

X-Ray Light Sources: An International Perspective

BESAC Meeting 23-24 Feb 2017

Persis S. Drell

Stanford



Helmut Dosch





Outline

Introduction

BESAC Contributions & Impact

- John Hemminger's Leadership
- Most recent recommendations on future BES light source facilities

Americas Perspective

- Science Results & Drivers
- New Rings & FELs

Asia & Europe Perspective

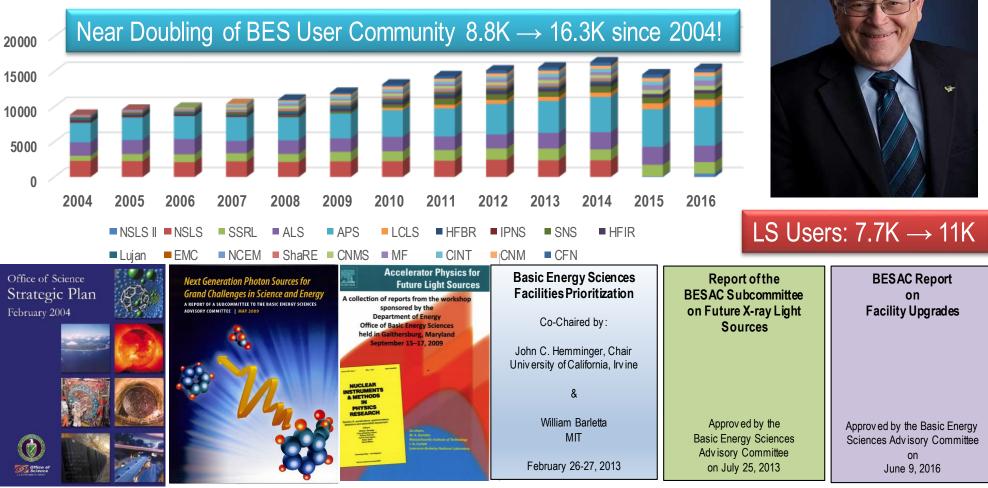
- Science Results & Drivers
- New Rings & FELs

Concluding Remarks



BESAC Contributions & Impact to BES Facilities

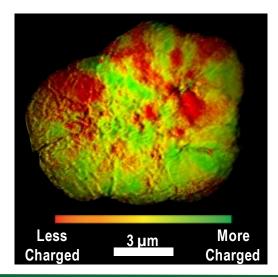
- Dr. John Hemminger: 13 years as BESAC Chairperson
 - Key BESAC & SC Strategic Planning Reports (See Below)
 - New Facilities: SNS, 5 NSRCs, LCLS, NSLS-II, LCLS-II, APS-U, ...





Motivation: Desire to Probe Nature at Atomic Length (Å) & Time (fs) Scales

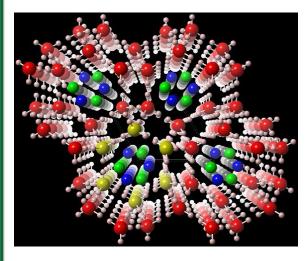
Seeing the Invisible in Real Materials



Compositional heterogeneity in a LiNi1/3Co1/3Mn1/3O2 battery hundreds of hours after charging

Adv. Materials (2016)

Where are the Atoms?



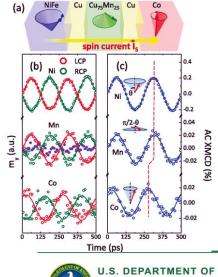
Newly discovered structure of a hydrogen-stuffed, quartz-like form of ice

JACS (2016)

Where are the Electrons & Spins?

Office of

Science

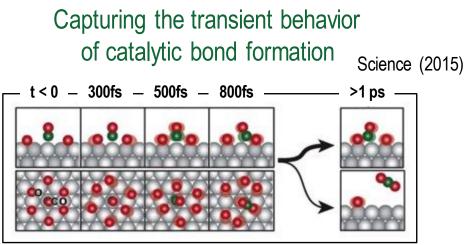


NERG

Direct measurements of "pure" ac spin currents (flow of spin angular momentum without flow of charge)

PRL (2016)

What are the Dynamics?



Goal: Control Matter & Energy on These Scales! 4

Light Sources Are Alive & Kicking: 60⁺ Facilities Worldwide & Growing



USA Response: BES Community Consensus Building Guided by BESAC



U.S. DEPARTMENT OF Office of Science

Subcommittee on BES Facility Upgrade Prioritization Agenda 14-16 April 2016

MEETING FORMAT:

- Lab Presentation of Upgrade (90 min)
- Subcommittee Q&A with Lab (60 min)
- Subcommittee Discussion of Upgrade (60 min)
- $\circ~$ Thu PM: LBNL ALS-U
- Fri AM: ANL APS-U
- o Fri PM: ORNL PPU/STS
- Sat AM: SLAC LCLS-II-HE
- Sat PM: Subcommittee Discussion & Closeout

Chair: John Hemminger

BESAC Report Also Included Neutron Sources

USA Response: BESAC Report on Light Source Facility Upgrades (June 2016)

	Storage	FEL	
Project	ANL APS-U	LBNL ALS-U	SLAC LCLS-II-HE
Project Scope	Hard X-ray ~Diffraction Limited 6 GeV Multi-Bend Achromat (MBA) Ring	Soft X-ray ~Diffraction Limited 2 GeV Multi-Bend Achromat (MBA) Ring	High Rep-Rate, High Energy X-ray FEL, 8 GeV SC Linac
Current Status of Facility	APS is operational since 1996; ring will be replaced	ALS is operational since 1993; ring will be replaced	LCLS is operational since 2010; LCLS-II is under construction
Worldwide Competition	EU ESRF Germany PETRA 3,4 Japan SPring-8-II China BLS	Sweden MAX-IV Brazil SIRIUS CH SLS-II	EU XFEL Japan SACLA Korea PAL XFEL CH Swiss FEL
Dark Time	~1 yr	~0.75 yr	0 yr
Status FY2017	CD-3b	CD-0	CD-0



