spiral, commensurate zig-zag phase
- Dispersing magnon identified for both spiral and zigzag
- First results with  $B \neq 0$  ( $\leq 2\text{T}$ ):  
softening of zigzag,  
hardening of spiral



# Magnetic Fields

- Small magnet assemblies for use in closed-cycle cryostats
- 1.5 ... 2 ... 3 T(?)



# Magnetic Fields

- Pulsed, DC magnets on 6-ID @ APS
- Trapped-field magnets  
(Z. Islam, APS)





# New Opportunities for IXS

- Polarization Analysis
- Imaging (of heterogeneous materials)
- Time-Resolved Measurements
- Improved Energy Resolution (in Resonant Techniques)
- **Meaningful In situ Sample Environments**
  - High-Pressure
  - Magnetic Fields
  - **Uniaxial Strain**

# Uniaxial Strain

Uniaxial pressure control of competing orders in a high-temperature superconductor

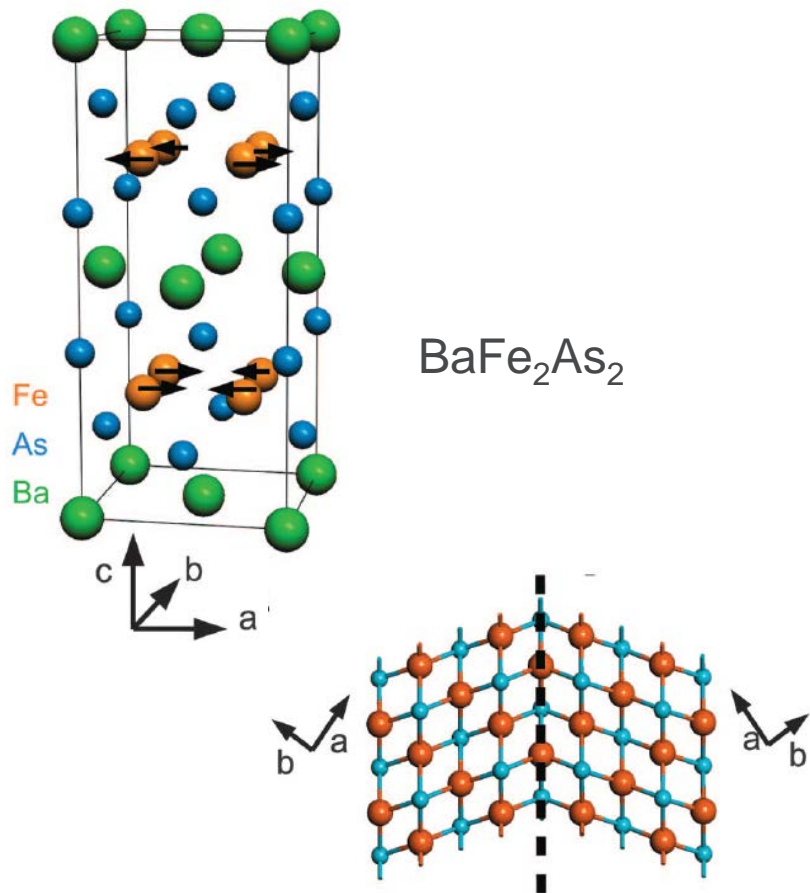
H.-H. Kim et al., Science 362 1040 (2018)

- Ground states of TMOs (High  $T_c$ , CDW, ...) can be tuned by doping, external fields
- Tuning might introduce disorder
- Application of strain can distinguish between competing orders

In-Plane Resistivity Anisotropy in an Underdoped Iron Arsenide Superconductor

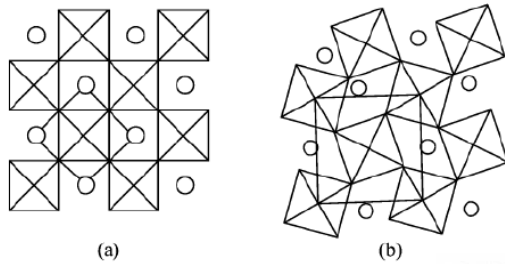
J.-H. Chu et al., Science 329 824 (2010)

