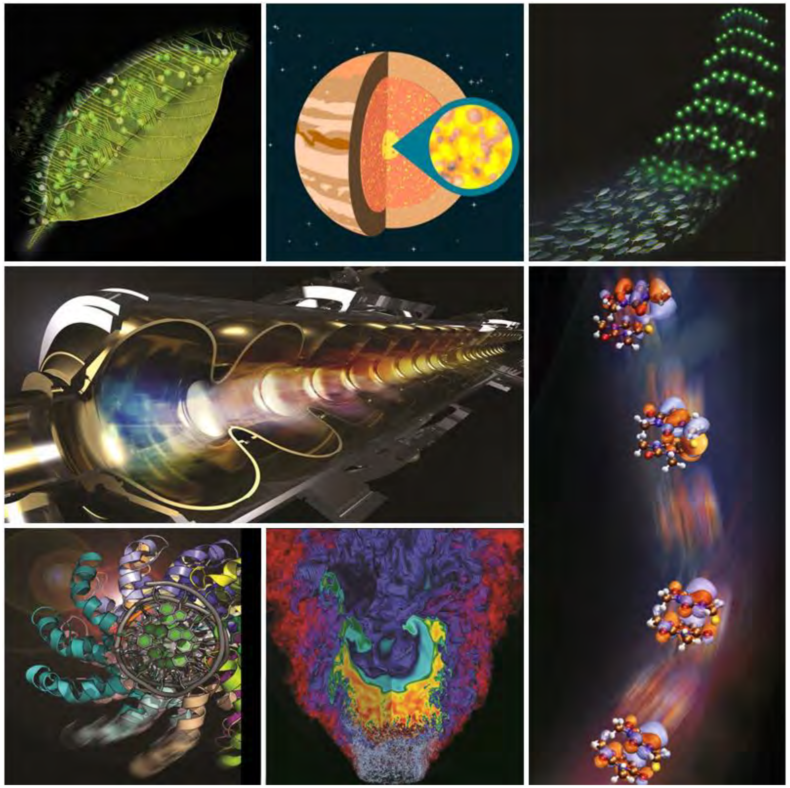
Science Opportunities for the LCLS-II X-ray Lasers

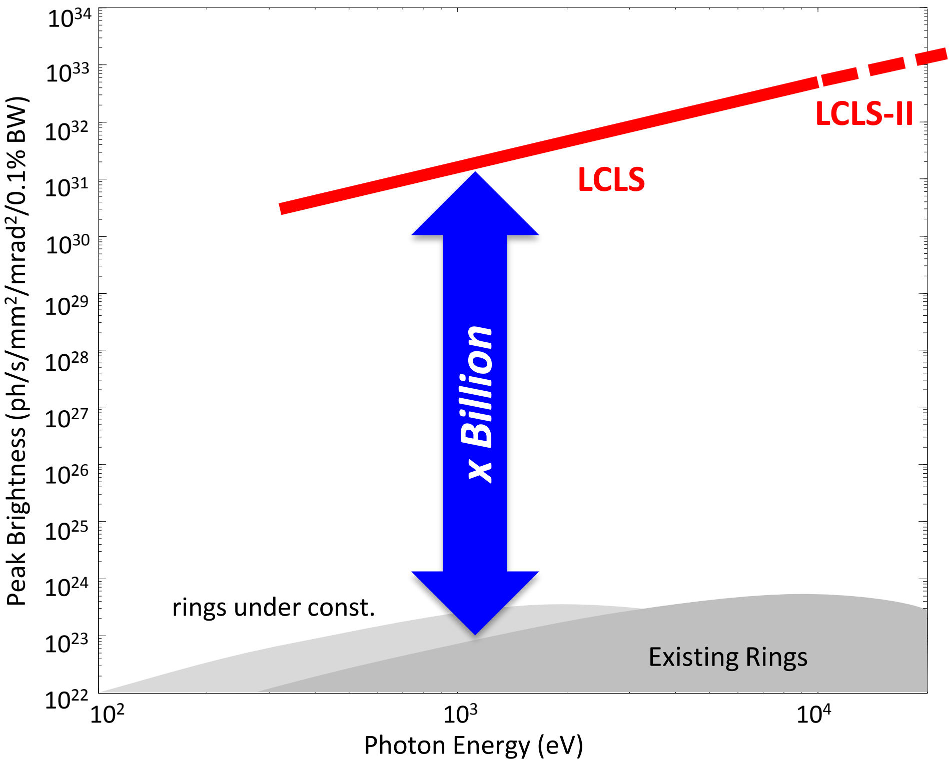


Robert Schoenlein
Jerome Hastings
William Schlotter
Phil Heimann

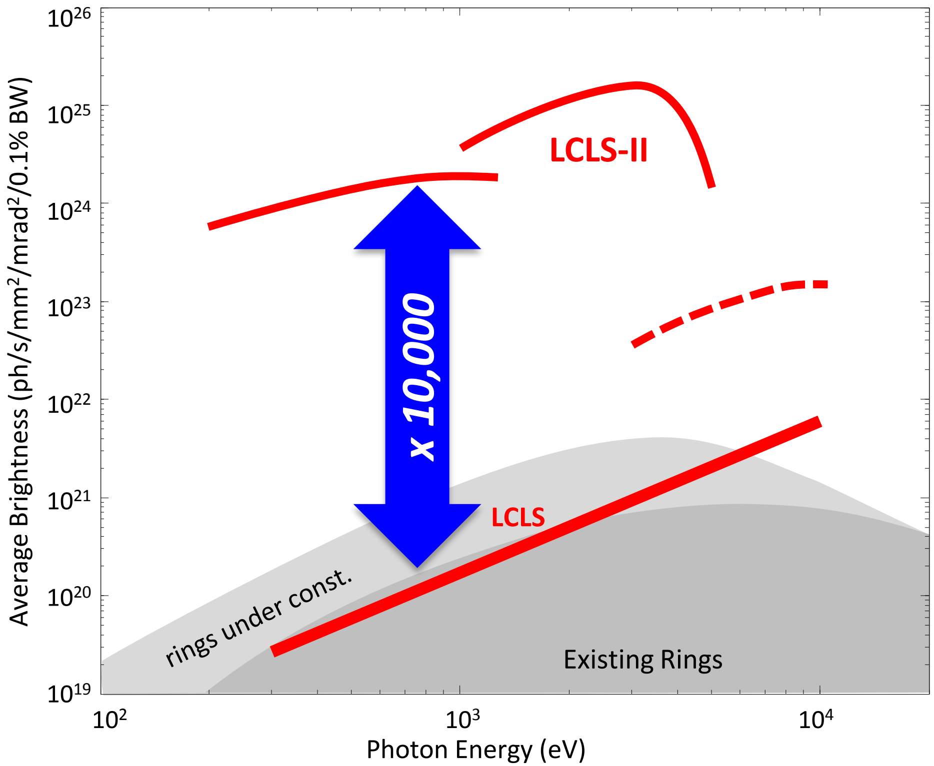
Nobel Symposium on Free Electron Laser Research
June 2015

X-ray FELs: A Revolution in X-ray Science

Peak Power



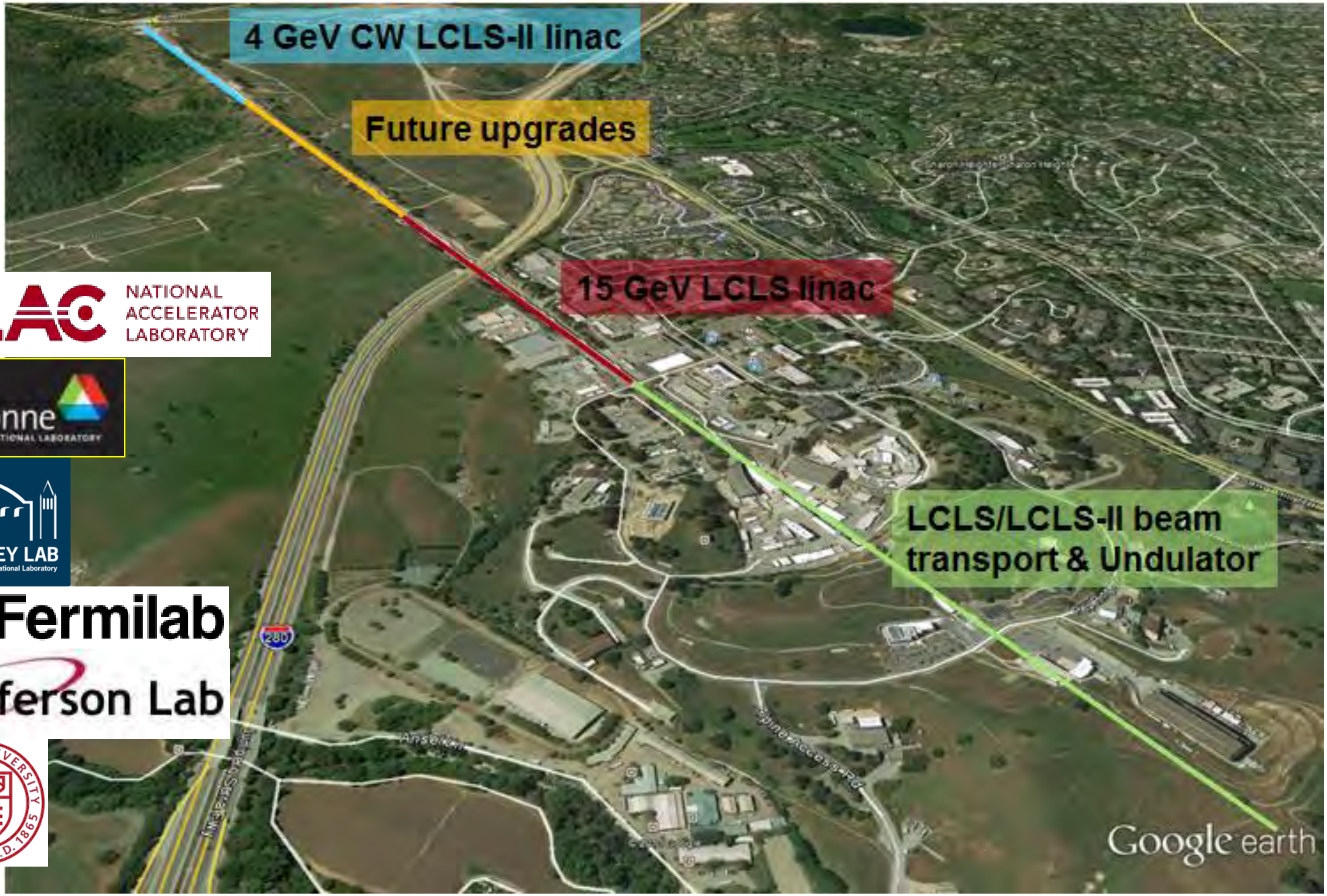
Average Coherent Power – Advanced FELs?



LCLS-II:

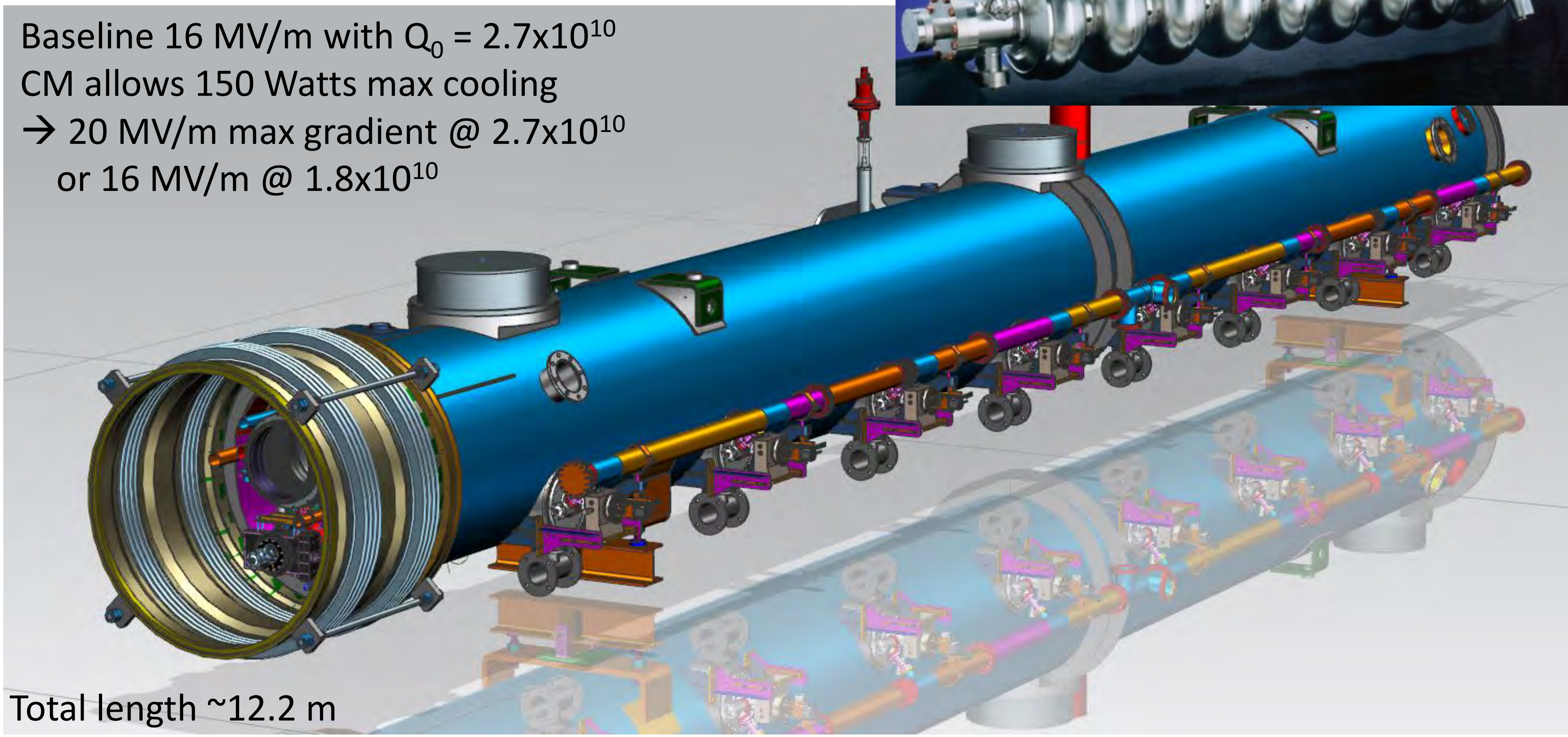
- Repetition rate
- Stability
- Coherence (seeding)
- Photon energy reach

LCLS-II Project
New SCRF linac in 1st km of SLAC linac, Two new tunable undulators



SLAC NATIONAL ACCELERATOR LABORATORY
Argonne NATIONAL LABORATORY
BERKELEY LAB Lawrence Berkeley National Laboratory
Fermilab
Jefferson Lab
Cornell University Founded A.D. 1865

LCLS-II 1.3 GHz Cryomodule
Similar to EuXFEL but modified for *CW RF operation*



Baseline 16 MV/m with $Q_0 = 2.7 \times 10^{10}$
CM allows 150 Watts max cooling
→ 20 MV/m max gradient @ 2.7×10^{10}
or 16 MV/m @ 1.8×10^{10}