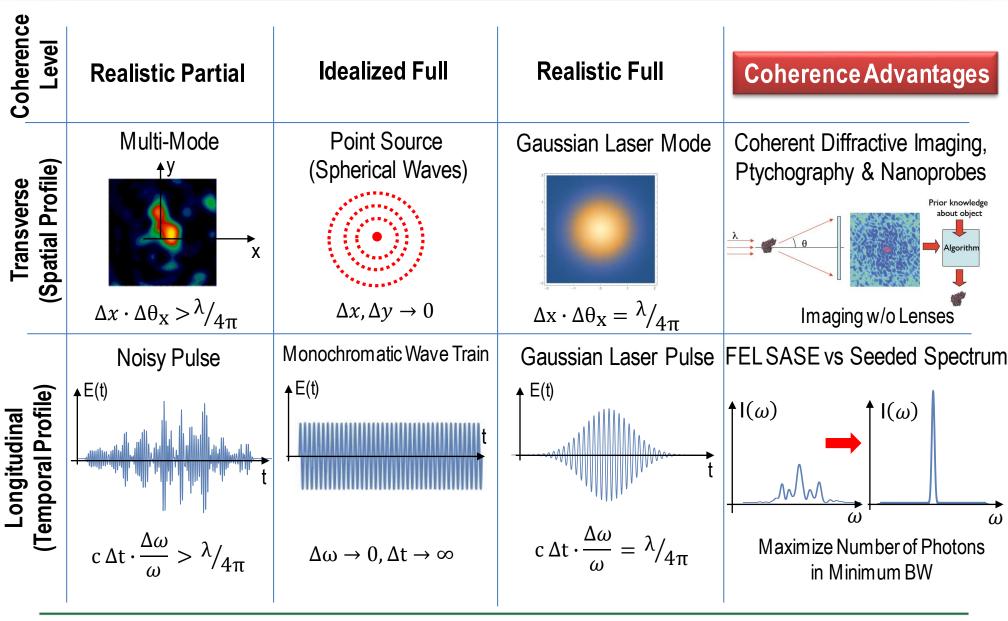
The ALS-U, APS-U & LCLS-II-HE proposals were each deemed "absolutely central to contribute to world leading science & ready to initiate construction"

Storage Rings & Free Electron Lasers are Complementary

Parameter	Storage Rings	FELs	
Beam Stability	Excellent	Very Good	
Number of Beamlines	Up to 70+	1-5	
Brightness (Ave, Peak)	(High, Low)	(Up to Very High, Extreme)	
Transverse Coherence	Partial-Full	Full (@ Saturation)	
Longitudinal Coherence	Poor	Moderate (SASE)-Very Good (seeding)	
Pulse Time Structure		<pre></pre>	
Pulse Energy	~nJ, 0.1%BW	Eu-XFEL ~mJ (FLASH) // ~fs // CLS-II → ~µsec ~0.1-1 mJ	



New Sources Will Provide Enhanced Transverse & Longitudinal Coherence

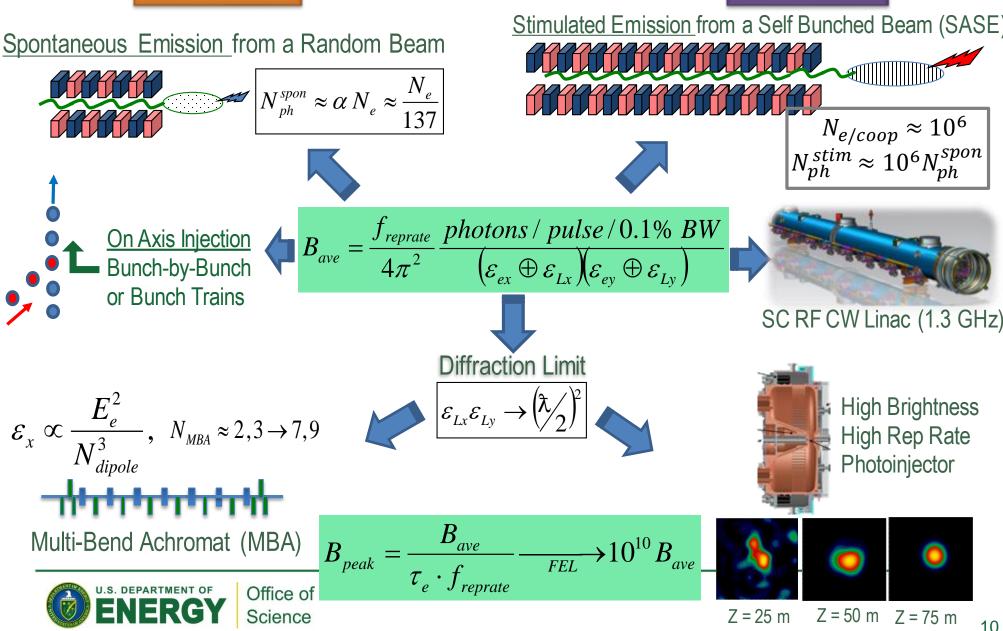




Physics & Technology for Maximizing the Photon Beam Brightness, Bave

Rings ~ 10²²



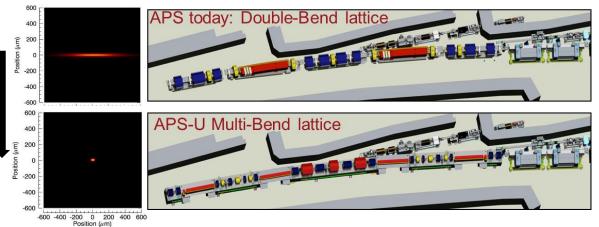


Advanced Photon Source Upgrade (APS-U) at ANL

Project Developments:

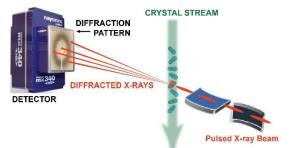
- Design optimized to provide penetrating highenergy x-rays
- MBA-7 lattice incorporating reverse bends to reduce emittance from 67pm to 41pm
- Beamline proposal selection and roadmap complete
- Technical prototypes well along; Preliminary Design Report underway; ready for next step

APS-U MBA-7 lattice uses 7 bending magnets/sector (was 2)



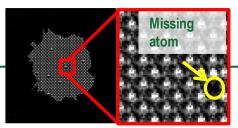
Small-Beam Scattering & Spectroscopy

- Nanometer imaging with chemical and structural contrast; fewatom sensitivity
- Room-temperature, serial, singlepulse pink beam macromolecular crystallography



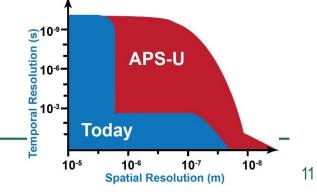
Coherent Scattering & Imaging

- Highest possible spatial resolution: 3D visualization; imaging of defects, disordered heterogeneous materials
- XPCS to probe continuous processes from nsec onward, opening up 5 orders of magnitude in time inaccessible today,