- Application of strain can remove twinning

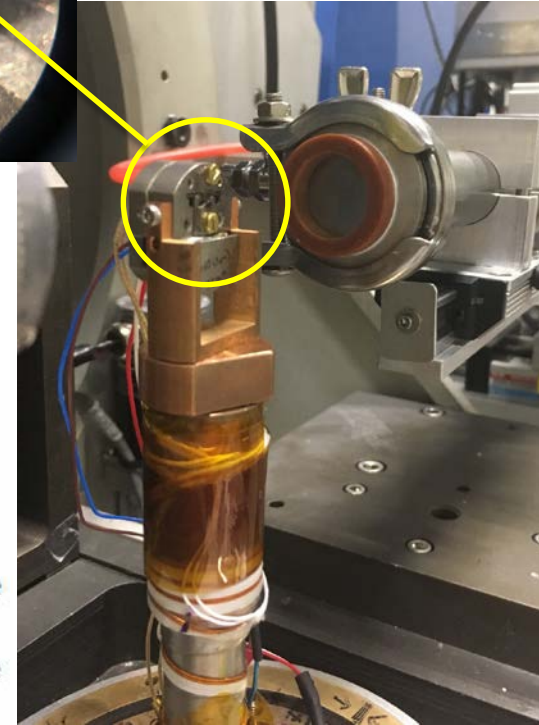
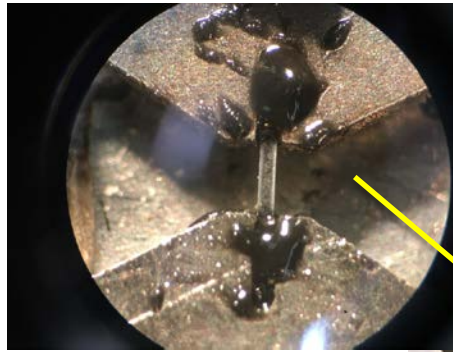
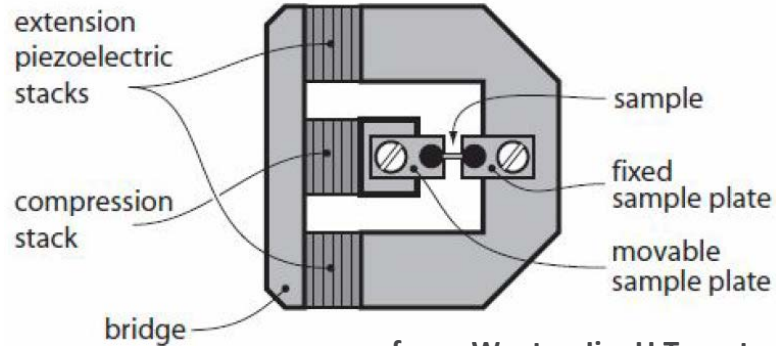


# Uniaxial Strain

- W. Jin et al.: RIXS in  $\text{Sr}_2\text{IrO}_4$
- Suppression of structural phase transition in STO



High T/ Low T



from: Wentao Jin, U Toronto

# Conclusions

- IXS has come a long way as a practical, efficient probe of elementary excitations in complex materials
- => Novel materials discovery, characterization
- Efficient polarization analysis possible and will further enhance IXS
- Imaging and time-resolved (ps,ns) measurements at Synchrotrons possible
- As probe of magnetic excitations, RIXS energy resolution has been greatly improved ( $\sim 10$  meV)
- ... but needs to improve even further ( $\sim < \cancel{5}$  1 meV) to be on “equal” footing with Inelastic Neutron Scattering
- Novel flat crystals optics and special spherical analyzers provide path to ultra-high resolution

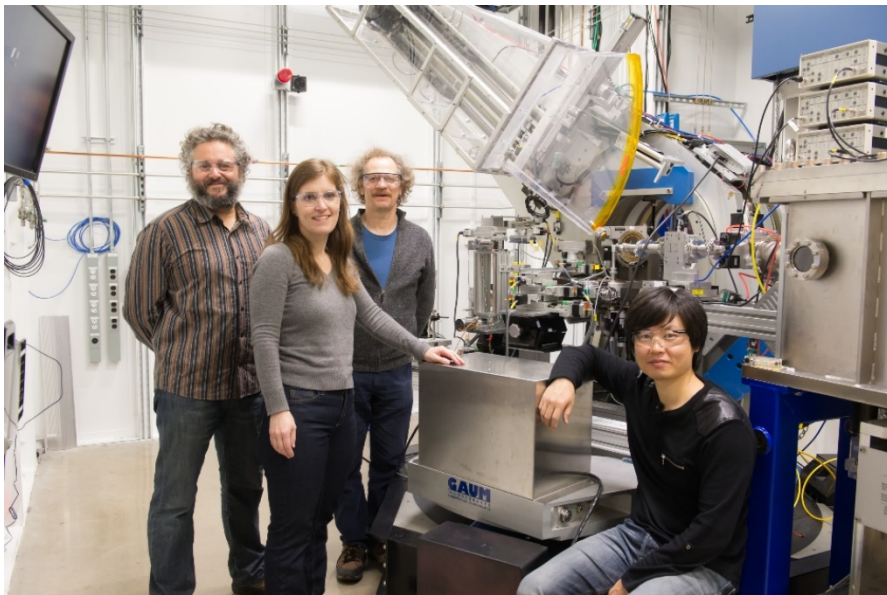
# Conclusions

- New multilayer optics / flat-crystal on the horizon / being implemented
- Meaningful in-situ sample environments

# People

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Jungho Kim ([jhkim@anl.gov](mailto:jhkim@anl.gov))

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Diamond Anvil Cells)



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(Scientific Assc.)

