# WG-1
# "Science needs"

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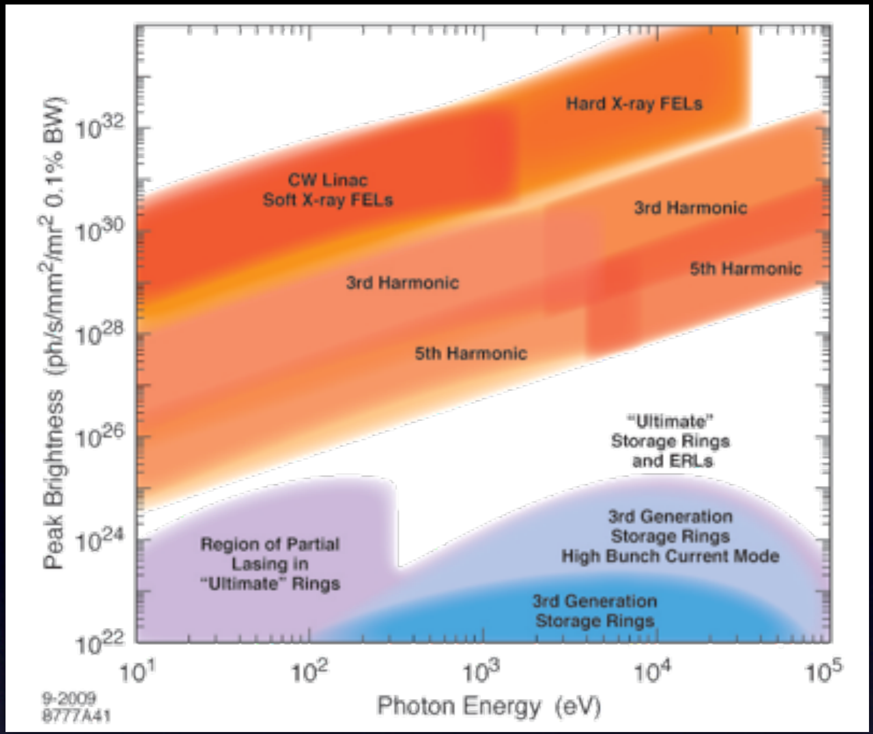
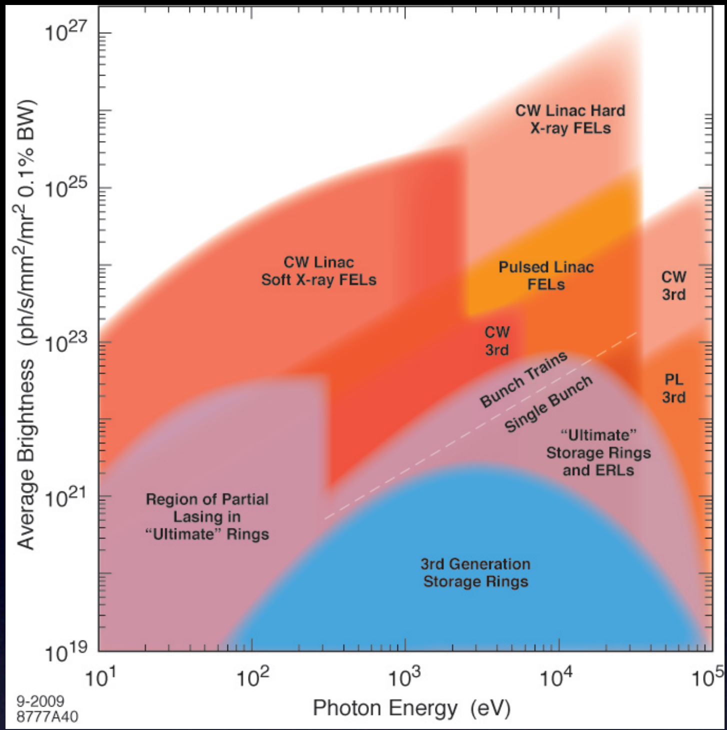
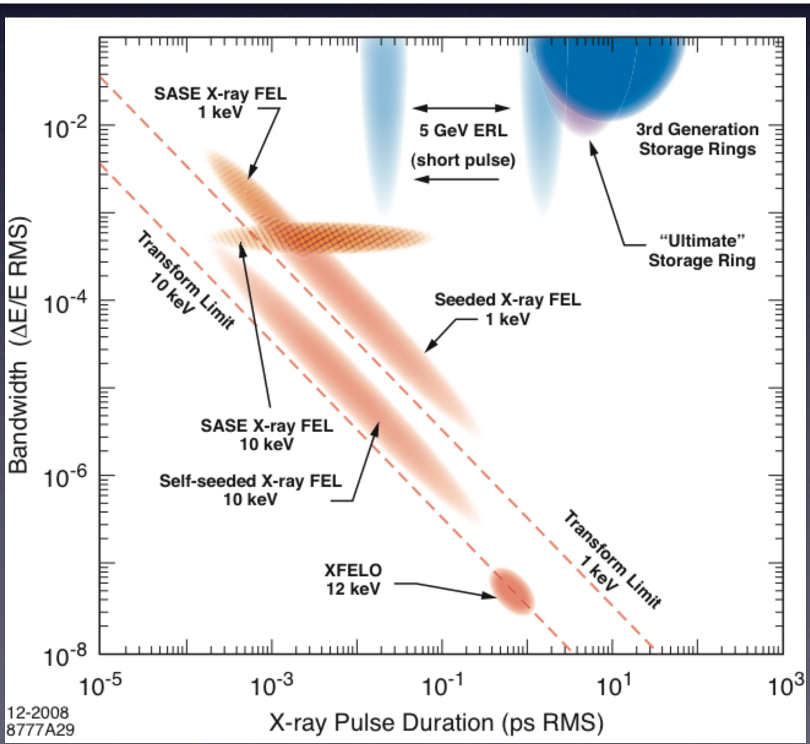