Resolution @ Speed

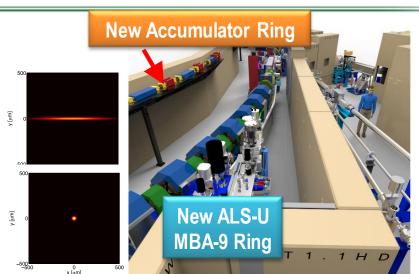
- Mapping all of the critical atoms in a cubic millimeter
- Detecting and following rare events
- Multiscale imaging: enormous fields of view with high resolution;



Advanced Light Source Upgrade (ALS-U) at LBNL

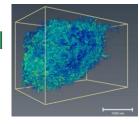
Goal: High CW soft x-ray coherent flux necessary to resolve nm-scale features & enable real-time observation of chemical processes & materials as they function **Project Developments:**

- Replace the existing MBA-3 ring with a new MBA-9 ring
- New accumulator ring for on-axis bunch train injection
- Critical Decision 0 approved on Sept 2016



Map nano-objects' 3D electronic, chemical, & magnetic structure Understand Roles of Heterogeneity Master Hierarchical Architectures

• Connect spatial, chemical, & temporal heterogeneity with real-time movies



 Potential benefit – optimize material processes & properties, e.g., low carbon footprint concrete



Control chemical kinetics in confined spaces

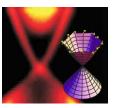
Reveal relationships between nanoscale chemical structures** & the kinetic processes they support

• Potential benefit – chemical catalytic reactors, solar fuel production, water purification

Deploy spin, quantum, and topological materials

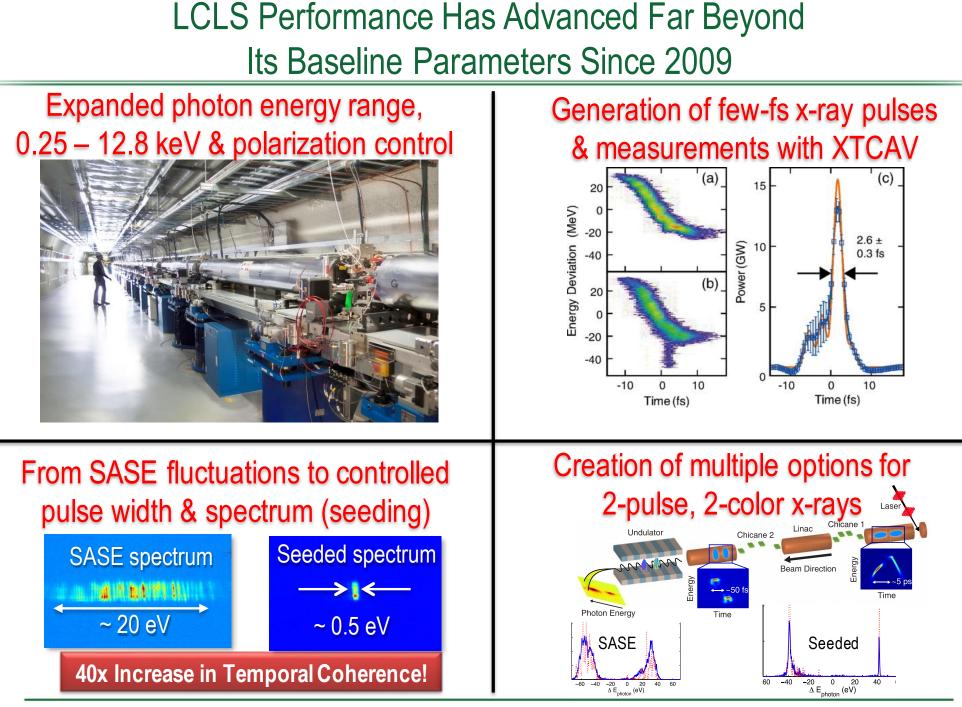
Harness Coherence in Light & Matter

 Probe electronic structure of single domains and gated structures of



complex materials

• Potential benefit – ultralow-power computing, new classes of sensors, spin-based devices





Linac Coherent Light Source II (LCLS-II) at SLAC

Project Scope & Status:

- 200-5,000 eV x-rays at up to 1 MHz (from 120 Hz)
- Double the energy reach of LCLS to 25 keV
- 4 GeV CW SC linac, 2 new variable gap IDs
- CD-2, CD-3 approved in 2016

Charge dynamics on fundamental timescales

- Reveal coupled electronic and nuclear motion in molecules
- Capture the initiating events of charge transfer chemistry with sub-fs resolution

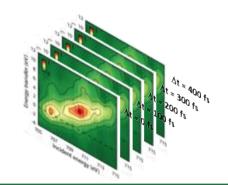
Mar Mar

Emergent phenomena in quantum materials

- Connect spontaneous fluctuations, dynamics and heterogeneities on multiple length- and time- scales to bulk material properties
- Study interacting degrees of freedom (e.g. unconventional superconductors)

Molecular dynamics with exquisite resolution

- Measure element-specific, local chemical structure and bonding
- Study efficient, robust, selective photo-catalysts



14

Fermilab Jefferson Lab



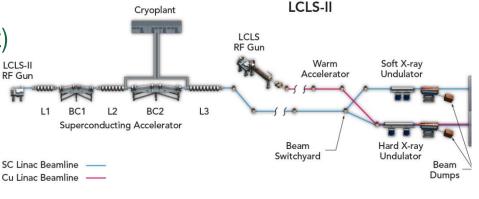




orbita

lattice

charge



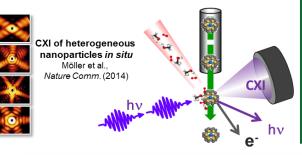
LCLS-II-HE is Needed to Probe Structural Dynamics at the Atomic Scale (~1 Å)

Project Scope & Status:

- Extend CW-SCRF linac from 4 to 8 GeV
- Provide high rep-rate capability beyond 1Å (>12 keV)
- Injector development to enable lasing up to 20 keV
- Average coherent x-ray power (spatial & temporal) is transformative
- CD-0 approved in Dec 2016

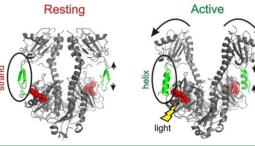
<u>Heterogeneity</u> & complexity in ground & excited states

