BESSY ^{VSR} : Science opportunities and current developments

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Contributors
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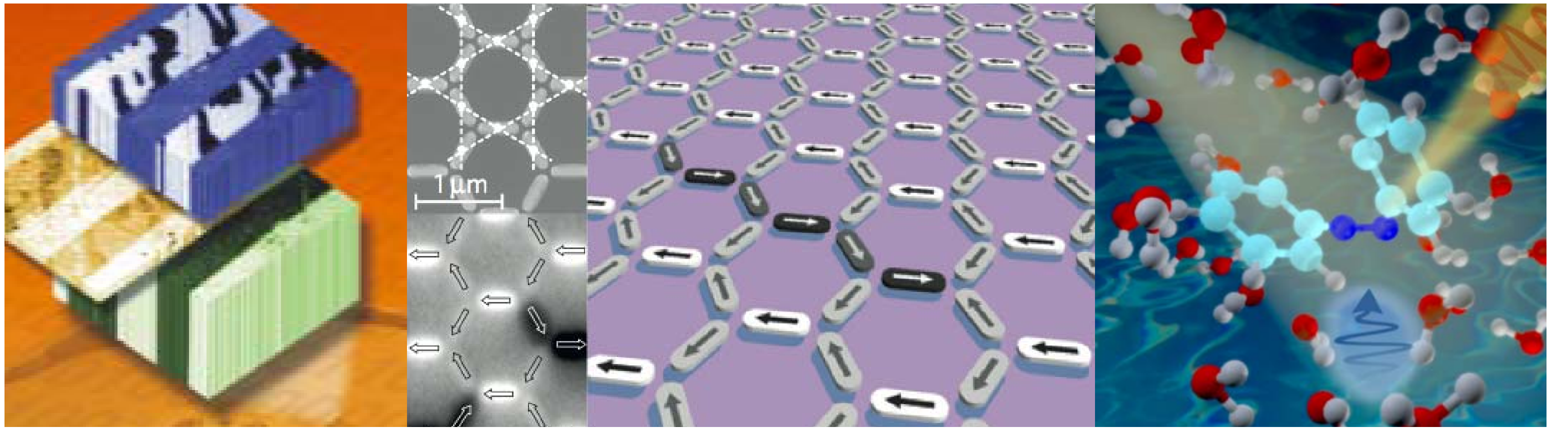
Grand challenges

How do we communicate and archive knowledge ?

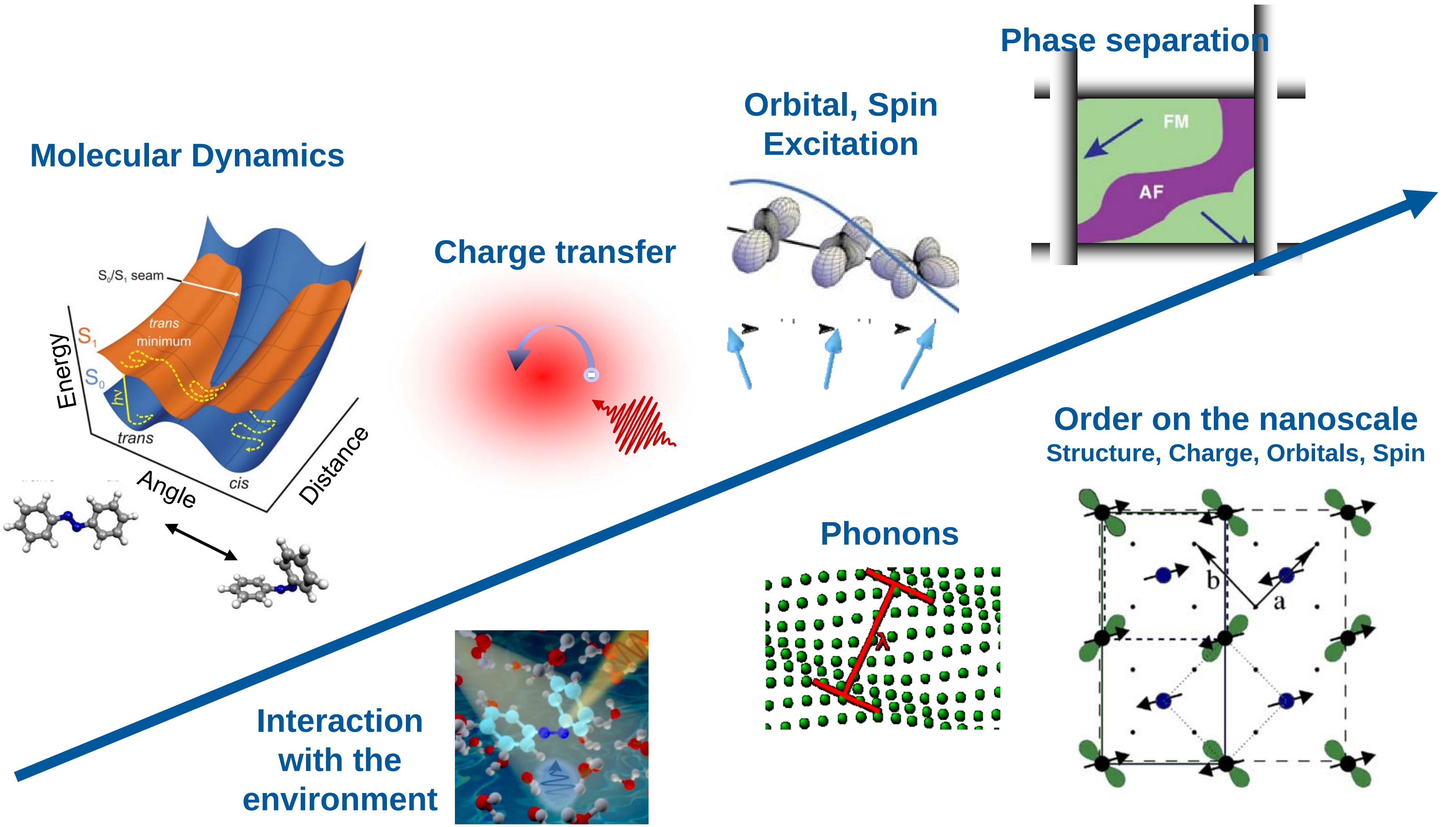
How do we harvest, convert and store energy ?

How do we govern selectivity and rate of chemical processes ?

Quantum materials and phase transitions
Molecular and chemical dynamics
Energy and charge transport



Governing principles of materials function : Coupled degrees of freedom



Fundamental Scales

Speed of Sound	1 nm	in	1 ps
Fermi Velocity	1 nm	în	1 fs
Speed of light	1 atom (3 A)	in	1 as

