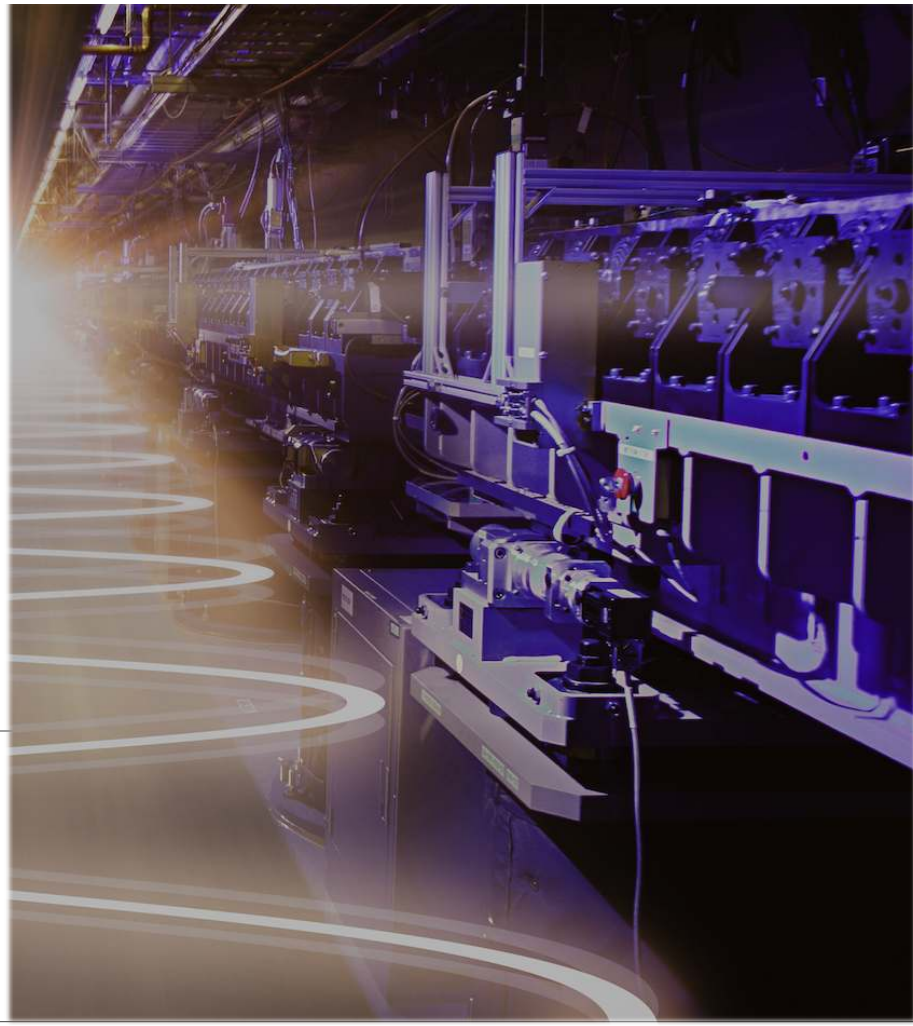
Accelerated massive data analytics for materials and semiconductors

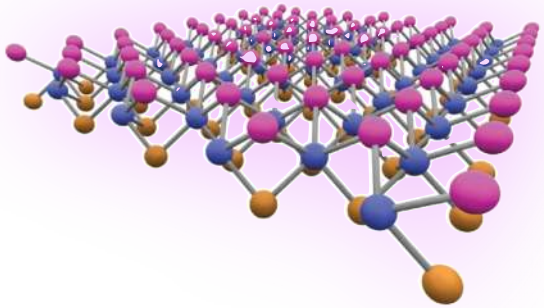
Quynh L. Nguyen

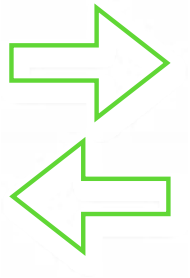
Linac Coherent Light Source
SLAC National Accelerator Laboratory

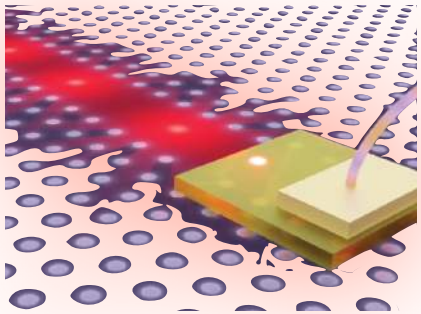
4 December 2024

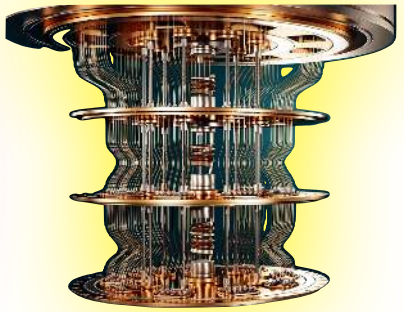


Materials for devices









Understanding and manipulating matter for practical applications

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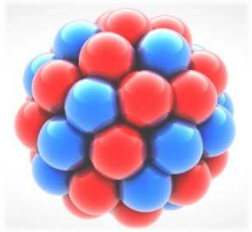
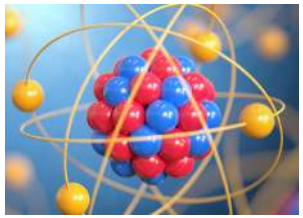
Wavelength and Matter Size

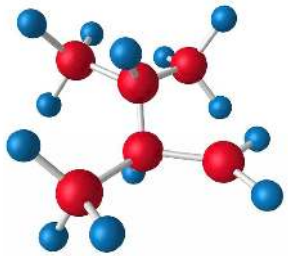
Gamma Ray	X-ray	Ultraviolet	Visible	Infrared	Microwave
10^{-12} m	10^{-10} m	10^{-8} m	10^{-6} m	10^{-5} m	10^{-2} m



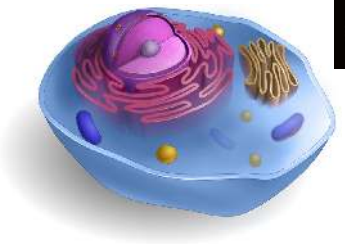
Atomic nuclei



Atom



Molecules



Cells

Sewing Needles

Honey Bees

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Wavelength and Matter Size

Gamma Ray
10^{-12} m

X-ray
10^{-10} m

Ultraviolet
10^{-8} m

Visible
10^{-6} m

Infrared
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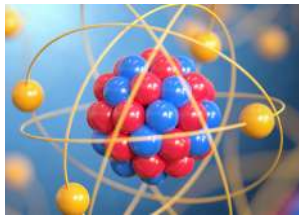
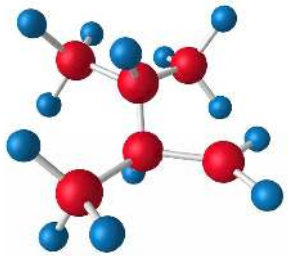
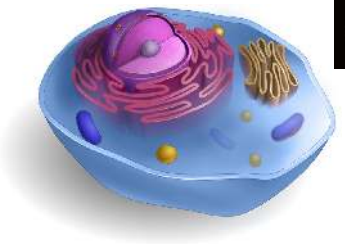
Microwave
10^{-2} m







