ERL Project
KEK/IMSS

Science cases on ERL as a synchrotron light source

ERL project Office, KEK

Hiroshi KAWATA

After Sol M. Gruner at the occasion of IMSS symposium 2012

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ERL Specifications[1]

- **Energy range: tunable, VUV to hard x-ray (30 eV to 100 keV)**
- **Spectral brightness: 10^{22} to 10^{23} x-rays/s/mr^2/mm^2/0.1%bw**
- **Highly Coherent Source: 60% at 10 keV in Hi-coherence mode**
- **Hi-flux mode: 100 mA, 25m undulators w/many short periods**
- **Tiny electron energy spread ($2\text{x}10^{-4}$) for 1000 period undulators.**
- **Very flexible operating modes, controlled by injector laser.**
- **Can run with non-recovered interleaved pulses (+ fast kicker)**
- **Short pulse: ~50 fsec**
- **Many simultaneously operating ID stations**
- **2 micron diameter round electron beam facilitates nanoprobe imaging**
- **High repetition rate avoids local sample heating, allow multiple exposures of a sample. Very important for materials science.**

The breadth of science and technology enabled is huge. ERL will be a resource for many sciences, especially materials science.

1. Different modes are not all simultaneous

Science at the Hard X-ray Diffraction Limit

A series of workshops devoted to science with diffraction-limited, high repetition rate, hard x-ray sources, e.g., Energy Recovery Linac and Ultimate Storage Ring sources

CHESS, Cornell Univ., June 2011

https://www.classe.cornell.edu/Research/ERL/ErlXDL2011.html

Science at the Hard X-ray Diffraction Limit (XDL-2011)

- Series of 6 workshops at Cornell in June, 2011
- Co-sponsored by SSRL, DESY, Photon Factory; funded by NSF & DOE
- Lots of interest and excitement
- Lots of ideas for great science enabled by continuous duty, coherent x-ray sources (ERLs & USRs)
- 488 participants

Science at the Hard X-ray Diffraction Limit

XDL 2011

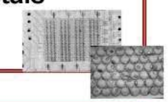
A series of workshops
Cornell University, Ithaca NY ◦ June 2011

A series of workshops devoted to science with diffraction-limited, high repetition rate, hard x-ray sources, e.g., Energy Recovery Linac and Ultimate Storage Ring sources.

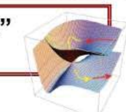
Location: **Robert Purcell Conference Center, Cornell University, Ithaca NY**

Diffraction Microscopy, Holography and Ptychography using Coherent Beams
June 6 & 7, 2011

Biomolecular Structure from Nanocrystals and Diffuse Scattering
June 13 & 14, 2011

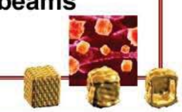


Ultra-fast Science with "Tickle and Probe"
June 20 & 21, 2011

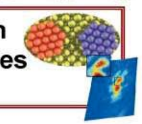


High-pressure Science at the Edge of Feasibility
June 23 & 24, 2011

Materials Science with Coherent Nanobeams at the Edge of Feasibility
June 27 & 28, 2011



Frontier Science with X-ray Correlation Spectroscopies using Continuous Sources
June 29 & 30, 2011



CHESS DESY SSRL PF Photon Factory

http://erl.chess.cornell.edu/gatherings/2011_Workshops/index.htm
For more information contact Kathy Dedrick, User Administrator – 607-255-0920

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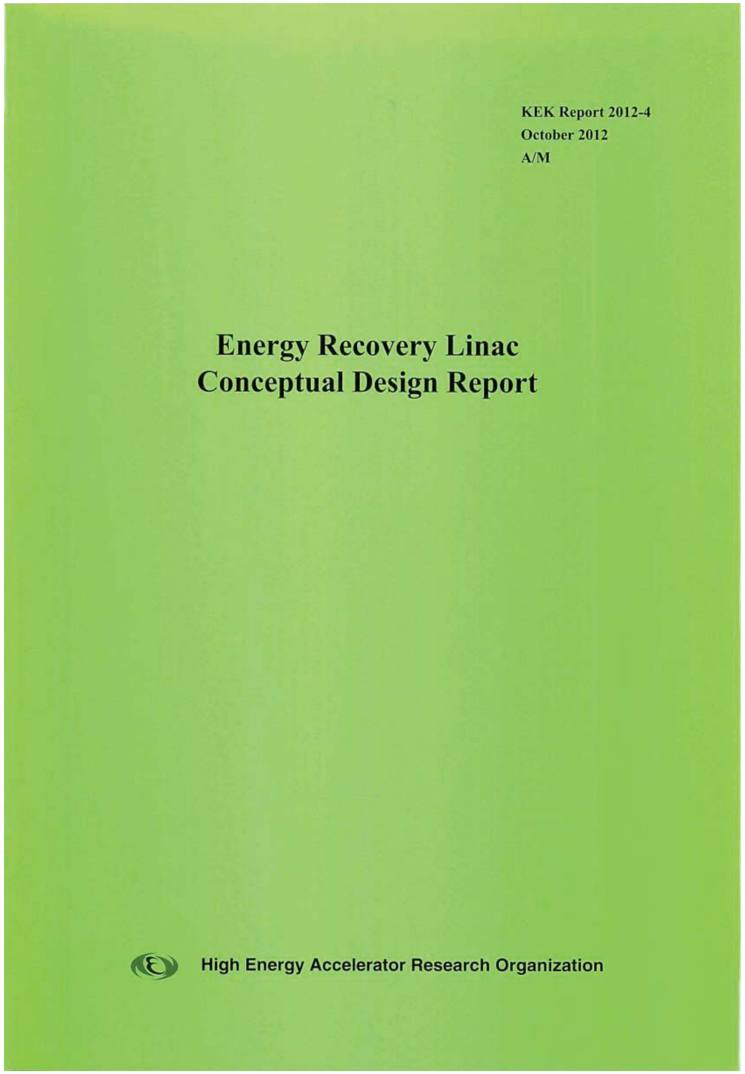
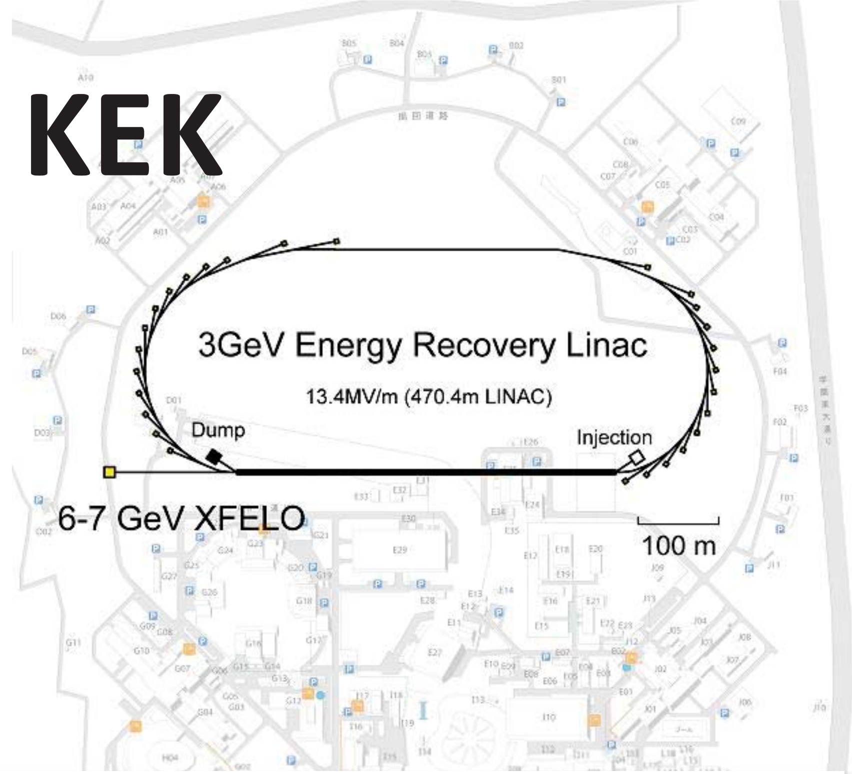


http://ccdb5fs.kek.jp/tiff/2012/1224/1224004.pdf

KEK Report 2012-4



- Beam energy
  - Full energy: 3 GeV
  - Injection and dump :10 MeV
- Geometry
  - Linac length : 470 m
- Straight sections for ID’s
  - 22 x 6 m short straight
  - 6 x 30 m long straight

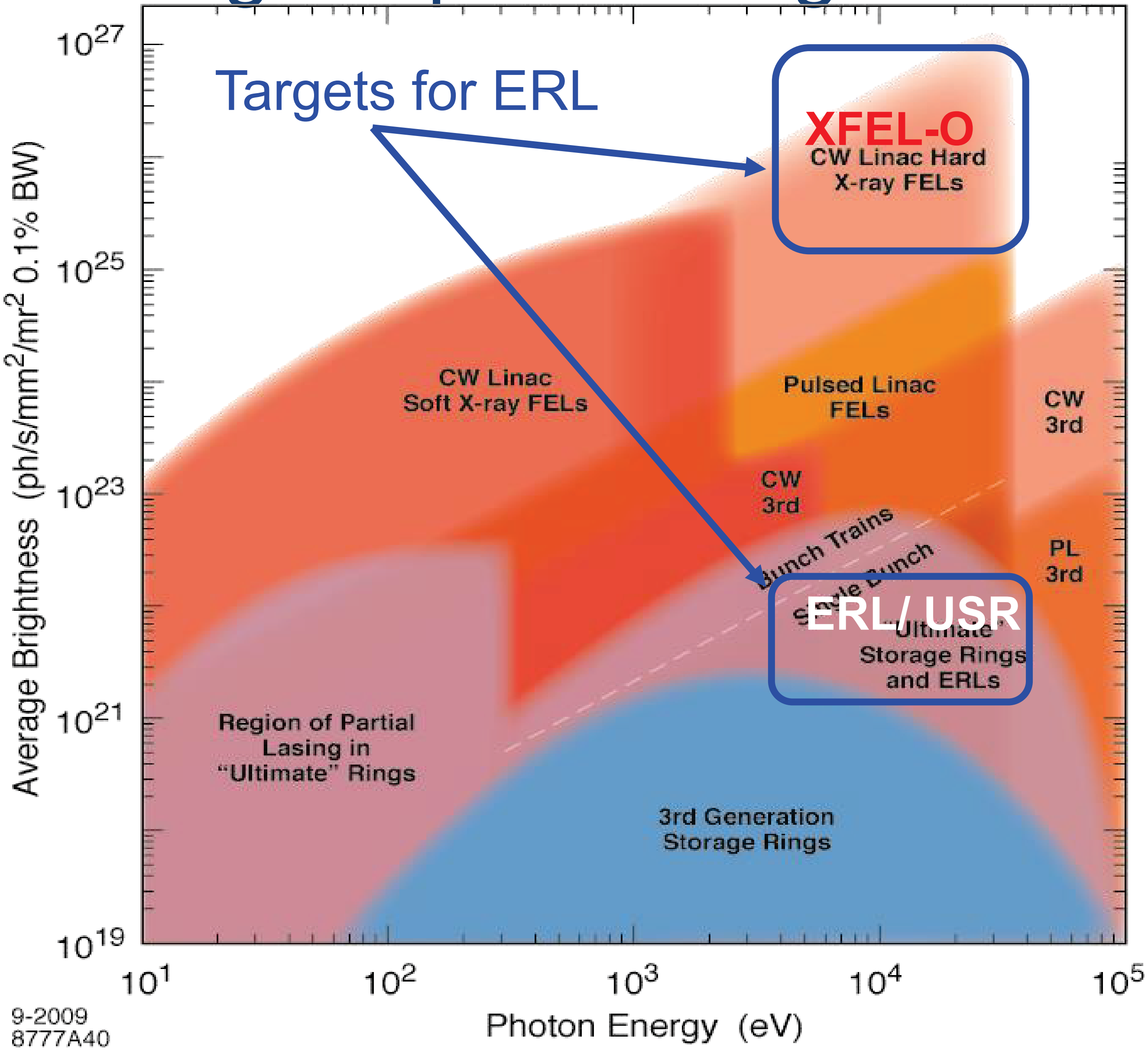
Chapter 1 Executive Summary (1)