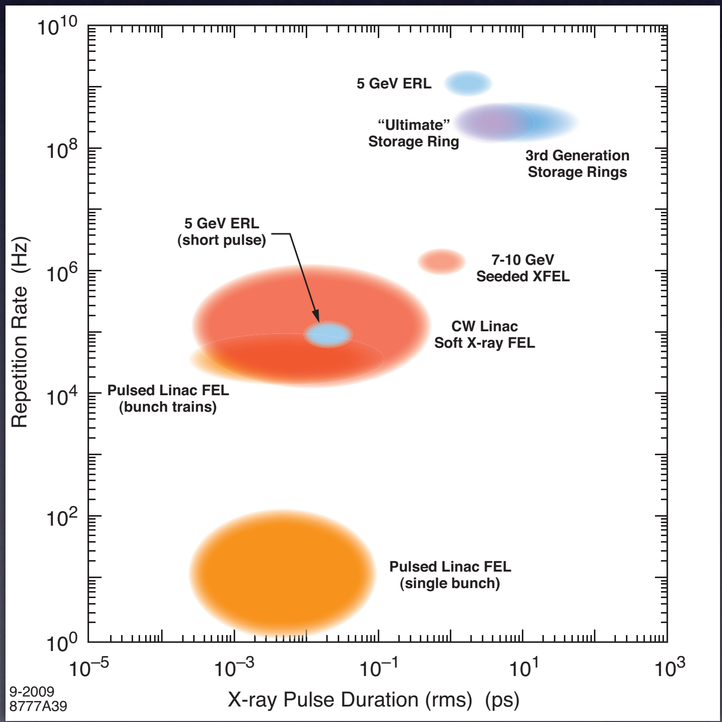
Hard X-ray FELs
CW Linac
Soft X-ray FELs
3rd Harmonic
3rd Harmonic
5th Harmonic
5th Harmonic
"Ultimate"
Storage Rings
and ERLs
Region of Partial
Lasing in
"Ultimate" Rings
3rd Generation
Storage Rings
High Bunch Current Mode
3rd Generation
Storage Rings
Peak Brightness (ph/s/mm²/mr² 0.1% BW)
Photon Energy (eV)
9-2009
8777A41

CW Linac Hard
X-ray FELs
CW Linac
Soft X-ray FELs
Pulsed Linac
FELs
CW
3rd
CW
3rd
PL
3rd
Bunch Trains
Single Bunch
"Ultimate"
Storage Rings
and ERLs
Region of Partial
Lasing in
"Ultimate" Rings
3rd Generation
Storage Rings
Average Brightness (ph/s/mm²/mr² 0.1% BW)
Photon Energy (eV)
9-2009
8777A40

SASE X-ray FEL
1 keV
5 GeV ERL
(short pulse)
3rd Generation
Storage Rings
"Ultimate"
Storage Ring
Transform Limit
10 keV
Seeded X-ray FEL
1 keV
SASE X-ray FEL
10 keV
Self-seeded X-ray FEL
10 keV
XFELO
12 keV
Transform Limit
1 keV
Bandwidth (ΔE/E RMS)
X-ray Pulse Duration (ps RMS)
12-2008
8777A29

5 GeV ERL
"Ultimate"
Storage Ring
3rd Generation
Storage Rings
5 GeV ERL
(short pulse)
7-10 GeV
Seeded XFEL
CW Linac
Soft X-ray FEL
Pulsed Linac FEL
(bunch trains)
Pulsed Linac FEL
(single bunch)
Repetition Rate (Hz)
X-ray Pulse Duration (rms) (ps)
9-2009
8777A39