Atomic nuclei

Atom

Molecules

Cells

Sewing Needles

Honey Bees

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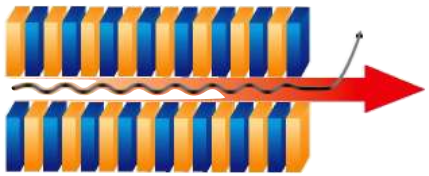

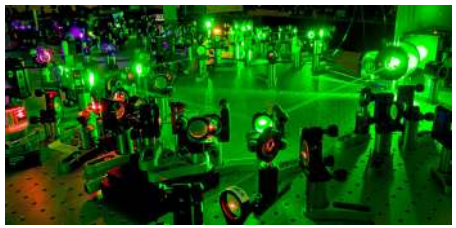

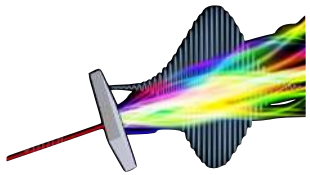

X-ray Large and Mid-scale Facilities

Table-top laser syste

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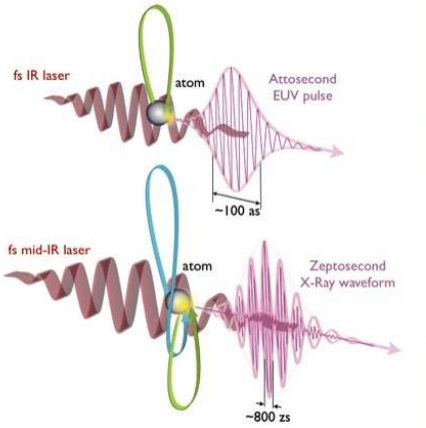
Ultrafast X-ray Light Sources: HHG, Synchrotron, FEL

VUV, EUV to soft-Xray (< 300 eV)
femto to attosecond (10^{-15} - 10^{-18} s)
10^{6} - 10^{8} photons/sec

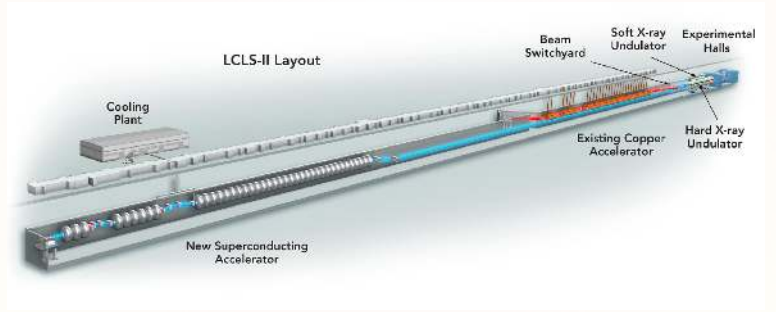


High-harmonic Generation

Soft x-ray (0.25 - 1.6 keV)
picoseconds (10^{-12} s)
10^{12} photons/sec

Synchrotron

Soft x-ray (0.25 - 1.6 keV), 1-MHz
femtoseconds (10^{-15} s)
10^{15} photons/sec



Free-Electron Laser

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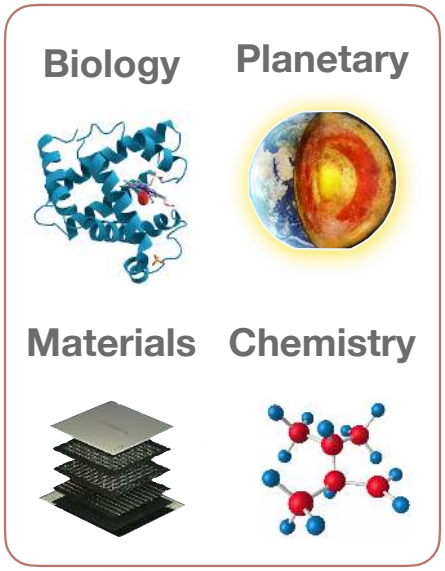
World's first X-ray Free Electron Laser

SLAC X-ray Free Electron Laser

- 3-km long tunnel under I-280 and close to Stanford campus
- Access angstrom-length-scales and electronic movements
- Unravel new scientific insights in matter

Applications



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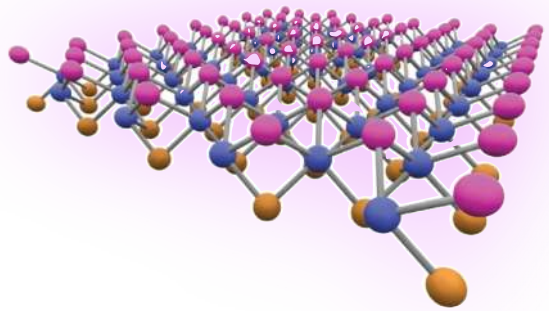
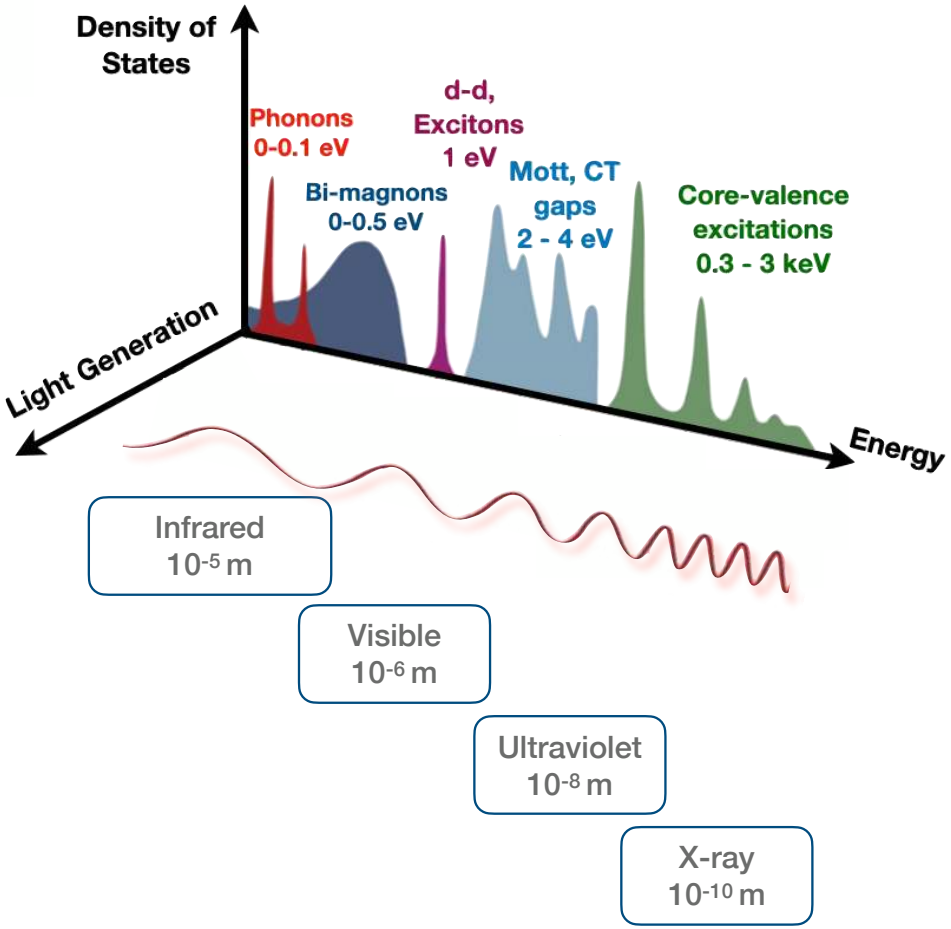
Ultrafast Excitation Driver