ERL is a future X-ray light source designed based on state-of-the-art superconducting linear accelerator technology, which will offer far higher performance than the existing storage ring. The **high repetition rate**, **short pulse**, **high spatial coherence and high brightness** of ERL will enable the filming of ultrafast atomic-scale movies and determination of the structure of heterogeneous systems on the nano-scale. These unique capabilities of ERL will drive forward a distinct **paradigm shift** in X-ray science from ***"static and homogeneous"*** **systems to** ***"dynamic and heterogeneous"*** **systems,** in other words, from ***"time- and space-averaged"*** **analysis to** ***"time- and space-resolved"*** **analysis.**

Chapter 1 Executive Summary (2)

This paradigm shift will make it possible to directly witness **how heterogeneous functional materials work in real time and space,** and will enable predictions to be made in order to design and innovate better functional materials which will eventually solve the grand challenges of society and support life in future. Such functional materials will continue to be used in indispensable technologies such as catalysts, batteries, superconductors, biofuels, random access memories, spintronics devices and photoswitches.

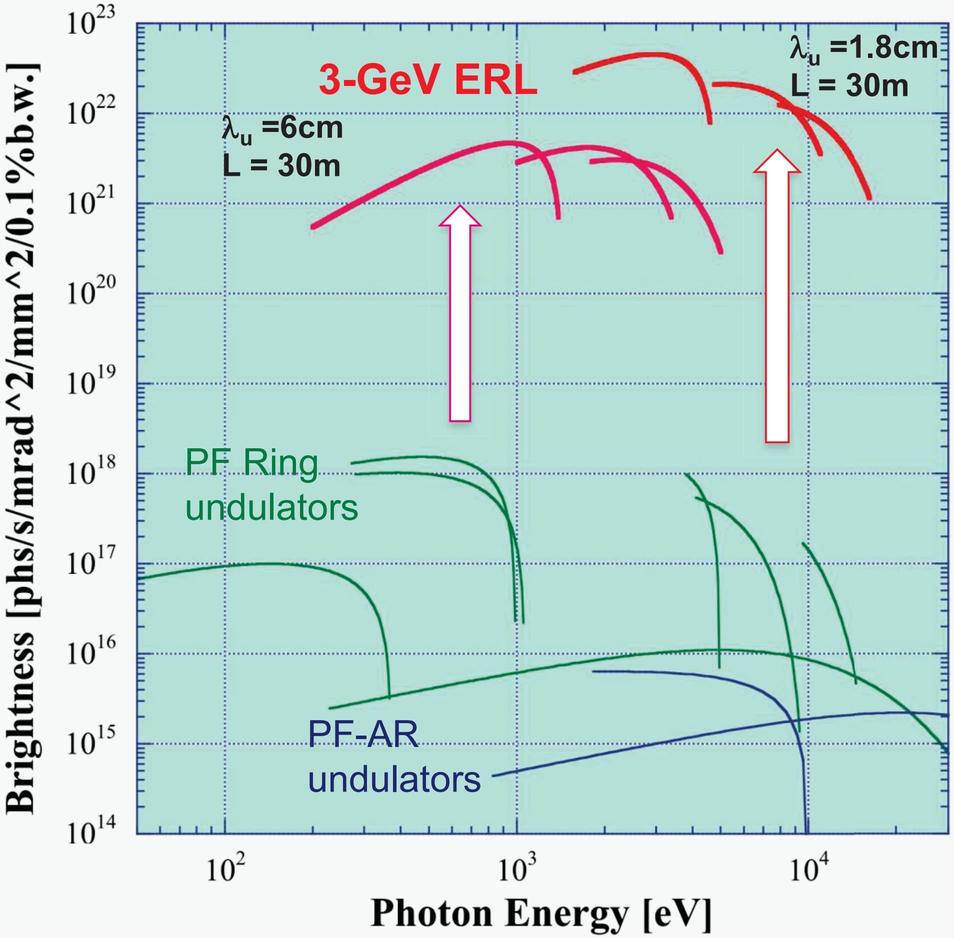
Target: spectral brightness



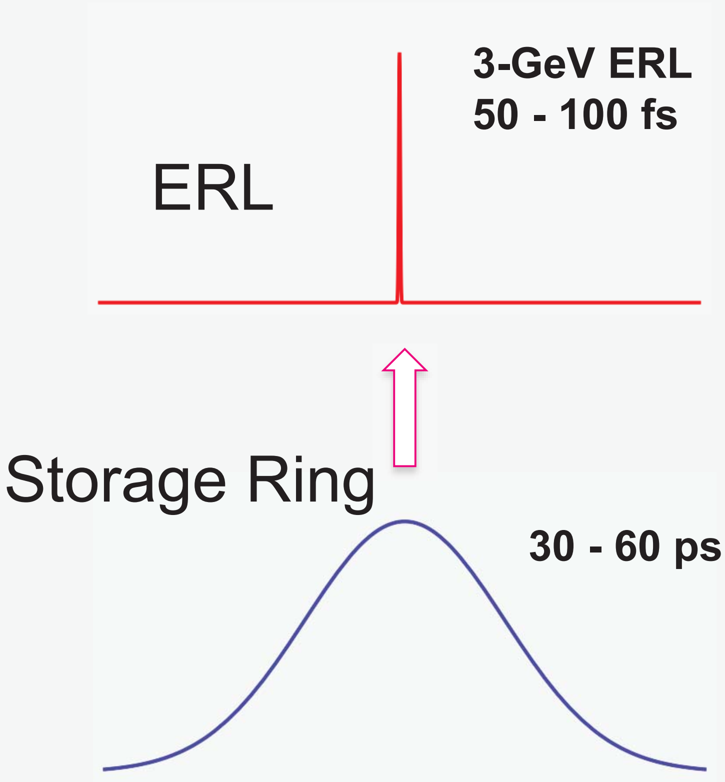
Figures are cited from: R. Hettel, "Performance Metrics of Future Light 13 Sources", FLS2010, SLAC, March 1, 2010.