# Agreeing on future light source needs can feel like...

# We identified 8 science driver areas for new light sources

- Hierarchical biology
- Molecular movies
- Correlated materials
- Materials at the mesoscale
- Atoms to materials
- Multi-component materials
- Matter in extreme conditions
- Understanding chemical reactions

# 1 - Understanding chemical reactions

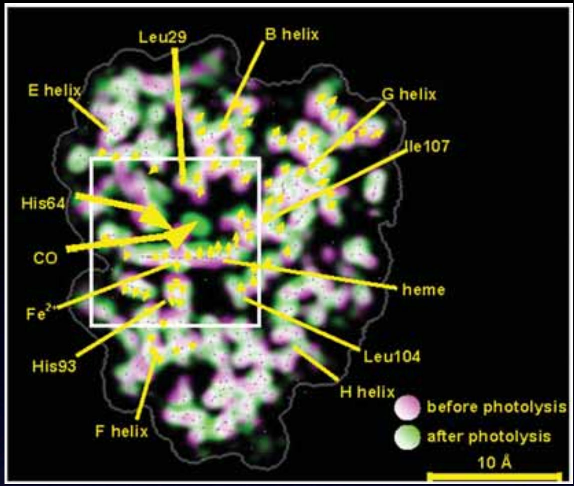
## Science drivers:

- Catalysis, interfaces, combustion
- Want to do it at high pressure, and as a function of time
- Examples:
  - combustion engines, evolution on ms time scales
  - VUV excitation of neutral species in flames,
  (measure emission to determine species that are present)

## Techniques:

- Spectroscopy, XAS, XES, RIXS, ion detection
- Various flavours of time-resolved pump-probe:
  - X-ray pump, X-ray probe
  - Optical pump, Xray probe
- Photon echo, two photon in – one photon out, 4 wave mixing with x-rays
- X-Pump- X-probe, optical pump, X-probe, 10fs time scales, sub-ps
- Various flavours of inelastic scattering

# 1 - Understanding chemical reactions




## Photon needs:

- 100 eV to 8 keV photons
- Monochromaticity, tunable to resonances

- 1-50 fs pulses (even as low as 100 as)
  - Auger time ~5fs, photoelectron times in as
- High peak X-ray intensity
- Pulse trains on demand (ideally different pulses to different experiments)
- Flexibility in bunch structure, pulse structure
- X-ray pulse shaping similar to optical lasers, chirping (chirped adiabatic passages)
- Rep rate of source commensurate with 10 fs optical pump lasers (<10kHz)

## Comments:

- Time resolved experiments are hard at synchrotrons –
  - single bunch, lower average current (makes other customers unhappy, takes too long, need better detectors, more flux, more flexibility in mode of operation).
  - Intense pulse every 100ms needed for some experiments, others need more frequent pulses. How do you serve all needs at once?
- Start and end of each e- bunch lases, but not the middle - fs X-ray time delay?

# 2 - Molecular movies

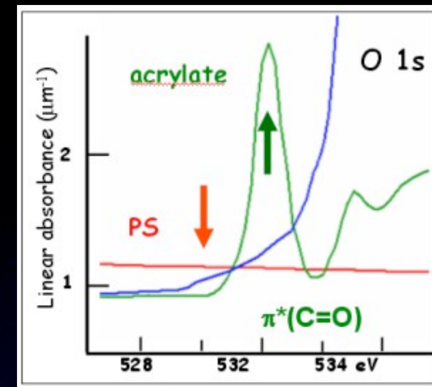
## Science drivers:

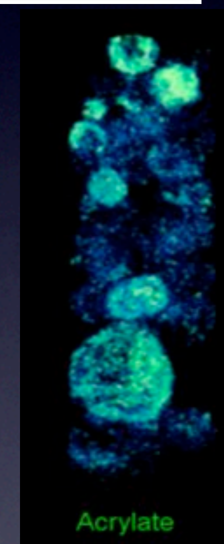
- Observe function of catalysts (zeolite based, metal organic frameworks, bio inspired enzymatic like catalysts) on molecular scale with time dependence
- Nanometers, inside e.g. liquid at high pressure/temperature
- 0.1 – 1000 fs time scales
- (Closely related to chemistry topic)

## Techniques:

- IXS spectroscopy
- Serial imaging
  - Coherent diffraction from molecules
  - XCS
- Core level spectroscopies
- See also techniques used for chemistry