Total length ~12.2 m

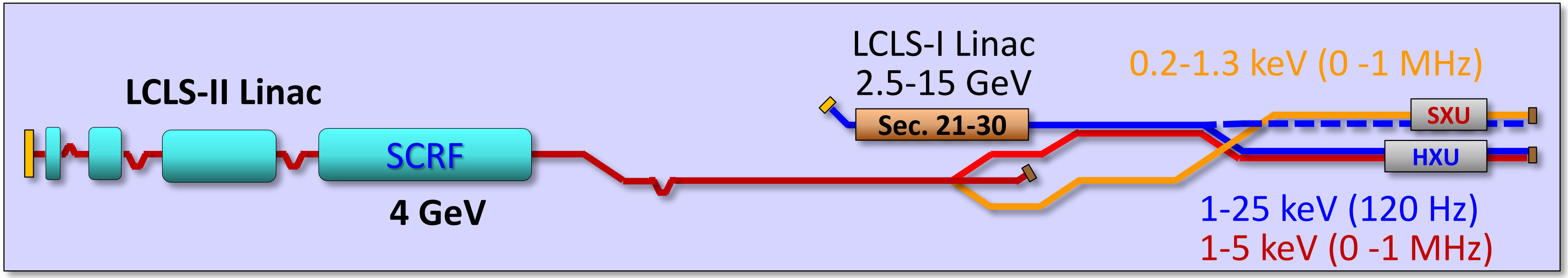
LCLS-II Accelerator Layout

New Superconducting Linac → Two new tunable undulators

- Two sources: high rate SCRF linac and 120 Hz Cu LCLS-I linac
- North (SXU) and South (HXU) undulators can operate simultaneously in any mode

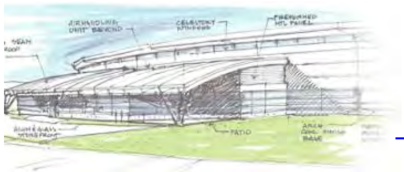
Undulator	SC Linac (up to 1 MHz)	Cu Linac (up to 120Hz)
North SXU	0.20 - 1.3 keV	(potential) >5 mJ 1-3 keV
South HXU	1.0 - 5.0 keV	up to 25 keV higher peak power pulses

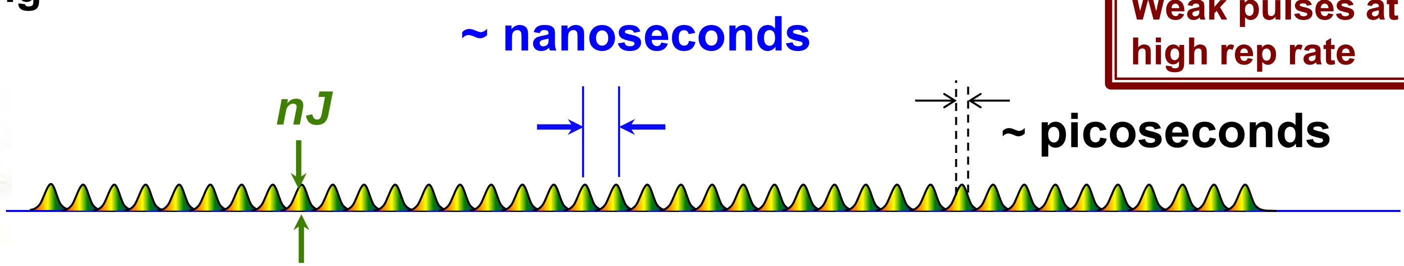
- Concurrent operation of 1-5 keV and 5-25 keV is not possible



Storage Rings and X-ray Lasers

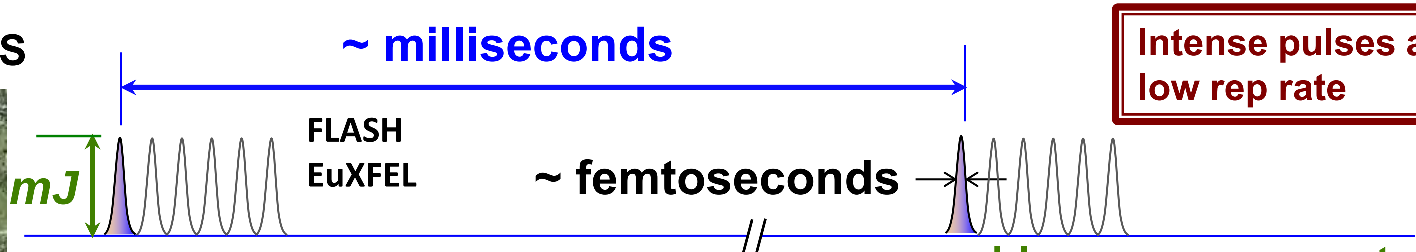
Today's storage ring X-ray sources





Weak pulses at high rep rate

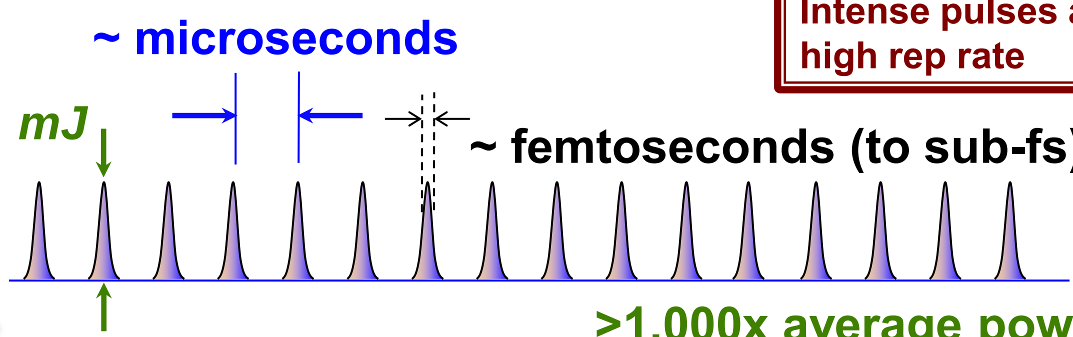
X-ray lasers - LCLS



comparable average power to SR

Intense pulses at low rep rate

2019 LCLS-II

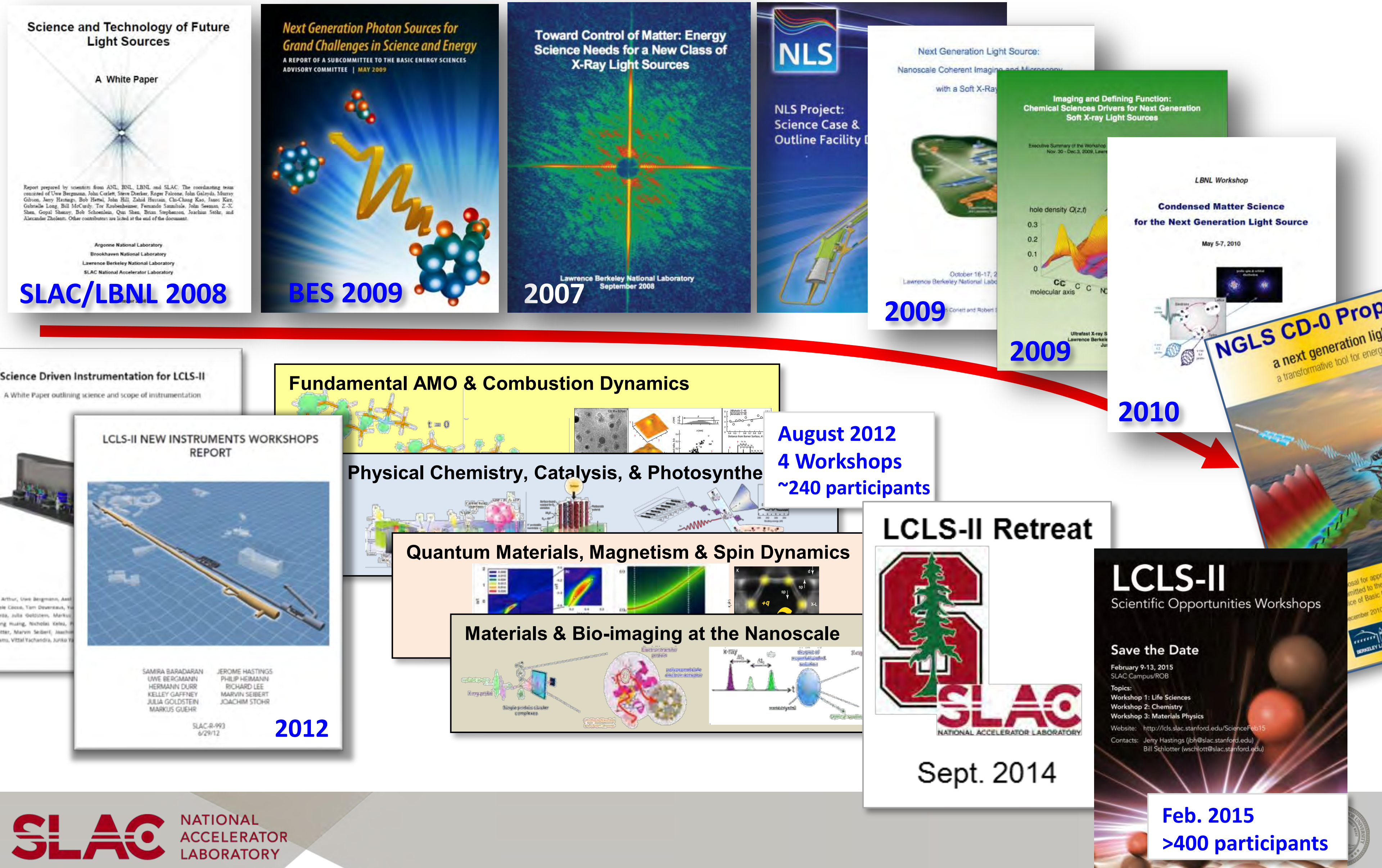


>1,000x average power

Intense pulses at high rep rate

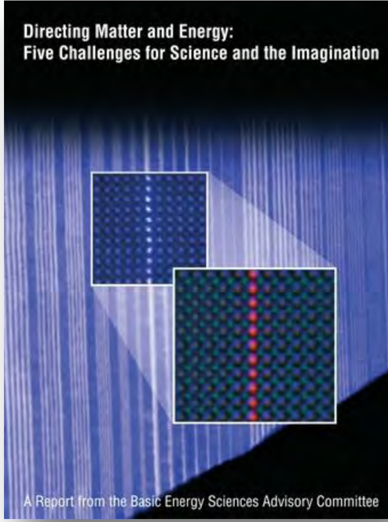
Science Drivers for a High-rep-rate X-ray FEL

Developed and supported by a diverse science community

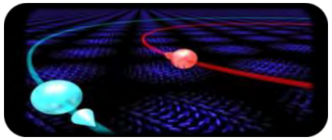


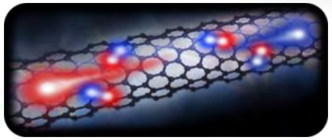
SLAC NATIONAL ACCELERATOR LABORATORY

Five Grand Challenges for Science and the Imagination (2007)

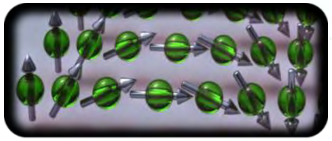


Emergent Properties from Complex Electronic and Atomic Correlations

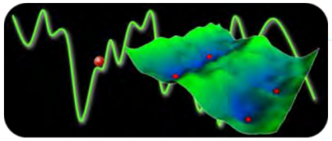




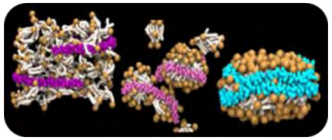
Master Energy and Information on the Nanoscale



Control Matter at the Level of Electrons



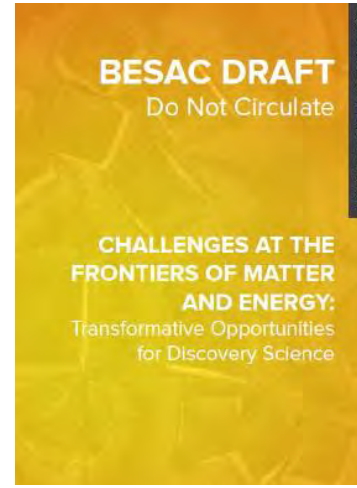
Characterize & Control Systems away from Equilibrium



Directed Synthesis of Matter with Tailored Properties

Instrumentation, Synthesis, People, Resources

Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science (2015)



Beyond Ideal Materials and Systems

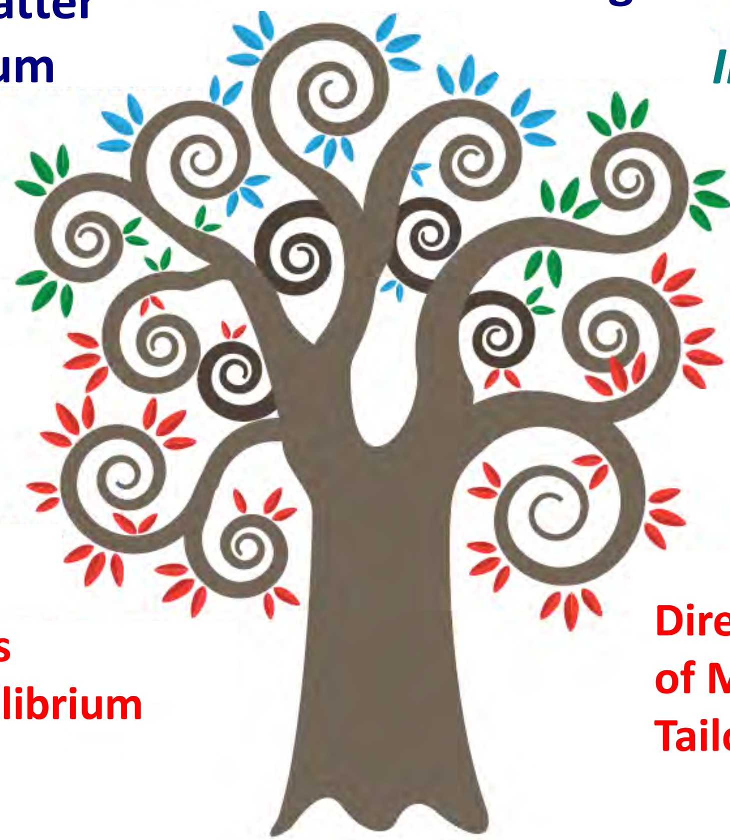
Harnessing Coherence in Light and Matter

Mastering Hierarchical Architectures in Matter Beyond Equilibrium

Imaging Matter across Scales

Emergent Properties from Complex Electronic and Atomic Correlations

Data, Algorithms and Computing



Control Matter at the Level of Electrons

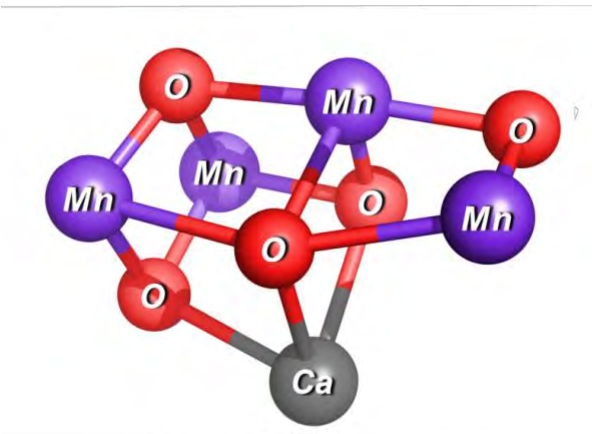
Master Energy and Information on the Nanoscale

Characterize & Control Systems away from Equilibrium

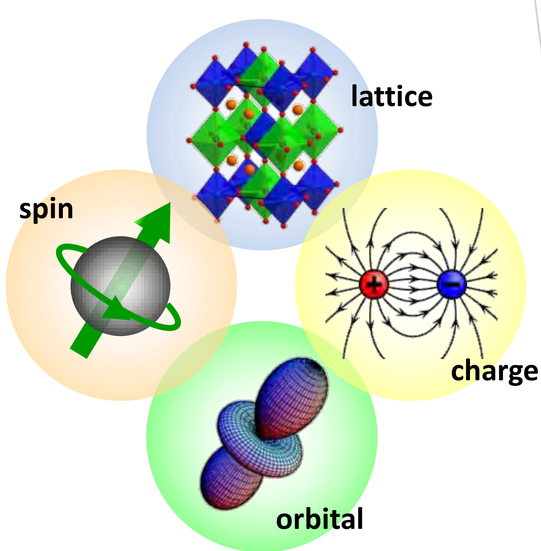
Directed Synthesis of Matter with Tailored Properties