Light Source Performance

Spectral Brightness



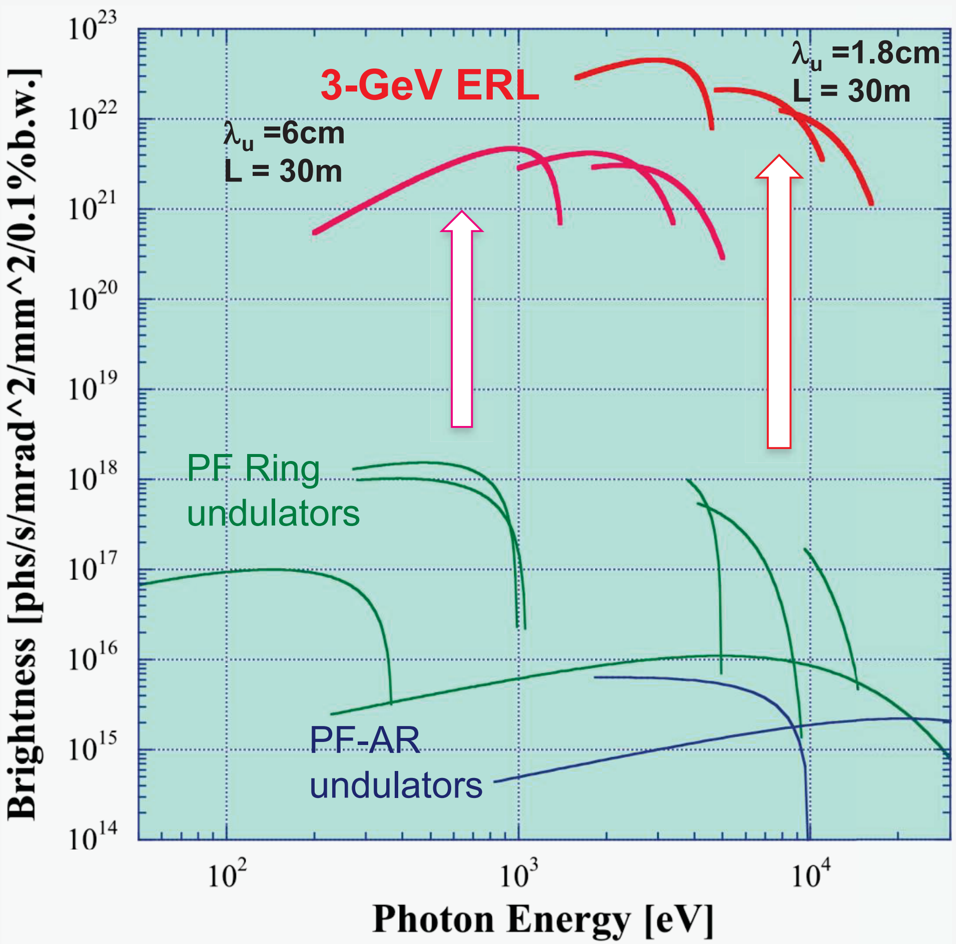
SR Pulse length



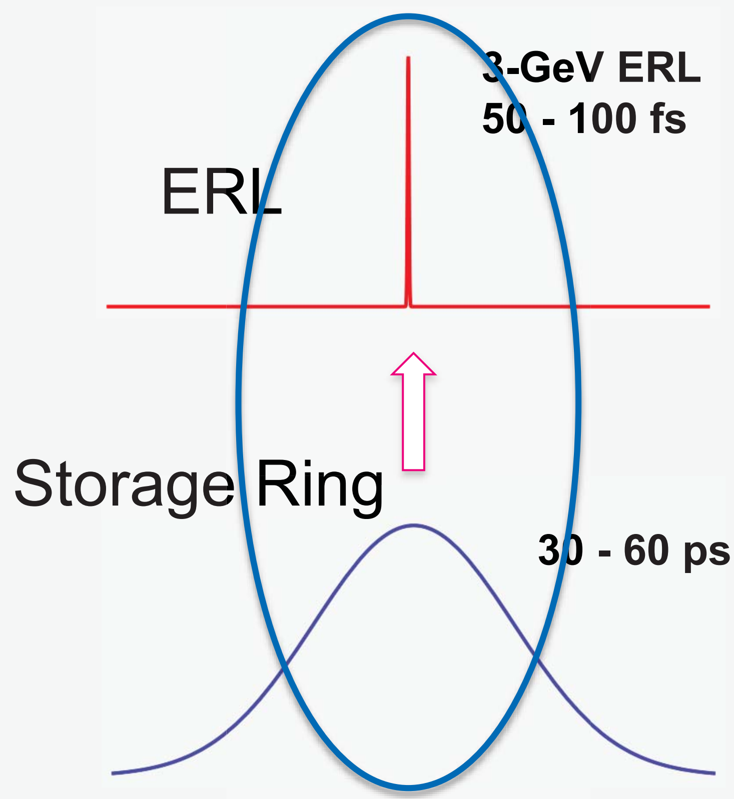
Calculated by K. Tsuchiya

Light Source Performance

Spectral Brightness



SR Pulse length



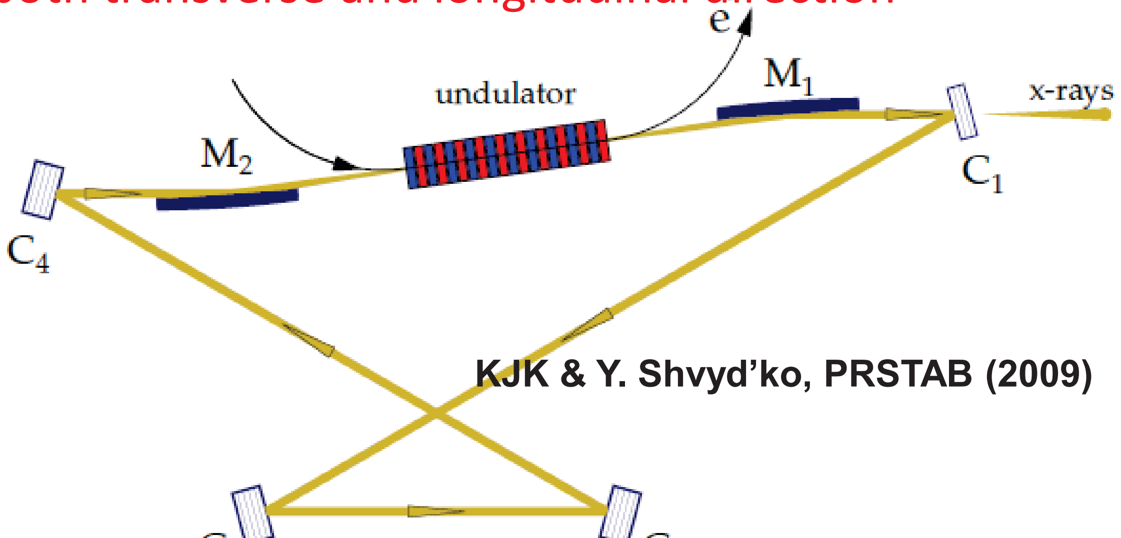
Calculated by K. Tsuchiya

Further possibility of upgraded ERL (1)

XFEL Oscillator and or (CW-FEL)

Super high flux and high energy resolution X-ray beam
full coherence X-ray in both transverse and longitudinal direction

- **10^{15} photons/s, or 10^{9} photons/pulse(@~10keV with a few meV b.w.)**
- **Single mode X-ray laser**



KJK & Y. Shvyd'ko, PRSTAB (2009)

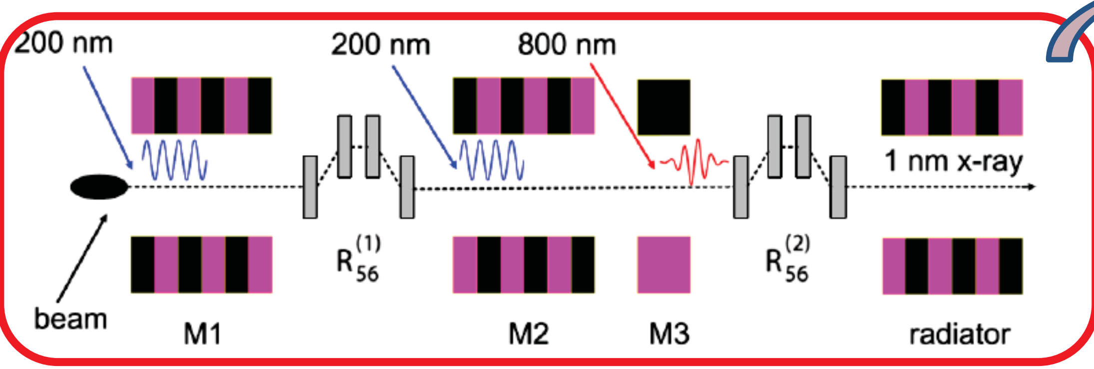
- **Revolution of the Inelastic X-ray scattering experiment (increase the photon number of 10^{6})**

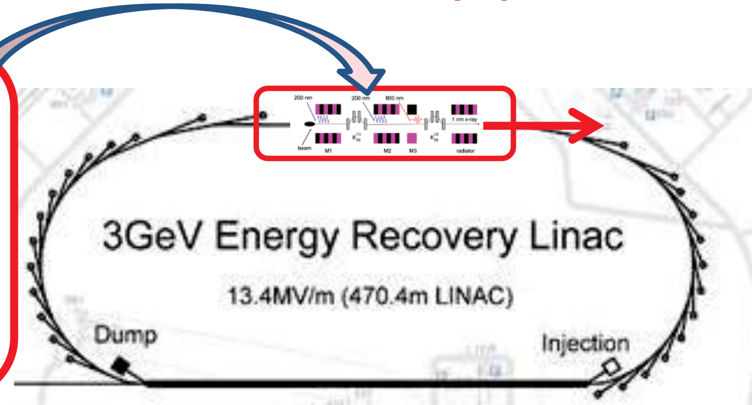
  nm-space resolved inelastic scattering (nucleation process of phase transition)
  From RIXS to NIXS to achieve the quantitative measurement
  Bulk-sensitive Fermi surface study with HX-TR-AR PES
  ....and new applications

Further possibility of upgraded ERL (2)

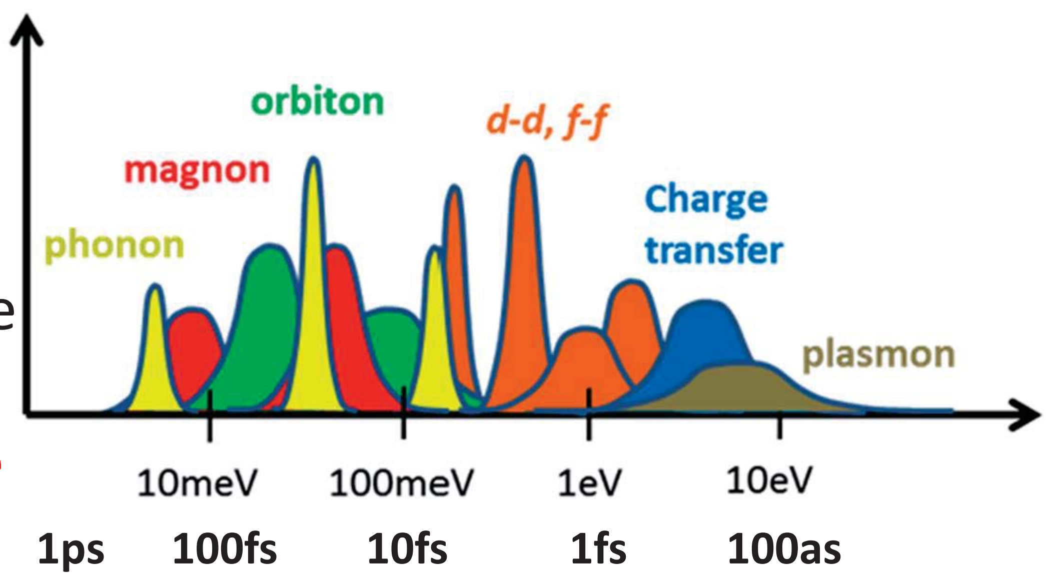
Echo-Enabled Harmonic Generation (EEHG)