1 mm

1 µm

1 nm

1 A

1 µs

Large amplitude Motion, folding

1 ns

Domain Dynamic

1 ps

Spin precession

Bond formation

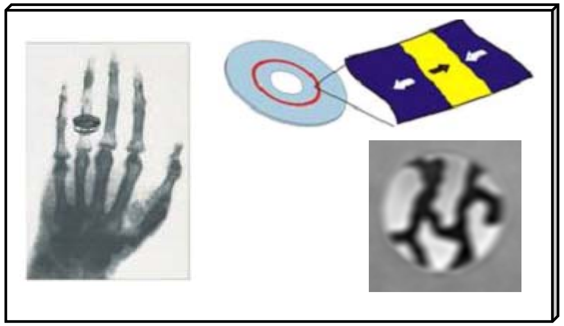
1 fs

Exchange
Charge transfer

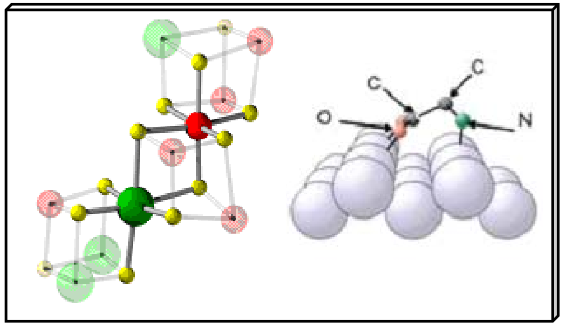
1 as

Science driven tools - X-rays

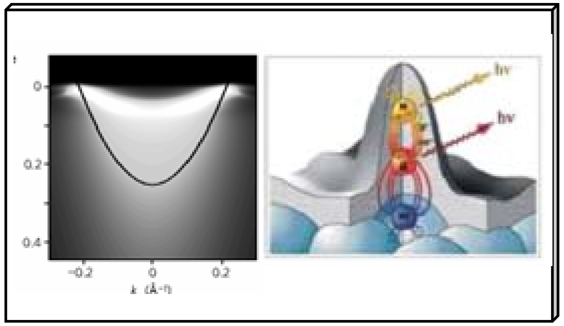
imaging - seeing the invisible



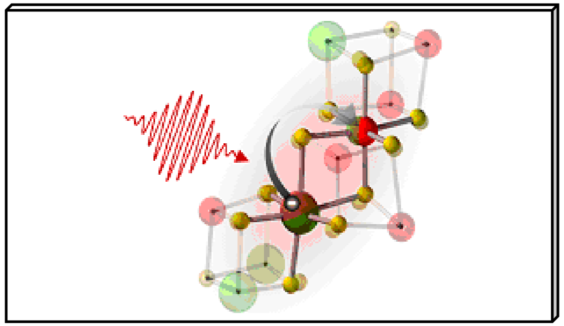
geometric structure
- where are the atoms -



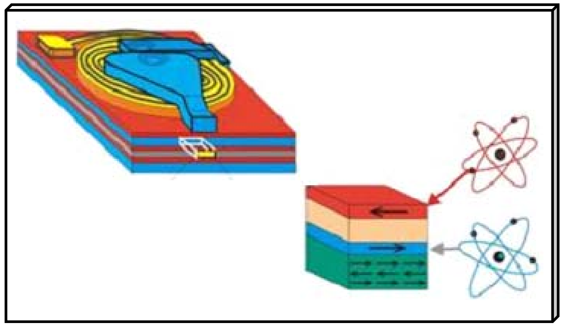
electronic structure and bonding
- where are the electrons -



dynamics and function
- how electrons and atoms interact -



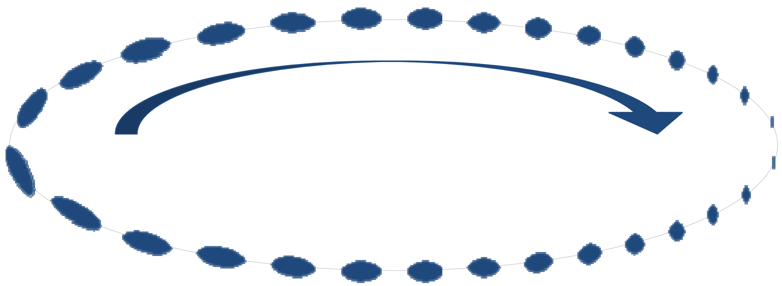
magnetic properties
- where are the spins -



Element, chemical state, orbital and spin selective
Atomic and nanoscale

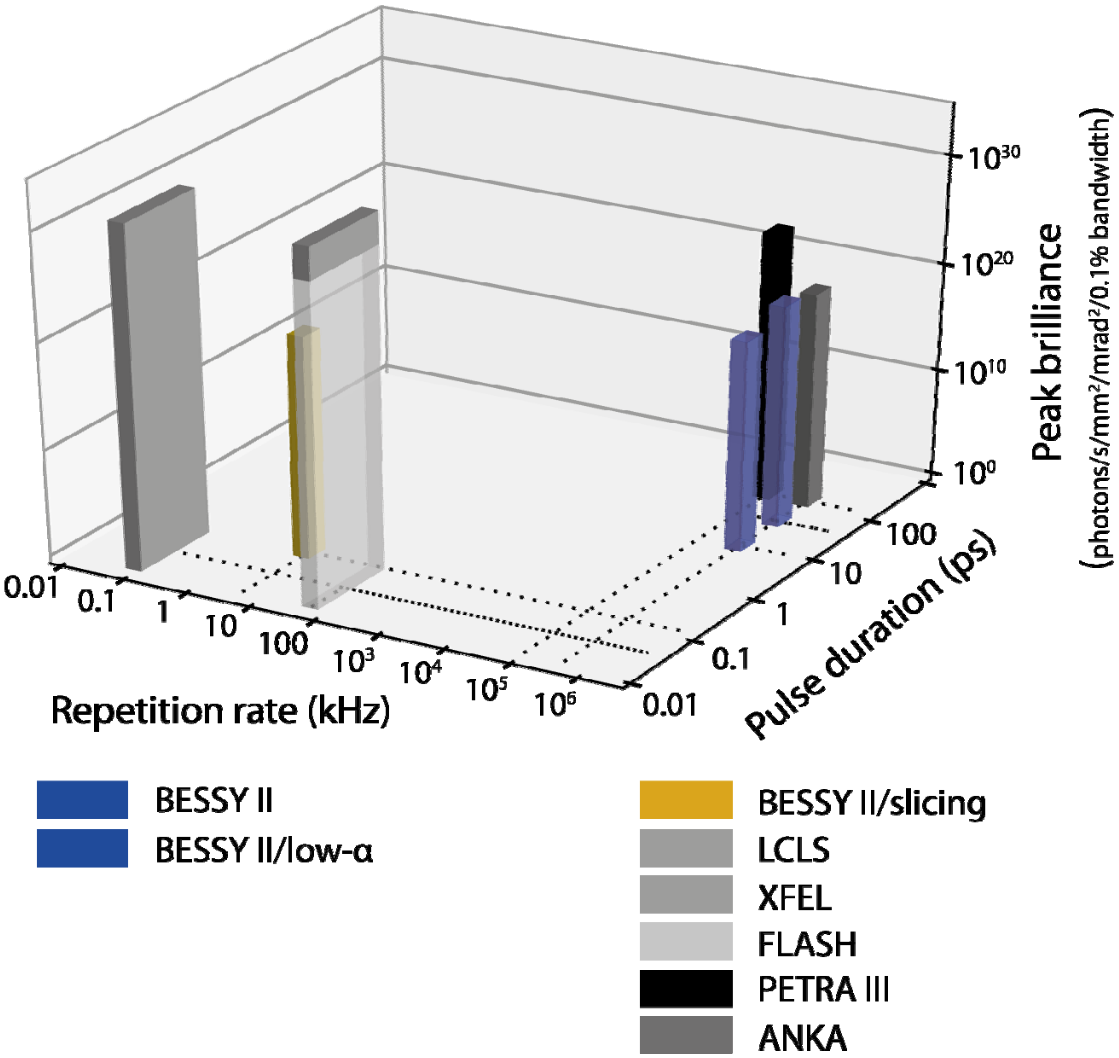
BESSY VSR The Variable pulse length Storage Ring