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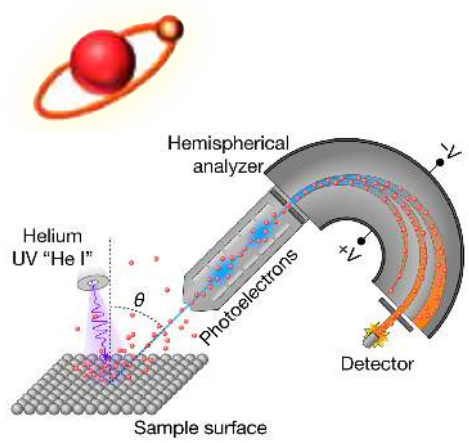
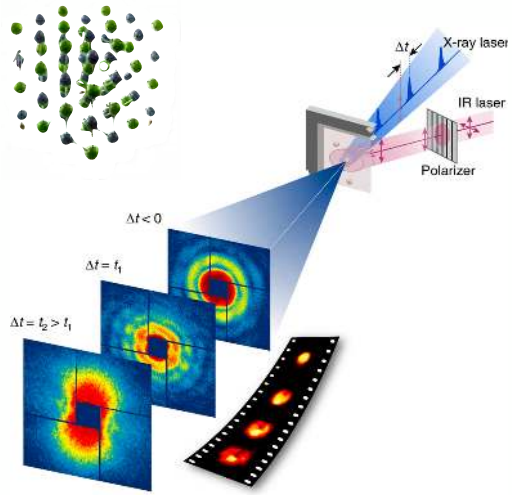
Ultrafast characterization approaches

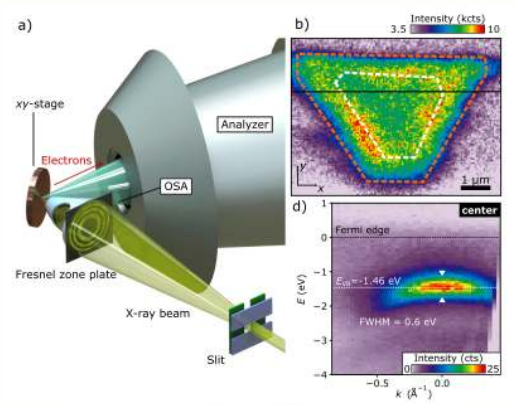
Electronic Structure



Atomic Landscape



Spectral Microscopy



Spectroscopy

Scattering

Spatial Imaging

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Time-resolved X-ray experiment schematic timeline