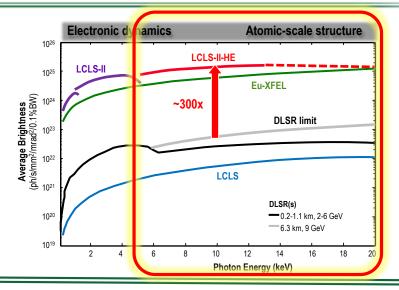
- Correlate catalytic reactivity and structure
- Real-time evolution with chemical specificity and atomic resolution



<u>Dynamics</u> of biomolecules and molecular machines

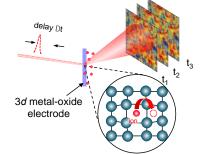
- Study large scale conformational changes via solution scattering
- Physiological conditions
- Dynamics ties structure to function





<u>Fluctuations</u> in the ground state and spontaneous evolution

- Characterize statistically dynamic systems without long-range order
- Inform directed design of energy conversion and storage materials





Сн₂он X-Ray Light Sources Europe and Asia

II H2A II

Helmut Dosch Deutsches Elektronen-Synchrotron DESY

HELMHOLTZ

The new Challenge

Long-ranged Ordered Structures Equilibrium Phenomena Phase Diagrams

1900

Locally Ordered Structures Nonequilibrium Phenomena Bio-Nano-Matter Transient States

Conventional X-ray probes

Coherent X-ray probes !! Time-Resolved X-ray probes !!

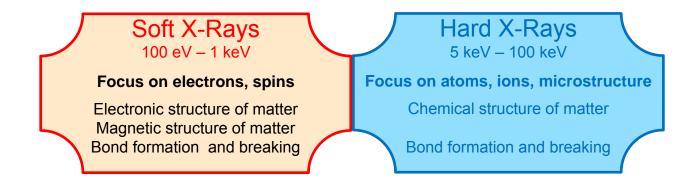
future

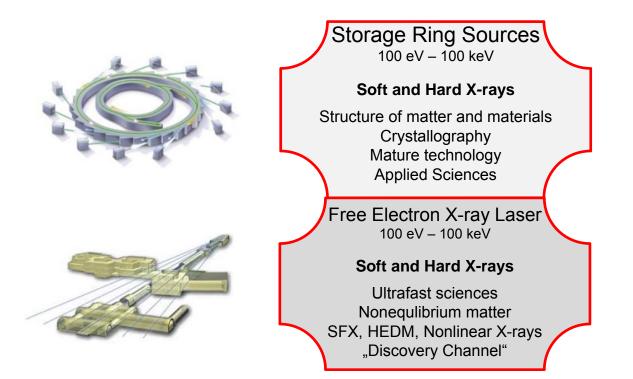
Era of Crystalline Matter

Era of Complex Matter

2000

European Strategy - X-Ray Sources 2000+







SR

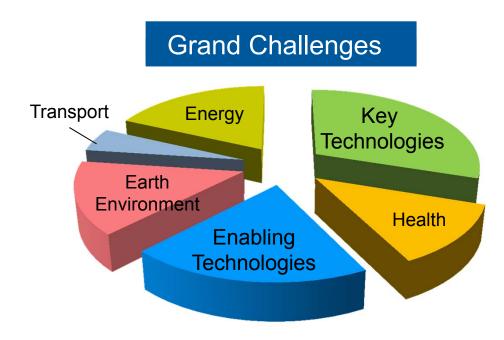
Mature Technology

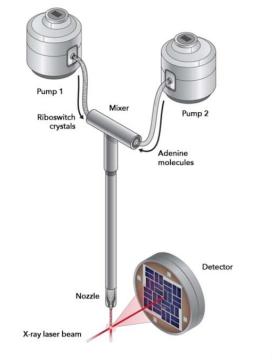
MBA → "Ultimate 4d Microscopes" In-situ, operando interrogation of matter Fundamental – applied - industry GC of our society

FEL

Novel Disruptive Technology

"Discovery Channel" Ultrafast Science, "Molecular Movie" Pathfinder of new technologies







Facility	Location	Energy	Lab Info	Comments		
Storage Rings						
ESRF	Grenoble/FR	6 GeV	Upgrade MBA 2018- 2020 "ESRF-EBS"	Hard Energy X-ray Facilities		
PETRA III	Hamburg/DE	6 GeV	Upgrade MBA 2022-24 "PETRA IV"			
ALBA	Barcelona/ ES	3,0 GeV	Not fully instrumented			
Diamond	Didcot/UK	3,0 GeV	Upgrade MBA planning phase	Medium Energy X-ray Facilities		
MAXIV	Lund/SE	3,0 GeV 1,5 GeV	7BA Lattice commissioning			
SOLEIL	Paris- Saclay/FR	2,75 GeV	Upgrade plans no details yet			
ANKA	Karlsruhe/DE	2,5 GeV	closes user ops in 2017			
SLS	Villigen/CH	2,4 GeV	Upgrade plans No details yet			
ELETTRA	Trieste/IT	2,0-2,4 GeV				
BESSY II	Berlin/DE	1,7 GeV	Upgrade VSR 2018	Soft X-ray Facilities		
SOLARIS	Krakow/PL	1,5 GeV	Under construction			
ASTRID2	Aarhus/DK	0,58 GeV	Operating, no upgrade plans			



Science Case : FEL

Fundamentals Holy Grails

- Disorder to Order
- Q-Control of Response Functions
- Transients in Catalytic reactions
- Crystallography of Local Order
- Real time Evolution of Electronic Correlations*)
- Nonlinear X-Ray Science

- Serial Nanocrystallograpy
- Single Molecule Diffraction
- Biochemical Reactions

Bio-Medical

Applied Sciences

- Materials under Extreme
 - Conditions
 - Crack Propagation ♦
 - Catalytic Reactions
- Ultrafast Switching of Materials