Production of Sub-femto second soft X-ray pulse





D. Xiang, Z. Huang, and G. Stupakov,
Phys. Rev. ST Accel. Beams 12, 060701 (2009)



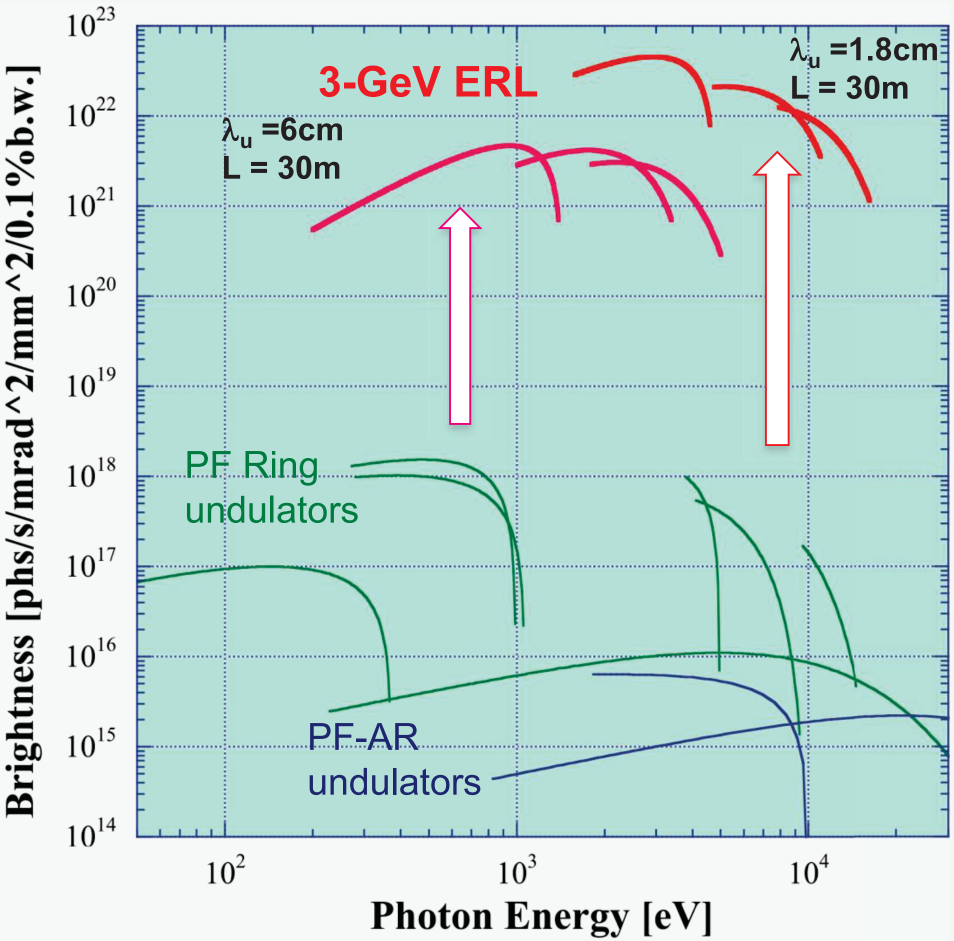
Measurement of excitation

Present: spectroscopy technique

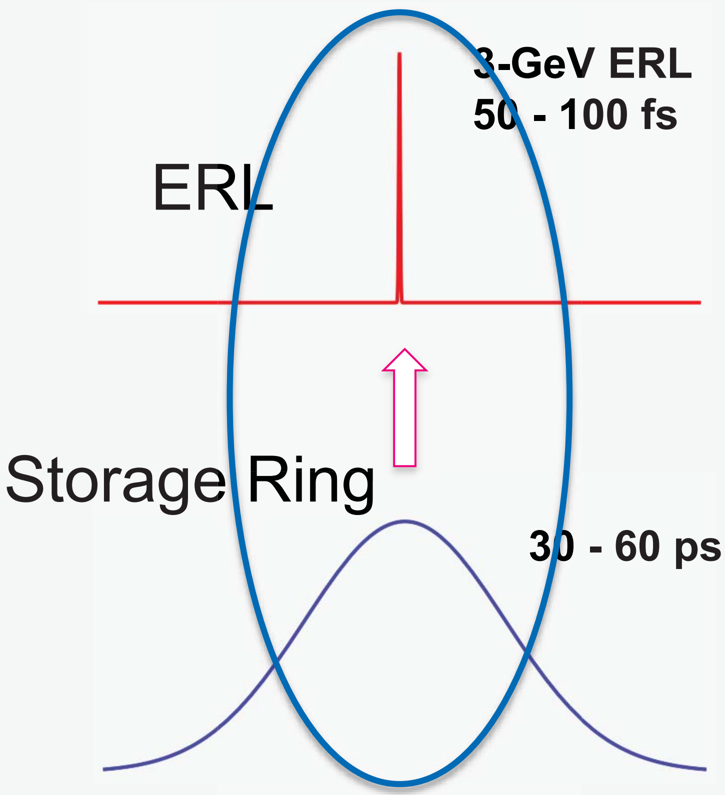
ERL: Direct observation of these excitation processes