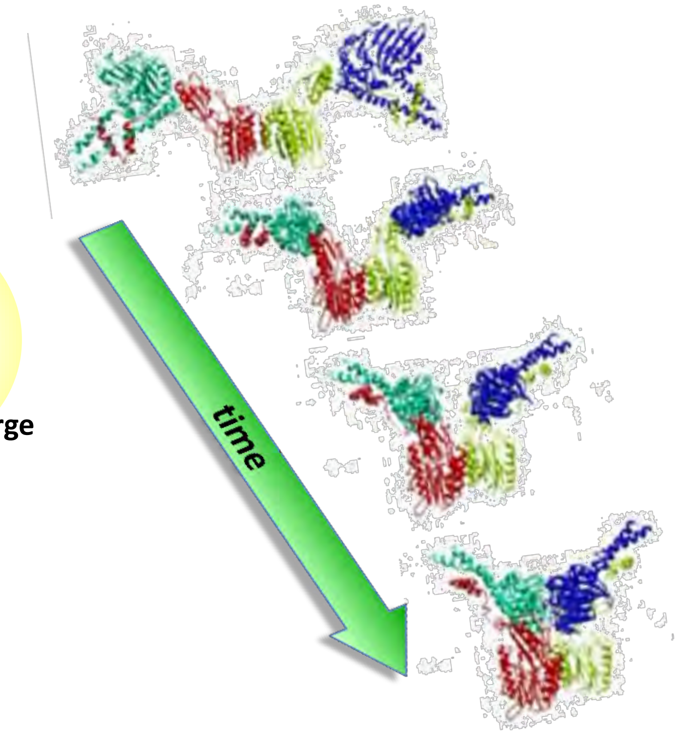
Instrumentation, Synthesis, People, Resources

Underlying questions from the electronic to the mesoscale



O_2 Evolving Catalyst:
Mn_4CaO_5





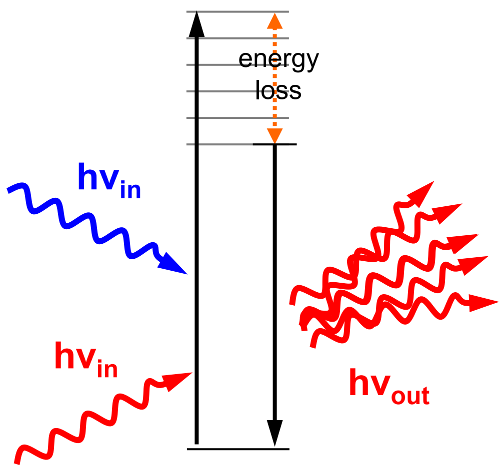
How can we understand the role of correlated electronic degrees of freedom and nuclear displacements in systems like multi-electron catalysts?

How do new material properties emerge from mesoscale ordering & dynamic coupling of charge, spins, & phonons?

How do nanoscale components assemble and operate in functional groupings and can we control this?

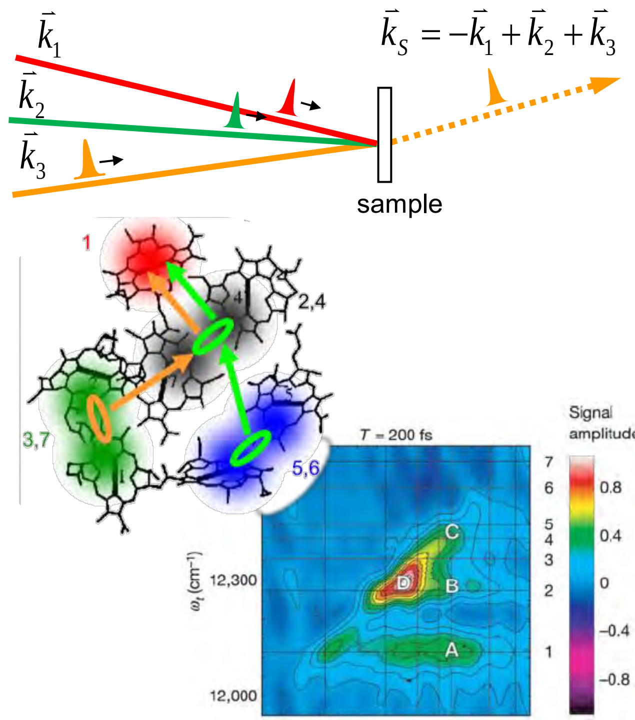
New approaches to interrogating molecules and materials are needed for these questions to be answered

Time-resolved X-ray Raman, stimulated emission



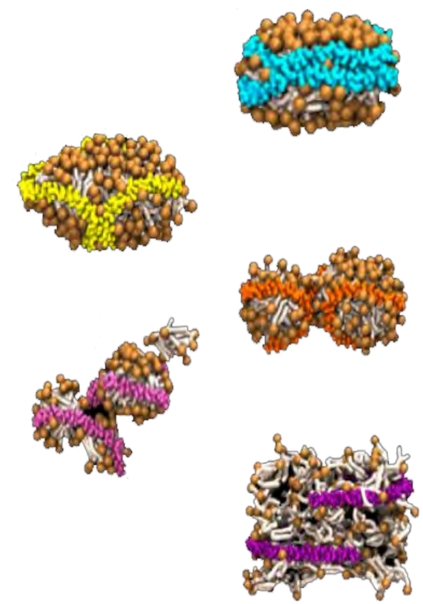
X-ray emission spectrum

Multi-dimensional nonlinear spectroscopy



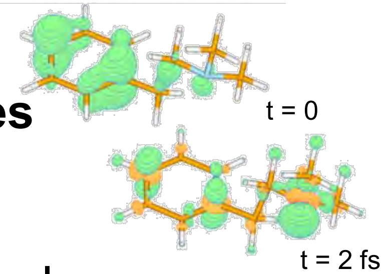
Pump-probe

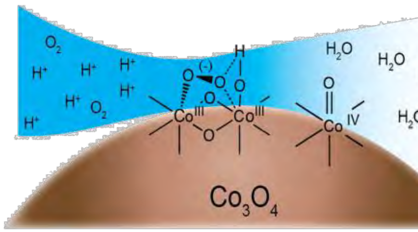
Macromolecular assembly & dynamics



Structure of single molecules

Outline

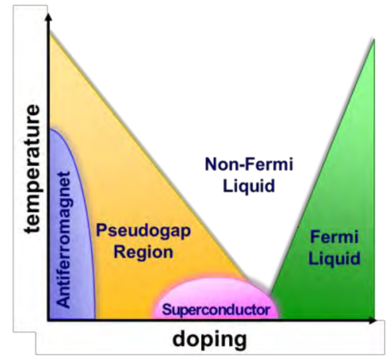




Brief Overview of LCLS-II Science Opportunities

Chemistry - example
- Coupled electronic & nuclear dynamics in molecules

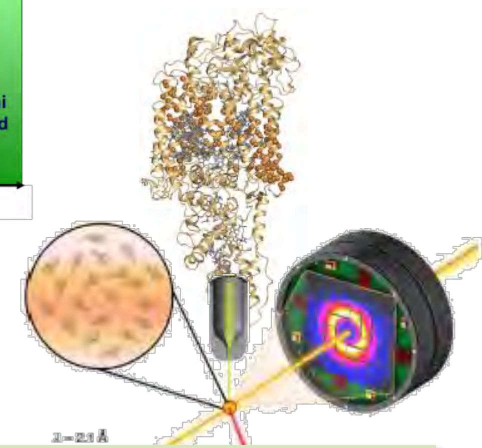
Materials Physics - example
- Emergent phenomena in quantum systems with interacting degrees of freedom



Nanoscale heterogeneity and fluctuations

Life Sciences - example
- Understanding the dynamics of biological complexes & molecular machines

in physiological environments & on natural time scales



LCLS-II Defining Capabilities:

High repetition rate (up to 1 MHz)
- Coherent X-ray power
- Rare events, Heterogeneity (sample entire phase space)

Extended energy range (up to 25 keV)
- Atomic resolution, dynamics, bulk penetration

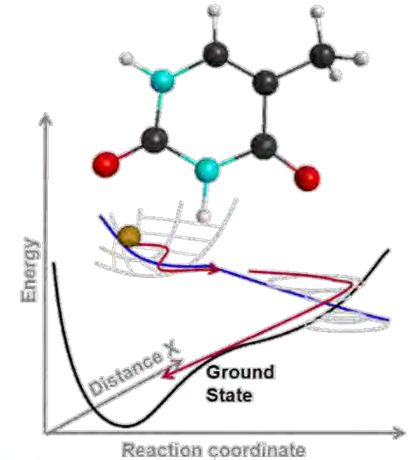
Transform: X-ray spec., scattering, imaging

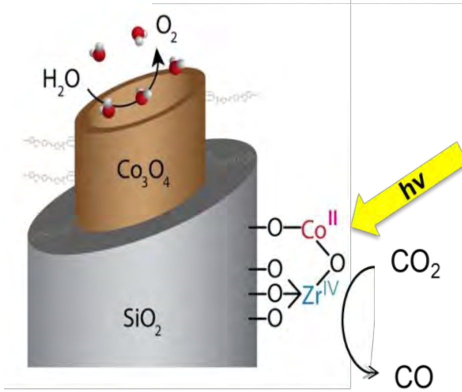
… from demonstration experiments in model systems

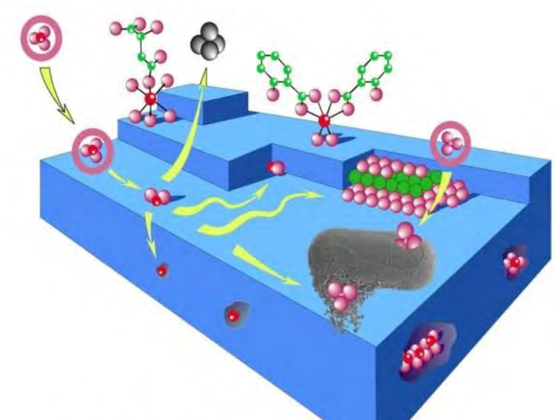
… to high-impact results in relevant systems & environments

Chemistry

- Fundamental charge migration & redistribution
  - Role of quantum coherence & evolution in chemistry
  - Light conversion & non Born-Oppenheimer dynamics
  - Following molecular transformations & bond formation
- Predictive understanding of photo-catalysis
  - Natural & artificial photo-catalytic systems
  - Fundamental light harvesting & charge separation
  - Charge migration channels & processes
  - Oxidation/reduction dynamics
- Heterogeneous catalysis - in real time & *operando*
  - Fundamental surface dynamics (electronic/nuclear) under relevant reaction conditions
  - Interfacial chemistry and charge-transfer in real time & under reactive conditions (environmental chemistry)
- Combustion & aerosol chemistry
  - Spatial, temporal & chemical characterization of reactive flows & byproducts





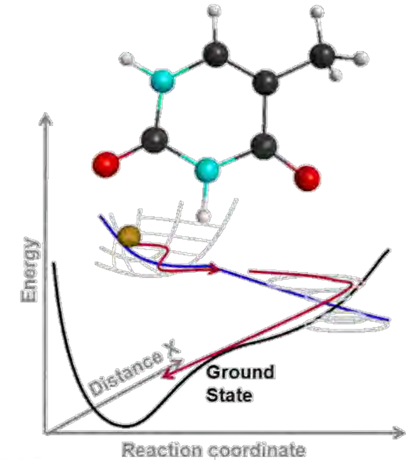


After Manceau et al. (2002)

Chemistry

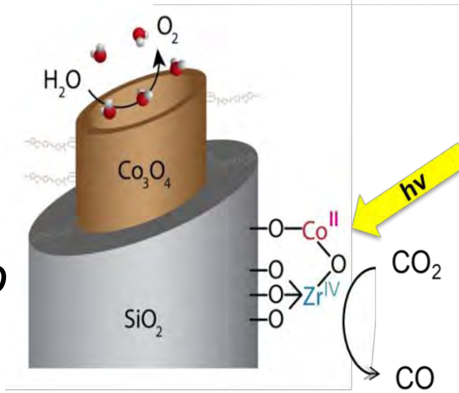
❑ Fundamental charge migration & redistribution

Dynamic reaction microscope	High rep rate
Stimulated X-ray Emission Spec.	Coherence (few fs), 2-color
Time-resolved Photoemission	Soft, tender X-rays
X-ray scattering	Hard X-rays



❑ Predictive understanding of photo-catalysis

Time-resolved X-ray Raman	High rep rate
(X-ray absorption/emission)	Soft, tender X-rays
Time-resolved photoemission	Coherence (FT limit), 2-color

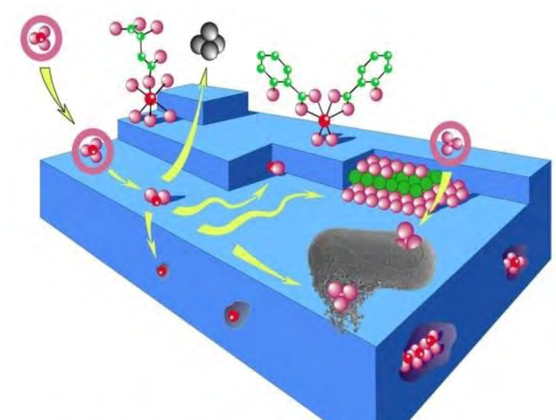


❑ Heterogeneous catalysis - in real time & *operando*

Time-resolved photoemission	High rep rate
(ambient pressure)	Soft, tender X-rays
Res. coherent X-ray scattering	Hard X-rays + soft X-rays

❑ Combustion & aerosol chemistry

Flash tomography	High rep rate
Stimulated X-ray Emission Spec.	Soft, tender X-rays
Coherent X-ray scattering	2-color

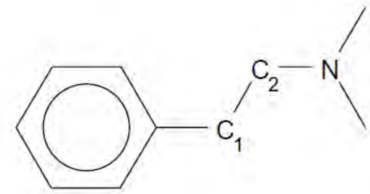


After Manceau et al. (2002)

Understanding coupled electronic & nuclear dynamics is essential to design efficient artificial photosynthetic and catalytic systems

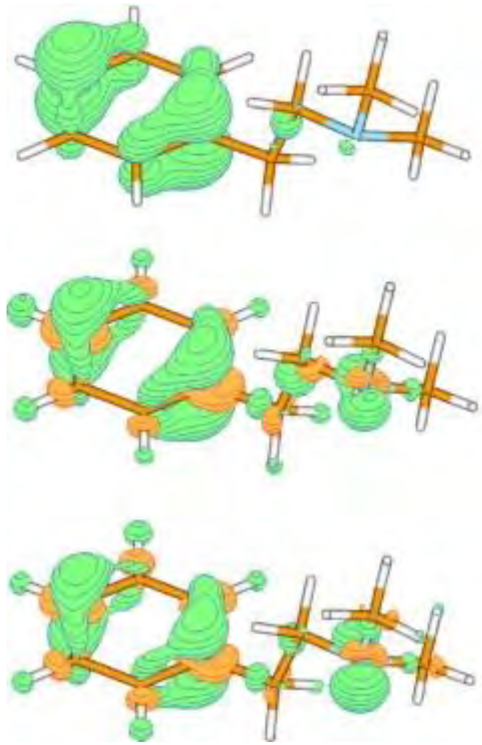
Charge migration is not just the movement of electrons

*The nuclei must also move to localize charge at a new location - **irreversibly***



PENNA chromophore

ground-state geometry



t = 0

t = 2 fs

t = 4 fs

Cederbaum (2008)

LCLS-II Science Opportunity:

- Map electron dynamics on sub-angstrom and sub-femtosecond scales and reveal coupled electronic and nuclear motion in molecules