# People

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## CNM

R. Divan  
S. Miller

Thank you

# Path to Ultra-High Energy Resolution

Compilation of viable  
Reflections in Si, Ge,  
Sapphire, Lithium Niobate,  
Quartz

[www.aps.anl.gov/Analyzer-Atlas/Analyzer-Atlas](http://www.aps.anl.gov/Analyzer-Atlas/Analyzer-Atlas)

www.aps.anl.gov/Sectors/Sector30/AnalyzerAtlas/AnalyzerAtlas.html

Argonne NATIONAL LABORATORY

Advanced Photon Source  
A U.S. Department of Energy, Office of Science,  
Office of Basic Energy Sciences national synchrotron x-ray research facility

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Introduction  
Staff  
HERIX  
MERIX  
Sample Environments  
Publications  
Useful Links

**Near-Backscattering, Spherical Analyzers for RIXS :  
A Compilation of Viable Reflections in Si, Ge, LiNbO<sub>3</sub>, Sapphire and Quartz  
(Under Construction)**

T. Gog, D. Casa, A. Said, M. Upton, Jung Ho Kim, I. Kuzmenko, Xianrong Huang, R. Khachatryan

[Introduction] - [Reflection Tables] - [Detector-Analyzer Geometry] - [Quantities Listed]

|    |    |    |    |    |    |    |    |    |               |    |    |     |    |     |    |     |     |  |
|----|----|----|----|----|----|----|----|----|---------------|----|----|-----|----|-----|----|-----|-----|--|
| H  |    |    |    |    |    |    |    |    |               |    |    |     |    |     |    |     | He  |  |
| Li | Be |    |    |    |    |    |    |    |               |    |    | B   | C  | N   | O  | F   | Ne  |  |
| Na | Mg |    |    |    |    |    |    |    |               |    |    | Al  | Si | P   | S  | Cl  | Ar  |  |
| K  | Ca | Sc | Ti | V  | Cr | Mn | Fe | Co | Ni            | Cu | Zn | Ga  | Ge | As  | Se | Br  | Kr  |  |
| Rb | Sr | Y  | Zr | Nb | Mo | Tc | Ru | Rh | Pd            | Ag | Cd | In  | Sn | Sb  | Te | I   | Xe  |  |
| Cs | Ba | Lu | Hf | Ta | W  | Re | Os | Ir | L1 13.419 keV |    |    | Tl  | Pb | Bi  | Po | At  | Rn  |  |
| Fr | Ra | Lr | Rf | Db | Sg | Bh | Hs | Mt | L2 12.824 keV |    |    | Uut | Fl | Uup | Lv | Uus | Uuo |  |
|    |    |    | La | Ce | Pr | Nd | Pm | Sm | L3 11.215 keV |    |    | Ho  | Er | Tm  | Yb |     |     |  |
|    |    |    | Ac | Th | Pa | U  | Np | Pu | Am            | Cm | Bk | Cf  | Es | Fm  | Md | No  |     |  |