Light Source Performance

Spectral Brightness



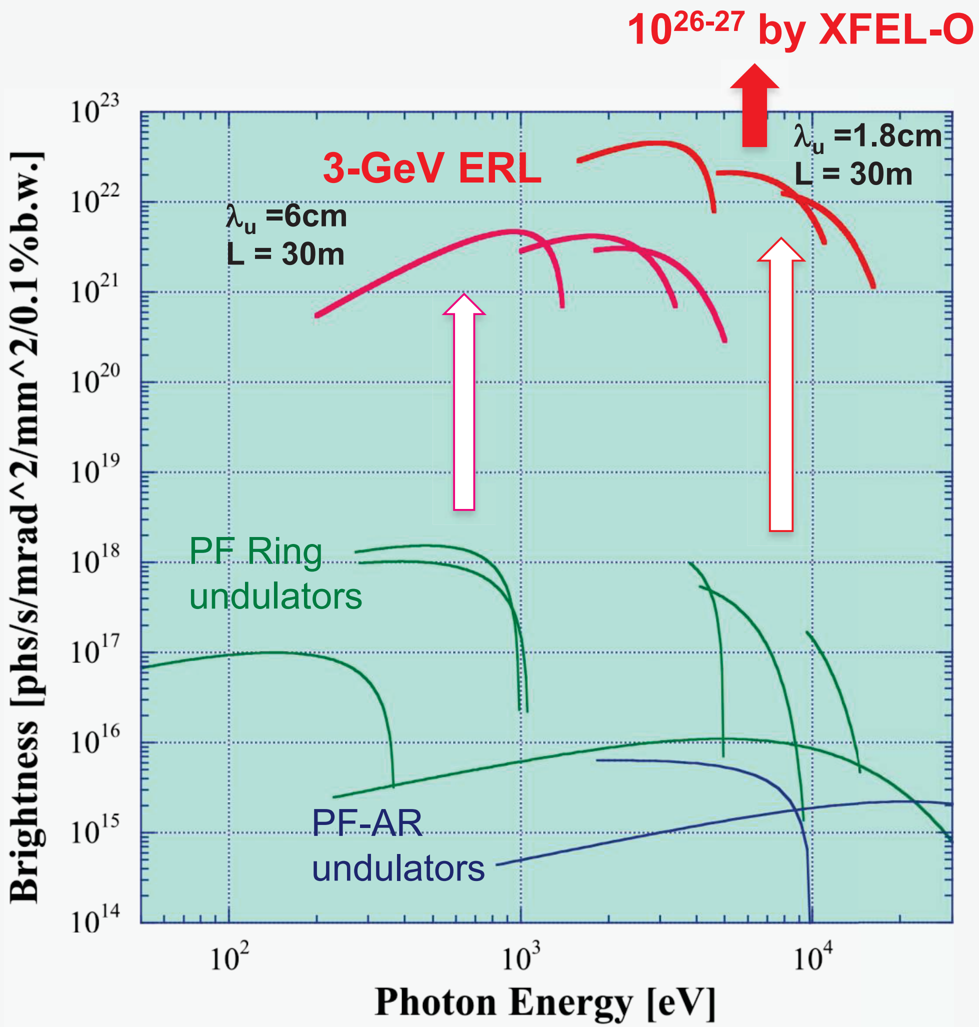
SR Pulse length



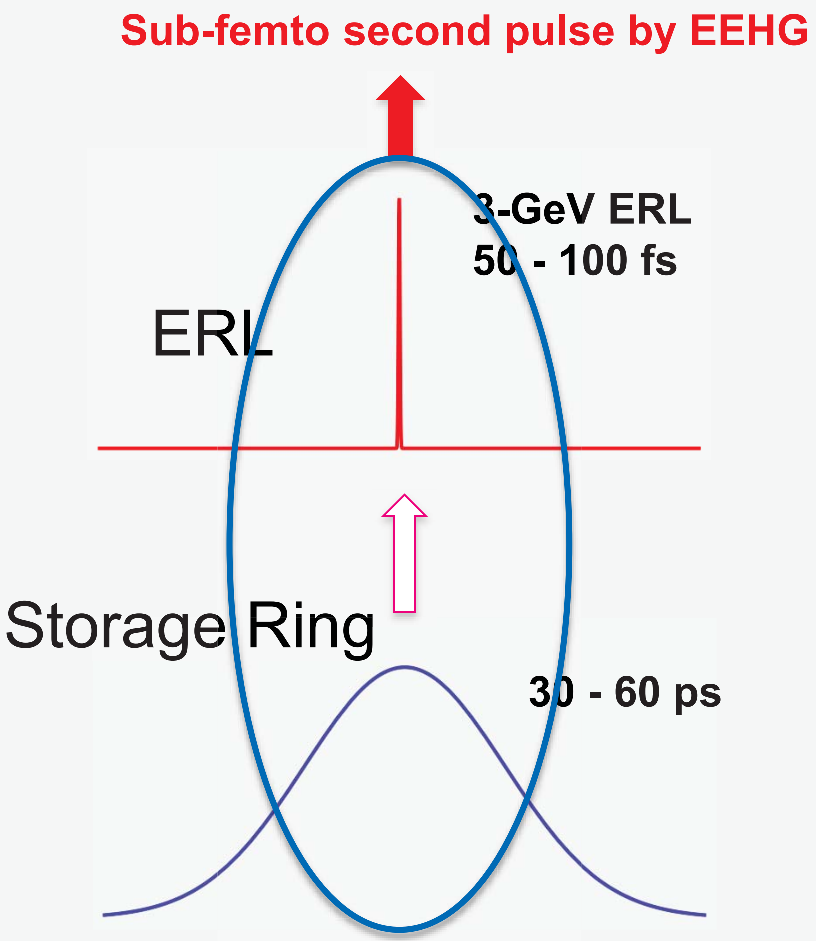
Calculated by K. Tsuchiya

Light Source Performance

Spectral Brightness



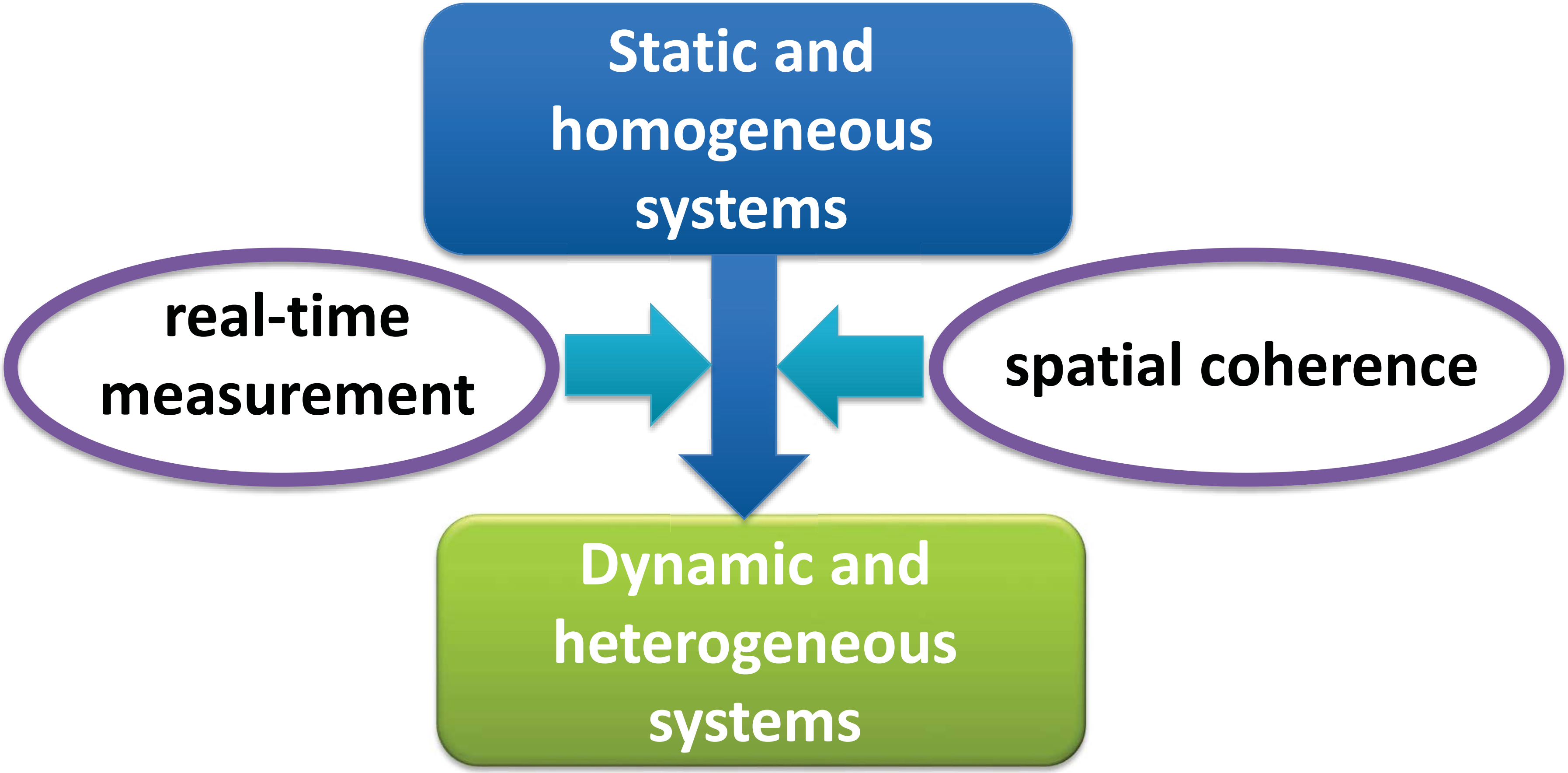
SR Pulse length



Calculated by K. Tsuchiya

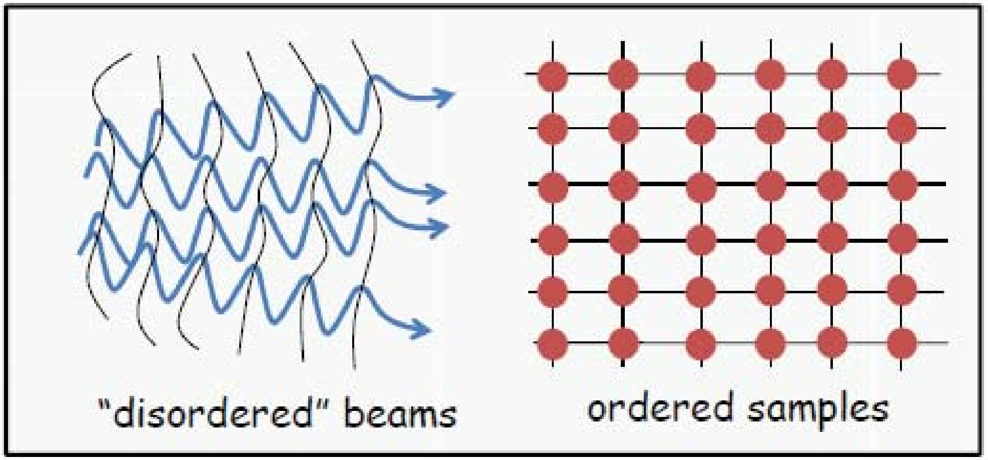
Strategy for new light sources

Our Goals: Characterizing heterogeneous and functional materials in action at nano-scale

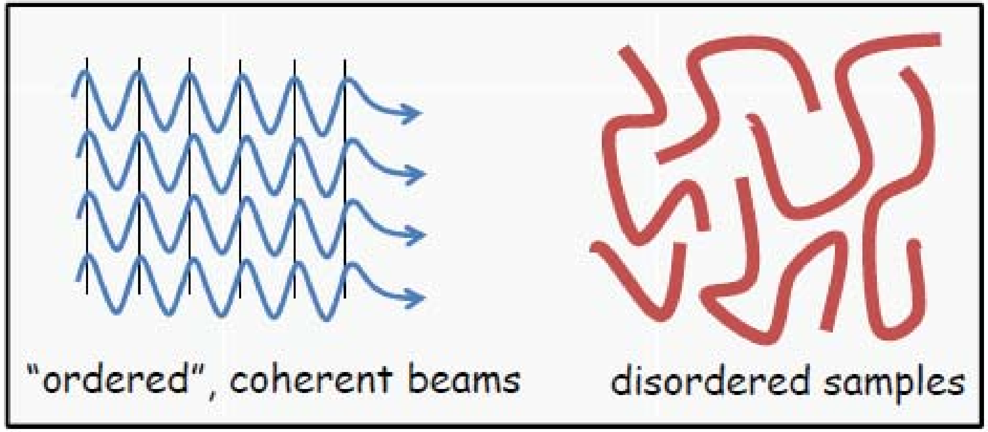


Incoherent vs. coherent X-ray beams

PAST & PRESENT:



FUTURE:



http://erl.chess.cornell.edu/gatherings/2011_Workshops/talks/WS1Shpyrko.pdf

Materials Overview

**Simon Billinge (Columbia), Paul Evans (U of Wisconsin)
& Reinhard Boehler (Carnegie Institution of Washington)**

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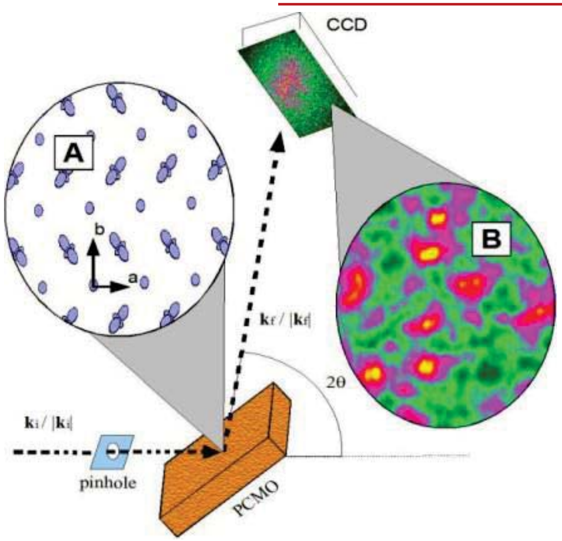

Coherent diffraction imaging of electronic textures in correlated materials. Information is available on nanometer spatial scale. Josh Turner et al., New J. Phys. 10 (2008) 053023.

“Advances in **materials science lie on the critical path of many technological solutions to mankind's most pressing problems, such as sustainable energy, environmental remediation and health**. Increasingly we seek materials that have directed functionalities, in analogy with enzymes in biological systems, that can be built up into more complicated devices. **This necessitates the study of materials of increasing complexity**, for example, larger unit cells, more complicated compositions, heterostructures on the nanometer and micrometer length-scales, and structural modifications on the nanoscale. **Nanostructured materials are at the heart of many of these proposed technologies.”, Simon Billinge**

“These emerging hard **x-ray sources can be focused to small spot sizes, at which they can provide high-resolution structural information via either diffractive imaging or scanning techniques. The fs to ps bunch duration of the electron bunches at these sources inherently allows such probes to provide time resolution simultaneously.** Key examples of the scientific impact of these developments will arise in the study of both reversible and irreversible materials processes. The scientific needs for these probes arises in the study of fundamental excitations, GHz mechanics, **dynamics in magnetic and spintronic devices, and dynamics and extreme conditions in complex oxides, etc.”, Paul Evans**

“**Melting at high pressure is of fundamental interest and plays a key role in estimates on temperatures in planetary interiors** and on the dynamics of dynamos creating magnetic fields and dynamics of motion in planetary mantles and plate tectonics. **Melting temperatures of both metals and silicates/oxides measured statically in laser-heated diamond cells are in serious disagreement with those obtained from shock experiments for transition metals. Diffraction measurements on a millisecond resolved time sequence could resolve this issue to follow the structural evolution during the melting-freezing event.**” **Reinhard Boehler**

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Dynamics of soft matter & complex fluids

Y. Shinohara[1], W. Burghardt[2], A. Fluerasu[3], S. Mochrie[4], L. Lurio[5]

Workshop 6: X-ray Correlation Spectroscopy using continuous beams

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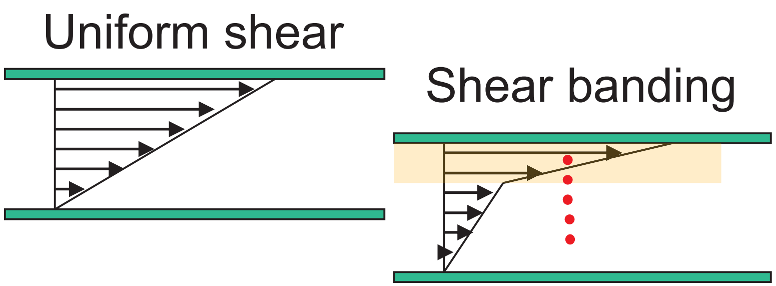
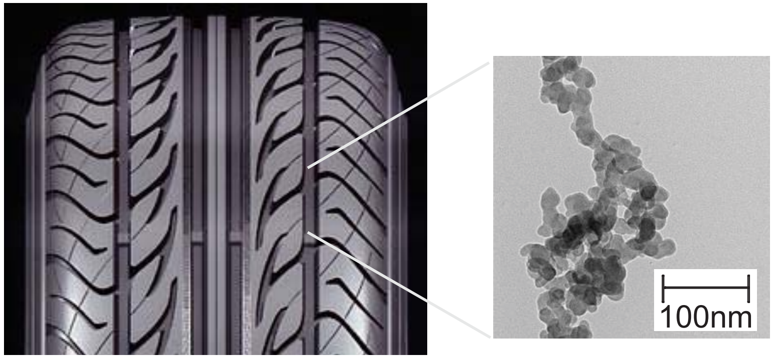
Nonlinear viscoelasticity



Many engineered and biological soft materials, such as polymers, colloids, emulsions, gels, etc., exhibit important but poorly understood behavior in non-equilibrium conditions, such as non-linear viscosity during flow (left). For example, although colloidal particles are often added to rubber to manipulate performance, the affect of such additives on elasticity and viscosity is difficult to predict.

Colloidal aggregates in soft-matter



The origins of such behavior involve molecular-scale fluctuations on length scales of 10-1000 nm and 10^{-6}-10^{-2} second time scales.

XPCS can directly measure these fluctuations, but such length and time scales require 2-3 orders of magnitude more coherence flux. ERL/USR sources should make such measurements routine, with potential impacts in many areas of application, such as improved tire performance.