Proposal

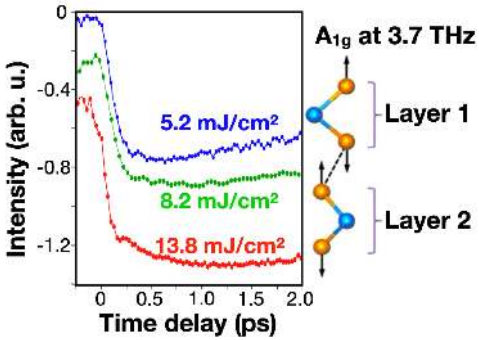
~1-year

60 hour

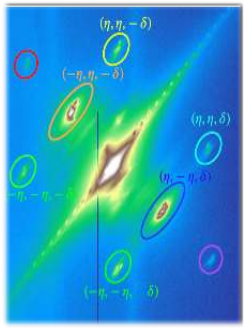
4. Decision Making

1. Data Collection

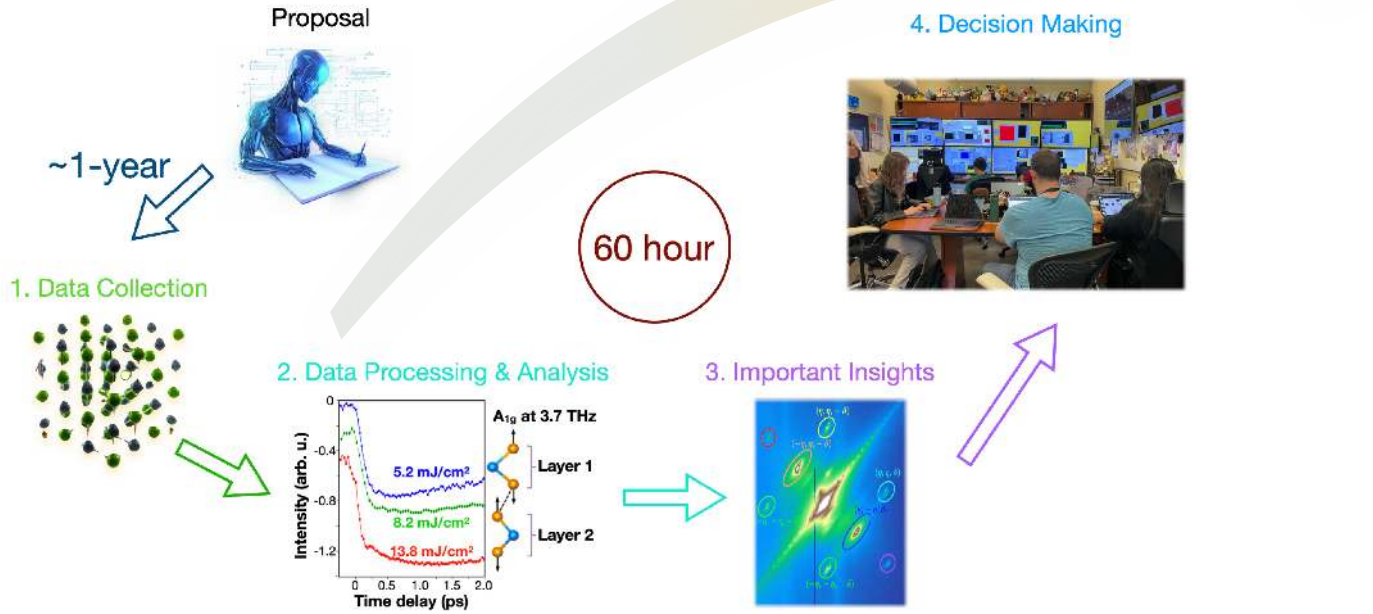
2. Data Processing & Analysis



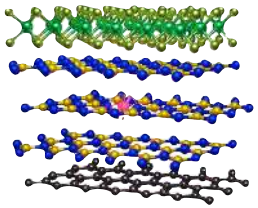
3. Important Insights

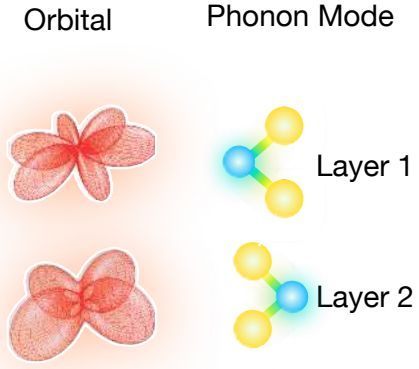


Time-resolved X-ray experiment schematic timeline



Science Discovery





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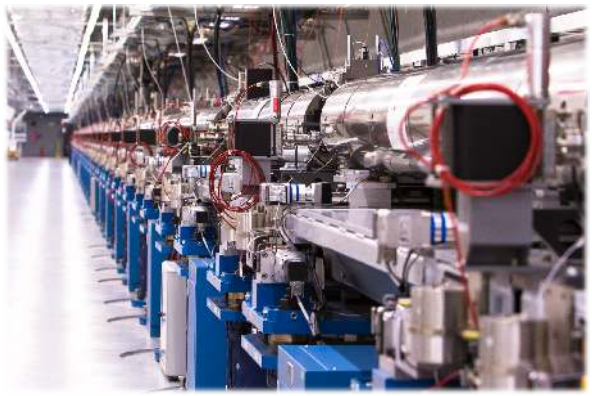
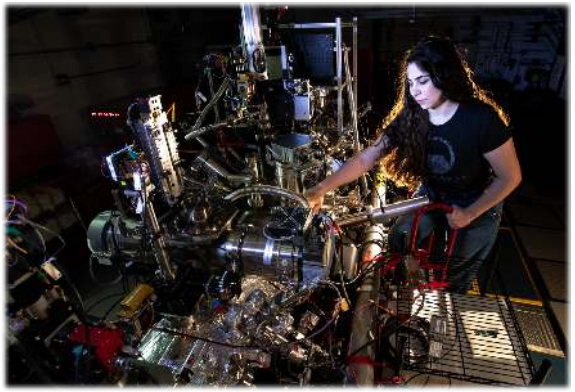
3-km beam line to complex instrumentations