# 2 - Molecular movies

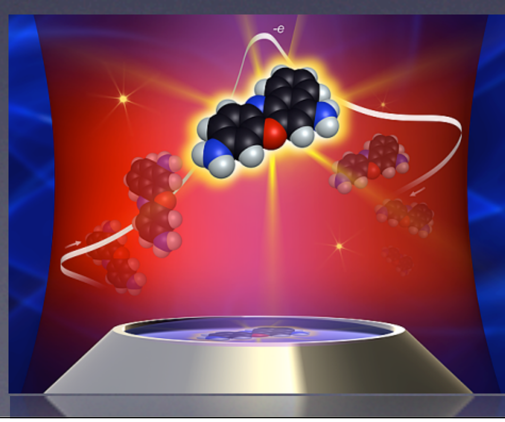


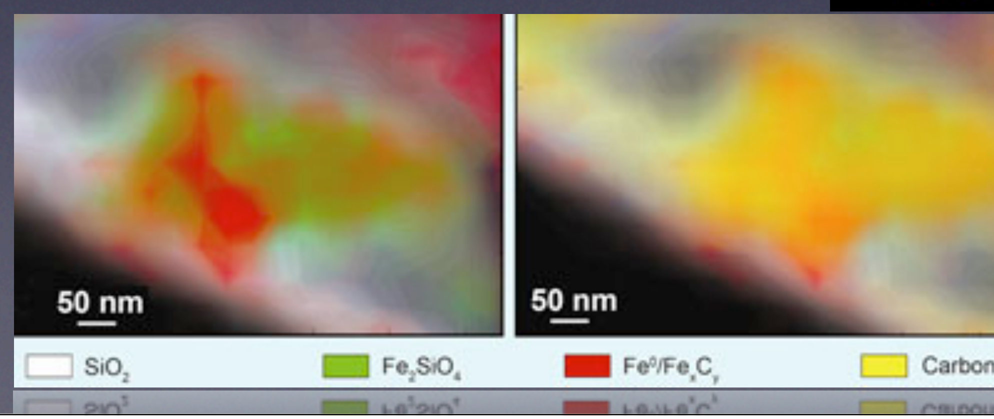




## Photon needs:

- 100 eV to 8 keV photons
- Monochromaticity, tunable to resonances, transverse coherence

- 1-50 fs pulses (even as low as 100 as)
  - Auger time ~5fs, photoelectron times in as
- High peak X-ray intensity, in other cases high average power
- Pulse trains on demand (ideally different pulses to different experiments)
- Rep rate of source commensurate with 10 fs optical pump lasers (<10kHz)





# 3 - Atoms to materials

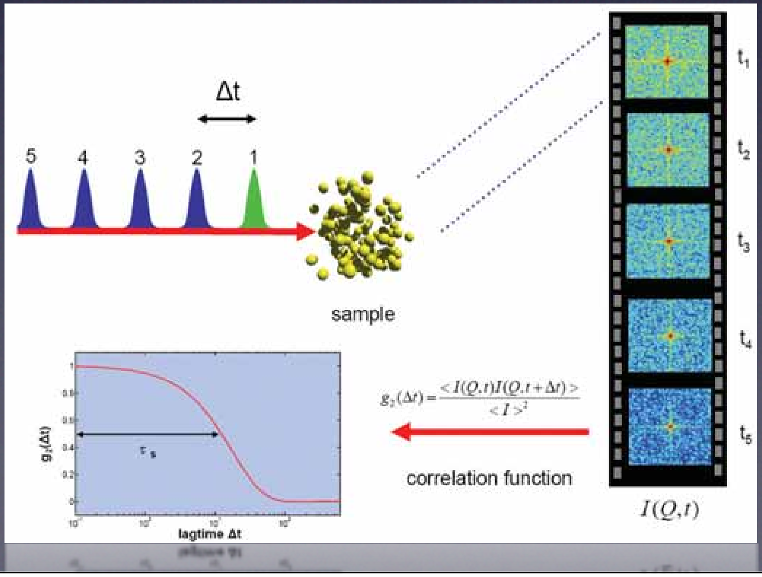
## Science drivers:

- Inorganic and bio clusters
- Electronics of magnetic clusters, movement from liquid to solid
- Superconductivity of systems, low-Z superconductors.
- Phase transition in mass-selected clusters: melting, metal-insulator (semiconductor) phase transitions, magnetic phase transitions.

What happens for 2,3,4 atoms, up to 100 atoms? Fill the gap between single atoms and bulk material. Emergence of solid state properties from collections of single atoms.