- Users switch individually between energy resolution and time information

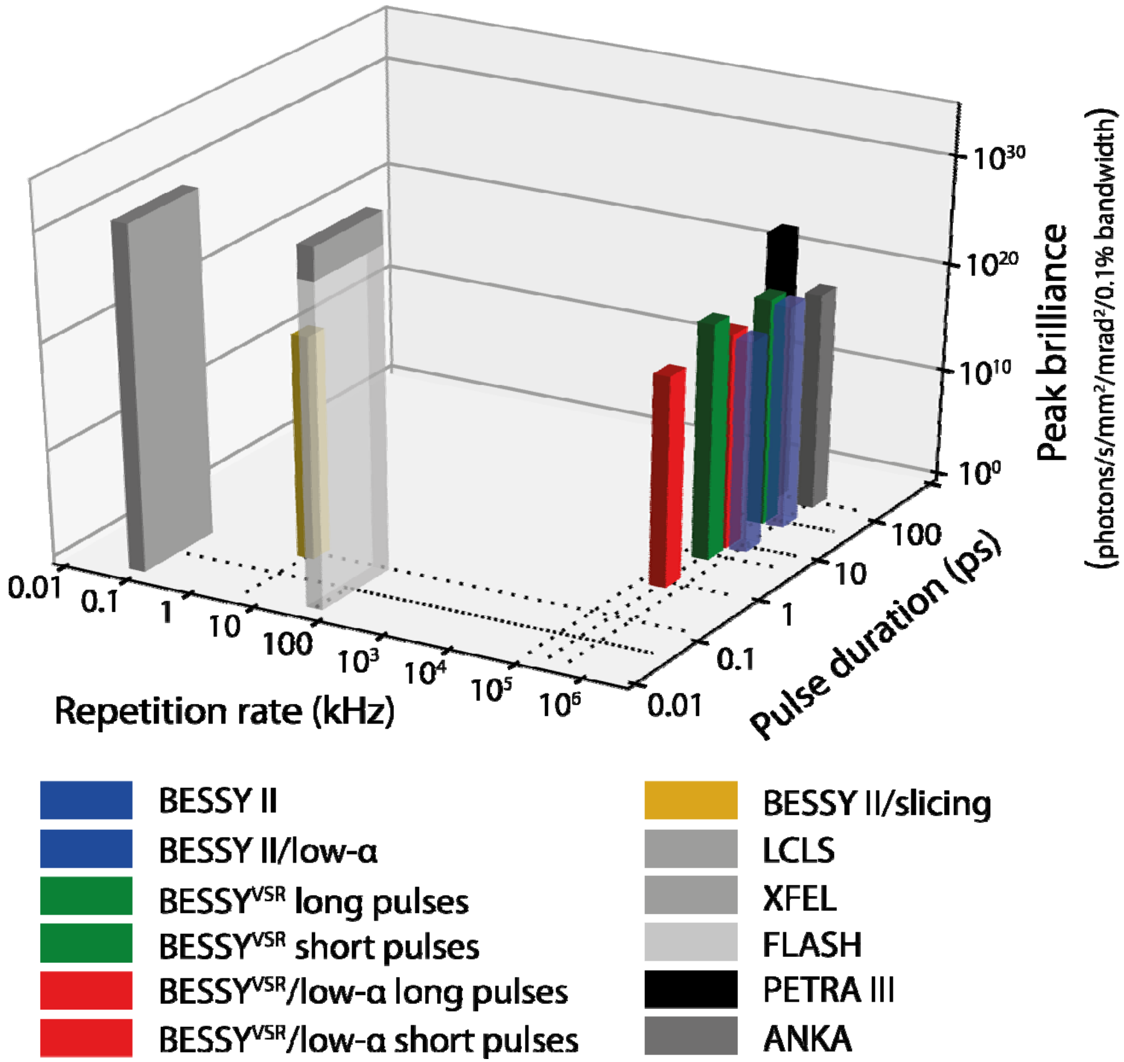


- High repetition rate ideal for repetitive/cyclic phenomena on ps timescales
- In combination with high resolution spectroscopy, scattering, microscopy

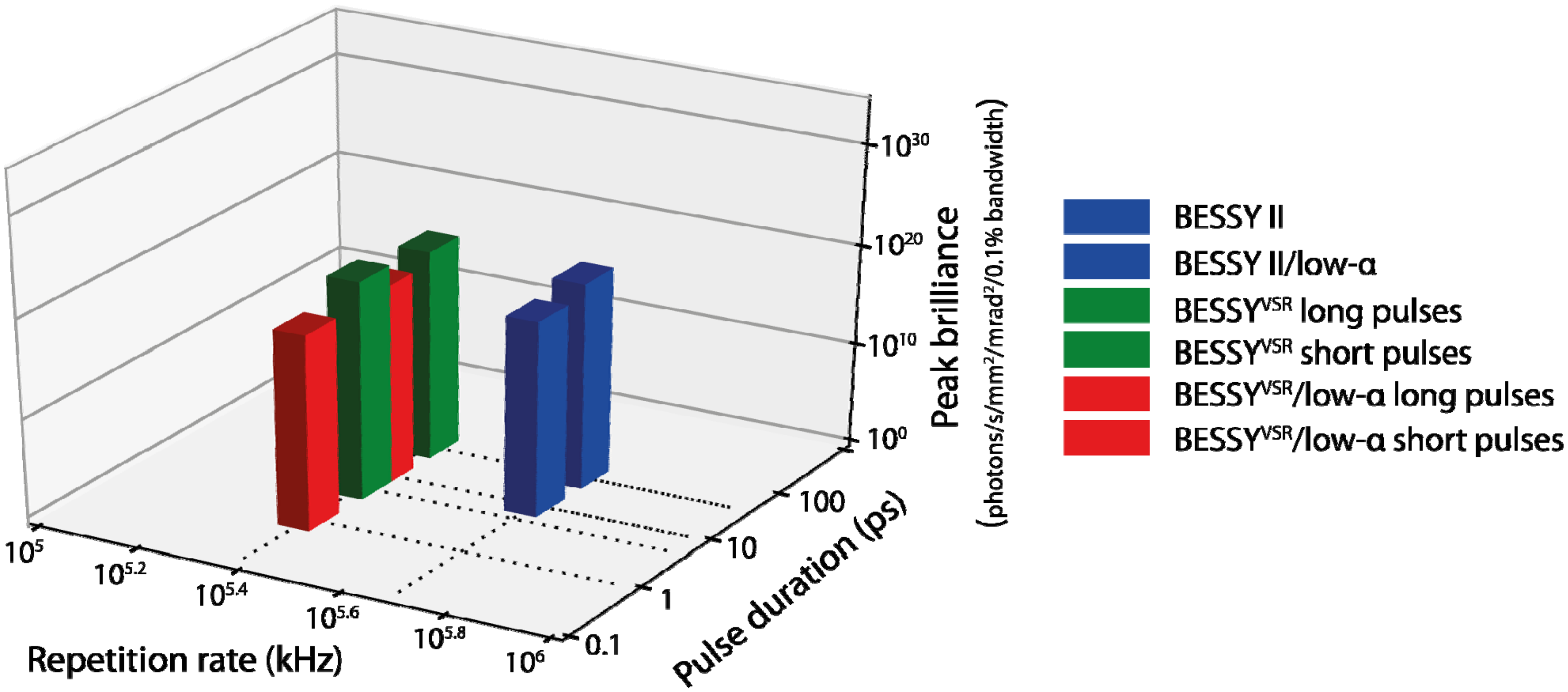
Synchrotron Radiation and FEL Sources Today



BESSY VSR Synchrotron Radiation Sources Today



BESSY II now – what BESSY ^{VSR} could be…..