Significance & Impact

- Charge migration initiates all charge transfer chemistry
- Dynamics on fundamental time scale have been invisible before this

LCLS-II Strengths & Challenges

- Coherent bandwidth and pulse intensity are essential for transient impulsive electronics
- Tunability and 2-color (element selectivity)
- High rep rate for rare events and coincidences

Understanding coupled electronic & nuclear dynamics is essential to design efficient artificial photosynthetic and catalytic systems

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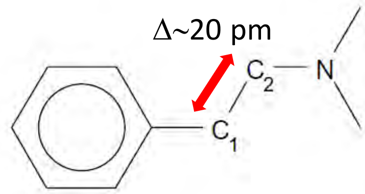
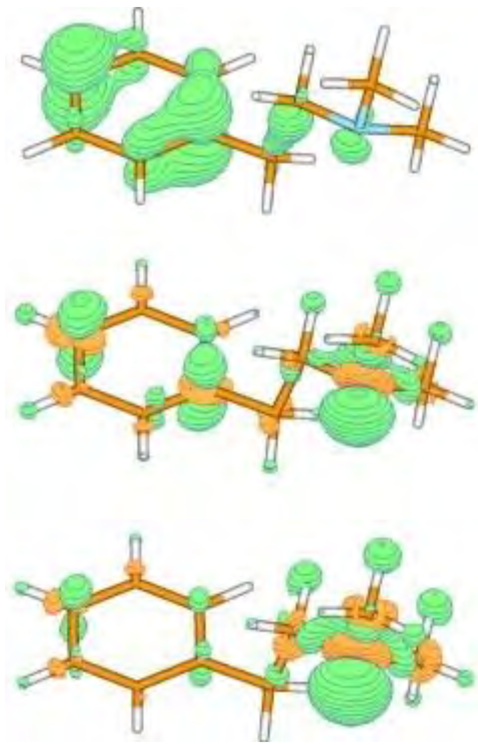


PENNA chromophore

excited-state geometry



Cederbaum (2008)

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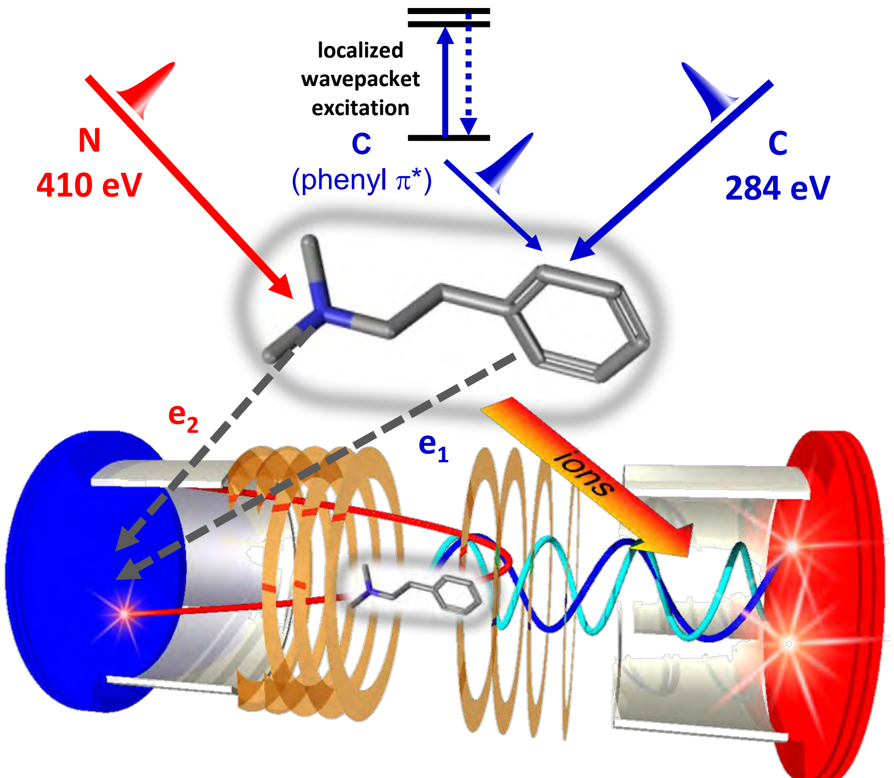
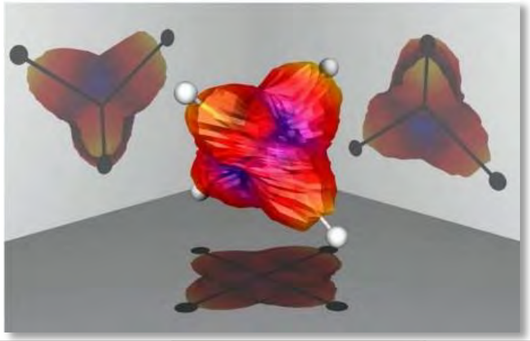
Example: X-ray FEL studies of dynamics in molecules

Dynamic Molecular Reaction Microscope for Coincidence Imaging

- Entanglement & correlation dynamics in many electron/nuclei systems
- Time-resolved energy & angular correlations between electrons & ions
- 2-color X-ray pump/probe is chemical/element specific
- Rare coincidence events ($\sim 10^{-5}$) $\Rightarrow$ high repetition rate



measures energy & momentum of electrons & ions



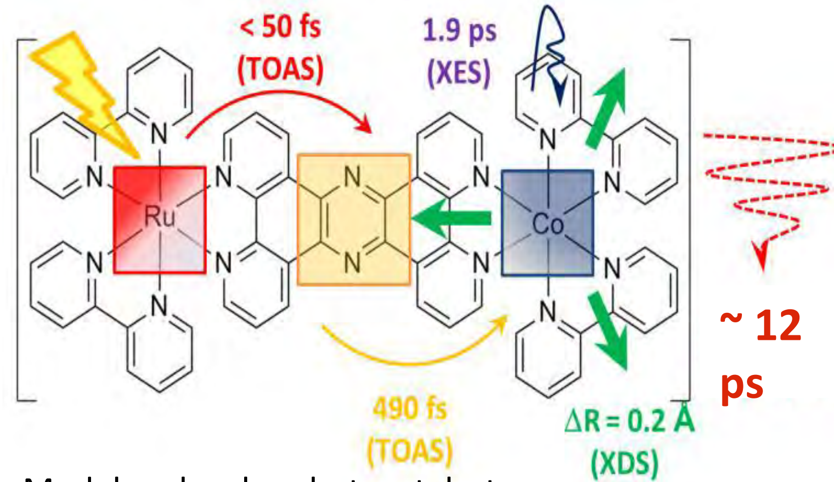
Ground-state electron distribution in molecular frame measured via coincidence

Deeper Understanding of Multi-electron Photo-catalysts

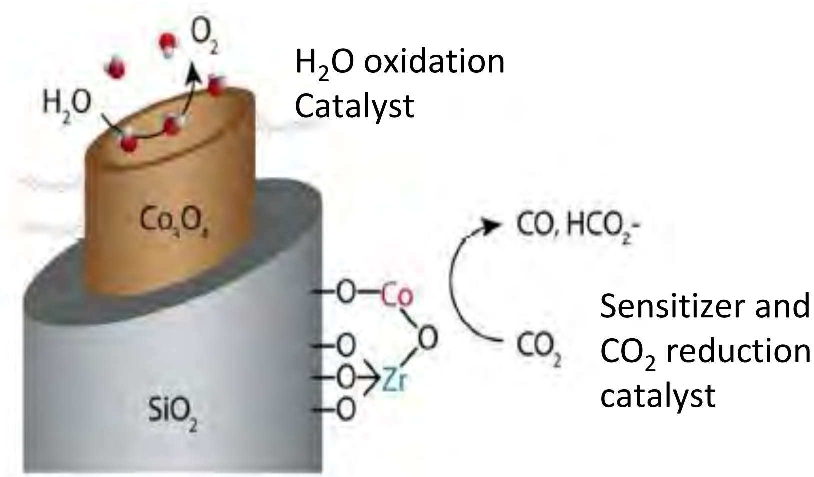
LCLS-II Science Opportunity:
- Map charge separation, transport & accumulation on fundamental time scales
- Element/chemical specificity
- Evolution of molecular orbitals, bonds, & relation to atomic structure

Significance & Impact
- Detailed insight will advance theory & inform synthesis efforts
- Efficient, robust, selective photo-catalysts
- Based on earth-abundant elements

LCLS-II Strengths & Challenges
- High average power at high rep rate (moderate peak power)
- Ultrafast time resolution
- Tunability & energy resolution near the transform limit
- 2D maps of evolving electronic structure under operating conditions



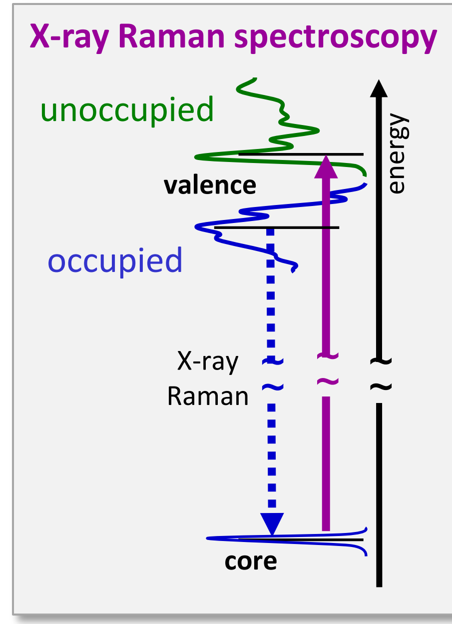
Model molecular photocatalyst
V. Sundström et al. *Nature Comm*. **6**, 6359 (2015)



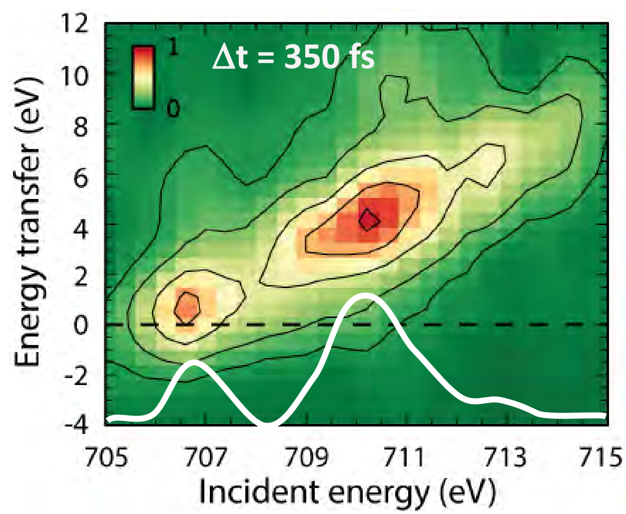
Inorganic water oxidation catalysts
H. Frei et al. *Nature Chem*. **6**, 362 (2014)

Example: X-ray Raman Studies of Molecular Dynamics

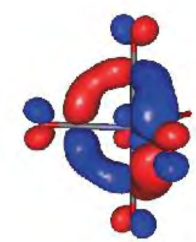
Ultrafast X-ray Raman Spectroscopy
(resonant inelastic X-ray scattering – RIXS)



- ❑ Soft X-ray RIXS maps frontier molecular orbitals & their evolution
- ❑ Element-specific: transition-metals & ligands
- ❑ Local chemical structure & bonding
- ❑ Current limitations:
  - Sensitivity - observe only large molecular changes, in model complexes, at high concentrations
  - Time/energy resolution - not at Fourier limit
  - Limited time information - average X-ray flux (rep rate)



$^1Fe(CO)_5^*$

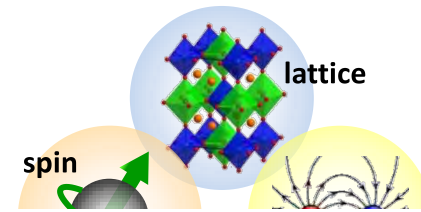


Fe 3*d* → CO π*

MLCT excitation

P. Wernet et al., *Nature*, 520, **78** (2015)

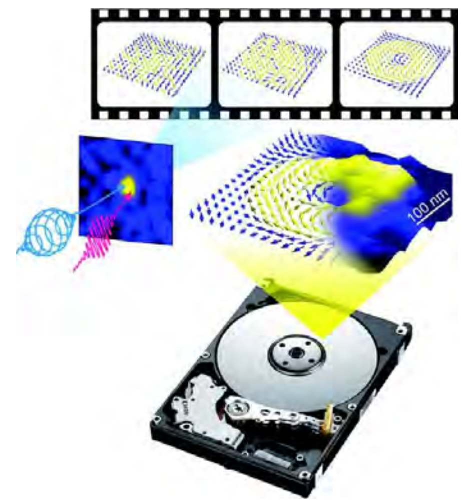
Materials Physics



- ❑ Understand & cc systems with inte
  - Unconventional
  - 2D materials & i
  - Transient fields
- ❑ Understand & cc at fundamental l
  - Spintronics at T
  - Emergence of n
  - Spin textures &
  - Disentangling/cc
- ❑ Nanoscale heter
  - Electronic, chen
  - Metastable mate
  - Energy conversi

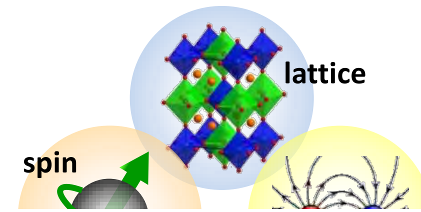
Emergence of magnetic order at ultimate length- & timescales

- **Science Challenge/Opportunity**
  - –Microscopic mechanism & transient states leading to all-optical switching are not understood
  - –Control magnetic interactions to generate topologically protected nanoscale spin textures
  - –Observe non-local nanoscale angular momentum exchange
  - –Observe spin-lattice angular momentum exchange
- **Significance & Impact**
  - \- Fundamentally: how does order emerge out of disorder?
  - -Technologically: what is the ultimate magnetic data storage & logic?
- **LCLS-II Strengths & Challenges**
  - –Probing spin dynamics at the exchange length (<10nm) and timescales (~10fs) with *high-resolution imaging and scattering*
  - –Probing lattice angular momentum (phonons)



Magnetism & Spin

Materials Physics



- ❑ Understand & cc
  systems with inte

  Time & momentum
  Time-resolved hard
  Time-, spin-, imaging

- ❑ Understand & cc
  at fundamental l

  Time-resolved X-ray
  Coherent, resonant
  Hard X-ray photoem

- ❑ Nanoscale heter

  X-ray photon correla
  X-ray scattering
  THz pump/X-ray pro

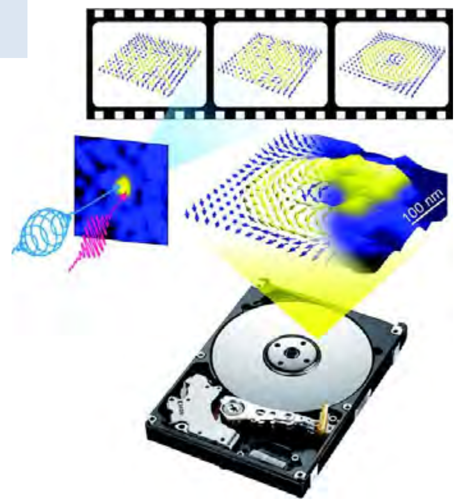
Emergence of magnetic order at ultimate length- & timescales

High rep rate
Soft, tender, hard (3ω) X-rays
Coherence (FT limit)

- **Science Challenge/**
  - –Microscopic mechanism &
    switching are not underst
  - –Control magnetic interactions to generate topologically protected nanoscale spin textures
  - –Observe non-local nanoscale angular momentum exchange
  - –Observe spin-lattice angular momentum exchange

- **Significance & Impact**
  - \- Fundamentally: how does order emerge out of disorder?
  - -Technologically: what is the ultimate magnetic data storage & logic?