Point to an element for available absorption edges / emission lines

contact: Thomas Gog, last updated: 16.Feb.2012



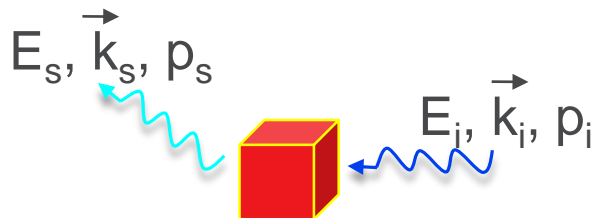
# Path to Ultra-High Energy Resolution

Compilation of viable  
Reflections in Si, Ge  
Sapphire, Lithium N  
Quartz

www.aps.anl.gov/A  
-Atlas/Analyzer-Atl

| www.aps.anl.gov/Sectors/Sector30/AnalyzerAtlas/AnalyzerAtlas.html         |                           |                    |                   |                                |                 |                               |                     |                                  |                                  |
|---|---------------------------|--------------------|-------------------|--------------------------------|-----------------|-------------------------------|---------------------|----------------------------------|----------------------------------|
| U.S. DEPARTMENT OF Office of  |                           |                    |                   |                                |                 |                               |                     |                                  |                                  |
| Ei =<br>Cryst   | 8.9805<br>Refl<br>(h,k,l) | keV<br>EB<br>[keV] | $\Theta$ B<br>[°] | $\int$ IR d $\Theta$<br>[μrad] | Width<br>[μrad] | Ei cot $\Theta$<br>[meV/μrad] | $\Delta$ E<br>[meV] | $\Delta$ Eg<br>2m, 50μm<br>[meV] | $\Delta$ Et<br>2m, 50μm<br>[meV] |
| Ge  | (3,3,7)                   | 8.969              | 87.14             | 80.2                           | 81.5            | 0.448                         | 36.51               | 5.6                              | 36.94                            |
| Ge  | (0,0,8)                   | 8.766              | 77.46             | 30.3                           | 28.2            | 1.998                         | 56.34               | 24.97                            | 61.62                            |
| Si  | (2,4,6)                   | 8.542              | 72.02             | 13.1                           | 11.5            | 2.915                         | 33.48               | 36.44                            | 49.48                            |
| Si  | (1,3,7)                   | 8.768              | 77.5              | 11.8                           | 10.8            | 1.991                         | 21.56               | 24.89                            | 32.93                            |
| Equiv. Refl.: (3,5,5)   |                           |                    |                   |                                |                 |                               |                     |                                  |                                  |
| LiNbO3  | (1,5,-10)                 | 8.941              | 84.6              | 58.1                           | 55.8            | 0.85                          | 47.45               | 10.62                            | 48.62                            |
| Equiv. Refl.: (5,-6,-10), (6,-5,-10), (-1,6,-10), (-5,-1,-10), (-6,1,-10) |                           |                    |                   |                                |                 |                               |                     |                                  |                                  |
| LiNbO3  | (1,-6,10)                 | 8.941              | 84.6              | 56.4                           | 55.8            | 0.85                          | 47.45               | 10.62                            | 48.62                            |
| Equiv. Refl.: (5,1,10), (6,-1,10), (-1,-5,10), (-5,6,10), (-6,5,10)       |                           |                    |                   |                                |                 |                               |                     |                                  |                                  |
| Quartz  | (-4,6,4)                  | 8.972              | 87.44             | 37.5                           | 34.4            | 0.401                         | 13.78               | 5.01                             | 14.66                            |
| Equiv. Refl.: (-4,-2,-4)  |                           |                    |                   |                                |                 |                               |                     |                                  |                                  |
| Quartz  | (6,-2,4)                  | 8.972              | 87.44             | 37.4                           | 34.4            | 0.401                         | 13.77               | 5.01                             | 14.65                            |
| Equiv. Refl.: (6,-4,-4), (-2,6,-4), (-2,-4,4)                             |                           |                    |                   |                                |                 |                               |                     |                                  |                                  |
| Quartz  | (4,-6,-4)                 | 8.972              | 87.44             | 36.3                           | 34.4            | 0.401                         | 13.78               | 5.01                             | 14.66                            |
| Quartz  | (2,4,-4)                  | 8.972              | 87.44             | 36.2                           | 34.4            | 0.401                         | 13.77               | 5.01                             | 14.66                            |
| Equiv. Refl.: (2,-6,4), (4,2,4), (-6,2,-4), (-6,4,4)                      |                           |                    |                   |                                |                 |                               |                     |                                  |                                  |
| Quartz  | (6,-2,-4)                 | 8.972              | 87.44             | 28.5                           | 26.9            | 0.401                         | 10.79               | 5.01                             | 11.89                            |

# Introduction

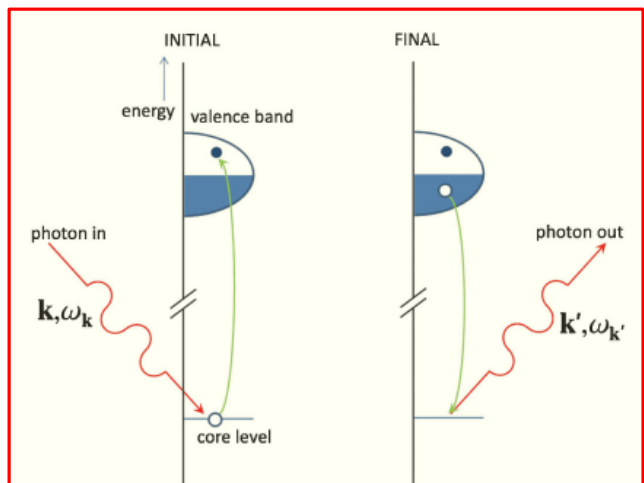


## Inelastic Scattering Cross Section

$$\frac{d^2\sigma}{d\Omega d\omega} \propto \left| \langle f | H_{\text{int}} | i \rangle + \sum_{|n\rangle} \frac{\langle f | H_{\text{int}} | n \rangle \langle n | H_{\text{int}} | i \rangle}{E_i - E_n + i\Gamma} \right|^2$$