 Properties

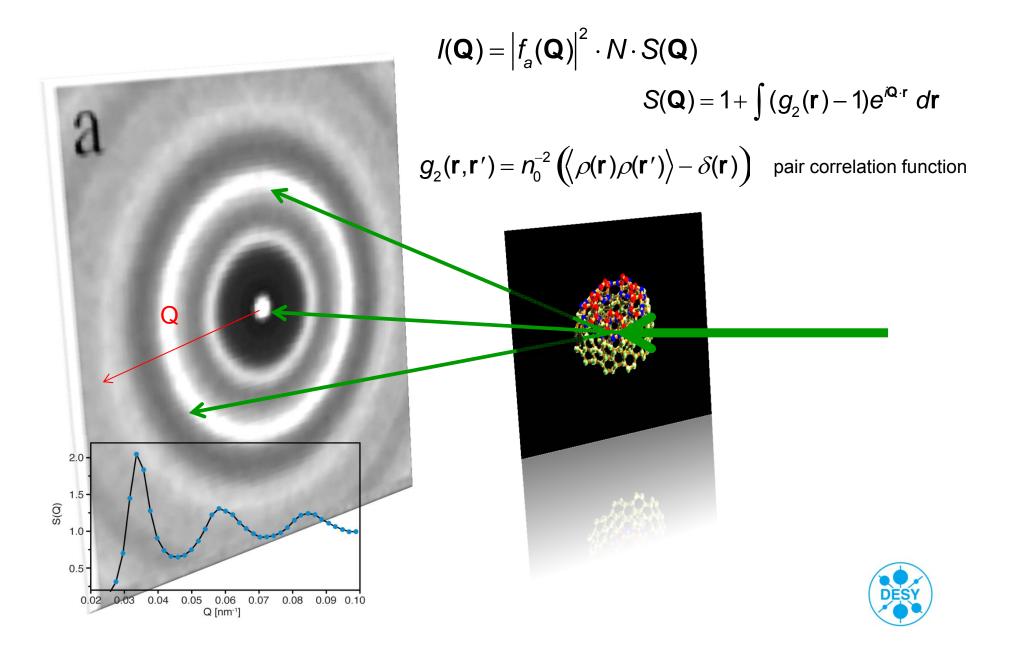
- Control of Friction
 - Catalysis ♦
 - Organic PV

itivedistort

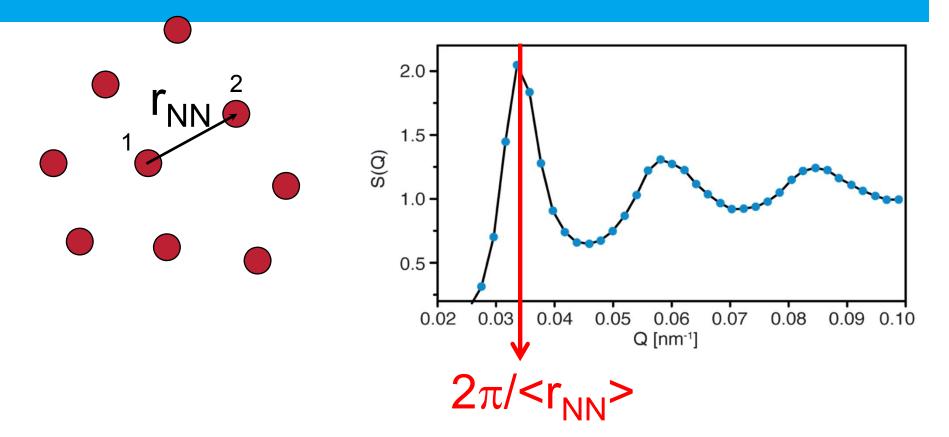
Ultrafast Switching of Materials
Functions

Opportunities for Industry

Conventional X-ray scattering from noncrystalline matter



2-Point Correlation Function



 $n_0 g_2(\mathbf{r}) d\mathbf{r}$ Average probability to find particle 2 at distance **r** from particle 1

$$g_{2}(\mathbf{r}_{1},\mathbf{r}_{2}) = n_{0}^{-2} \left\langle \sum_{i}^{N} \sum_{j \neq i}^{N-1} \delta(\mathbf{r}_{1} - \mathbf{R}_{i}) \delta(\mathbf{r}_{2} - \mathbf{R}_{j}) \right\rangle$$

• *g*₂(**r**) independent of bond angles !! no information on local structure/symmetry



Local Symmetry in Disordered Matter From Higher Order Correlation Function

 $n_0 g_2(\mathbf{r}) d\mathbf{r}$ probability to find particle 2 at distance **r** from 1 in d**r**

$$g_2(\mathbf{r}_1,\mathbf{r}_2) = n_0^{-2} \left\langle \sum_{i}^{N} \sum_{j \neq i}^{N-1} \delta(\mathbf{r}_1 - \mathbf{R}_i) \delta(\mathbf{r}_2 - \mathbf{R}_j) \right\rangle$$

- $g_2(\mathbf{r})$ independent of bond angles
- n-point distribution function depend on angles
 e.g.: g₃(r₁, r₂, r₃₎

 $n_0 \int g_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) d\mathbf{r}_3 = (N-2)g_2(\mathbf{r}_1, \mathbf{r}_2)$

• N-2 different arrangements with same g₂(**r**)

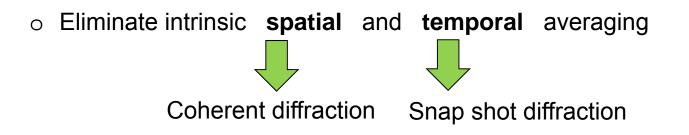
bond angles r₃ 3

> local nano-angle in matter coherent position of >3 atoms



Higher Order Correlation functions

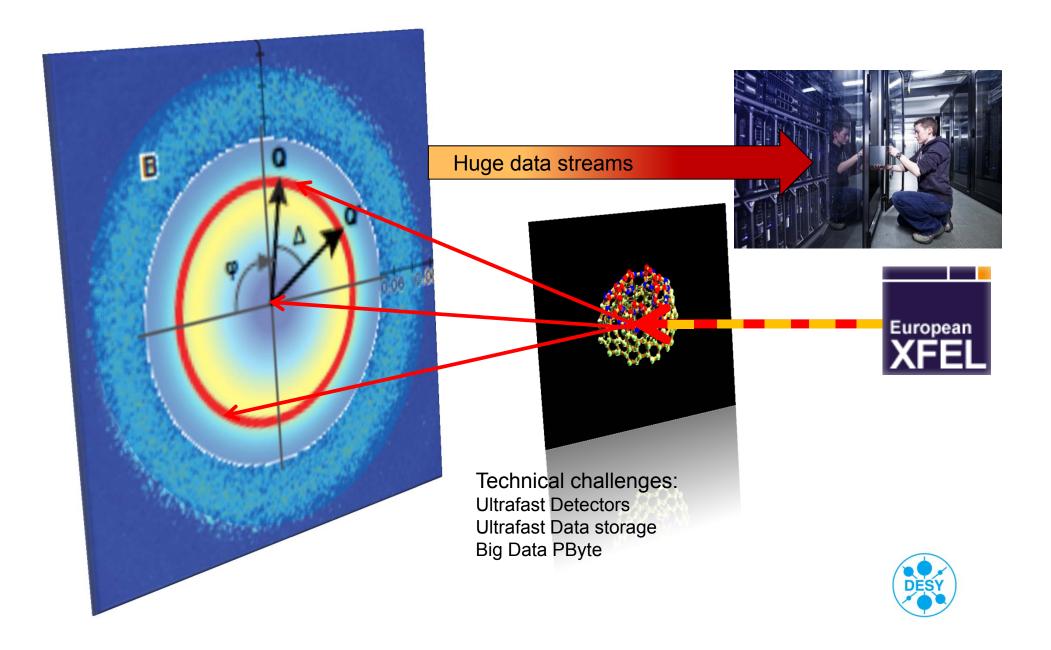
$$g_{2}(\mathbf{r}_{1},\mathbf{r}_{2}) = n_{0}^{-2} \left\langle \sum_{i}^{N} \sum_{j \neq i}^{N-1} \delta(\mathbf{r}_{1} - \mathbf{R}_{i}) \delta(\mathbf{r}_{2} - \mathbf{R}_{j}) \right\rangle$$