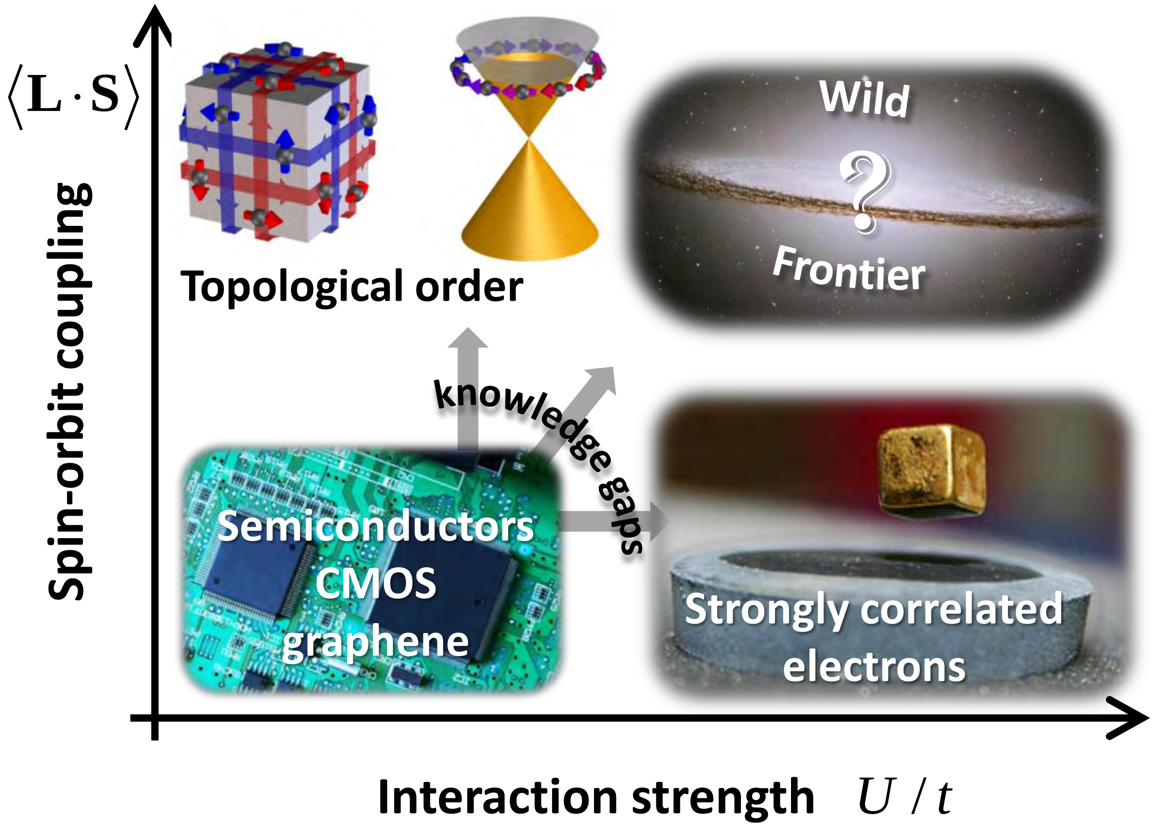
- **LCLS-II Strengths & Challenges**
  - –Probing spin dynamics at the exchange length (<10nm) and timescales (~10fs) with *high-resolution imaging and scattering*
  - –Probing lattice angular momentum (phonons)



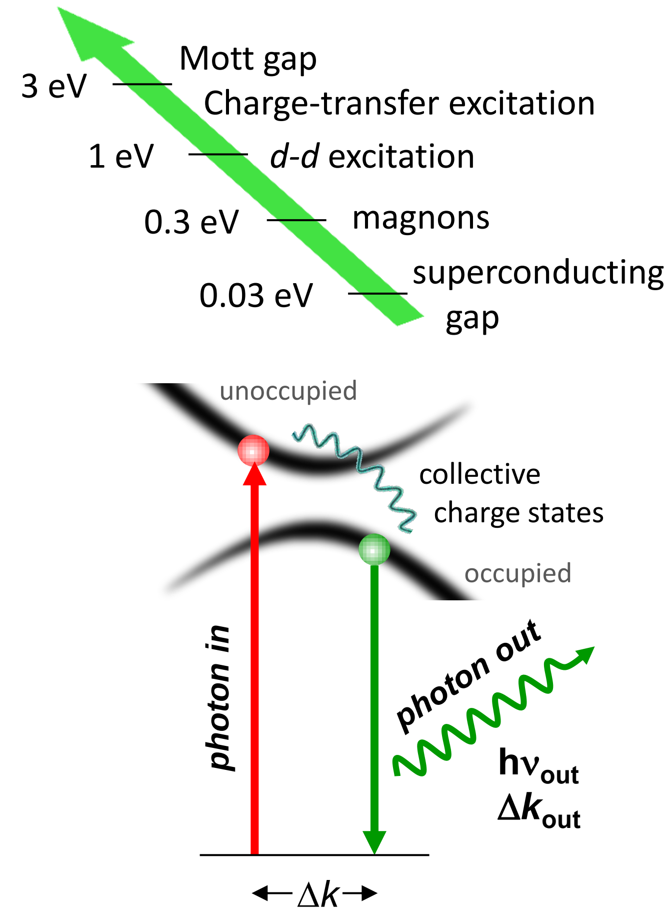
Magnetism & Spin

Understanding Emergent Properties in Complex Materials

Resonant Inelastic X-ray Scattering (RIXS) X-ray Raman
$\Rightarrow$ density-density correlation function: $S(\boldsymbol{q},\omega)$



Collective Modes in Complex Materials



Example: Emergent Properties in Complex Materials

RIXS (X-ray Raman) & Dynamic RIXS – Driven Emergent Properties

LCLS-II Science Opportunity:

- ***High-resolution*** RIXS probes critical collective charge modes (element specific)
- ***Dynamic*** RIXS reveals response of collective modes to control fields and tailored excitations (60 fs ⇔ 30 meV)
  - ***- light-induced superconductivity***
  - ***- vibrationally-driven ins./metal transition***

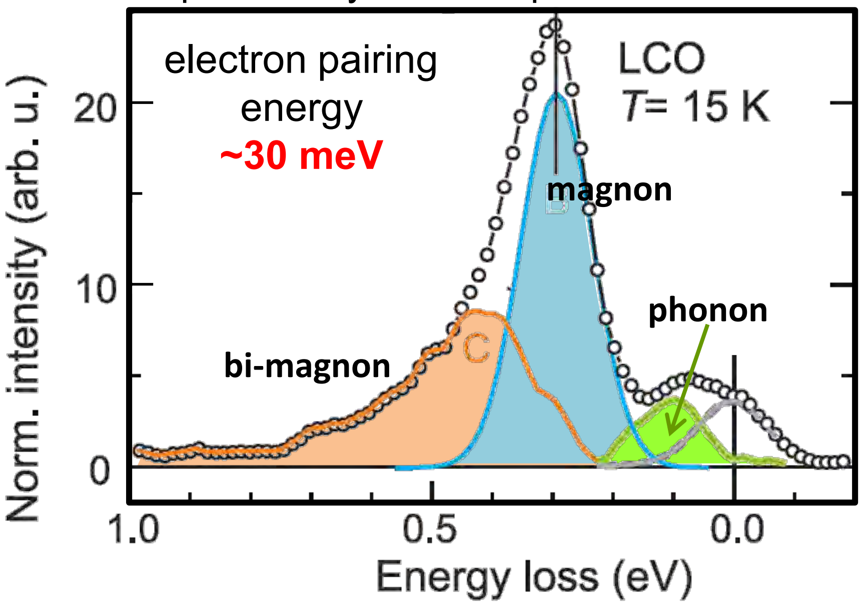
Significance & Impact

- Detailed insight will advance theory & inform synthesis efforts
- Toward control of emergent properties

LCLS-II Strengths & Challenges

- High average power at high rep rate (moderate peak power)
- Coherence (energy resolution) near the transform limit
- Ultrafast time resolution
- 2D maps of collective mode dynamics

Cuprate X-ray Raman Spectrum



Present Limitations:

- Energy resolution
- Momentum Resolution
- Dynamics

Example: Emergent Properties in Complex Materials

RIXS (X-ray Raman) & Dynamic RIXS – Driven Emergent Properties

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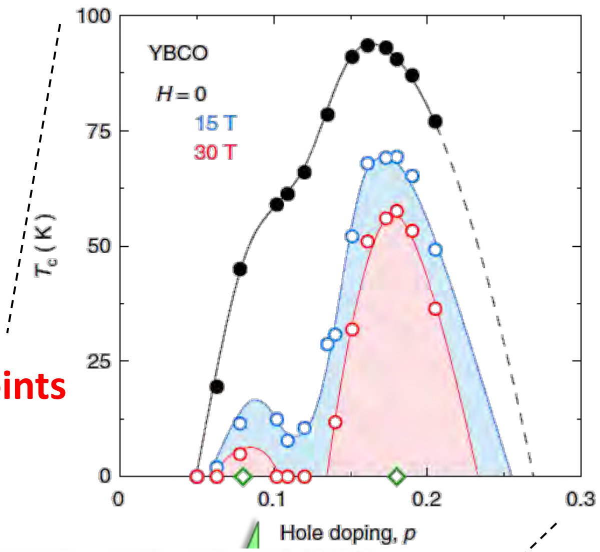
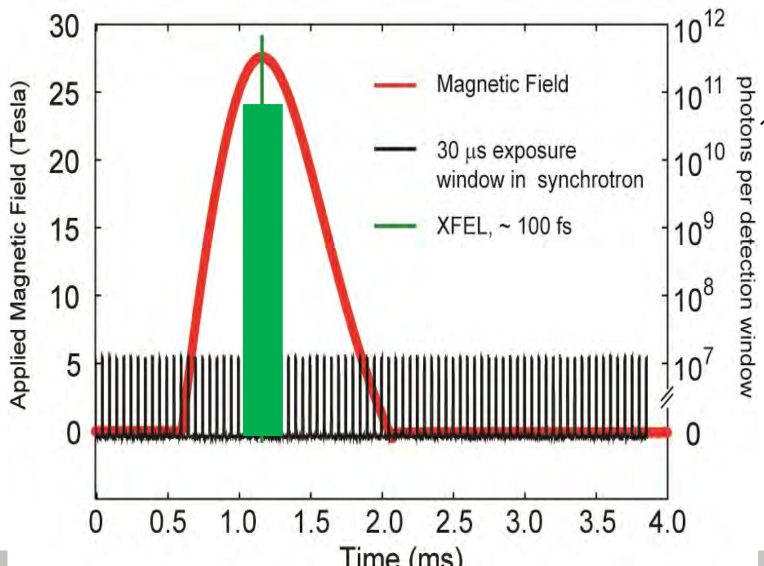
- Coherence (energy resolution) near the transform limit
- Ultrafast time resolution
- 2D maps of collective mode dynamics

- **Phase competition**
- **Quantum critical points**

Conductivity - Superconducting Dome





Example: Emergent Properties in Complex Materials

RIXS (X-ray Raman) & Dynamic RIXS – Driven Emergent Properties

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LCLS-II Strengths & Challenges

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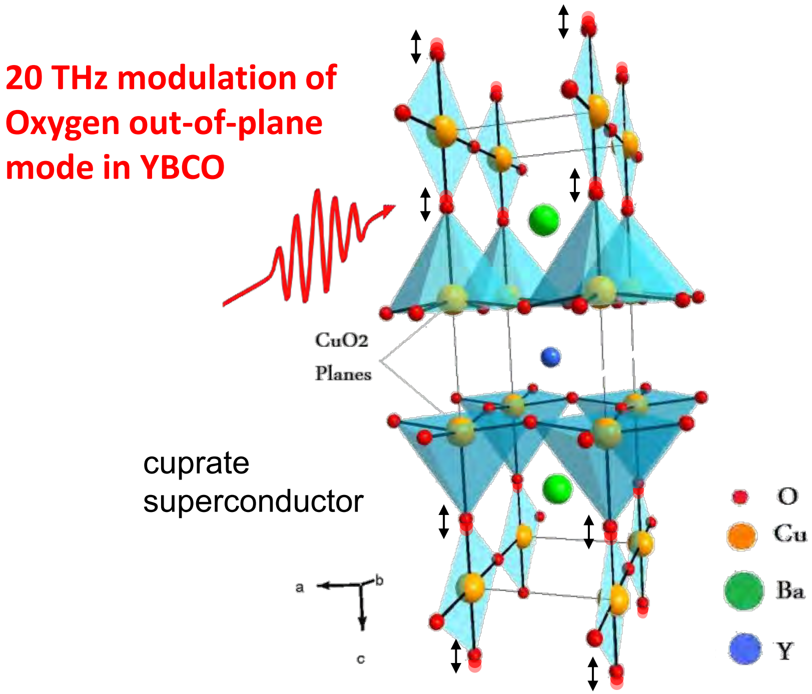
- Coherence (energy resolution) near the transform limit
- Ultrafast time resolution
- 2D maps of collective mode dynamics

THz-Driven Superconductivity Enhanced T_c ?

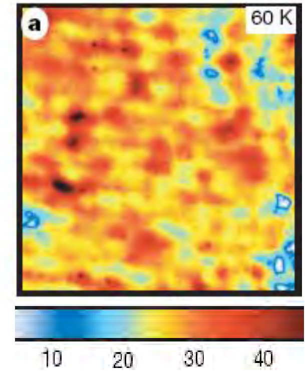


A. Cavalleri

Spontaneous Ground-state Dynamics of Complex Materials

nanoscale heterogeneity, fluctuations, & dynamics

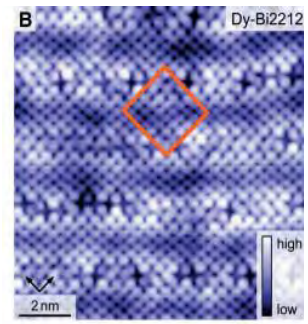
- Connect spontaneous fluctuations, dynamics and heterogeneities on multiple length- and time-scales to material properties
- Spontaneous (ground-state) dynamics complement stimulated (excited-state) dynamics of pump-probe
- Electronic structure dynamics
- Chemical heterogeneity/dynamics
- Phase transitions
- Energy conversion and transport on the nanoscale



Δ(meV)

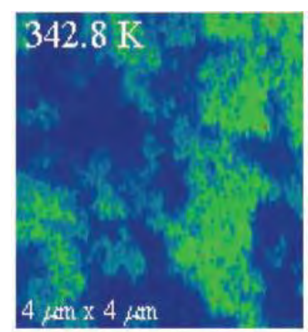
SC Gap in BSCCO

Gomes et al., *Nature* **447**, 569 (2007) (Yazdani Group, Princeton)



SC Gap in Dy-Bi2212

Kohsaka et al., *Science* **315**, 1380 (2007) (Davis Group, Cornell)



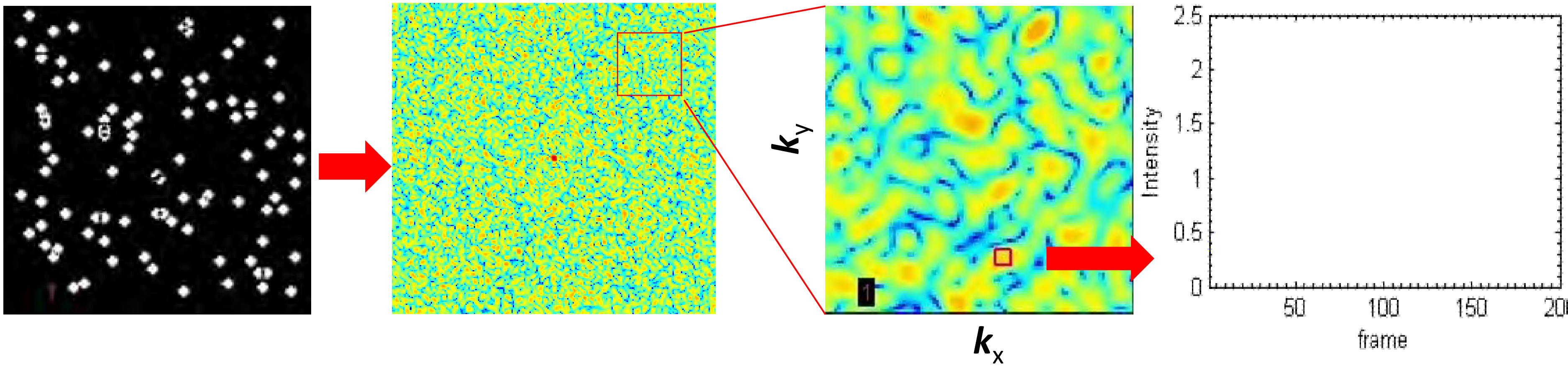
Metal-Insulator Transition in VO_2

Qazilbash et al., *Science* **318**, 1750 (2007) (Basov Group, UCSD)