[1]*Department of Advanced Materials Science, University of Tokyo*
[2]*Department of Chemical and Biological Engineering, Northwestern University*
[3]*NSLS-II, Brookhaven National Laboratory*
[4]*Department of Physics, Yale University*
[5]*Department of Physics, Northern Illinois University*

After Sol M. Gruner at the occasion of IMSS symposium 2012

Structures of biological cells with < 10 nm resolution in 3D

Chae Un Kim, Cornell University

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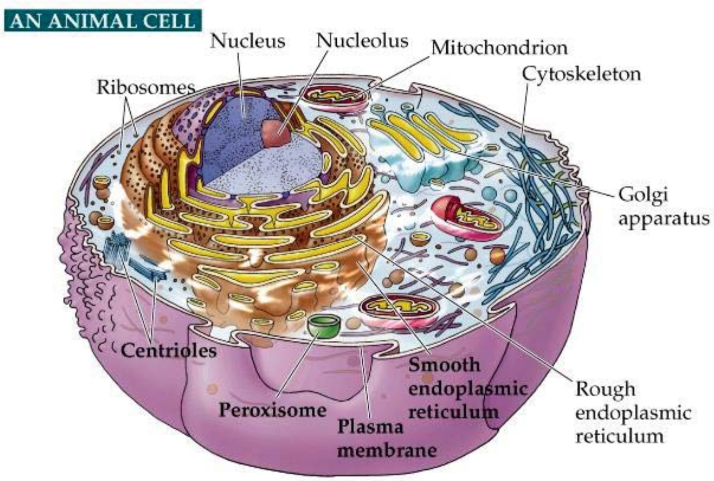
Workshop 1: Diffraction Microscopy, Holography and Ptychography using Coherent Beams



Visualization of sub-cellular components in 3D at high resolution is essential to understanding how cells function. However, the currently existing microscopic techniques have limitations for this purpose. Optical microscopy cannot provide high enough resolution (typically worse than 200 nm) and electron microscopy is poorly suited for thick cellular samples, requiring >1,000 sections.

X-ray diffraction microscopy (XDM) is a lensless microscopic technique and uses the high penetration power of X-rays to image biological cell (of a few microns in size) at high resolution in 3D. **XDM offers potential to image whole cancer cells or the structure and connectivity of the sub-cellular organelles in 3D at 5-10 nm resolution.**

The fundamental image resolution of XDM for biological samples is set by radiation damage. A variety of cryopreservation methods have been developed, including ambient plunge-freezing and high-pressure cryocooling techniques. The cryopreservation of hydrated samples replaces water with either low-density amorphous (LDA) or high-density amorphous (HDA) ice. Both LDA and HDA ice exhibit density fluctuations, whose structure and origins are presently poorly understood, which limit the use of cryopreservation for XDM.

Probing local structures of HDA/LDA ice requires highly brilliant/coherent nano-focused X-ray beams. The X-ray sources such as ERLs/USRs provide an ideal X-ray probe for this types of study. After better accounting for these density fluctuations, we anticipate that **the highly brilliant and coherent X-ray beams from ERLs/USRs will allow, for the first time, study of cellular structures in 3D with 5 to 7 nm spatial resolution .**

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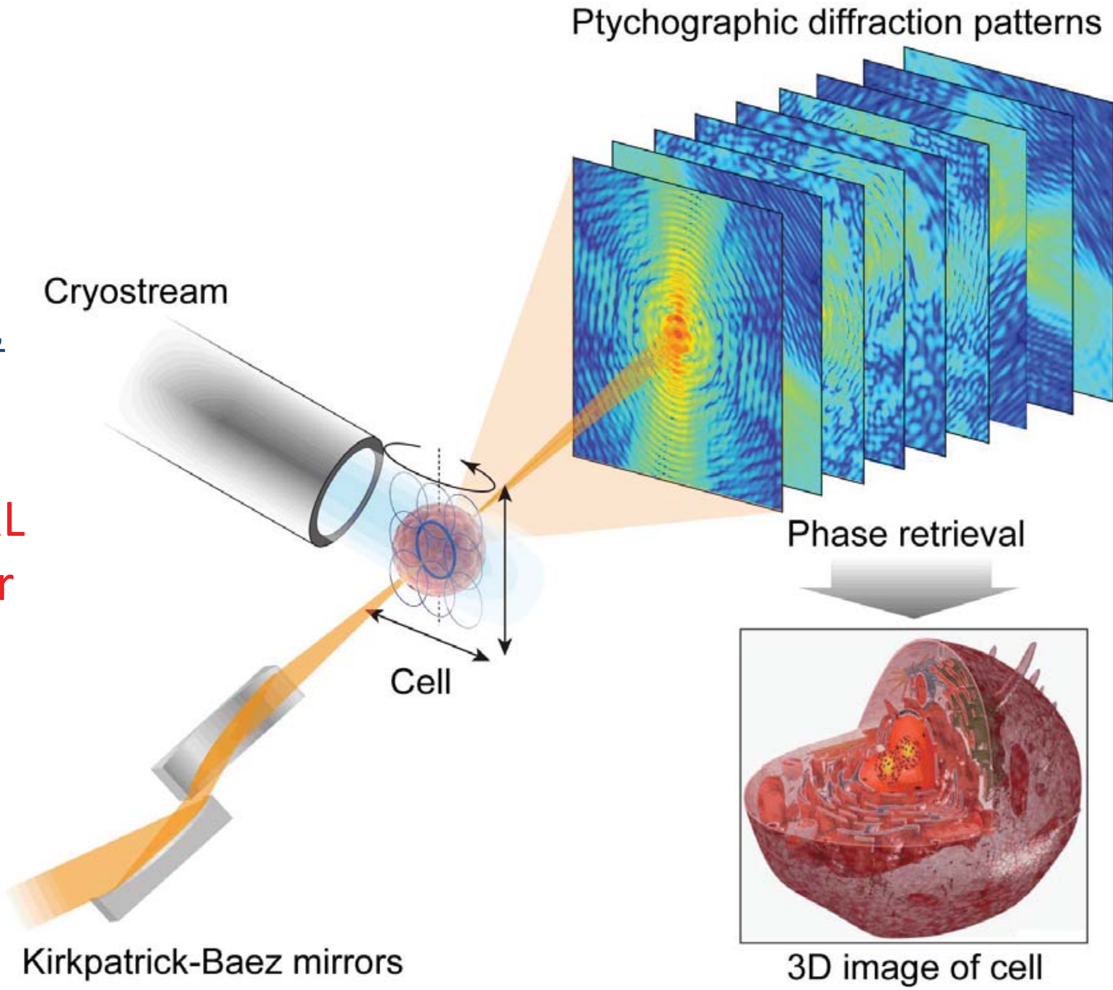
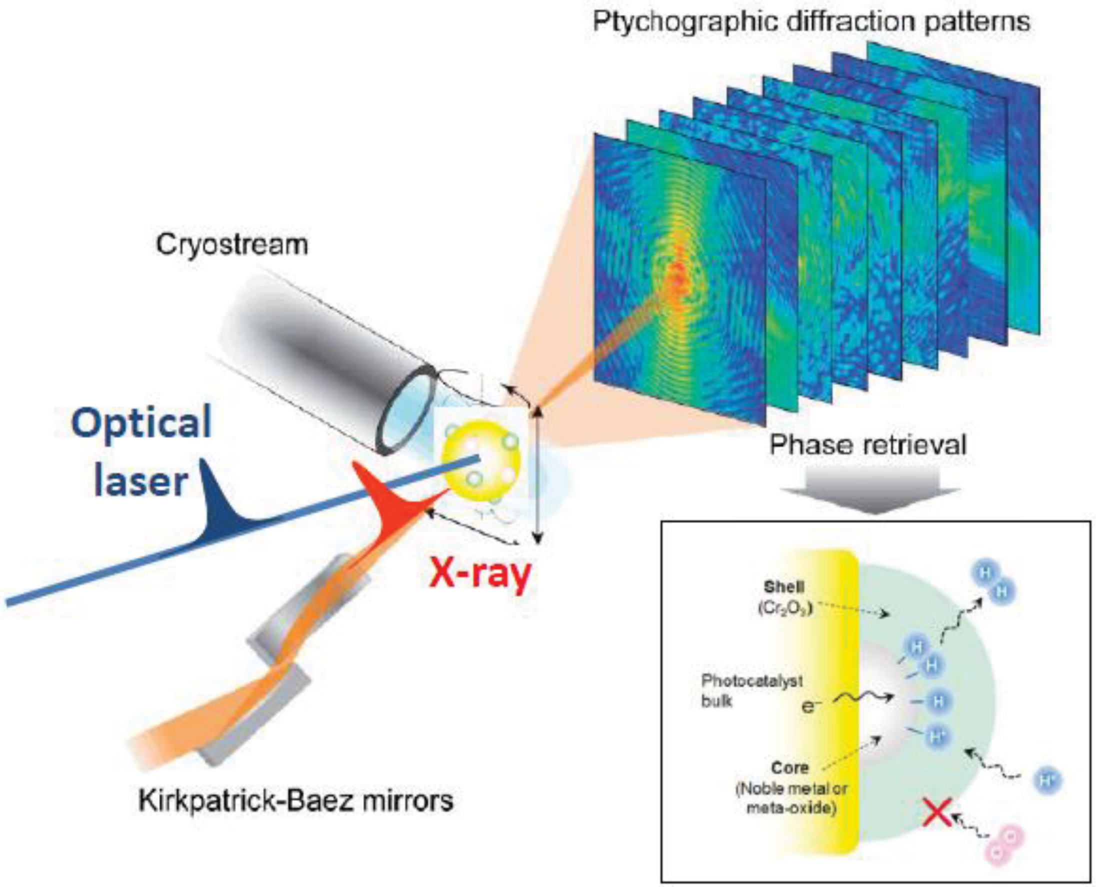
3D Imaging of whole cell

It is expected that the CXDI of single particles using the single-shot **"diffract and destroy"** approach in XFELs will break the resolution limit due to the radiation and hence can achieve atomic resolution. However, this approach limits the types of samples, i.e., the samples must be reproducible. On the other hand, ERL provides orders of-magnitude higher coherent flux than the third-generation synchrotron radiation. Then, ERL can realize **"ultimate nondestructive"** CXDI. CXDI with XFEL and CXDI with ERL should be complementary techniques.