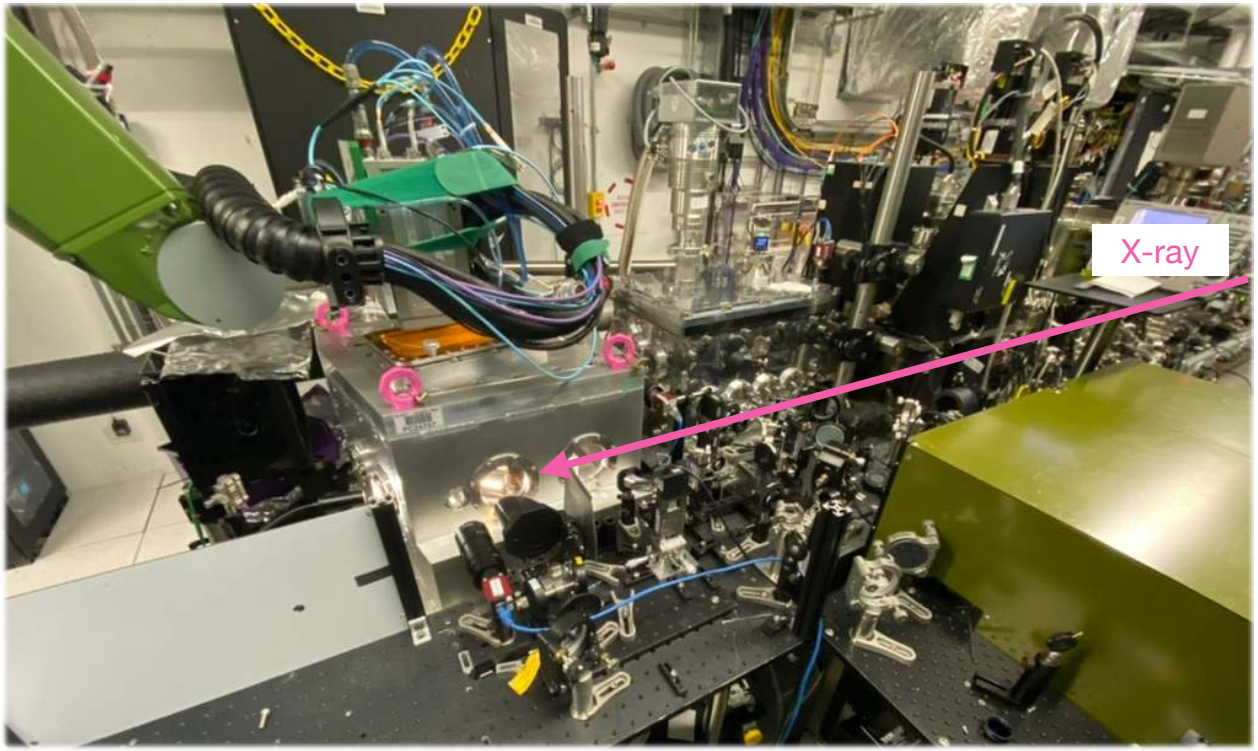
Undulator

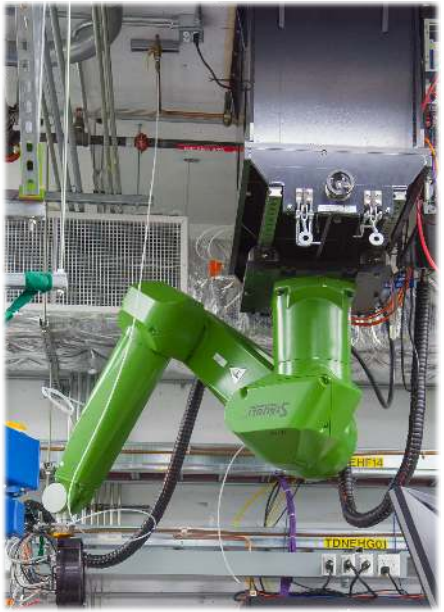


Experimental Hutch

Control Room

Cryogenic Time-resolved Scattering Experimental Setup





Robot Detector

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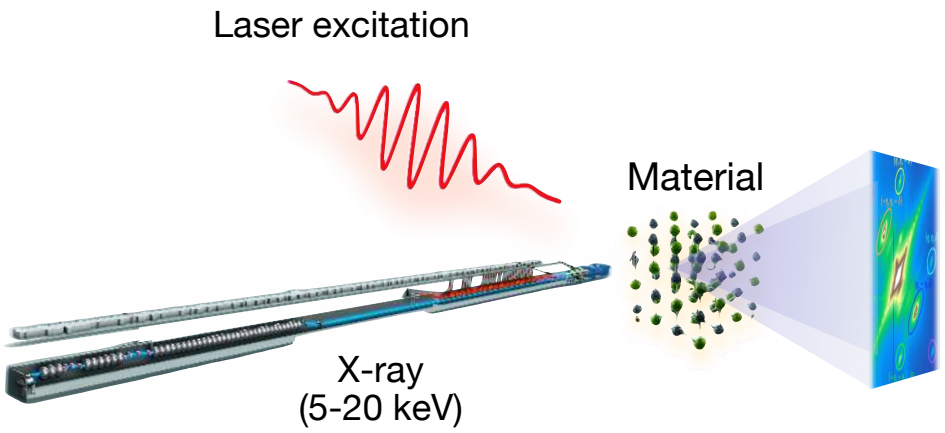
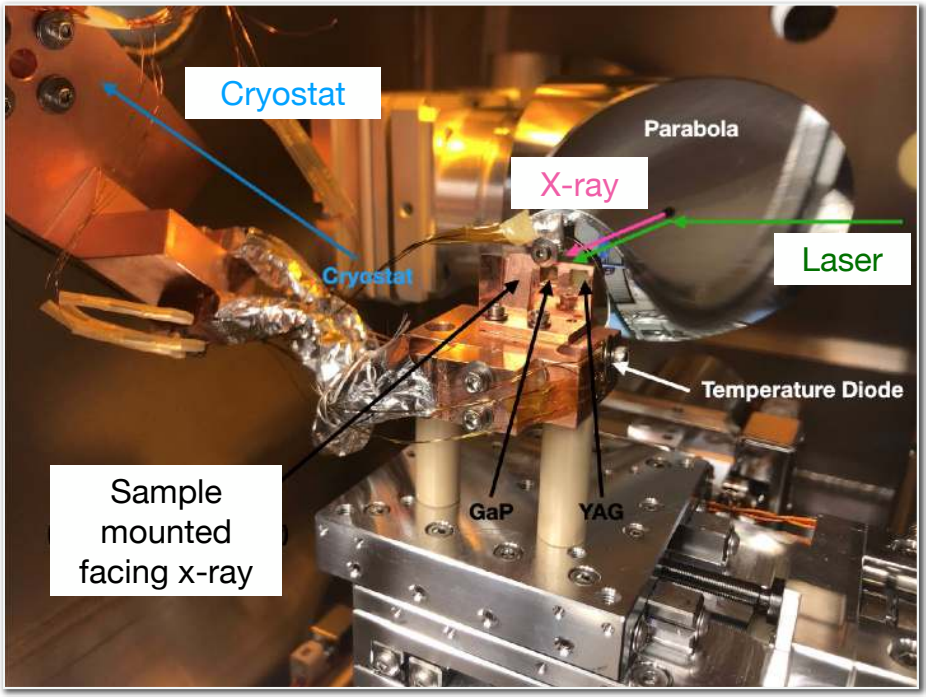
Multidimensional Tuning Parameters to Access Material Properties





Making material movies by varying parameters

- Sample geometry => Momentum range
- X-ray/laser energy
- Time delay
- Temperature

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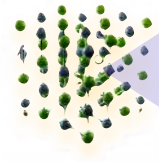
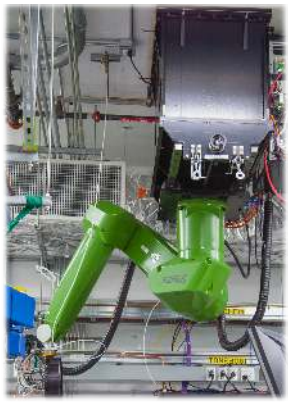
Data Structure