X-ray Photon Correlation Spectroscopy (XPCS)

measures dynamic structure Factor : $S(\boldsymbol{q},t)$

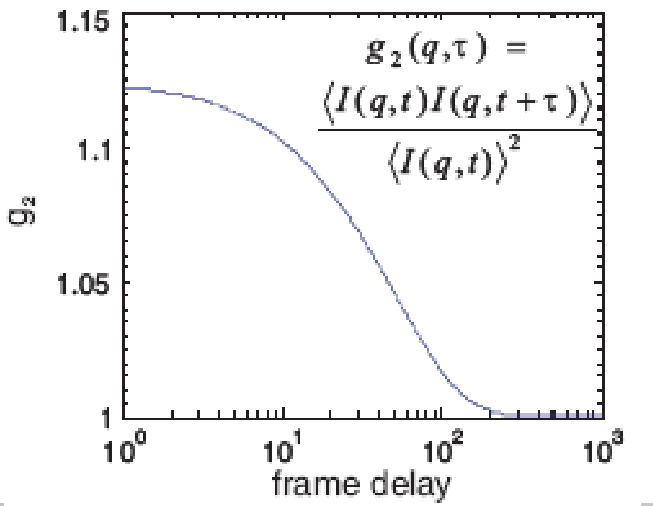
Brownian motion (100 particles, real-space) | **Diffraction Pattern Fourier (*k*) space** | **Speckles (coherent X-ray peaks)**



$$g_2(q,t) = \frac{\langle I(q,\tau) I(q,\tau+t)\rangle_\tau}{\langle I(q,\tau)\rangle_\tau^{\,2}}$$

$$= 1 + A\left|\frac{S(q,t)}{S(q,0)}\right|^2$$

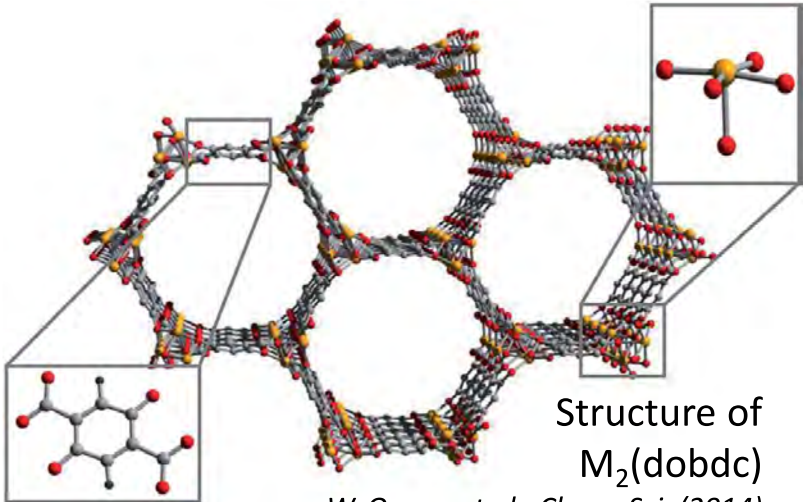
Intensity-intensity Auto-correlation $g_2(\boldsymbol{q}, t)$



Oleg Shpyrko

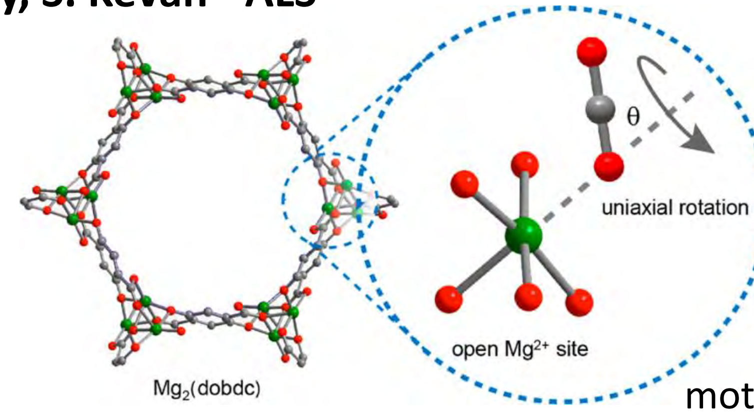
Example: Chemical Diffusion – CO_2 Adsorption in MOFs

S. Roy, S. Kevan - ALS



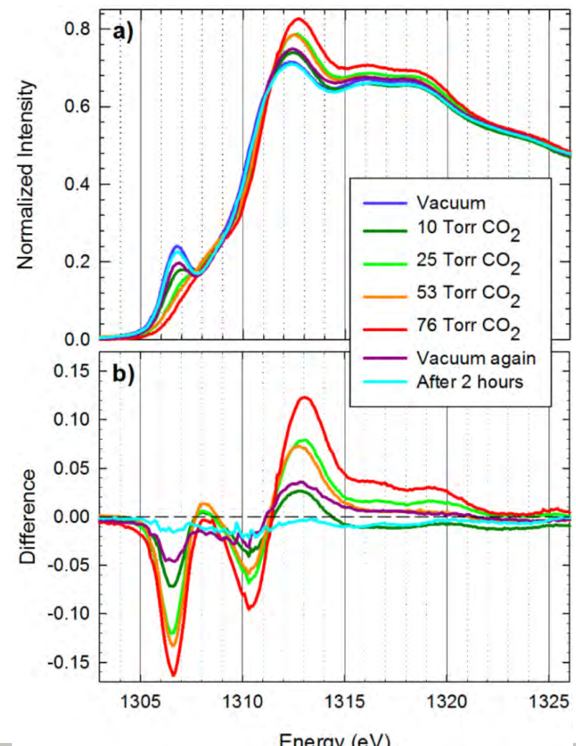
Structure of M_2(dobdc)

W. Queen et al., Chem. Sci. (2014)



CO_2 rotational motion in M_2(dobdc)

X. Kong et al, JACS (2012)



XAS at Mg K-edge

W. S. Drisdell et al, J. Am. Chem. Soc. (2013).

Local structure and symmetry variations have been studied.

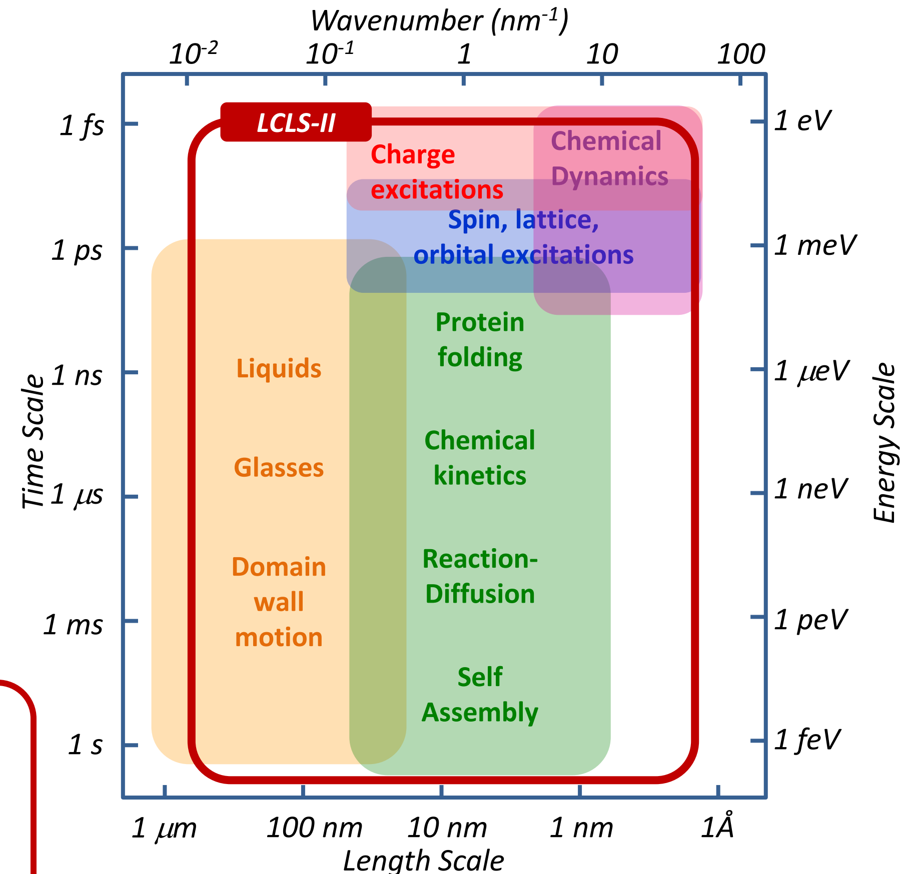
What is the temporal nature of these symmetry variations?

What are the chemical fluctuation and diffusion properties?

XPCS: site specificity, chemical selectivity

Ground-state Dynamics of Complex Materials

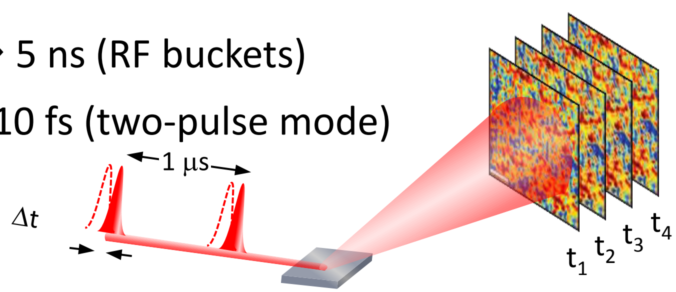
- Element specific
- Nano-scale resolution
- Charge, orbital, spin order
- Chemical bonding
- Photon in/out:
  in situ/operando,
  applied fields



LCLS-II Programmable Pulse Structure

2-pulse XPCS:

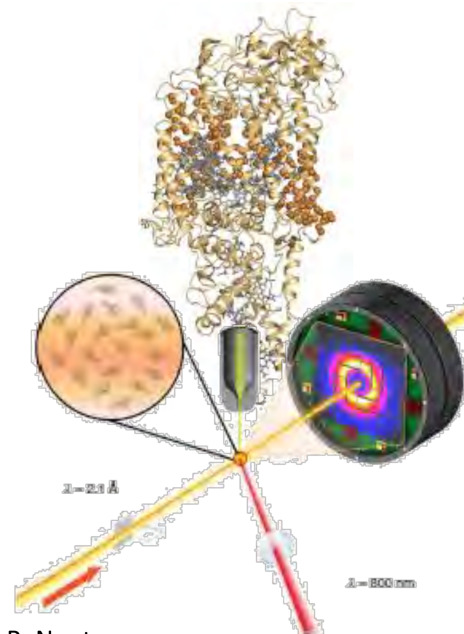
- >1 μs ➜ 5 ns (RF buckets)
- 1 ps ➜ 10 fs (two-pulse mode)



Time resolution scales as square of average brightness:

$$S/N_{XPCS} \sim t^{1/2} B \sigma_{X\text{-ray}}$$

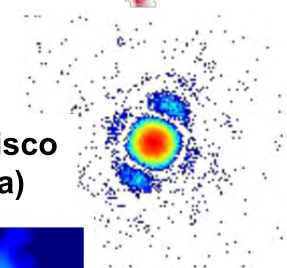
Life Sciences

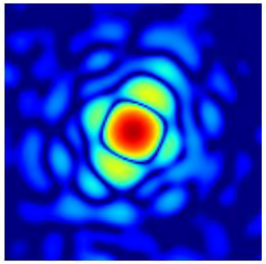


R. Neutze

- Understanding the dynamics of biological complexes & molecular machines
  - In physiological environments & on natural time scales
    structure alone provides limited insight to biological function
- Small-scale structural dynamics at Å resolution
  - Serial nano-crystallography
- Large scale conformational dynamics
  - Molecular movies – single particle imaging (2-6 keV)
  - Solution scattering – fluctuation SAX
- Electronic structure and biological function
  - Metallo-enzymes
  - Photosynthesis

2 keV Rubisco (550,000 Da)





J. Hajdu

Life Sciences

- Understanding the dynamics of biological complexes & molecular machines
  - In physiological environments & on natural time scales
    structure alone provides limited insight to biological function
- Small-scale structural dynamics at Å resolution

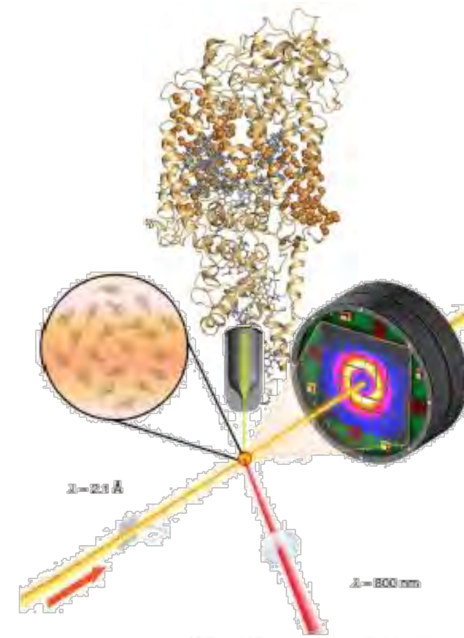
Anomalous phasing (Se – 12.5 keV)	Hard X-rays
Native phasing (S – 2.5 keV)	2-color
Resonant scattering (Na, Mg, P, Cl)	Tender X-rays

- Large scale conformational dynamics

Single-particle imaging	Tender X-rays
• Single-shot	High intensity (>5 mJ/pulse)
• Multi-shot	High rep rate
Fluctuation SAXS	High rep rate, tender X-rays

- Electronic structure and biological function

Time-resolved RIXS	High rep rate
Time-resolved XES, XAS	Soft, tender, hard X-rays
X-ray scattering	Coherence (FT limit), 2-color



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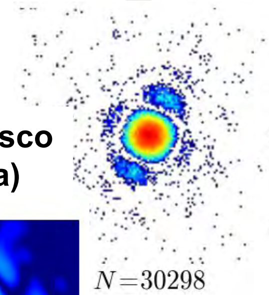
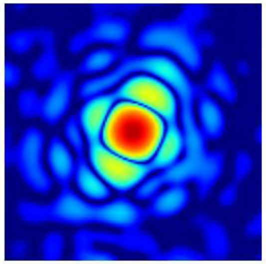
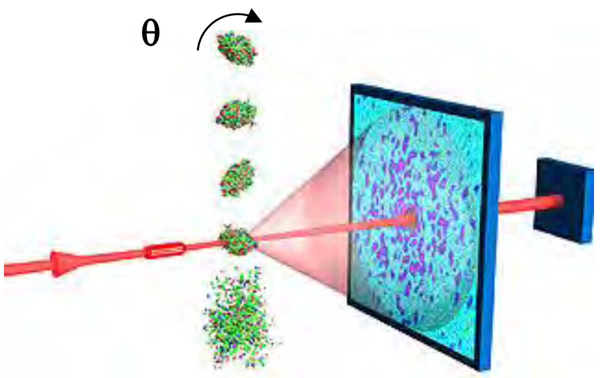




LCLS-II: Imaging Biological *Function* (biology in action)

Imaging heterogeneous, non-periodic objects

1 Billion X-ray snapshots captured by LCLS-II
Sample all molecular shapes



LCLS – single-particle imaging
Diffract before destroy
Single-shot orientation

- Diffract before destroy works
- Progressing rapidly toward full potential
- LCLS-II: ~7 mJ/pulse at 2 keV will advance single-particle imaging at sub-nm scale
- Nano-crystallography emerged as an important area of bio-science (LCLS-II: Se phasing)

Heterogeneity?