ERL experiment

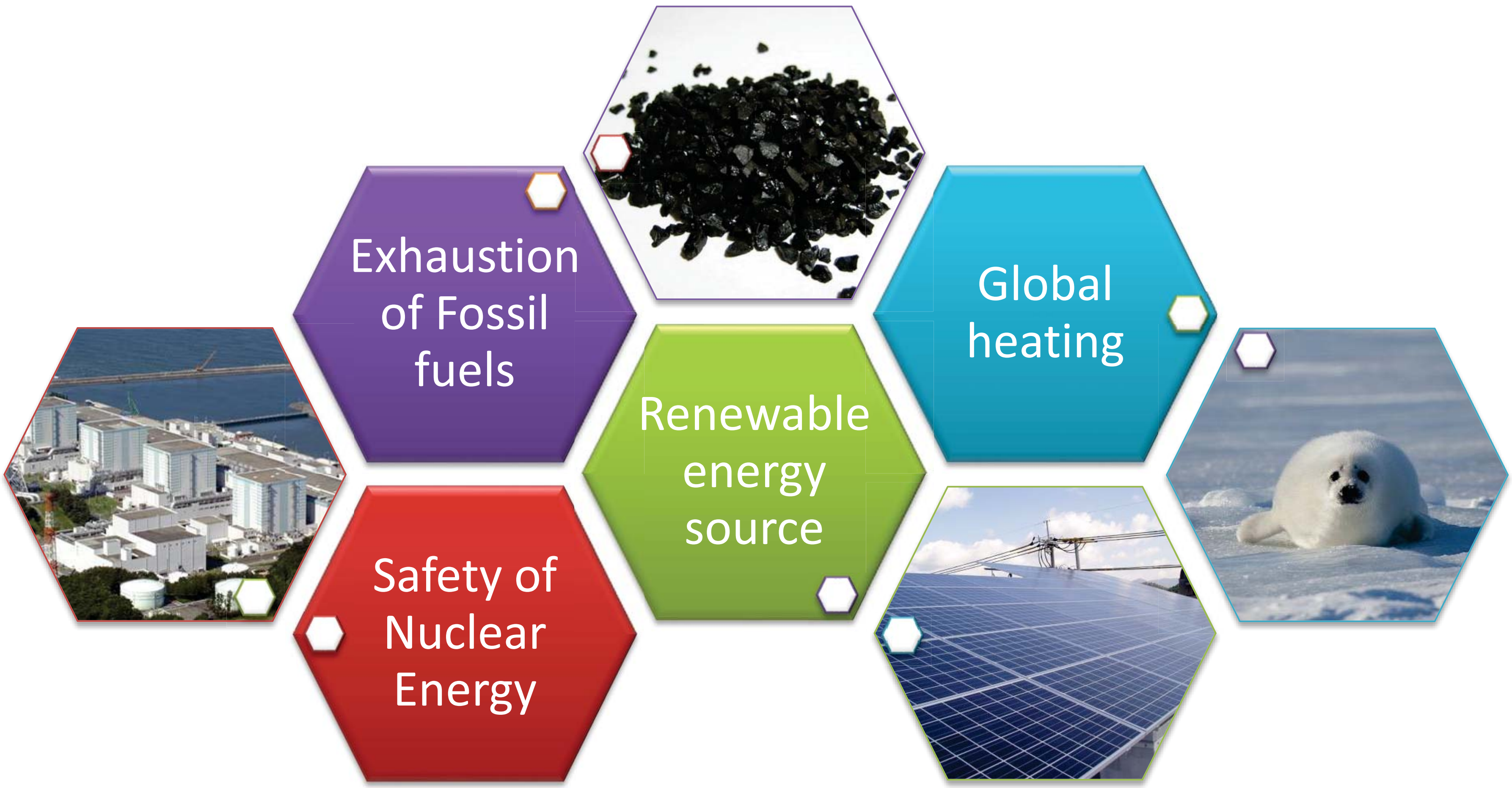
femtosecond pump-probe X-ray coherent diffraction imaging of single photo-catalyst particle



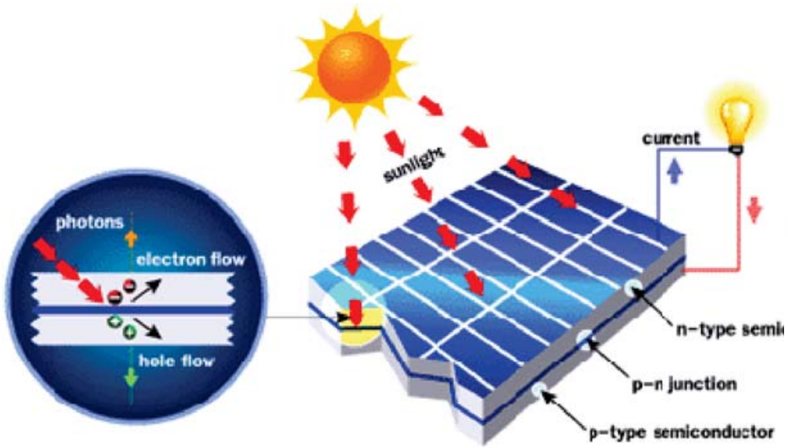
Courtesy of Prof. Yukio Takahashi
(Osaka Univ.)
(ERL Conceptual Design Report)

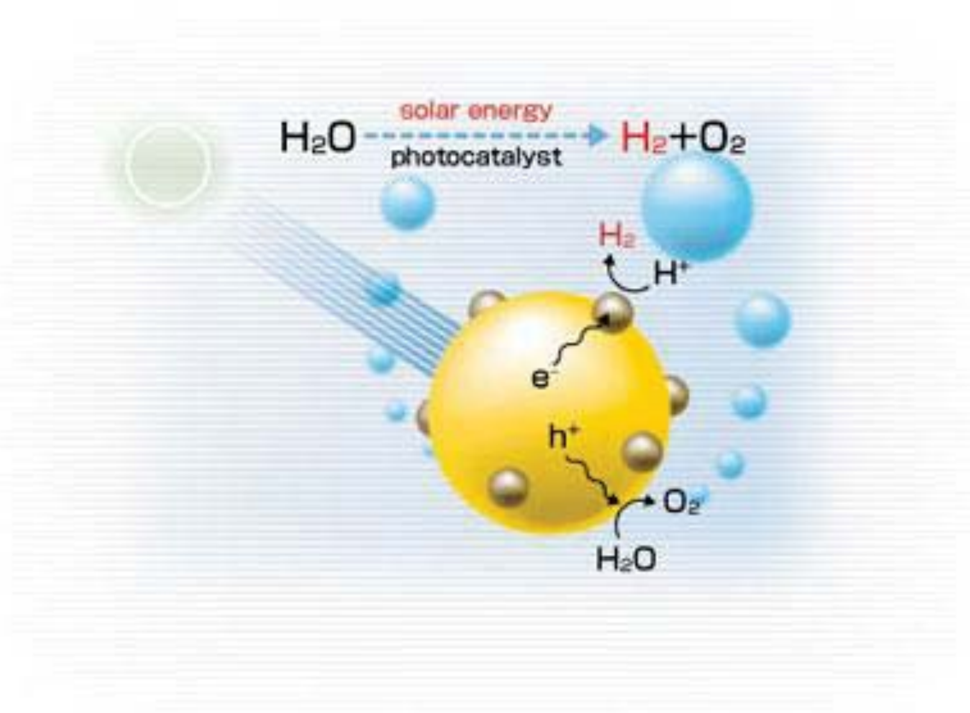
Femtosecond 3D movie of Photo-catalyst in action!

Future challenges
ERL for sustainable society



Key players
Solar Cell and Photocatalyst



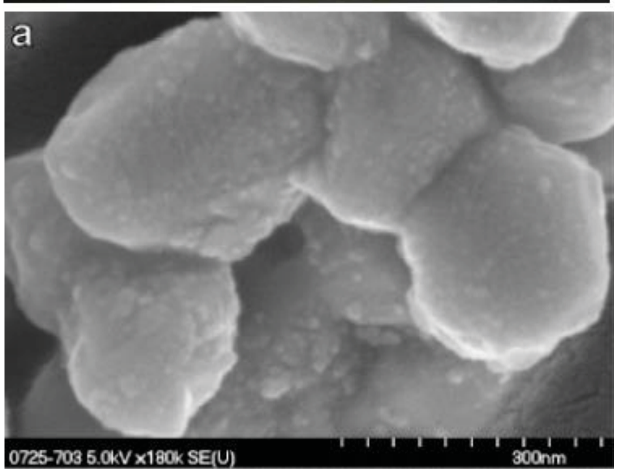


- Converts light energy to electricity
- Large-scale battery is needed for storage
- Quantum efficiency : ~20%

- Converts light energy to chemical energy
- Easily stored as hydrogen or hydrocarbons
- Quantum efficiency: ~5%

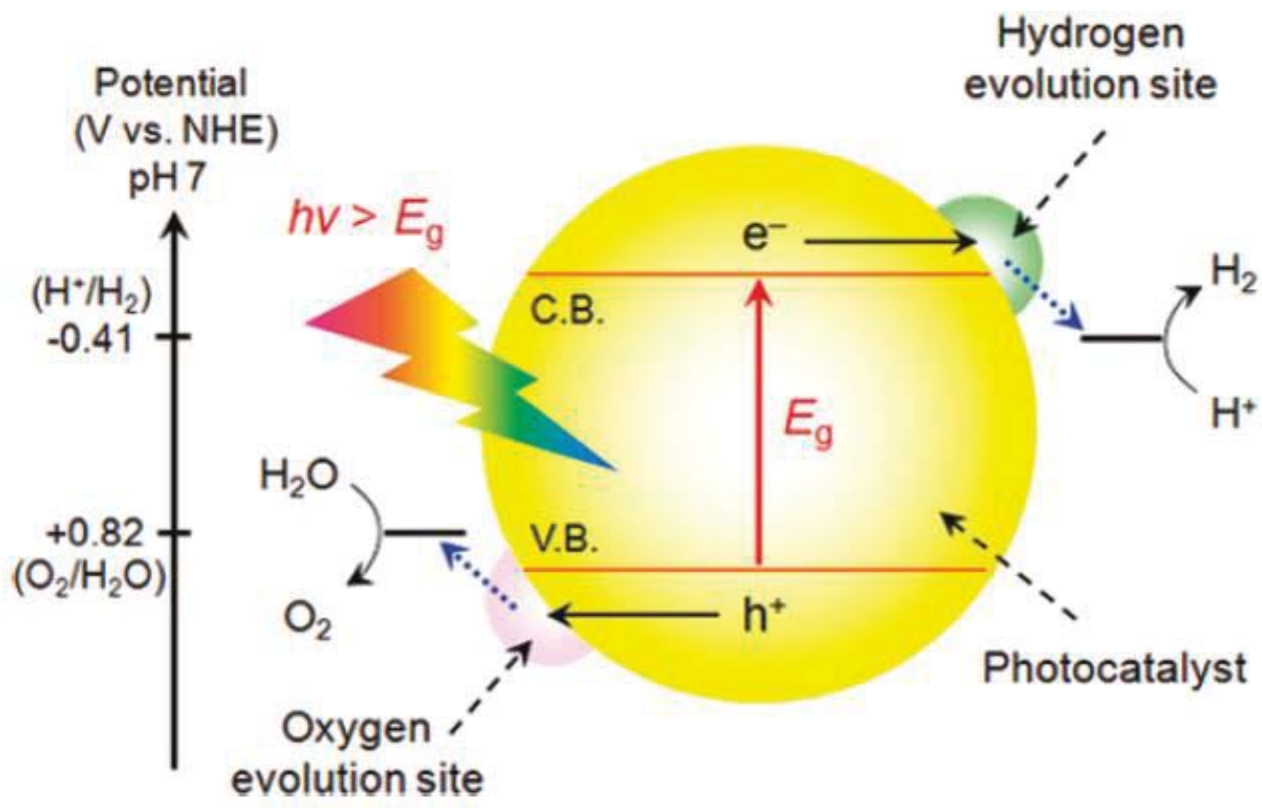
Toward artificial photosynthesis (2)

Hydrogen generation from water by photocatalyst $(Ga_{1-x}Zn_x)(N_{1-x}O_x)$



Maeda K. et al. (2006) *Nature* **440**, 295

Toward artificial photosynthesis (1)
Ultrafast dynamics of photocatalyst



Maeda, K. and Domen K. (2010) *J. Phys. Chem. Lett*. **1**, 2655.