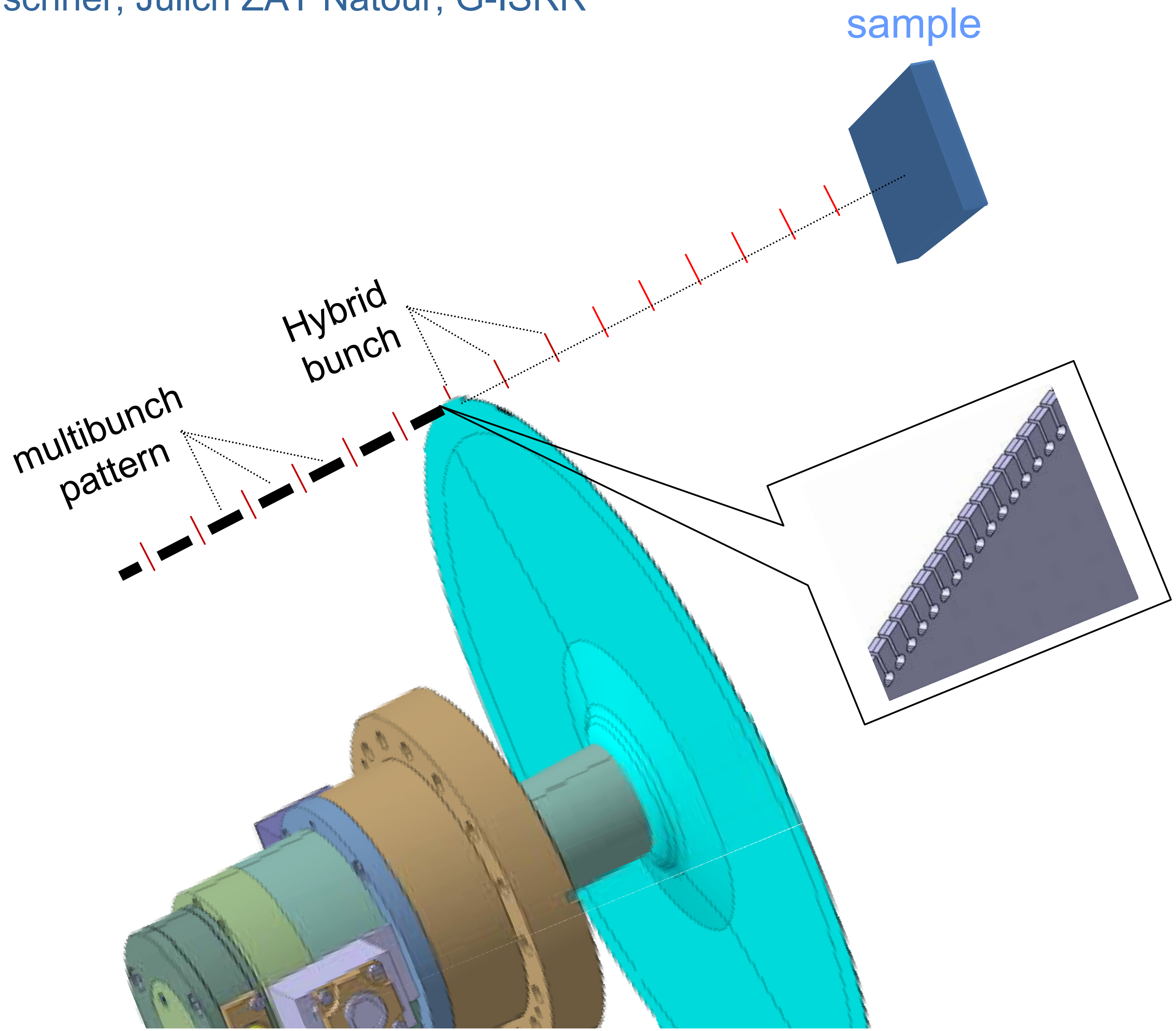


optics type	Hor. Emittance (nm mrad)	peak brilliance (number of buches)	average brilliance (multi bunch current)	Repetition rate (kHz)	pulse duration in ps/FWHM
BESSY II	5	6.1E20 (350)	8E18 (100mA)	5E5	30
BESSY II/ low-α	40	5.2E19 (350)	1.6E17 (100mA)	5E5	7.0
BESSY II/slicing	5	6E20 (4)	3.6E10	6	0.1

Interlaced 1.25 MHz single bunch operation: pulse-picking

From conceptual stage to operation Summer 2013

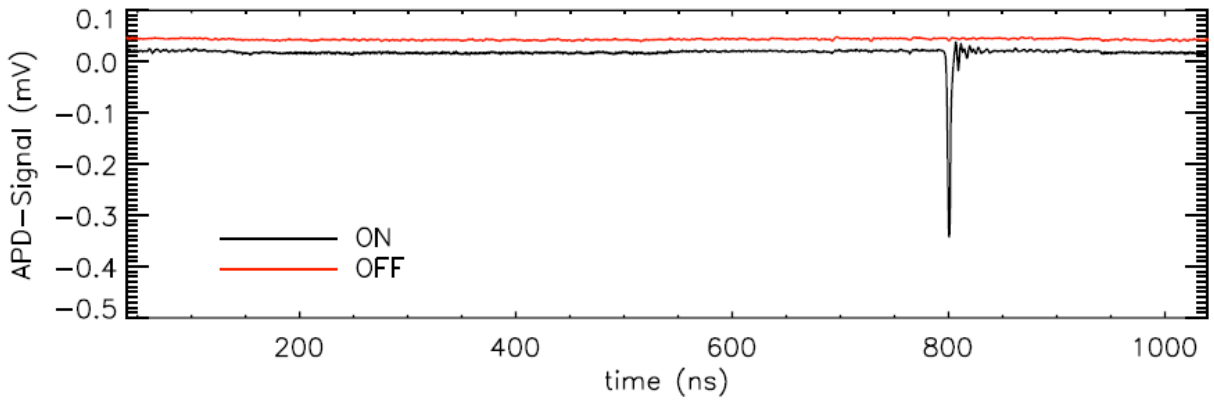
MPI Kirschner, Jülich ZAT Natour, G-ISRR

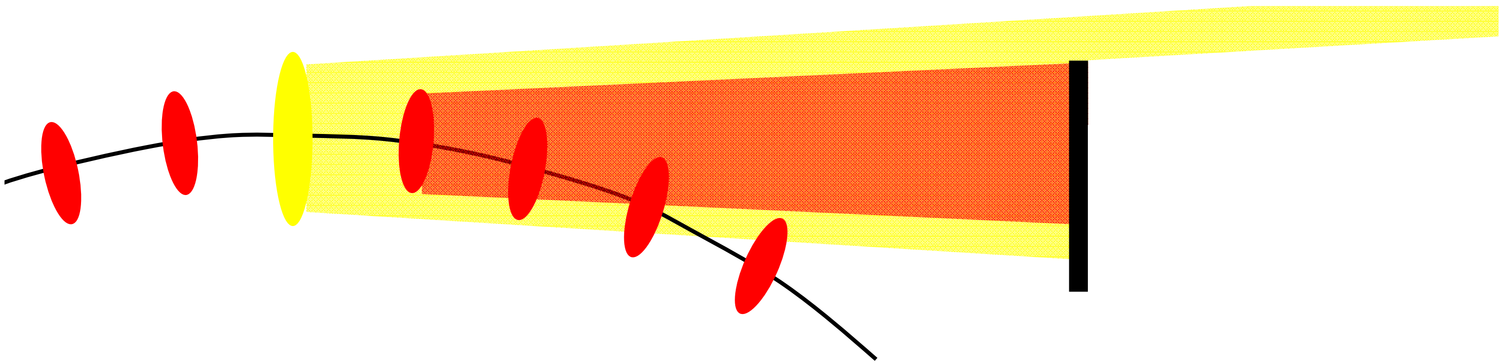


Interlaced 1.25 MHz single bunch operation: orbit-separation

K. Holldack, P. Kuske, R. Müller, R. Ovsyannikov, A. Schälicke et al.
By using the digital bunch by bunch feedback
one single bunch horizontally excited, which
allows to separate