## Techniques:

- XAS, XMCD, XMLD,
- Scattering, optical spectroscopy
- PES, Spin-resolved PES
- Coherent imaging



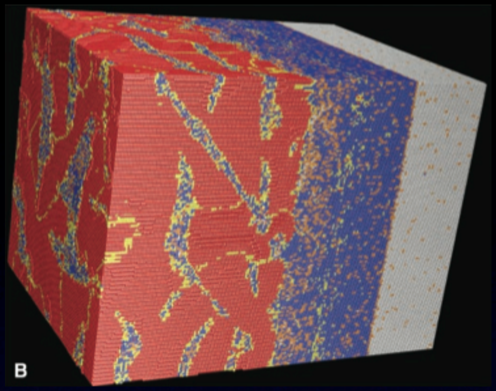
# 3 - Atoms to materials

## Photon needs:

*Need very bright X-rays to get any measurable signal.*

| | |
|---|---|
| • Photon energy range | EUV to Hard-x-rays (10 eV- 10 keV) |
| • Photon flux | > 10^14 ph s-1 mm-2 mrad-1 0.1%bw |
| • Coherence | full transversal and FTL |
| • Polarization | Circular and Linear (variable) |
| • Tunability | fast ( 1kHz) |
| • Pulse duration | from as to ps ( possibly variable) |
| • Beam stability (intensity) | high |
| • Beam stability (energy) | compatible with FTL |
| • Pulse to pulse jitter | < 500 as |
| • Beam divergence | diffraction limited |
| • Repetition rate | from ~10 Hz to ~ 1 MHz |

# 4 - Materials at the mesoscale

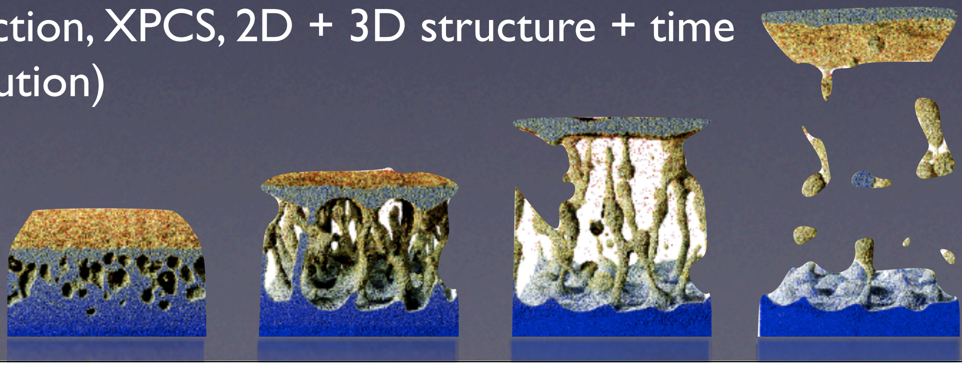



## Science drivers:

- Material fatigue, fracture, strain
- Multiple length/time scales
- Carbon capture / sequestration
- cm-size samples, more realistically mm, potentially high-Z
- Straining a pillar reproducible at >10kHz.  Strains are dynamic, must be done at natural frequency of the system.
- Mesoscale dynamics in disordered materials (liquids, amorphous)
- Nuclear reactor, aging effect on materials – changing structural material, fuel material, changing of failure rates, will it collapse under own weight?
- Nucleation of voids from radiation damage, how does it start at atomic scale then grow into mesoscopic damage.

## Techniques:

- Radiography (high energies)
- Coherent X-ray imaging, Coherent diffraction, XPCS, 2D + 3D structure + time
- Inelastic X-ray scattering (sub-meV resolution)



# 4 - Materials at the mesoscale

## Photon needs

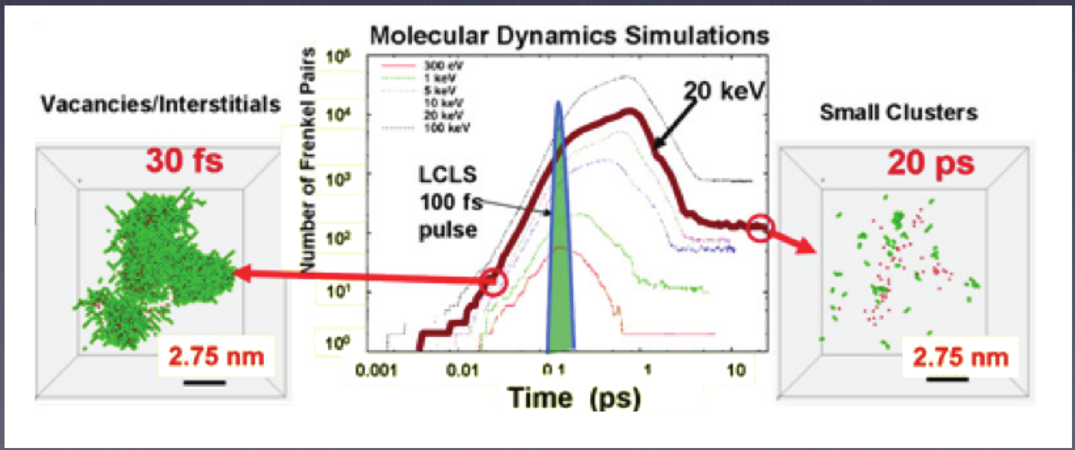
- Hard X-rays: >20keV 100s of keV (penetration!)
- In some cases very high energy X-rays (to Uranium k-edge at 115 keV)
  "We need a hard X-ray flame thrower" (thanks Lou!)
- "Short pulses" on ~ps scales (ps phenomena at these length scales)
- Rep rate from single shot to kHz (eg: mapping strain deformations)