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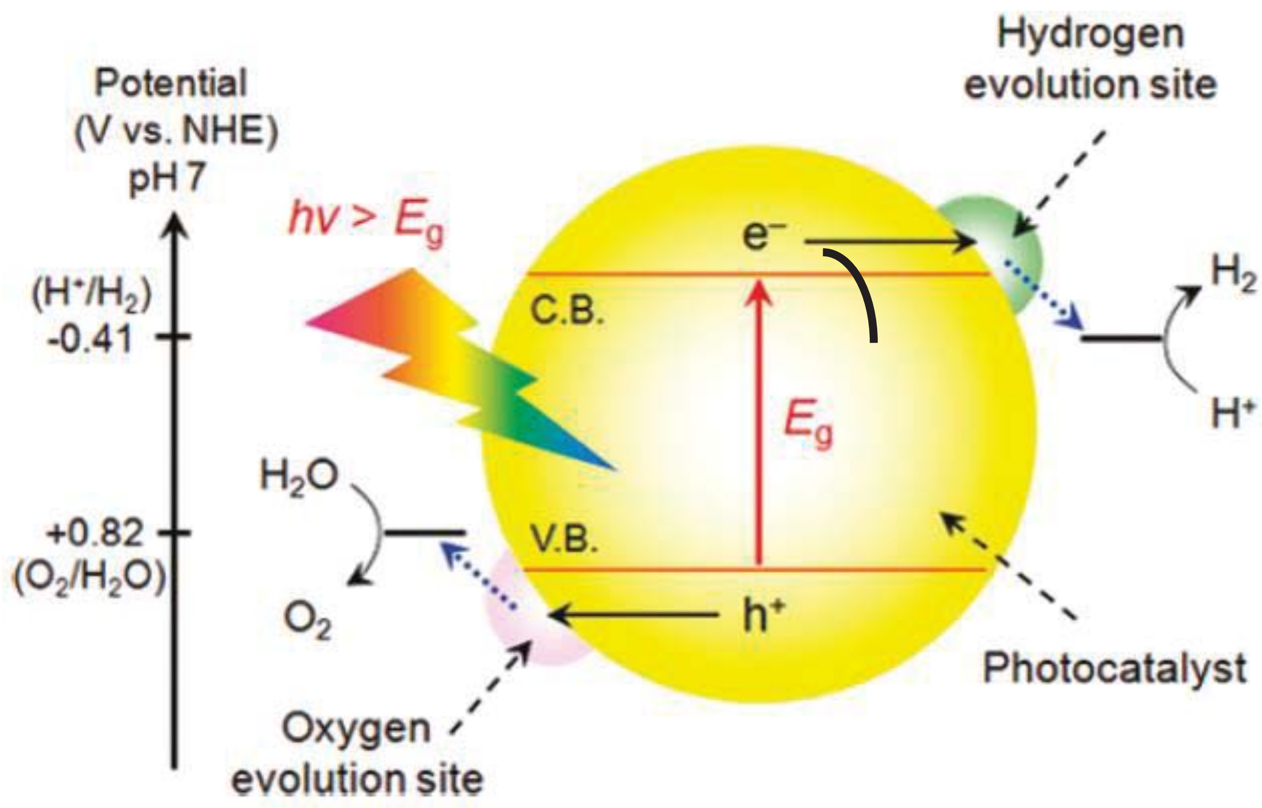

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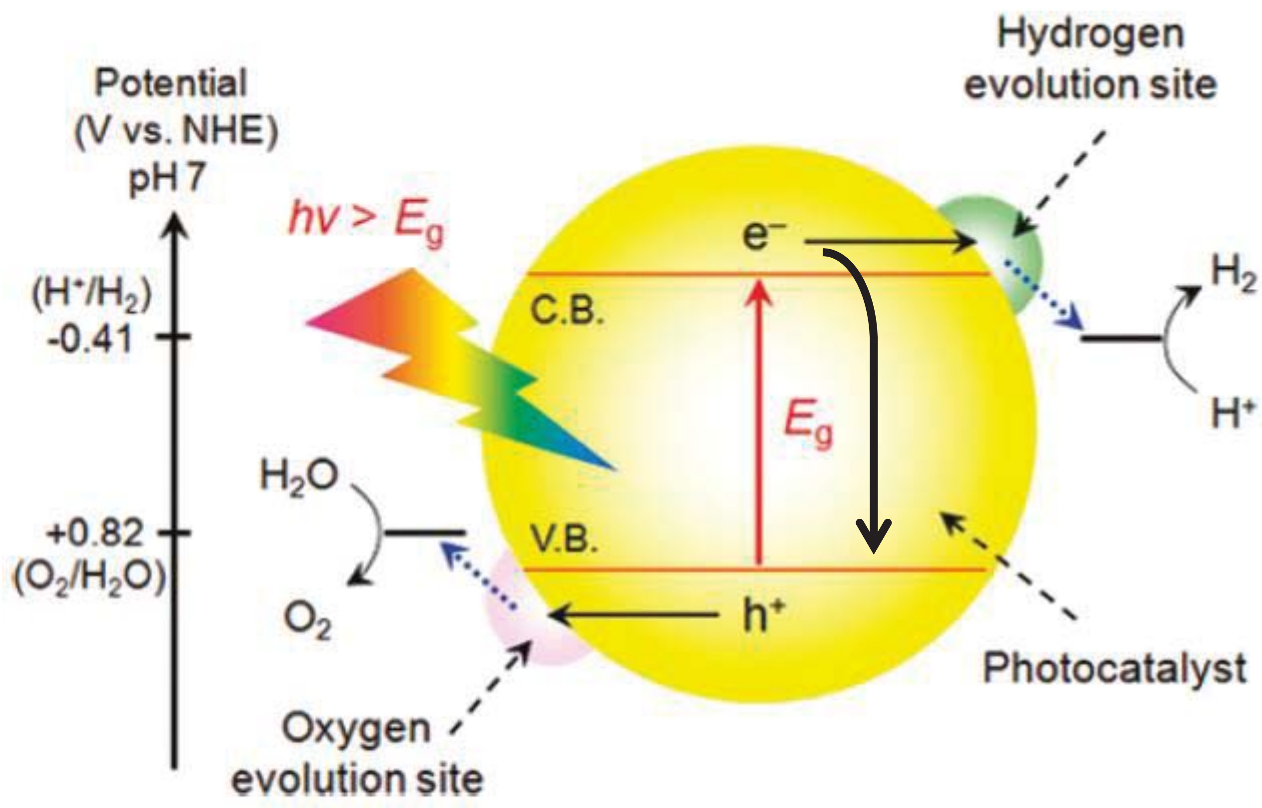

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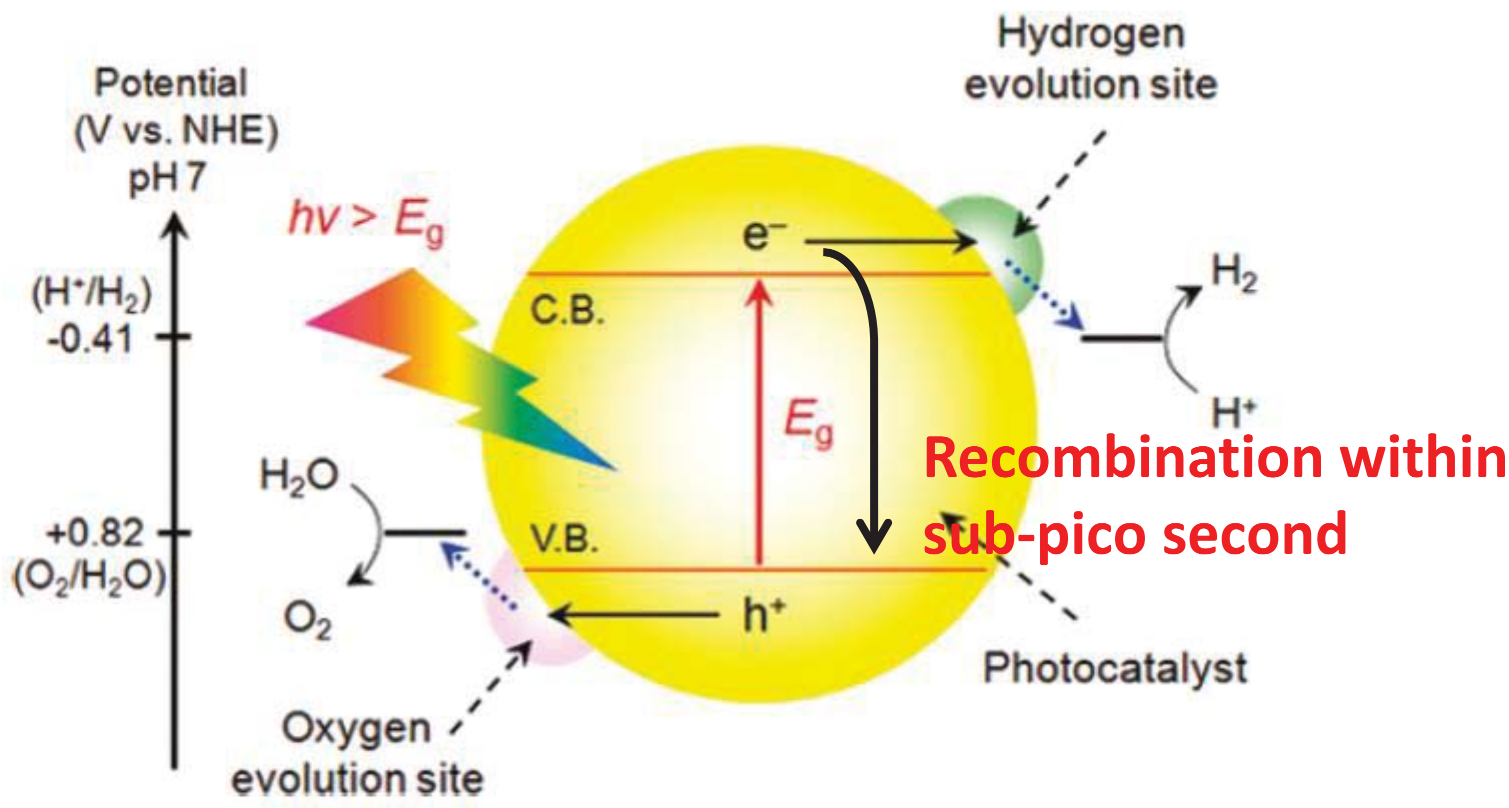

Maeda, K. and Domen K. (2010) *J. Phys. Chem. Lett*. **1**, 2655.

Toward artificial photosynthesis (1)
Ultrafast dynamics of photocatalyst

One of the most important information should be the recombination process of the electron and hole before arriving these activation sites.

<u>Sub-pico second dynamics!!</u>

Summary (1)

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Summary(2)

This paradigm shift will make it possible to directly witness **how heterogeneous functional materials work in real time and space,** and will enable predictions to be made in order to design and innovate better functional materials which will eventually solve the grand challenges of society and support life in future. Such functional materials will continue to be used in indispensable technologies such as catalysts, batteries, superconductors, biofuels, random access memories, spintronics devices and photoswitches.