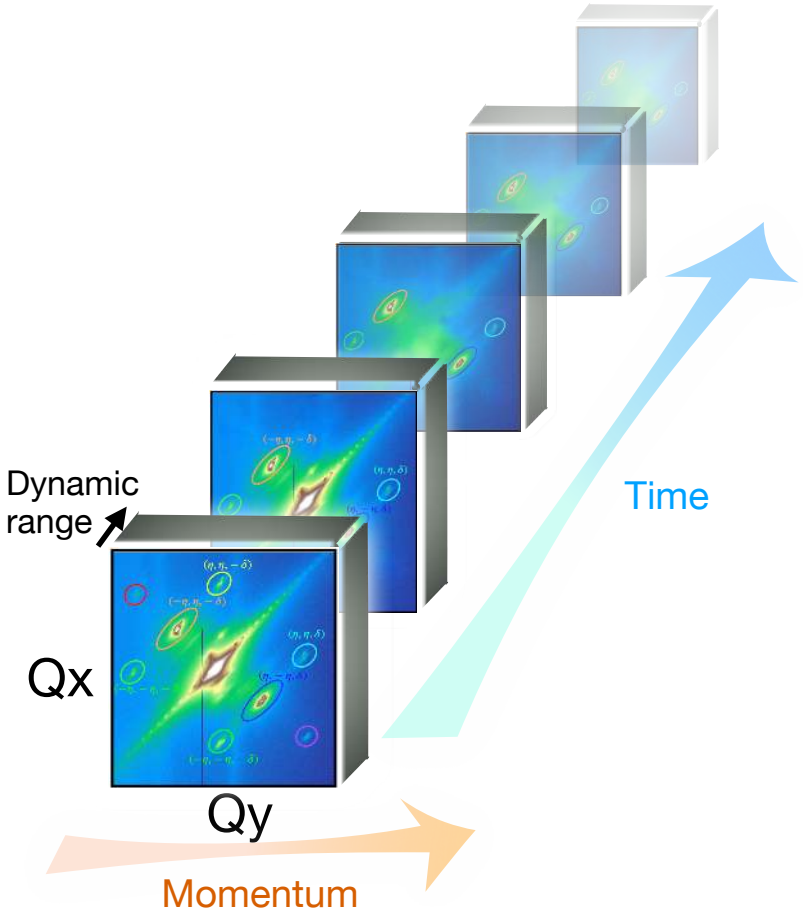


Detector

- 1024 x 512 pixels
- 75 um/pixel
- 120 Hz
- 10 Gps



Multidimensional Data



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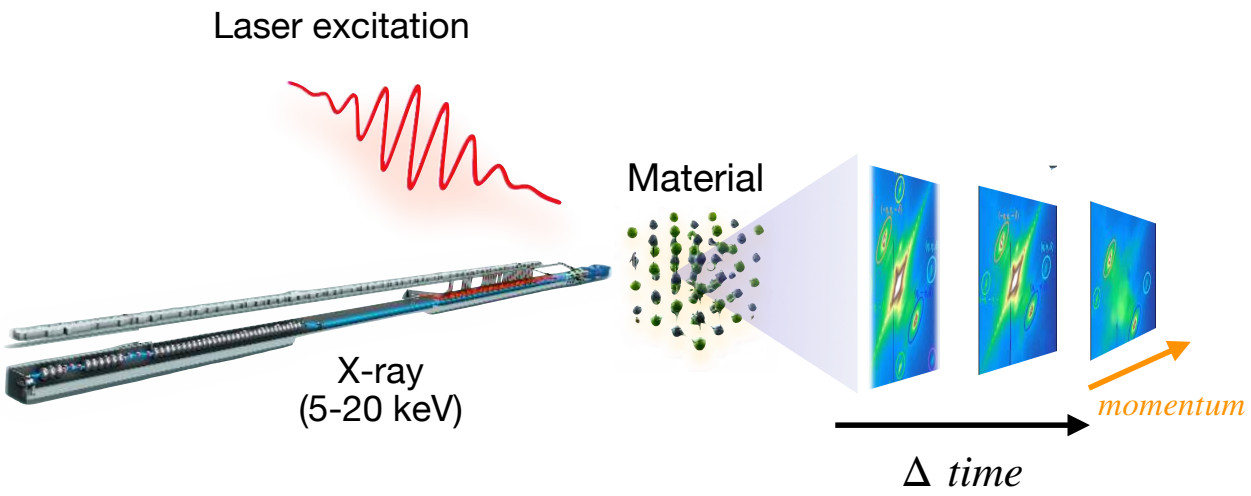
Multidimensional Data Structure



Making material movies by varying parameters

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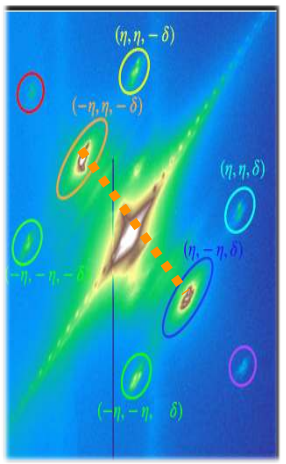
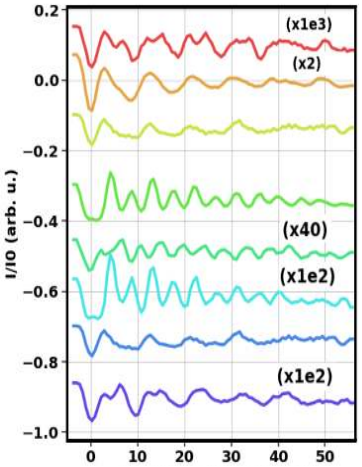
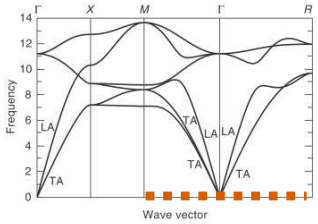
tr-XRD: q-dependence dynamics