For coherent imaging techniques

- Monochromaticity of better than 10^-4 (large field-of-view at high resolution)
- Good transverse coherence length

For inelastic X-ray scattering:

- High spectral monochromaticity <10^-7 (energy resolution), high flux



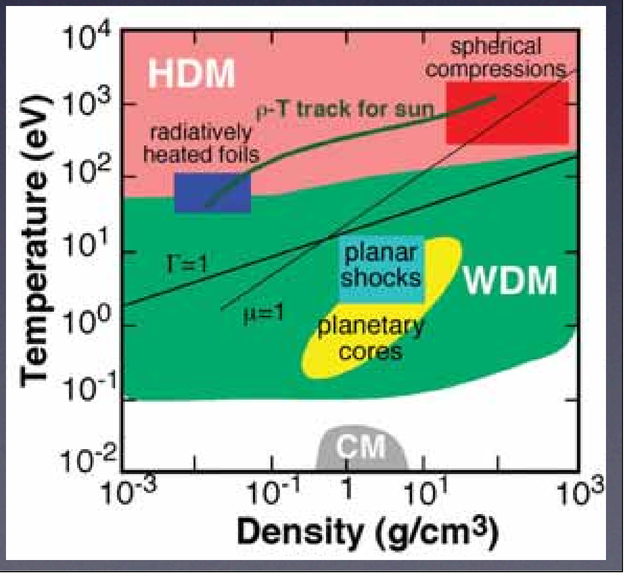
# 5 - Matter in extreme conditions

## Science drivers:

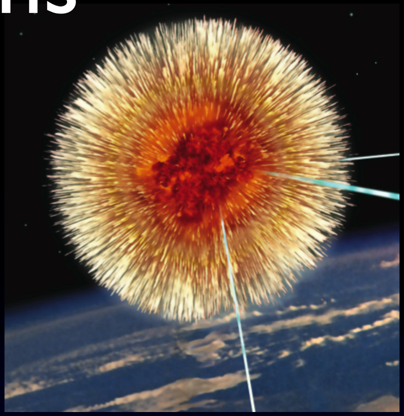

- Plasmas
- Geological science
- Fluids, pressure, radiation damage
- Oxides of high-Z materials, time domain evolution.
- Nucleation of voids on atomic scales, comparison to MD models (ideal for FELs)
- Voids nucleate formation of propagating cracks
- Extreme conditions = border of conventional phase diagrams, end of the scales
- Distinguish crack propagation below 10eV, electron shocks at keV temperatures.
- Material temperatures comparable to binding energies.
- Laboratory astrophysics: Compact objects, accretion disks, etc.
- Spectroscopy on materials in different states, towards spectroscopy on highly charged ions.
- Understanding high pressure phases for new materials design and control

## Techniques:

- Inelastic Xray scattering (IXS).
- Pump-probe fluorescence
- Nuclear resonant scattering
- Spectroscopy, XES, XAS, RIXS
- Coherent diffraction (time-resolved imaging and SAXS)
- Thompson scattering, diffraction
- Clusters: eTOF; Films: surface spectroscopy



# 5 - Matter in extreme conditions



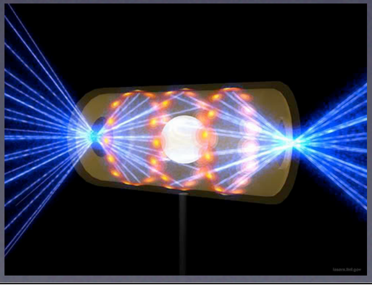
## Photon needs:

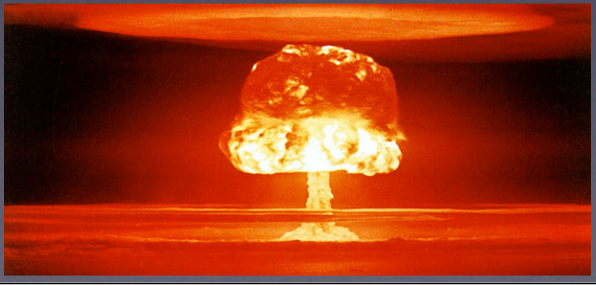
- Higher photon energy (20-80 keV!) short pulse, high intensity.
- High pulse-to-pulse stability
- Two time regimes
  - atoms: femtosecond time scales (XP-XP to within fs)
  - mesoscale dynamics: picosecond to nanosecond time scales
- Synchronisation of external drivers to X-ray pulses
- IXS and nuclear scattering requires high monochromaticity: 1e-7 and less.
  - Development of highly monochromatic sources for higher efficiency.
  - Very small beam size, stability of beam (micron stability)