Non-Resonant (weak)

Resonant Enhancement (x 50 ... 100)

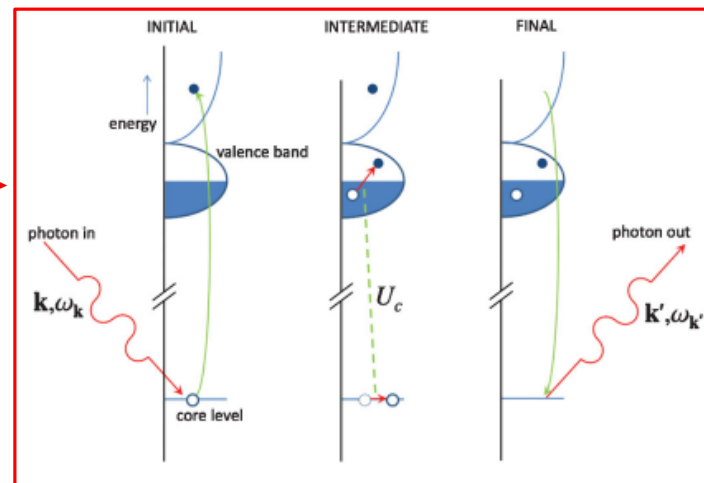


## RIXS Processes

direct

Indirect

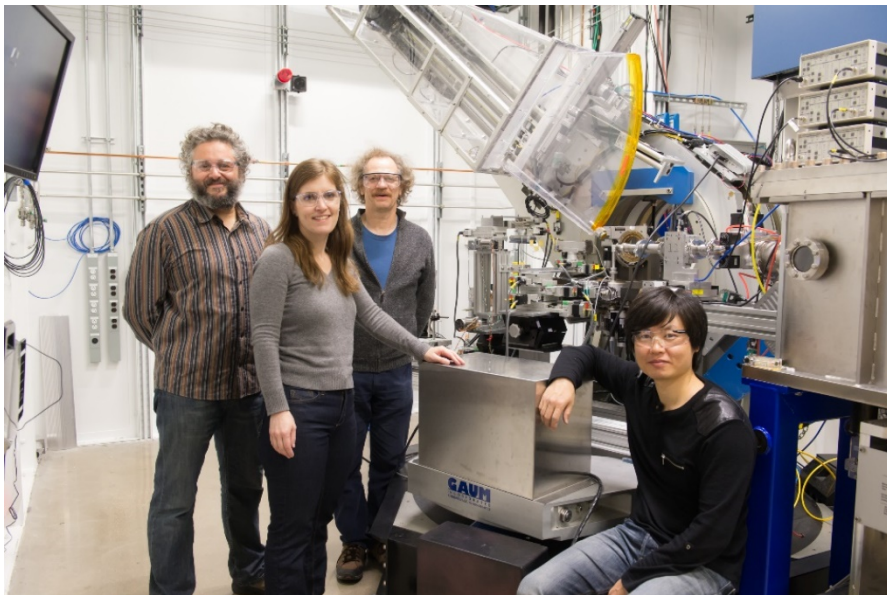
Ament, van Veenendaal, Devereaux, Hill, van den Brink, Rev. Mod. Phys. **83**, 705 (2011)



# People

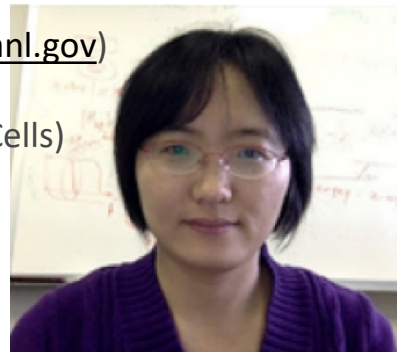
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Jungho Kim ([jhkim@anl.gov](mailto:jhkim@anl.gov))

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(Spherical Analyzers)



Tom Toellner ([toellner@anl.gov](mailto:toellner@anl.gov))  
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Rick Krakora  
(Scientific Assc.)