10^9 photons / s From multi-bunch batch with **10^4 suppression of background!**





BESSY ^{VSR} will be best in class…

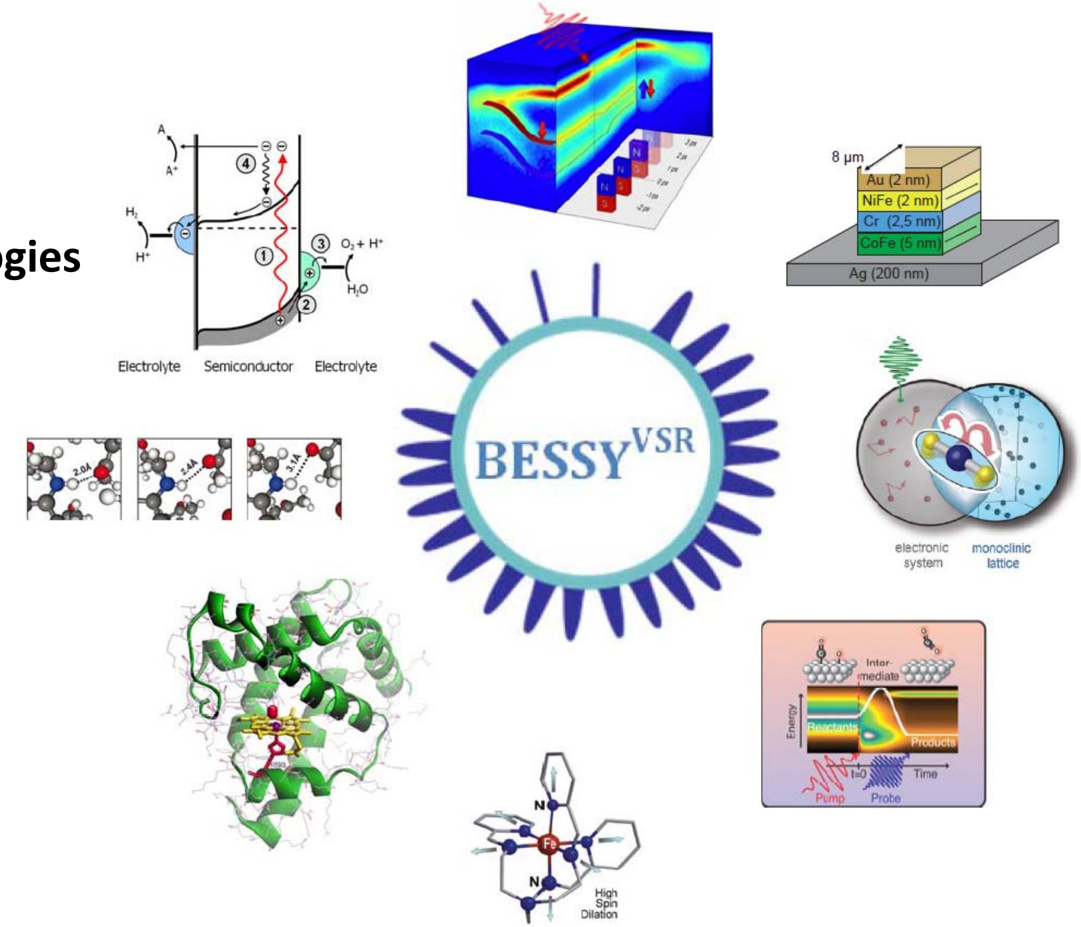
Static and dynamics down to the sub-ps

- Ideal for charged particle spectroscopy and microscopy
- Electron Spectroscopy and PEEM
- Absorption Spectroscopies
- Resonant elastic and inelastic Scattering
- Diffraction on big Crystals

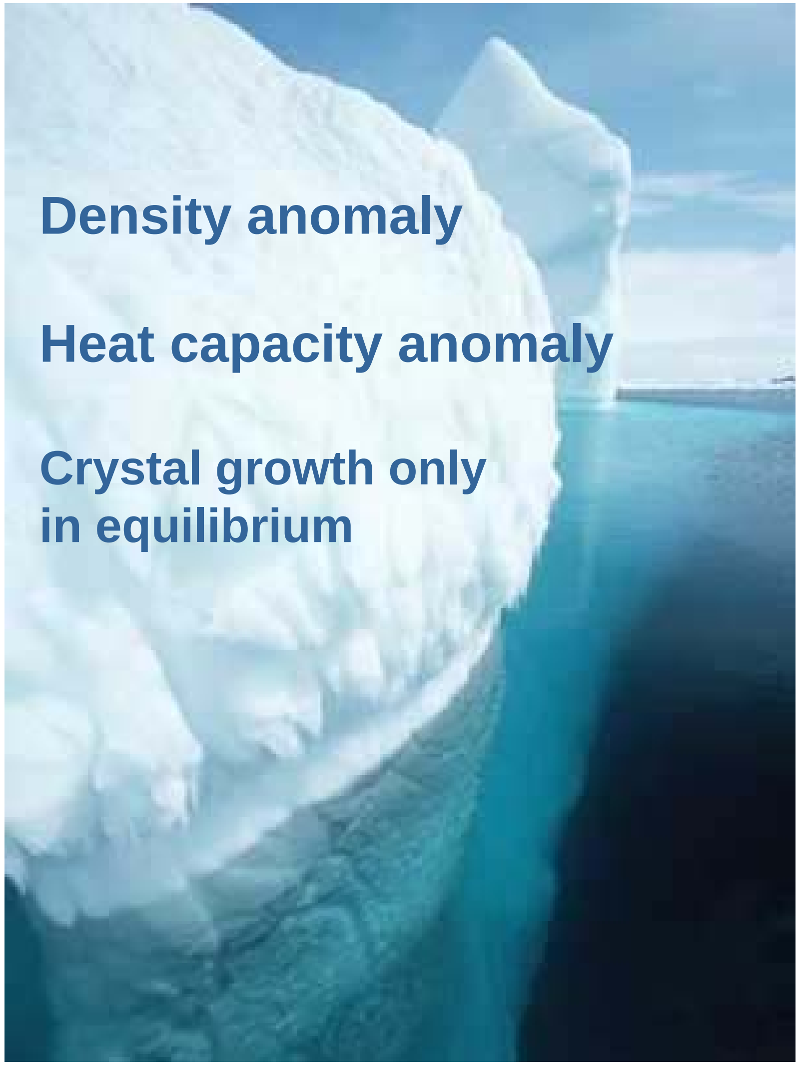
… as long as we have no multi-user
seeded MHz Rep-Rate
tuneable X-ray laser

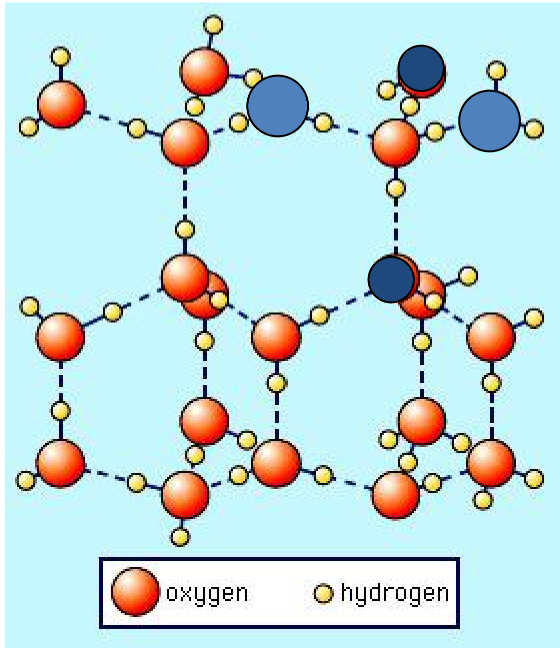
BESSY ^{VSR} – Scientific Case

1. **BESSY^{VSR} – Science drivers**
   1. **Quantum materials for energy**
      1. Superconductivity
      2. Photovoltaics
      3. Topological insulators
      4. Nanoscale materials
   2. **Future information technologies**
      1. Magnetism dynamics
      2. Phase transitions
      3. Molecular electronics
      4. Spintronics
   3. **Basic energy science**
      1. Photochemistry
      2. Photosynthesis
      3. Catalysis
      4. Solar fuels