## Comments:

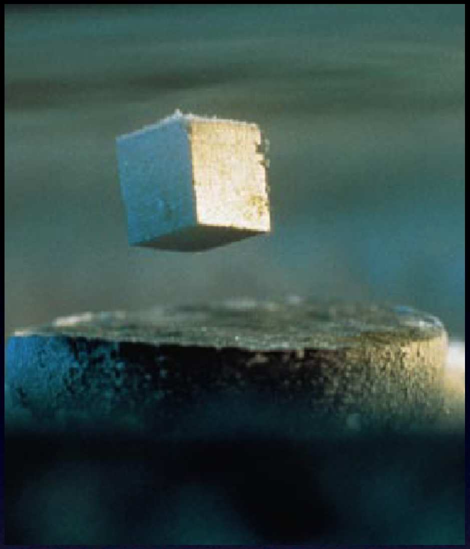
- Single-shot shocked material experiments at the APS: current experiments limited by Z of materials being looked at (eg: Tony van B's shocked porous Aerogel materials).
- Meanwhile mesoscale validation might be another type of source: Crack propagation through diffractive imaging, can be at different length scales and higher energies. Picosecond time scales.

Anvil cell





# 7 - Correlated materials



## Science drivers:

- "Emergence" phenomenon, phase transition
- High Tc superconducting materials
- CMR materials
- Magnetic Materials
- Topological insulators
- Thermal electric material and other Energy-related application.
- Heterojunction of the correlated materials
- Electronic dynamics when the system is driven out of equilibrium.
- Mode-selective pump-probe experiment -> ultrafast control of the electronic states
- The knowledge is not only fundamental important, but also feed back to the materials Synthesis and device engineering.

## Techniques

- High-resolution-ARPES, Spin-resolved ARPES, Time-resolved ARPES, nano-ARPES
- High-Resolution-RIXS, Time-resolved RIXS, Time-Resolved Resonant Diffraction, Time-Resolved XMCD, High spatial resolution of XMCD.

# 7 - Correlated materials

## Photon needs:

TR-ARPES:

-Tunable photon energy between 10 eV and ~10 keV

-pulse duration (sub fs and fs)

-control of the polarisation, photon density per pulse

-control of the repetition rate (from few kHz to 10 MHz regime)

-Tunable "pump" photon sources

HR-RIXS

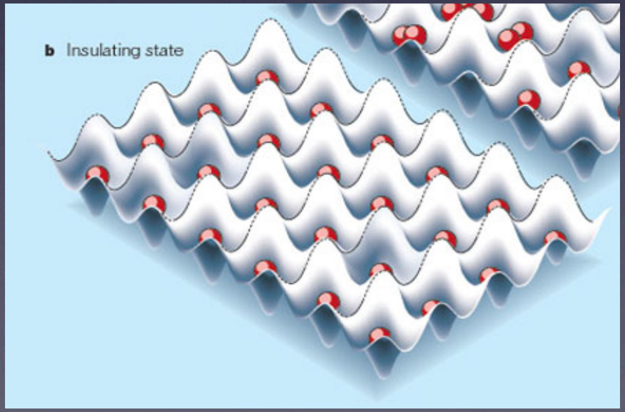
Tunable photon energy in Soft X-ray regime (250 eV to 2 KeV)

High repetition rate and beam stability.

Narrow bandwidth of the monochromatic beam

Small beam spot on sample in sub-micron range: (1) sample in-homogeneous (2) domain physics (3) enhance detection efficiency without sacrifice resolution.

Control of polarization.




TR-RIXS:

Tunable Energy in Soft X-ray (250 eV to 2 keV)

Tunable Pulse duration (sub fs to 100 fs)

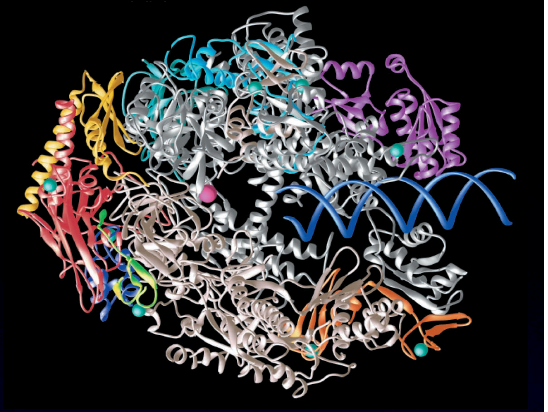
Requires very stable radiation sources

control of the polarisation, photon density per pulse

control of the repetition rate (up to 10 MHz)