 $\circ~$ Construct new higher order correlations by hand

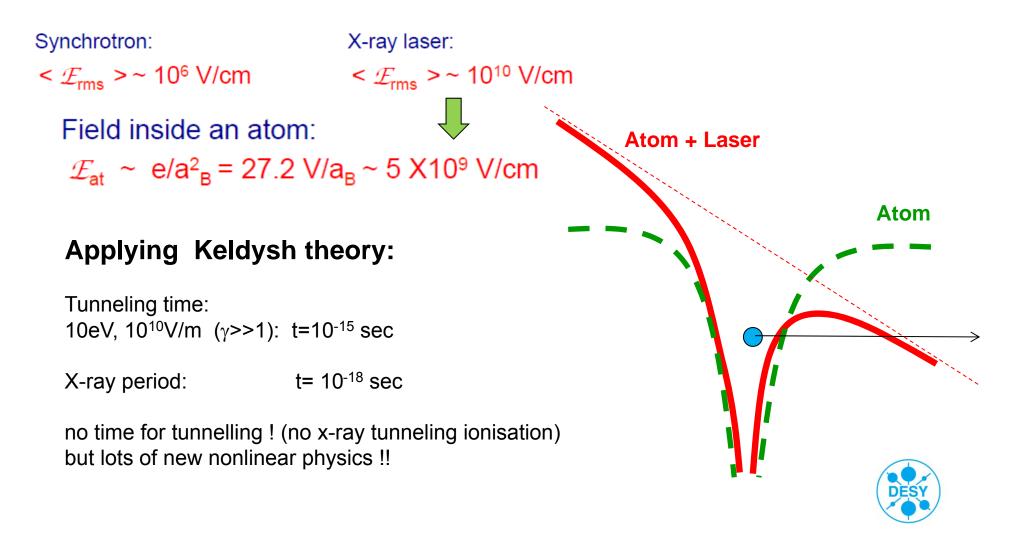


21st century challenge: Crystallography of noncrystalline matter



XFELs: Welcome to Nonlinear X-ray Physics !

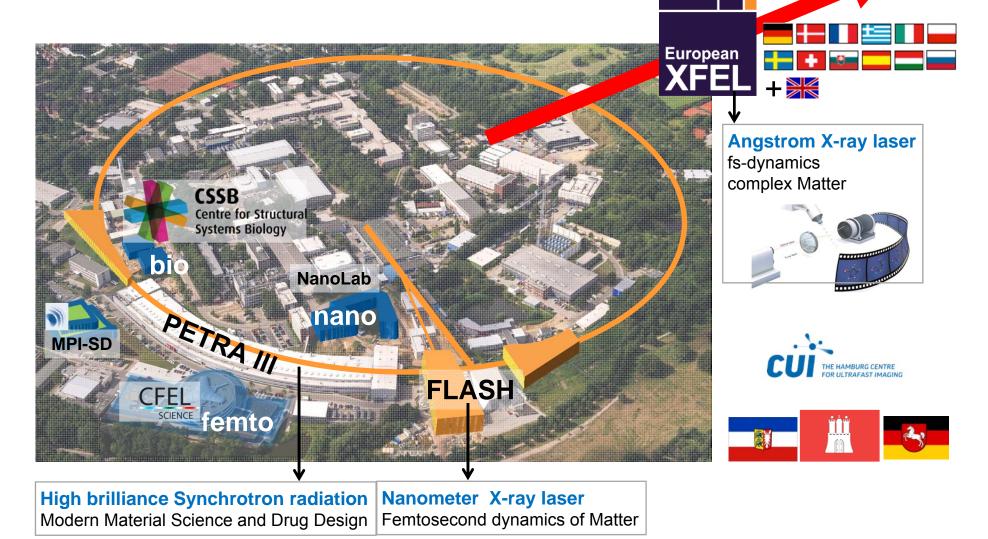
- Synchrotron 10⁵ ~1 keV photons/ 10⁻¹¹s on a μm² spot
- X-ray FEL 10¹² ~1 keV photons / 7 10⁻¹⁴ s on a μm² spot



Status in Europe: FELs

Facility	Location	Energy	Lab Info	Details	Comments	
X-ray Lasers						
EU.XFEL	Hamburg	17,5 GeV	Commissiong First beam fall 2017	Europ. X-ray Laser D, RUS, and EU countries	Soft and Hard Yrova	
Swiss FEL	Villigen	2,1-5,8 GeV	commissioning	National facility 2 branches: soft and hard	Soft and Hard Xrays	
FLASH	Hamburg	1,8 GeV	Upgrade 2020 Seeding, cw	1 st (soft) x-ray FEL Soft x-ray laser upgrade FLASH II National facility		
FERMI-1	Trieste	1,5-1,8 GeV	λ= 100nm-10nm 20-90fs, 10-50 Hz	2012 HGHG laser	Soft X-rays	
FERMI-2	Trieste	1,5-1,8 GeV		2016 HGHG Laser		
ELBE	Dresden	100- 150 MeV	Upgrade Plans "DALI"	IR/THz-FEL	IR and THz	
FELIX	Nijmegen	10-50 MeV	λ= 3-1500 μm	IR/THz-FEL		

DESY Photon Science





On the way to the International Photon Science Mekka.