- Non-identical objects, dynamic structure
- Molecular machines, interacting bio-complexes, conformational dynamics

LCLS-II: Imaging Biological *Function* (biology in action)

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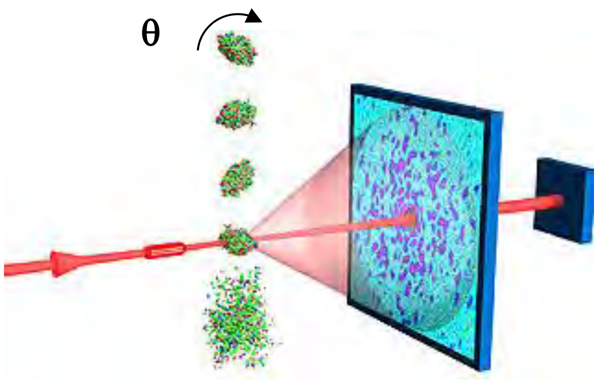
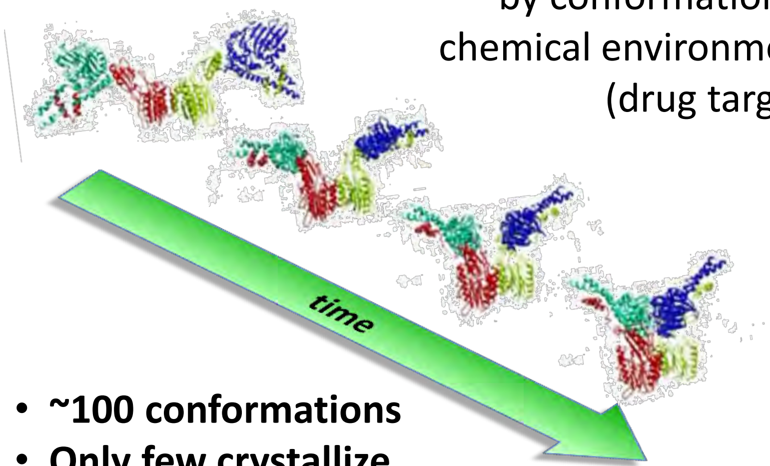
Sample all molecular shapes



LCLS – single-particle imaging
Diffract before destroy
Single-shot orientation

Hexameric Protein Complex

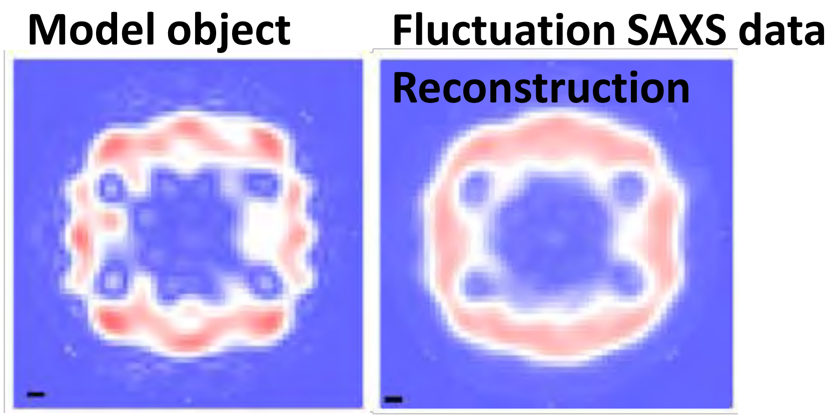
DNA repair role determined by conformation & chemical environment (drug target)

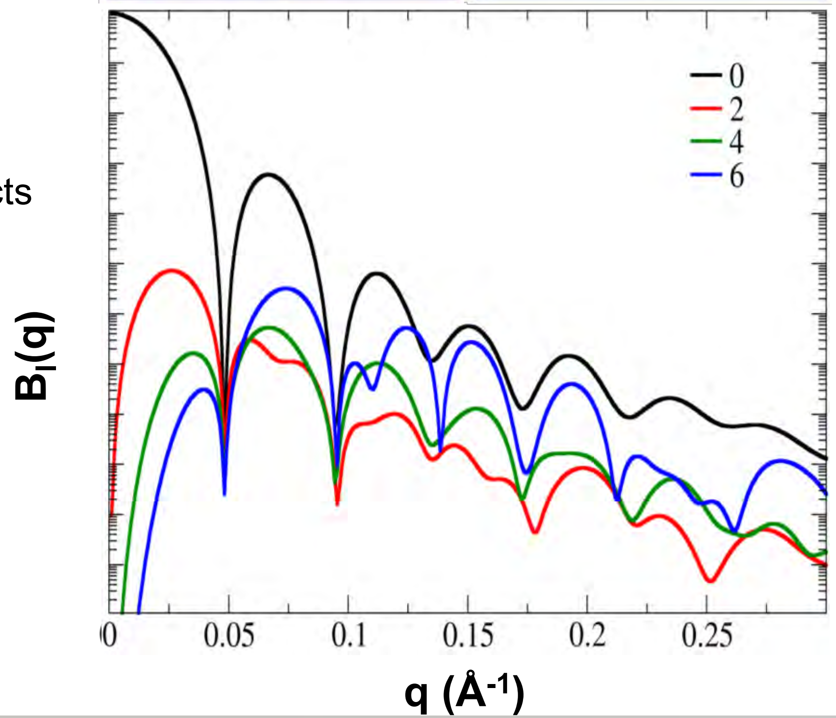


- **~100 conformations**
- **Only few crystallize**
- **Limited protein quantities**

LCLS-II: new approaches to visualize biology in action

- **"fluctuation" SAXS 100x greater information content $\tau_{pulse} < \tau_{rotation}$**
- **New computational approaches**
  (10^9 snapshots – mutual information content)
  - fSAXS + reverse monte carlo
  - Manifold mapping approaches
  - Iterative phasing approaches
- **Coherent diffraction imaging – sub-nm single-molecule "optimum" ~2-5 keV**
  - High flux/pulse ⇒ classification of non-identical objects
  - Reconstruct intermediate steps
- **Native phasing and resonant contrast for membrane proteins**
  P (2.1 keV), S (2.5 keV)
- **High hit rates with X-ray pulse-on-demand**





Life Sciences

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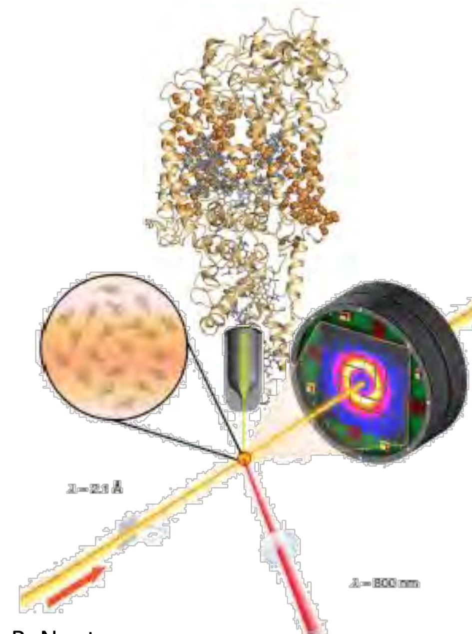
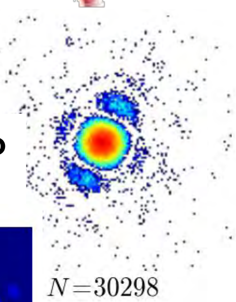


R. Neutze



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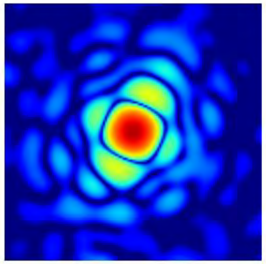
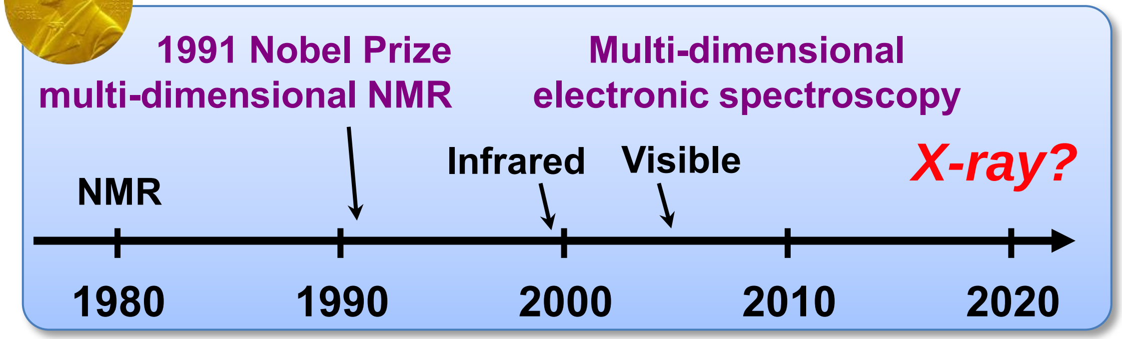


J. Hajdu

Nonlinear & Multidimensional X-ray Spectroscopy Reveals Fundamental Charge Flow & Couplings



LCLS-II:

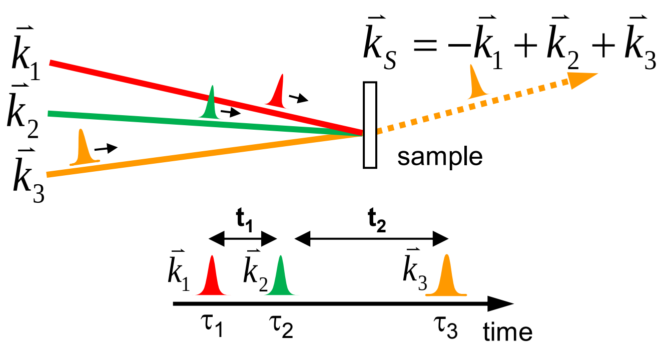
- Ultrafast (faster than Auger)
- 2-color (fully coherent)
- High repetition rate for:
  - small X-ray nonlinearities
  - controlled nonlinearities
  - small signals (low count rates)

NMR

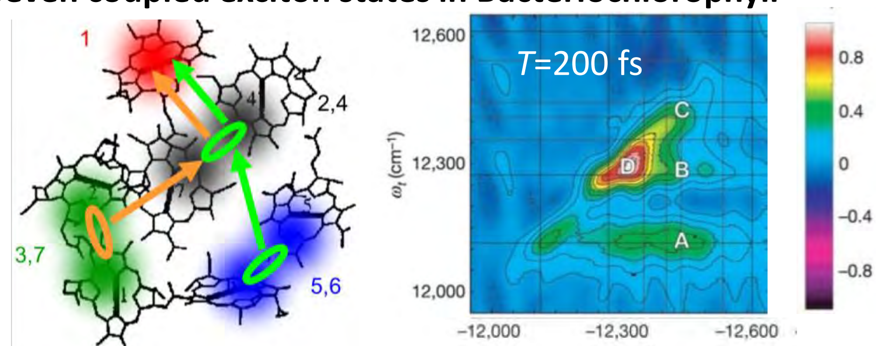
- RF pulse sequences couple to nuclear spins
- Measure ***nuclear resonances***, correlations
- Map ***molecular structures*** & spatial relationships

Multi-Dimensional Spectroscopy

- Pulses sequences couple to ***valence*** states
- Measure ***elect. resonances***, and correlations
- Map of ***valence elect. structure & dynamics***

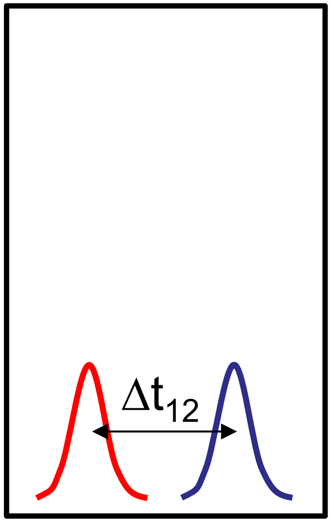


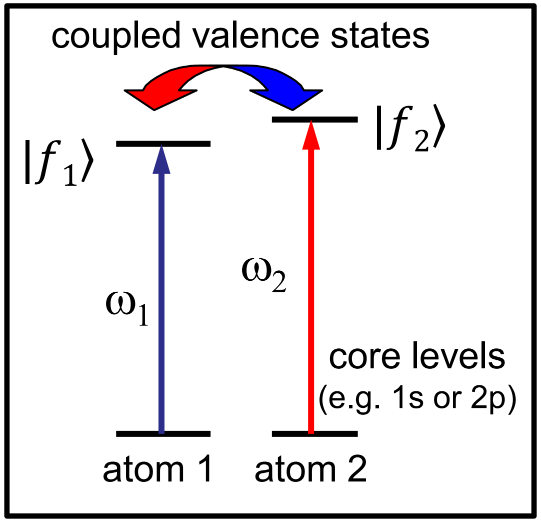
Seven coupled exciton states in Bacteriochlorophyll



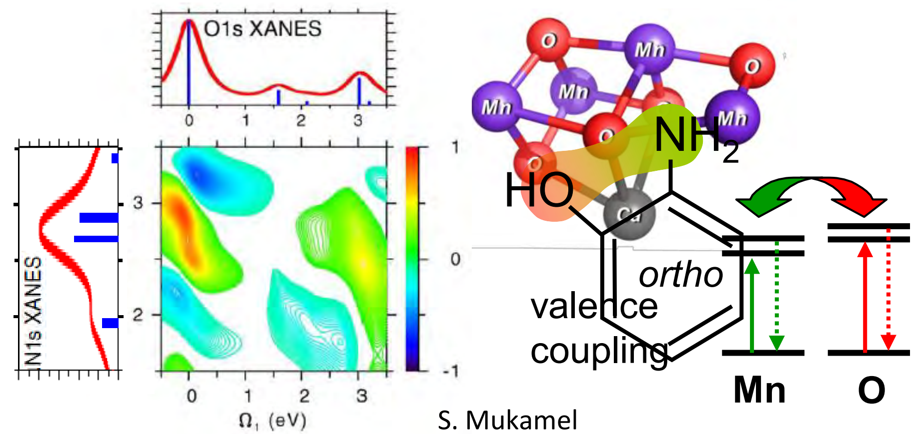
G. Fleming et al.