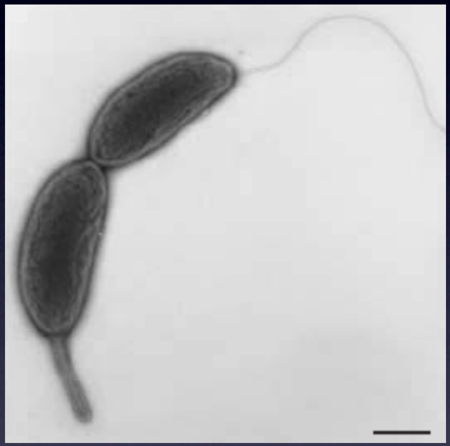
FT limited pulses for the measurements in the time domain

# 8 - Hierachical biology



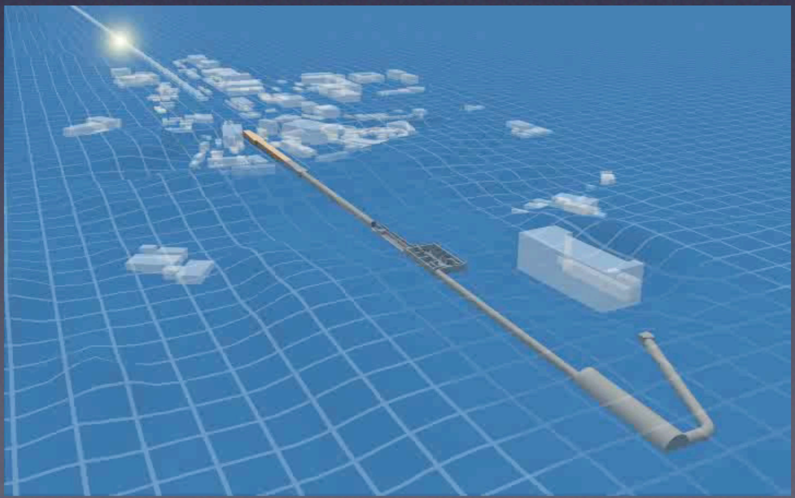
## Science drivers:

- spatio-temporal studies
- phase-transitions
- Biological water
- Protein folding
- Multi-scale
  - Spatial - atomic/molecular/macro-molecular/cellular
  - Temporal - reactions to cell division
  - Optical triggering / seeding



## Techniques:

- Multi-beam, multi-angle
- Spatial and temporal imaging
- Microsopy, tomography
- Dynamic cellular imaging
- Coherent imaging beyond crystallography
- IXS, nuclear resonant scattering
- Spectroscopies
- Solution and fluctuation scattering



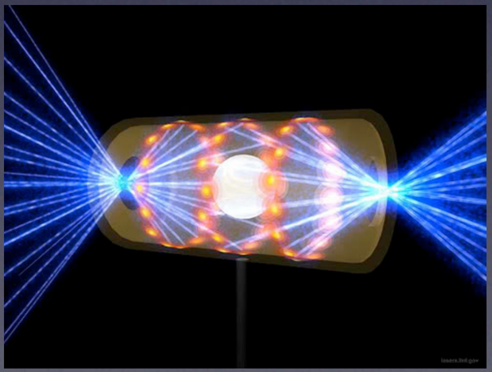
# 8 - Hierachical biology

## Photon needs:

*Many complementary sources*

- Energy regime:
  - from water window (300eV) to whole animal imaging at hard X-rays (50 keV)
- Coherent imaging:
  - high rep rate, high brightness
  - Full transverse coherence
  - Longitudinal coherence (FTL) - 10000l, field of view
  - Short pulses (10fs diffract-destroy)
  - CW, or quasi-CW ps pulses (static microscopy)
- Full field microscopy
  - Bright, incoherent source for full field microscopy, CW, narrow bandwidth, <2keV
- Diffract and destroy: LCLS++
  - More photons, 10fs pulses, transform limited temporal coherence bandwith
- IXS, nuclear resonant scattering need
  - Highly monochromatic 1e-7 and less
  - More flux!

- Flexibility of pulse trains, high rep rate
- Synchronisation of triggers (photons) with pulses



# Recurring themes*

## 1. Ultra-short pulse X-rays:

- Attosecond to10s of fs pulse lengths, 200 eV - 15 keV range
- Sufficient coherent power for single-shot measurements
- Programmable pulse trains, pulse shaping, ability to serve multiple users
- Synchronisation with fs pump lasers

## 2. Quasi-CW X-ray source

- 200 eV - 15 keV range
- Bright, high average flux, monochromatic, coherent, tunable
- Ability to serve multiple users

## 3. Picosecond very hard X-rays:

- 30 - 50 - 150 keV
- Picosecond pulses
- Transverse and longitudinal coherence

* Dangerous! Highly oversimplified - talk to us first!!!