XFEL 2017 PETRA IV 2025 FLASH 2020 Image: Storage Ring Image: Storage Ring Image: Storage Ring

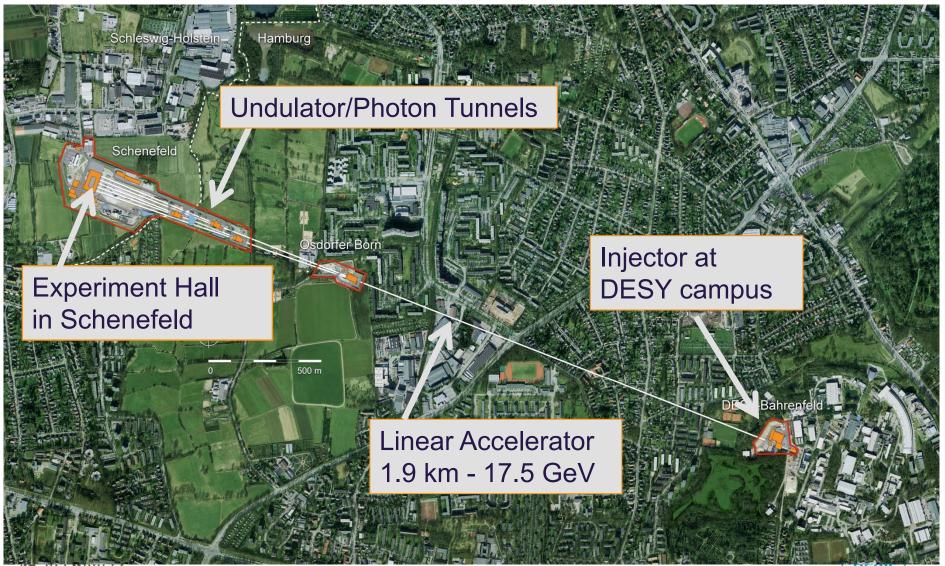


Photon Science Research Centers

Photon Science Facilities



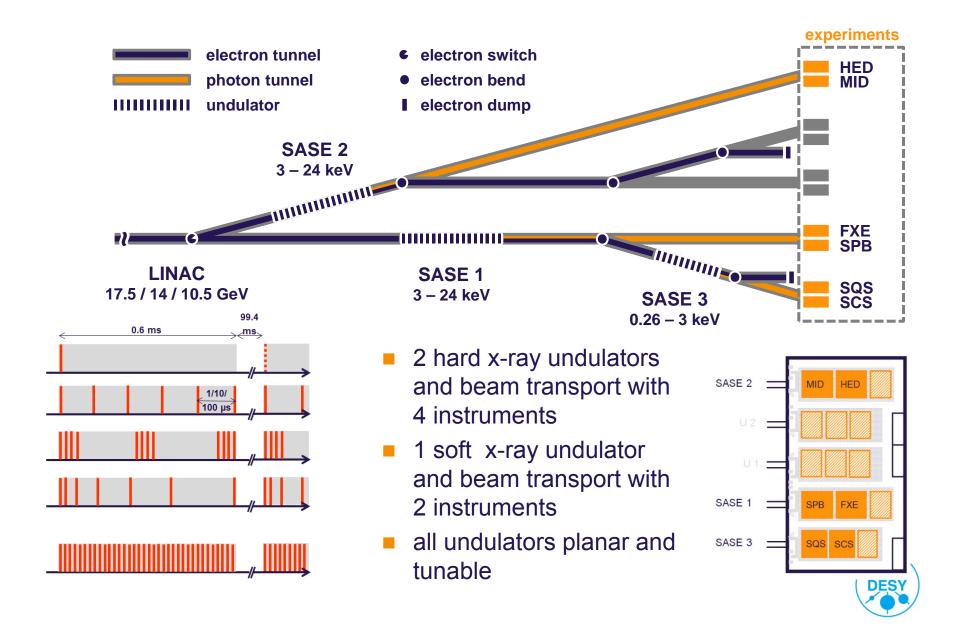
European XFEL Layout



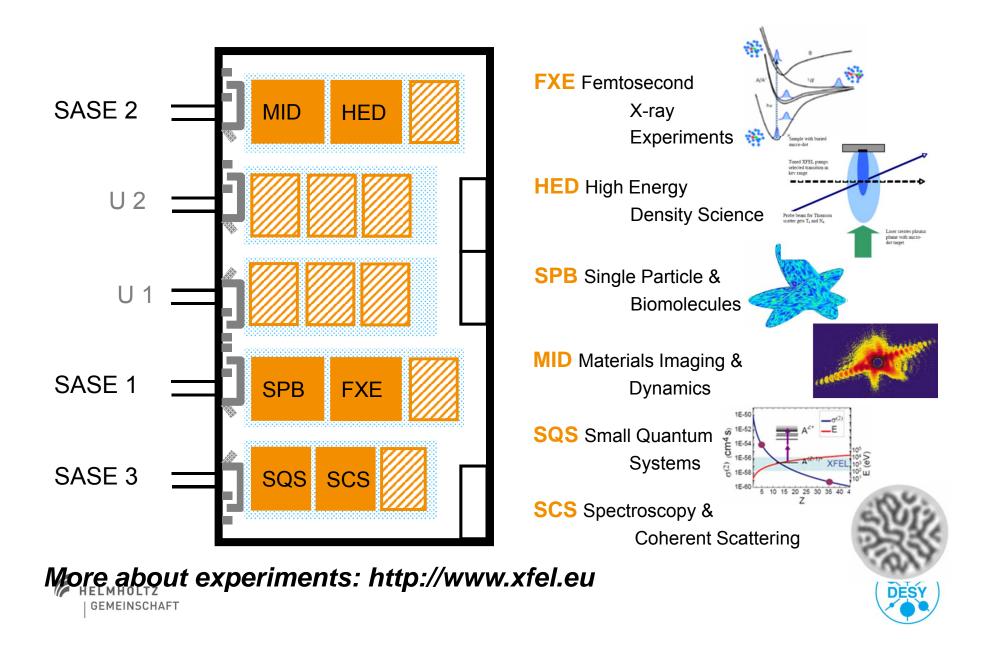
GEMEINSCHAFT



Layout European XFEL



The Suite of Instruments



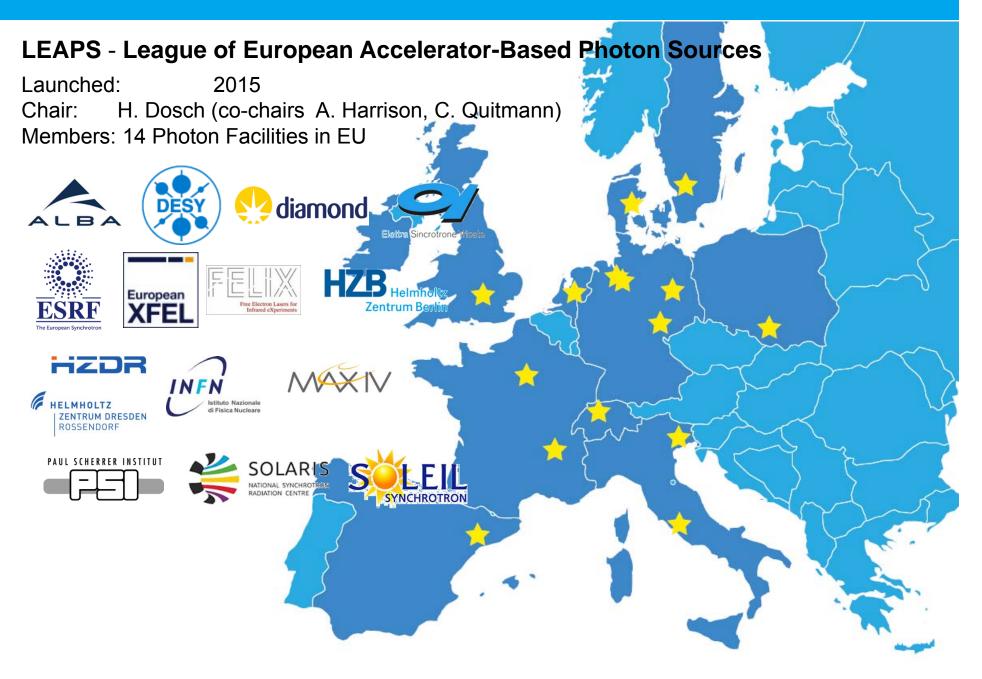


European Commission View

- More integration between RI ("smart specialisation") and the e-infrastructures and with other parts of Horizon 2020, to exploit synergies and complementarities
- New and reinforced emphasis on long term sustainability, innovation, and contribution to the EOSC
- Support to large scale initiatives for innovation
- Continuation of the different approach between Starting and Advanced Communities for integrating activities, and potential launch of pilot actions in 2020
- Training of future lab managers



LEAPS initiative



LEAPS initiative

LEAPS - League of European Accelerator-Based Photon Sources

Goals:

- Coherent Roadmap of SR and FEL facilities in EU
- Better Integration:
- Standardized Proposal System
- Standardized Facility Performance Metrics
- Joint Technology Roadmaps (data management, detectors, optics, ...)
- Joint Education and Training

LEAPS Charter LEAPS Strategy Doc Nov 2017

Input to EC FP 9 2020-2026

First and Last Name | Title of Prese Date | Page 21

China Strategy

Beijing

- Beijing Synchrotron Radiation Facility BSRF at IHEP
 - ~1990ies, various upgrades, 2.5 GeV, 12 beamlines, parasitic
- Beijing Free Electron Laser BFEL at IHEP ~1990ies, 30 MeV RF-Linac, mid-Infrared-FEL
- New: High Energy Photon Source HEPS Approved project, will be 50 km north from IHEP Beijing 6 GeV SR, 1.3 km circumference, 7BA, 60pm-rad ~700M\$ approved, earliest operation in 2022

Plans for a XFEL as well

Shanghai

- Shanghai Synchrotron Radiation Facility opened in 2012
 3.5 GeV, 432 m circumference, DBA lattice, 3.9 nm-rad
 13 beamlines in operation, 20 more to come over the next years (until 2022)
- SXFEL at SINAP/Shanghai