Order-Disorder Phase transitions



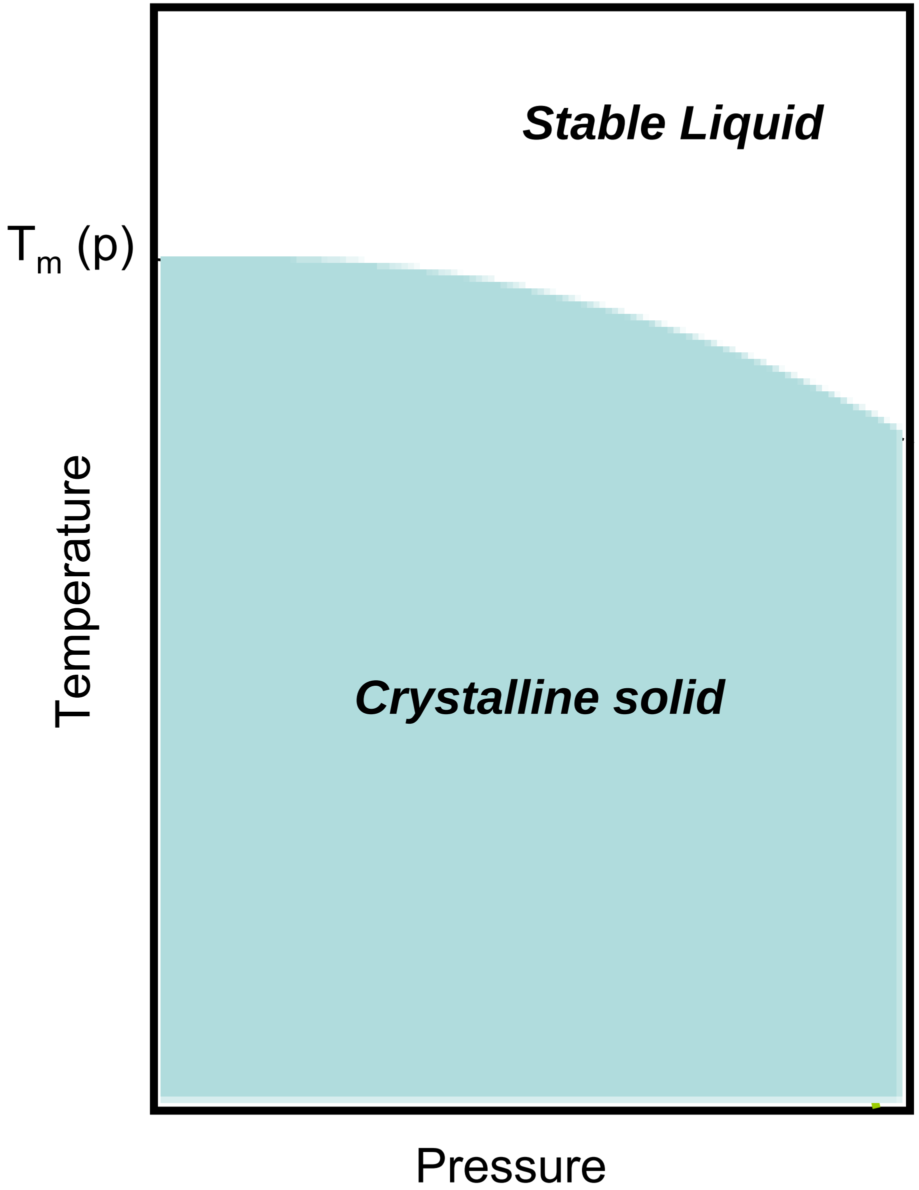


Melting destroys space consuming tetrahedral lattice

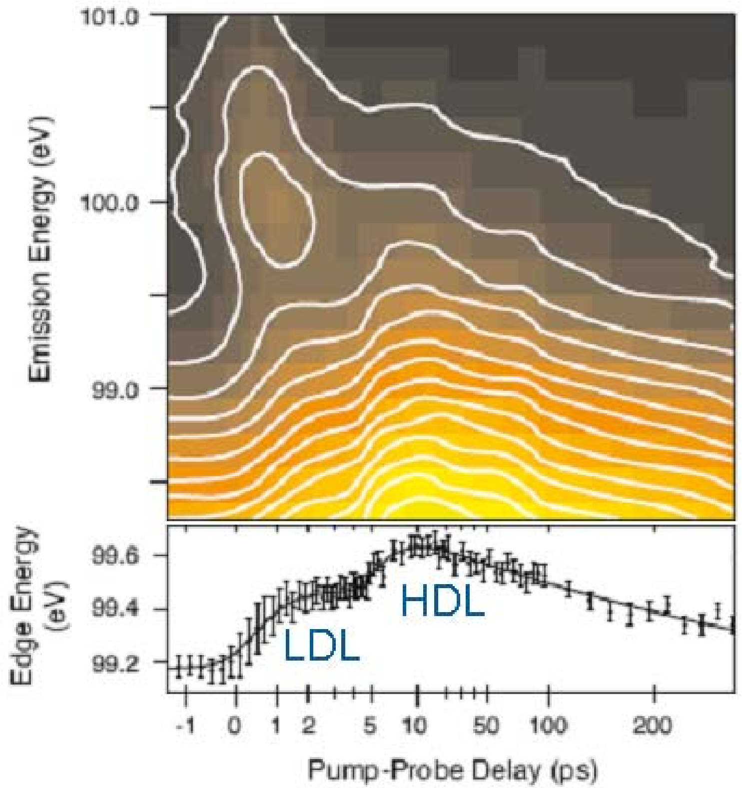
Rapid freezing creates glass

J. Angell et al, Water and its anomalies in perspective:tetrahedral liquids with and without liquid-liquid phase transitions *Phys. Chem. Chem. Phys.* **2**, 1559–1566 (2000).

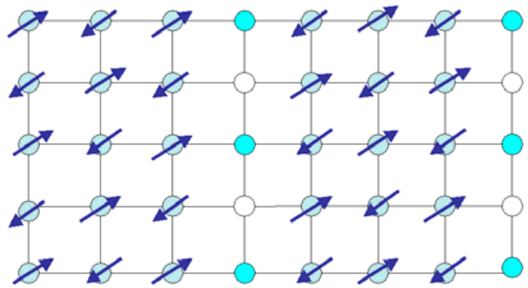
Coexistence of tetrahedral solids and supercooled liquids!