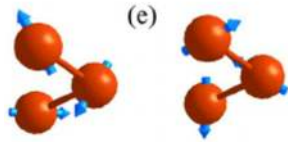


Phonon dynamics

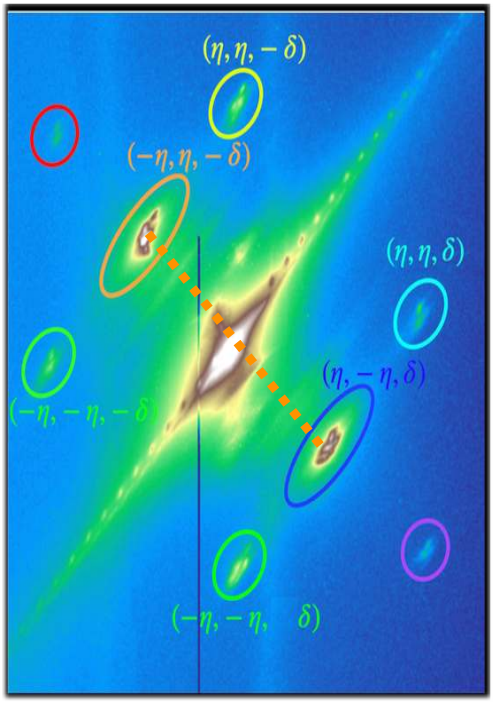




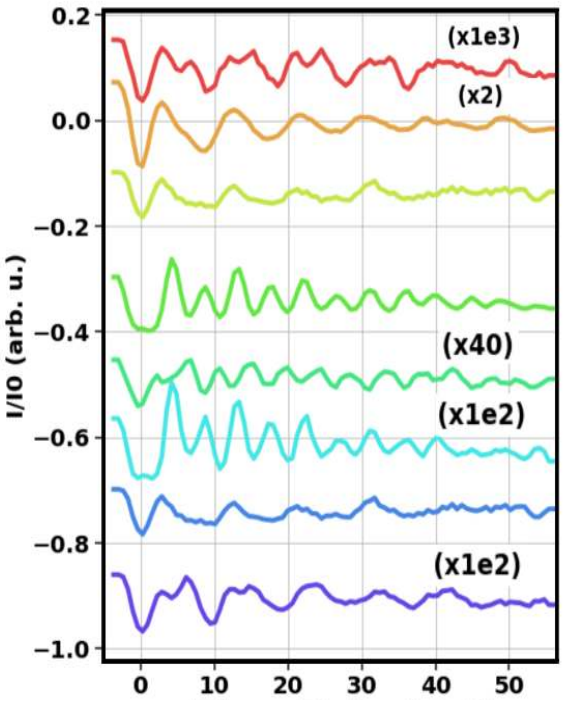
Phonon Dispersion



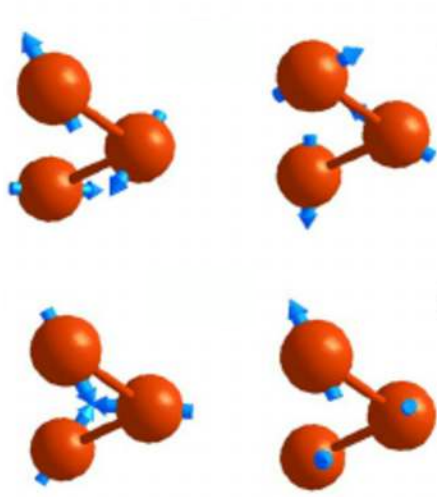
Multidimensional Data Structure



Phonon dynamics



Phonon Modes



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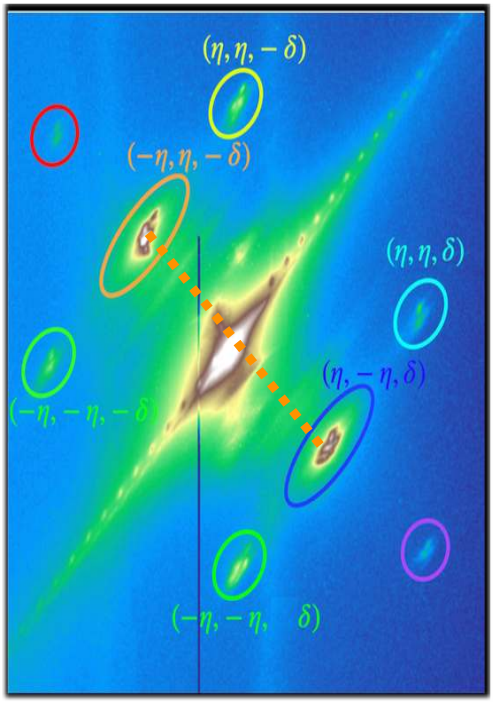
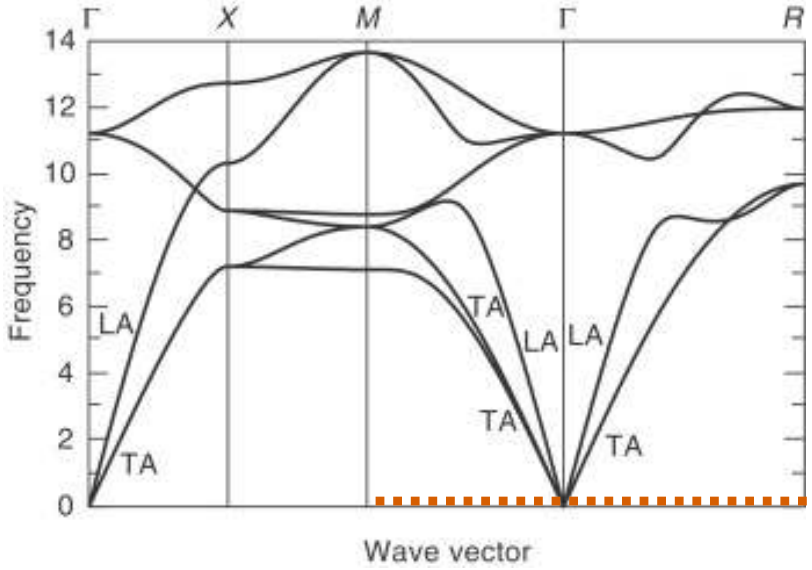
QL Nguyen et al. Physical review letters 131 (7), 076901 (2023)

Multidimensional Data Structure

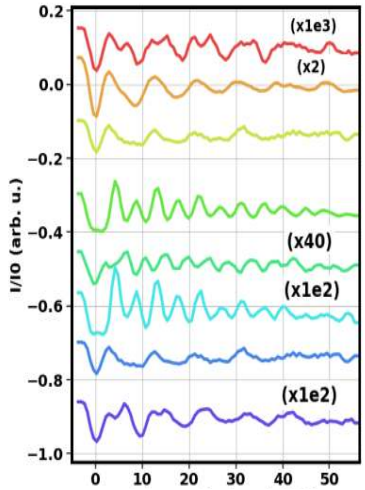


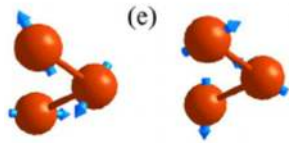
Phonon Dispersion



Fourier Transform

Phonon dynamics





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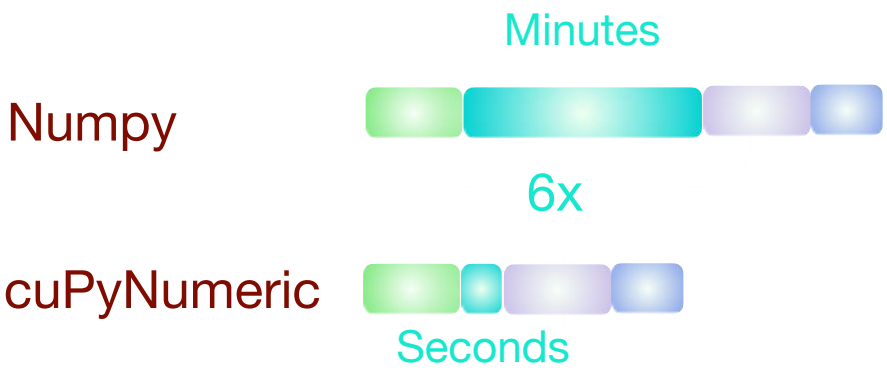
Data analytics with cuPyNumeric



- Extract new scientific insights from massive data at high efficiency
- Enable fast live-feedback for smart experiment steering by speeding up data analytics at 6x

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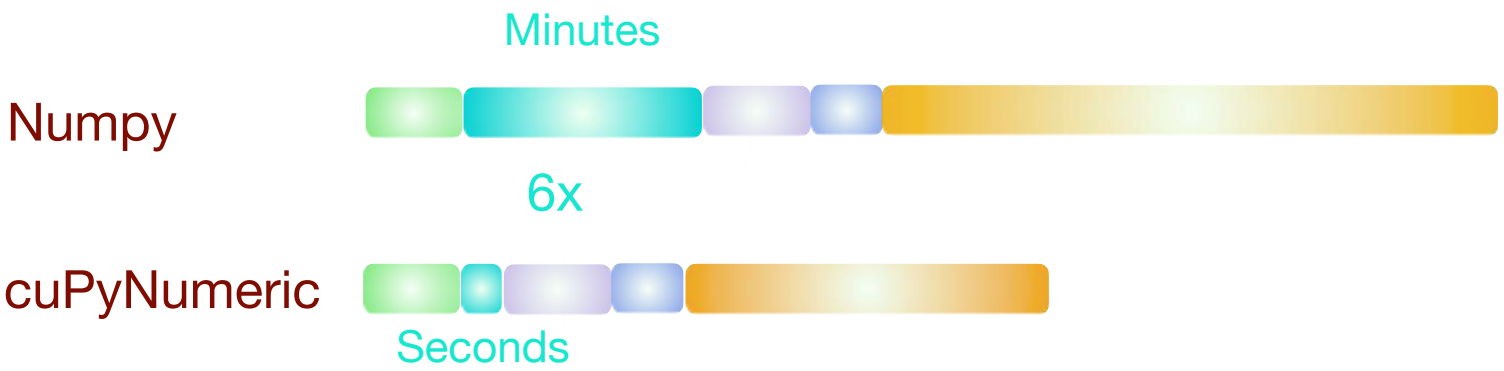
Data analytics with cuPyNumeric



- Extract new scientific insights from massive data at high efficiency
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$B 1-MHz LCLS-II just turned on after 10 years in the making!