Started as test facility in 2014

40 MeV linac, (C-band, S-Band) 8.8nm seeded FEL, 1-10 Hz

Upgrade to 1.6 GeV with undulator halls and 4-5 experimental stations to soft x-ray user facility

- Future extension to hard x-ray possible
- Dalian Coherent Light Source (University in cooperation with Max Planck Society) 300 MeV LINAC, VUV-FEL, 50-150 nm Developed together with SINAP Lasing by end of 2016

Other: National Synchrotron Radiation Laboratory, Hefei (University) 1991, various upgrades, 800 MeV SR





Korea Strategy

Pohang

Pohang, PLS-II SR Upgrade from PLS in 2011 to 3.0 GeV, 32 beamlines DBA, 5.8 nm Currently, no further upgrade planned

Pohang, PAL-XFEL

Just recently commissioned, lasing/saturation at 0.15nm achieved in November last year First call for proposals published in February/March 2017 10 GeV S-Band LINAC, 60Hz, 0.1nm FEL wavelength

Beamlines:

Soft x-ray scattering & spectroscopy X-ray scattering & spectroscopy nano-crystallography, coherent diffraction







Japan Strategy

Harima

 Spring-8: High performing 3rd generation SR 8 GeV

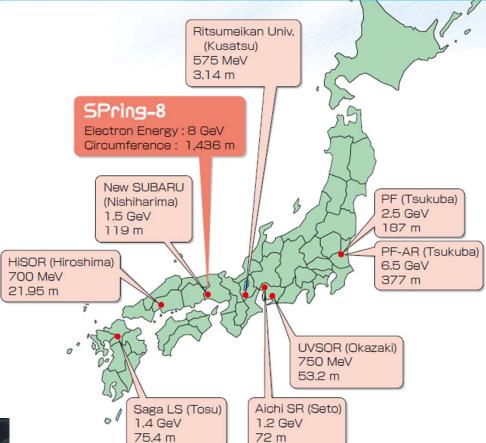
Upgrade Plans USR next years

 SACLA: 60 Hz, one beam line hard x-ray FEL Upgrade SACLA additional injector and additional undulators

Tsukuba (KEK)

- Photon Factory 2,5 GeV SR machine (Tsukuba) no upgrade plans known
- cERL 20 MeV in operation since 2013
- Plans for EUV-FEL for Lithography







- Light sources are generating exciting breakthrough science around the globe
 - BES user community has nearly doubled since 2004 to over 16,000 users including the 11,000 light sources users
 - New & upgraded facilities are driving the frontiers
- John Hemminger has provided a steady hand of leadership throughout these developments
 - As chair of BESAC he has shepherded the US light source strategy
 - The US light source strategy has influenced the international landscape
- Given the wealth of new ideas, new technology and the scientific opportunities, we anticipate light sources around the globe to be a continuing source of discovery for decades to come