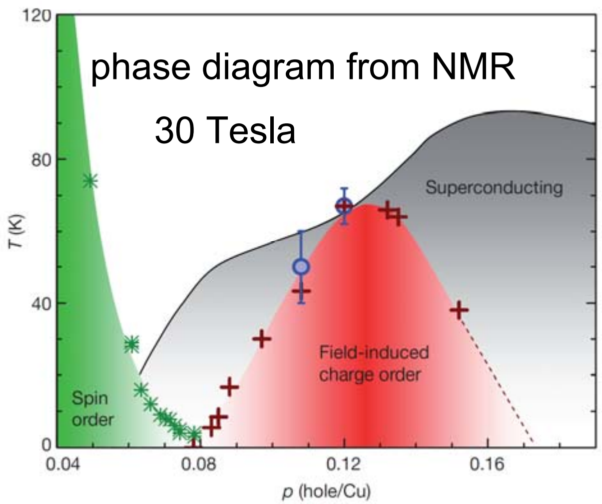


The transitions occur on the ps-timescale



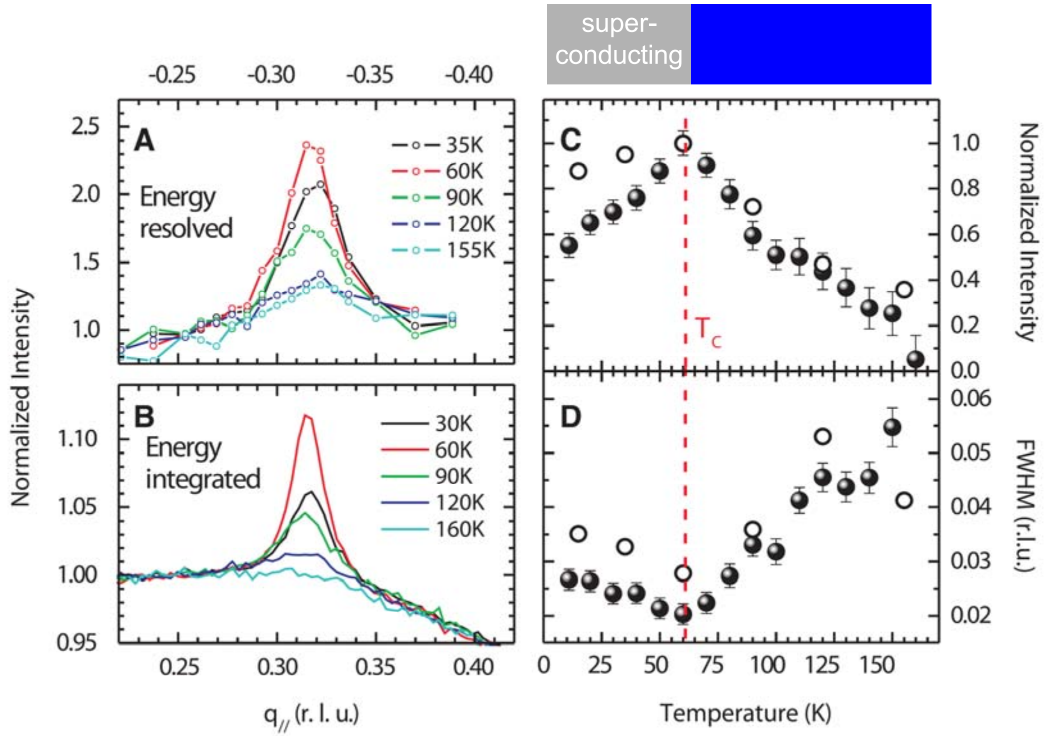
Quantum materials for energy: Ordering phenomena in correlated-electron materials charge order in superconducting cuprates: $YBa_2Cu_3O_{6-}$





T. Wu et al., Nature 477, 191 (2011)

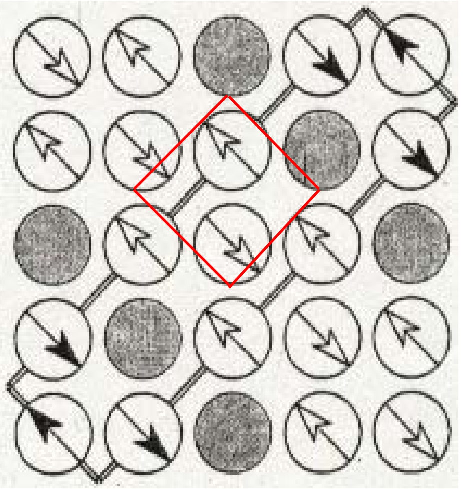
resonant soft x-ray diffraction at Cu-L_3 resonance (UE46)



G. Ghiringhelli, E. Weschke et al., Science 337, 821 (2012)

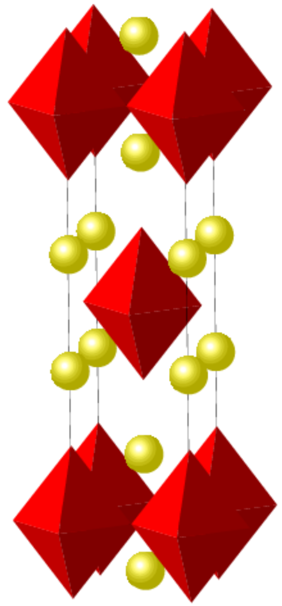
- first observation of charge order in YBCO without magnetic field
- charge order competes with superconductivity
- explains dip in the phase diagram
- charge order generic property of CuO planes

Quantum materials for energy: Non-equilibrium for spin and charge stripe order in La_2NiO_4 from RSXRD



Tranquada et al.

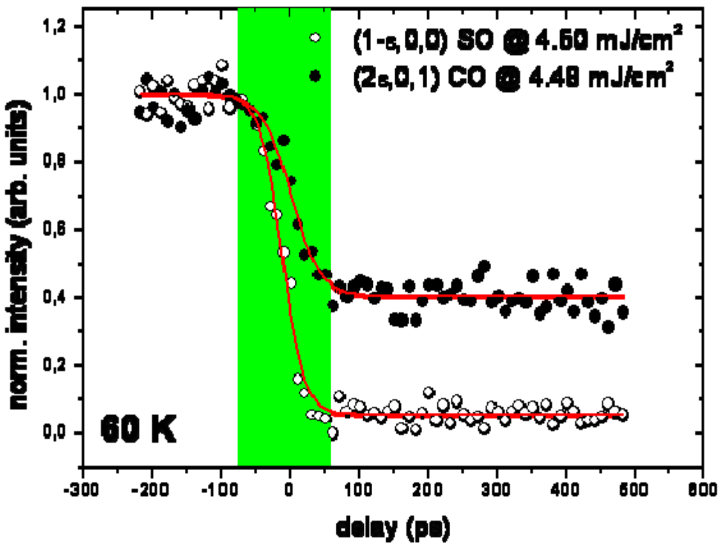
- first neutron study of stripe order
- isostructural with $La_{2-x}Sr_xCuO_4$
- not superconducting
- stripe phase at low temperatures

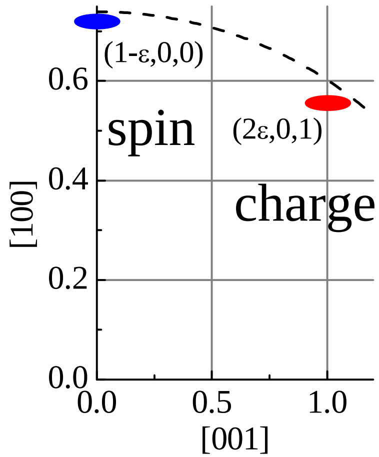


equilibrium: SO and CO simulteneous/ pump removes SO

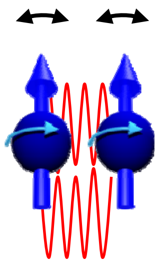
HZB:
Christoph Trabant
Christian Schüßler-Langeheine, J. Schlappa
Niko Pontius
Torsten Kachel
Alexander Föhlisch