Core-hole Correlation Spectroscopy

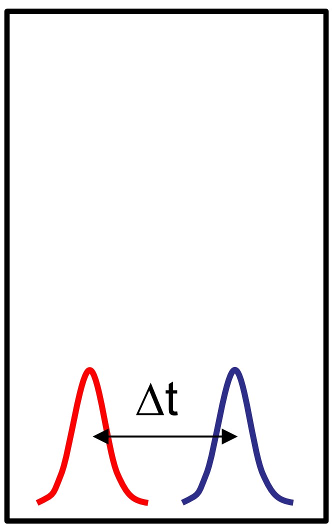


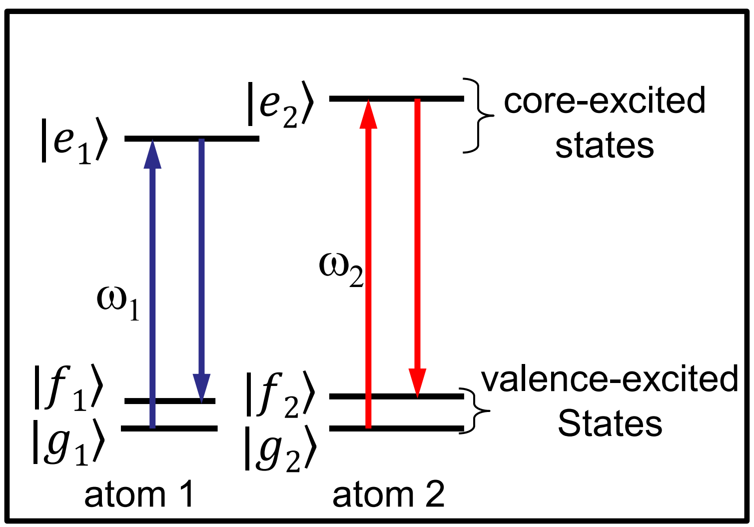


- τ_{pulse} < core-hole lifetime
- Δt_{12} < core-hole lifetime (few fs)

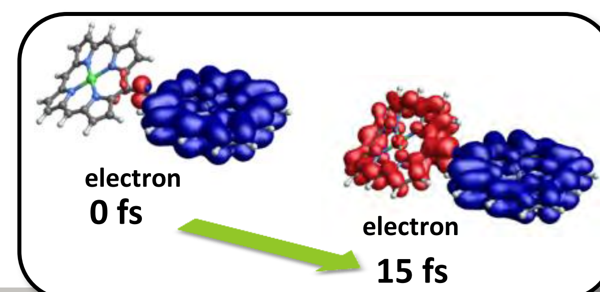


Stimulated X-ray Raman Spectroscopy - SXRS





- Localized (atom-specific) superposition of valence-excited states (e^- wave packet)
- Requires few eV BW excitation
- Follow charge flow

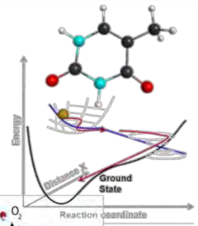


Compelling Science Opportunities – LCLS-II X-ray Lasers

Chemistry

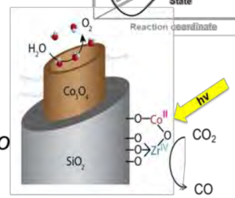
❑ Fundamental charge migration & redistribution

Dynamic reaction microscope	High rep rate
Stimulated X-ray Emission Spec.	Coherence (few fs), 2-color
Photoemission	Soft, tender X-rays
X-ray scattering	Hard X-rays



❑ Predictive understanding of photo-catalysis

Time-resolved X-ray Raman	High rep rate
(X-ray absorption/emission)	Soft, tender X-rays
Time-resolved photoemission	Coherence (FT limit), 2-color

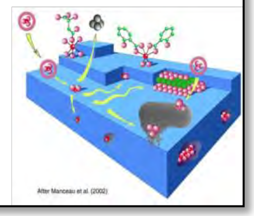


❑ Heterogeneous catalysis - in real time & *operando*

Time-resolved photoemission	High rep rate
(ambient pressure)	Soft, tender X-rays
Res. coherent X-ray scattering	Hard X-rays + soft X-rays

❑ Combustion & aerosol chemistry

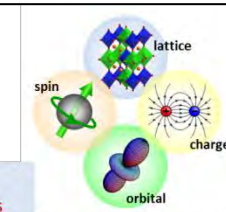
Flash tomography	High rep rate
Stimulated X-ray Emission Spec.	Soft, tender X-rays
Coherent X-ray scattering	2-color



Materials Physics

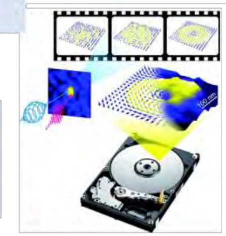
❑ Understand & control emergent phenomena in quantum systems with interacting degrees of freedom

Time & momentum resolved X-ray Raman	High rep rate
Time-resolved hard X-ray photoemission	Soft, tender, hard (3ω) X-rays
Time-, spin-, imaging- photoemission	Coherence (FT limit)



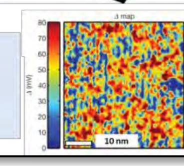
❑ Understand & control nonequilibrium spin states at fundamental length & time scales

Time-resolved X-ray dichroism	High rep rate
Coherent, resonant scattering	Soft, hard (3ω) X-rays
Hard X-ray photoemission (time/spin)	Polarization



❑ Nanoscale heterogeneity, fluctuations, & Dynamics

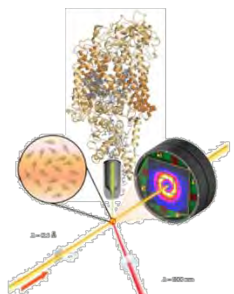
X-ray photon correlation (XPCS)	High rep rate
X-ray scattering	Soft, tender, hard (ω, 3ω) X-rays
THz pump/X-ray probe	Programmable pulse sequences



Life Sciences

❑ Understanding the dynamics of biological complexes & molecular machines

- In physiological environments & on natural time scales
  structure alone provides limited insight to biological function

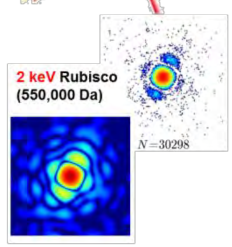


❑ Small-scale structural dynamics at Å resolution

Anomalous phasing (Se – 12.5 keV)	Hard X-rays
Native phasing (S – 2.5 keV)	2-color
Resonant scattering (Na, Mg, P, Cl)	Tender X-rays

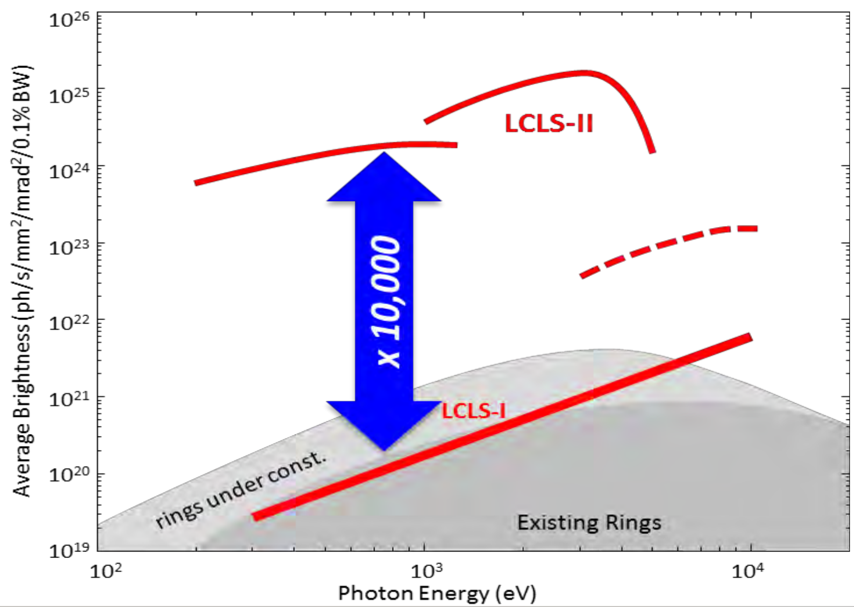
❑ Large scale conformational dynamics

Single-particle imaging	Tender X-rays
• Single-shot	High intensity (>5 mJ/pulse)
• Multi-shot	High rep rate
Fluctuation SAXS	High rep rate, tender X-rays



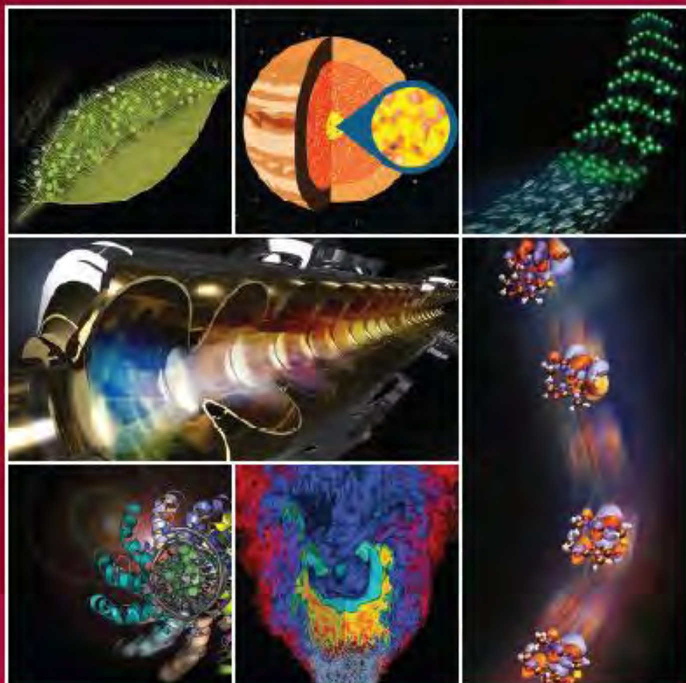
❑ Electronic structure and biological function

Time-resolved RIXS	High rep rate
Time-resolved XES, XAS	Soft, tender, hard X-rays
X-ray scattering	Coherence (FT limit), 2-color



SLAC-R-1053

NEW SCIENCE OPPORTUNITIES ENABLED BY LCLS-II X-RAY LASERS



June 1, 2015

LCLS SLAC NATIONAL ACCELERATOR LABORATORY U.S. DEPARTMENT OF ENERGY Office of Science

Contributors

P. Abbamonte[53] F. Abild-Pedersen[35] P. Adams[17] M. Ahmed[17] F. Albert[18] R. Alonso Mori[35]
P. Anfinrud[27] A. Aquila[35] M. Armstrong[18] J. Arthur[35] J. Bargar[35] A. Barty[6,7] U. Bergmann[35]
N. Berrah[46] G. Blaj[35] H. Bluhm[17] C. Bolme[19] C. Bostedt[35] S. Boutet[35] G. Brown[35,37]
P. Bucksbaum[35,37] M. Cargnello[37] G. Carini[35] A. Cavalleri[25,52,55] V. Cherezov[56] W. Chiu[3]
Y. Chuang[17] D. Cocco[35] R. Coffee[35] G. Collins[18] A. Cordones-Hahn[17] J. Cryan[35] G. Dakovski[35]
M. Dantus[22] H. Demirci[35] P. Denes[17] T. Devereaux[35,37] Y. Ding[35] S. Doniach[37] R. Dörner[15]
M. Dunne[35] H. Durr[35] T. Egami[57] D. Eisenberg[43] P. Emma[35] C. Fadley[17,41] R. Falcone[17,40]
Y. Feng[35] P. Fischer[17] F. Fiuza[35] L. Fletcher[35] L. Foucar[21] M. Frank[18] J. Fraser[45] H. Frei[17]
D. Fritz[35] P. Fromme[2] A. Fry[35] M. Fuchs[54] P. Fuoss[1] K. Gaffney[35] E. Gamboa[35] O. Gessner[17]
S. Ghimire[35] A. Gleason[19] S. Glenzer[35] T. Gorkhover[35] A. Gray[39] M. Guehr[35] J. Guo[17] J. Hajdu[60]
S. Hansen[33] P. Hart[35] M. Hashimoto[35] J. Hastings[35] D. Haxton[17] P. Heimann[35] T. Heinz[35,37]
A. Hexemer[17] J. Hill[4] F. Himpsel[58] P. Ho[1] B. Hogue[2] Z. Huang[35] M. Hunter[35] G. Hura[17]
N. Huse[25,52] Z. Hussain[17] M. Ilchen[8,37] C. Jacobsen[1] C. Kenney[35] J. Kern[17,35] S. Kevan[17] J. Kim[35]
H. Kim[36] P. Kirchmann[35] R. Kirian[2] S. Kivelson[37] C. Kliewer[33] J. Koralek[35] G. Kovácsová[21]
A. Lanzara[17,40] J. LaRue[35] H. Lee[35] J. Lee[35] W. Lee[35] Y. Lee[35,37] I. Lindau[37] A. Lindenberg[35,37]
Z. Lin[34] D. Lu[35] U. Lundstrom[37] A. MacDowell[17] W. Mao[35,37] J. Marangos[14] G. Marcus[35]
T. Martinez[35,37] W. McCurdy[17,41] G. McDermott[17,45] C. McGuffey[44] H. Michelsen[33] M. Minitti[35]
S. Miyabe[32] S. Moeller[35] R. Moore[35] S. Mukamel[42] K. Nass[21] A. Natan[35] K. Nelson[23] S. Nemšák[9]
D. Neumark[17,40] R. Neutze[12] A. Nilsson[35,38] D. Nordlund[35] J. Norskov[35,37] S. Nozawa[29]
H. Ogasawara[35] H. Ohldag[35] A. Orville[4] D. Osborn[33] T. Osipov[35] A. Ourmazd[59] D. Parkinson[17]
C. Pellegrini[35,43] G. Phillips[31] T. Rasing[30] T. Raubenheimer[35] T. Recigno[17] A. Reid[35] D. Reis[35,37]
A. Robert[35] J. Robinson[35] D. Rolles[16] J. Rost[24,37] S. Roy[17] A. Rudenko[16] T. Russell[47]
R. Sandberg[19] A. Sandhu[50] N. Sauter[17] I. Schlichting[21] R. Schlögl[10] W. Schlotter[35] M. Schmidt[59]
J. Schneider[6,7] R. Schoenlein*[17,35] M. Schoeffler[15] A. Scholl[17] Z. Shen[35] O. Shpyrko[44] T. Silva[26]
S. Sinha[44] D. Slaughter[17] J. Sobota[35] D. Sokaras[35] K. Sokolowski-Tinten[51] S. Southworth[1]
J. Spence[2] C. Stan[35] J. Stohr[35] R. Stroud[45] V. Sundstrom[20] C. Taatjes[33] A. Thomas[48] M. Trigo[35]
Y. Tsui[49] J. Turner[35] A. van Buuren[18] S. Vinko[55] S. Wakatsuki[35,37] J. Wark[55] P. Weber[5]
T. Weber[17] M. Wei[11] T. Weiss[35,37] P. Wernet[13] W. White[35] P. Willmott[28] K. Wilson[17]
W. Wurth[6,7,52] V. Yachandra[17] J. Yano[17] D. Yarotski[19] L. Young[1] Y. Zhu[4] D. Zhu[35] P. Zwart[17]

[1]Argonne National Laboratory
[2]Arizona State U.
[3]Baylor College Medicine
[4]Brookhaven National Laboratory
[5]Brown U.
[6]Center for Free Electron Laser Science
[7]DESY
[8]European XFEL
[9]Forschungszentrum Jülich
[10]Fritz-Haber-Institut - MPG
[11]General Atomics
[12]Goetheburg U.
[13]Helmholtz-Zentrum Berlin
[14]Imperial College London
[15]Institut für Kernphysik Goethe U. Frankfurt
[16]Kansas State U.
[17]Lawrence Berkeley National Laboratory
[18]Lawrence Livermore National Laboratory
[19]Los Alamos National Laboratory
[20]Lund U.
[21]Max Planck Inst. for Medical Research
[22]Michigan State U.
[23]MIT
[24]MPI Physics Complex Systems Dresden
[25]MPI Structural Dynamics
[26]National Institute Standards and Tech.
[27]National Institutes Health
[28]Paul Scherrer Institute
[29]Photon Factory, Japan
[30]Radboud U.
[31]Rice U.
[32]RIKEN Center for Advanced Photonics
[33]Sandia National Laboratories
[34]SIMIT, CAS, Shanghai Tech Univ.
[35]SLAC National Accelerator Laboratory
[36]Sogang U.
[37]Stanford U.
[38]Stockholm U.
[39]Temple U.
[40]U. California, Berkeley
[41]U. California, Davis
[42]U. California, Irvine
[43]U. California, Los Angeles
[44]U. California, San Diego
[45]U. California, San Francisco
[46]U. Connecticut
[47]U. Massachusetts Amherst
[48]U. Michigan
[49]U. Alberta
[50]U. Arizona
[51]U. Duisburg-Essen
[52]U. Hamburg
[53]U. Illinois
[54]U. Nebraska Lincoln
[55]U. Oxford
[56]U. Southern California
[57]U. Tennessee
[58]U. Wisconsin-Madison
[59]U. Wisconsin-Milwaukee
[60]Uppsala U.

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