SLAC NATIONAL ACCELERATOR LABORATORY

BERKELEY LAB

U.S. DEPARTMENT OF ENERGY | Office of Science

Fermilab

Argonne NATIONAL LABORATORY

Jefferson Lab
Thomas Jefferson National Accelerator Facility

Challenges: Massive Data Generation from Superconducting LINAC

LCLS-II Accelerator

Petabytes

LCLS

Terabytes

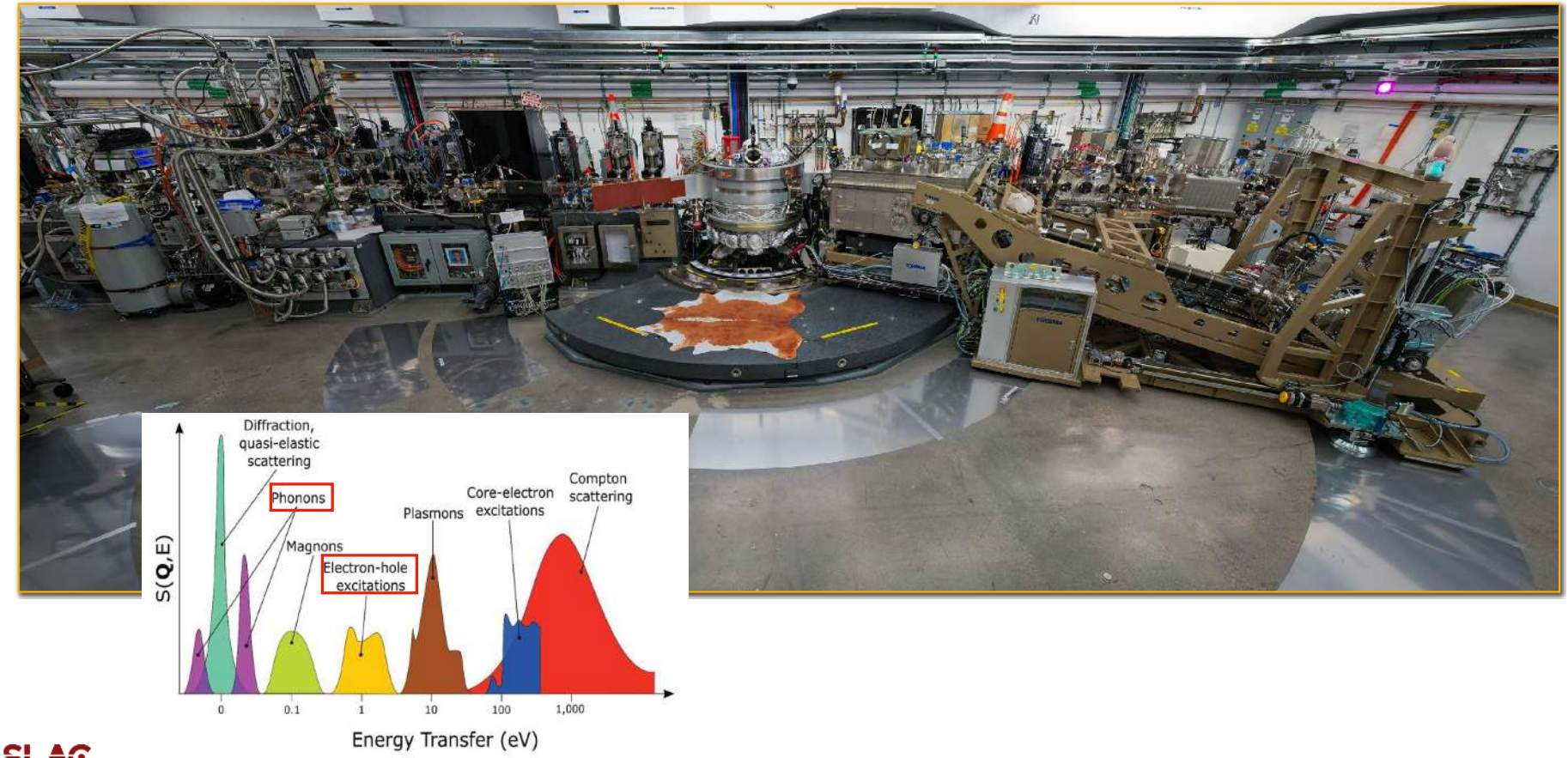
92x football fields

4000/day for life

SLAC

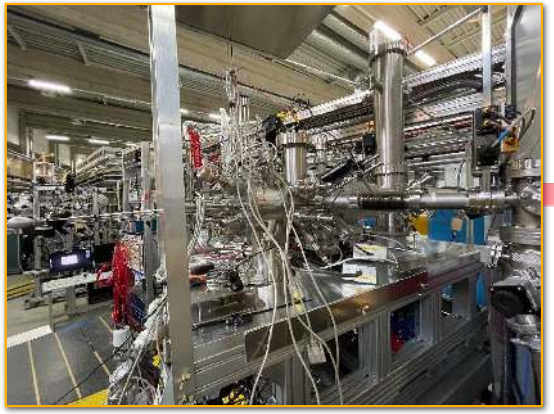
Soft X-ray FEL Probe at LCLS-II

ChemRIXS / Resonant inelastic Xray scattering (qRIXS) Instruments



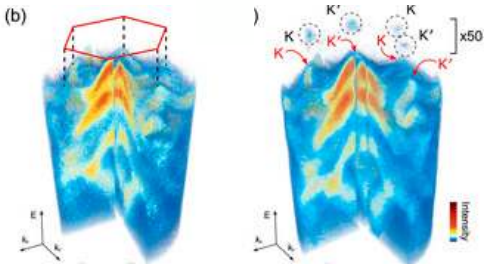
DOE BES Roundtable Report (2017)

Soft X-ray FEL Probe at LCLS-II: roll-in end stations



Momentum Microscope Instrument

Resonant inelastic Xray scattering (qRIXS) Instrument



Pump off Pump on

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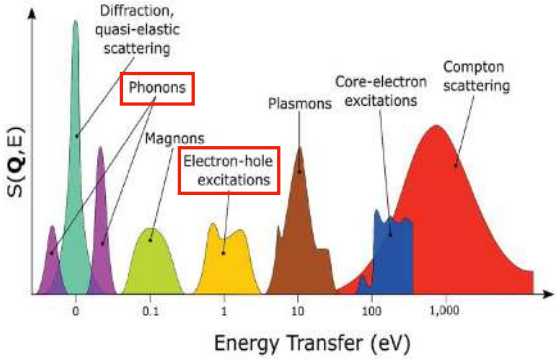

DOE BES Roundtable Report (2017)

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- Seshu Yamajala
- Alex Aiken
- Jana Thayer

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