Uni Köln:
Pascal Vogt
Chun-Fu Chang
Marcel Buchholz





Reversible magnetic manipulation/switching highly relevant in magnetic storage



Spin excitation

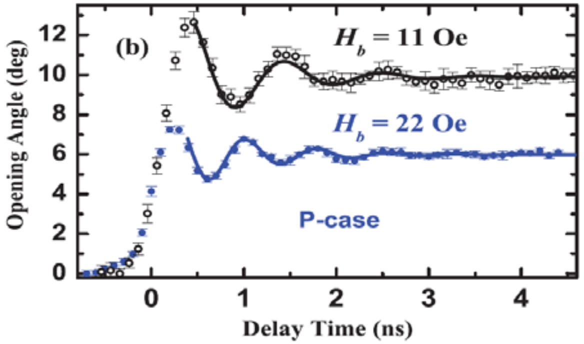
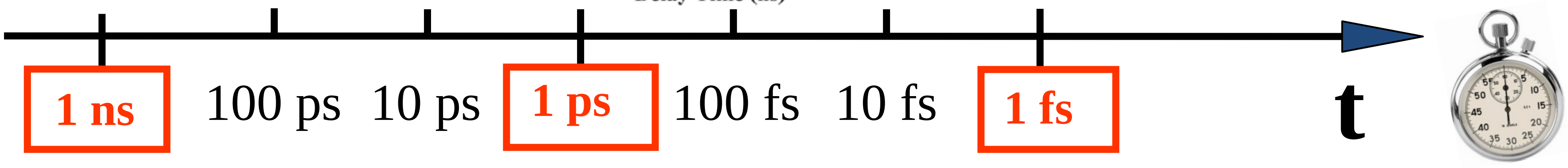
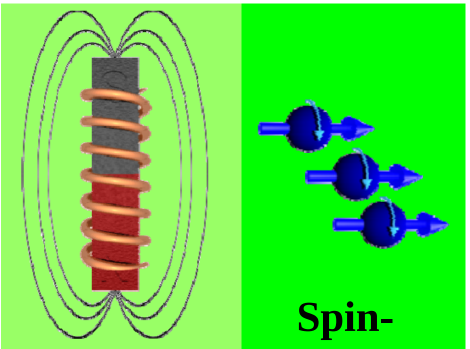


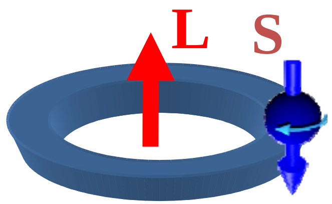
Figure 9. *Time resolved precessional dynamics of Fe in a Py/Cu/Fe spin valve determined by pump-probe methods at the Fe L_3 - edge. Taken from ref. 14, R. Salikhov et al., Phys. Rev. B* ***86****, 144422 (2012).*



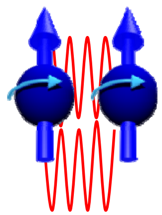


Magnetic field

Spin-polarized current



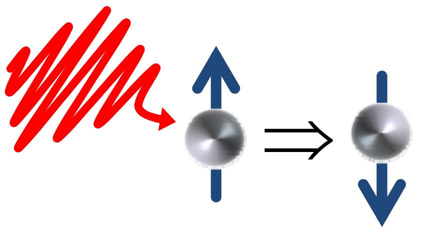
Spin-orbit (LS) interaction



Exchange interaction

Local and long range contributions to ultrafast demagnetization

direct photon-spin interaction

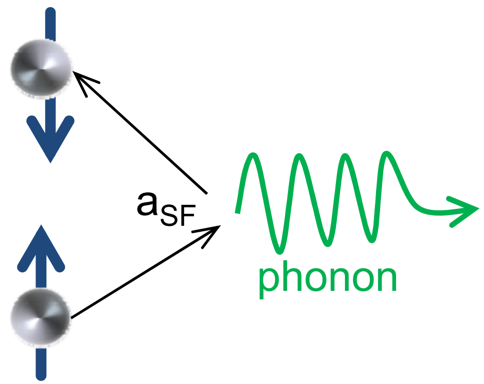


only at very high excitation densities

G.P. Zhang and W. Hübner, Phys. Rev. Lett. **85**, 3025 (2000)

J.-Y. Bigot et al., Nature Phys. **5**, 515 (2009)

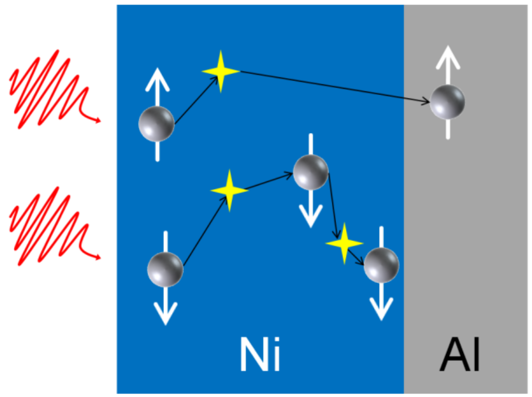
electron-phonon spin-flip scattering



B. Koopmans et al., Nature Mater. **9**, 259 (2010)

electron-magnon:
E. Carpene et al., Phys. Rev. B **78**, 174422 (2008)
electron-electron:
M. Krauß et al., Phys. Rev. B **80**, 180407 (2009)

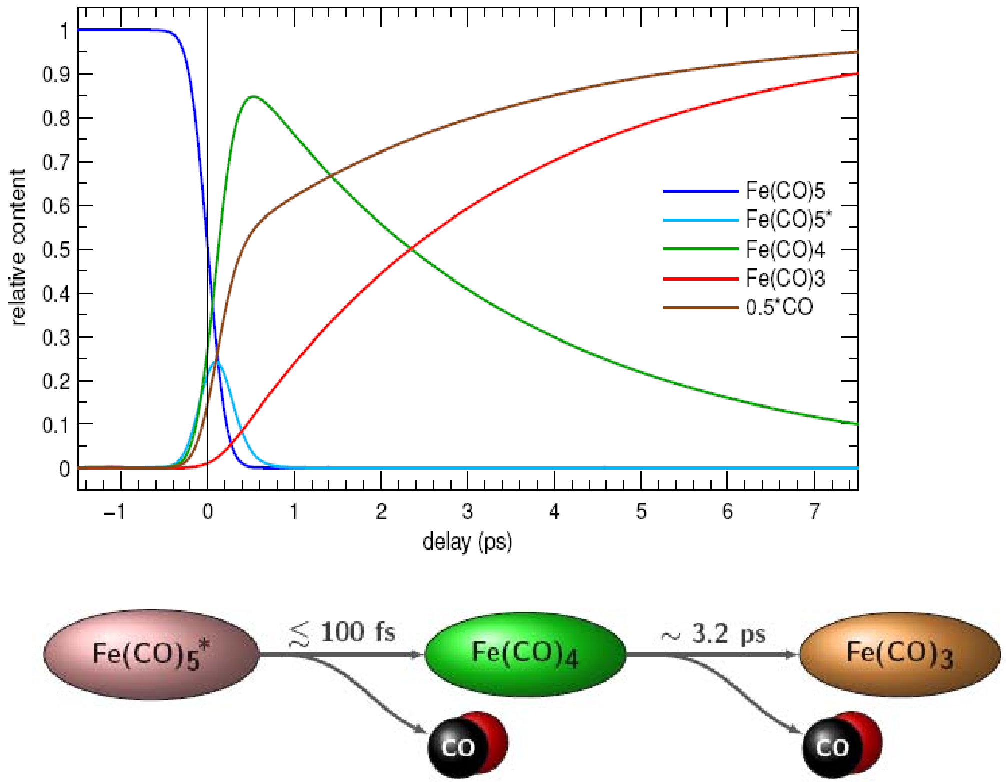
superdiffusive spin transport



M. Battiato et al., Phys. Rev. Lett. **105**, 027203 (2010)

Basic Energy Science: photochemistry, coherent wavepackets

Bondbreaking/creation   Isomerisation   Tautomerisation   Solvation



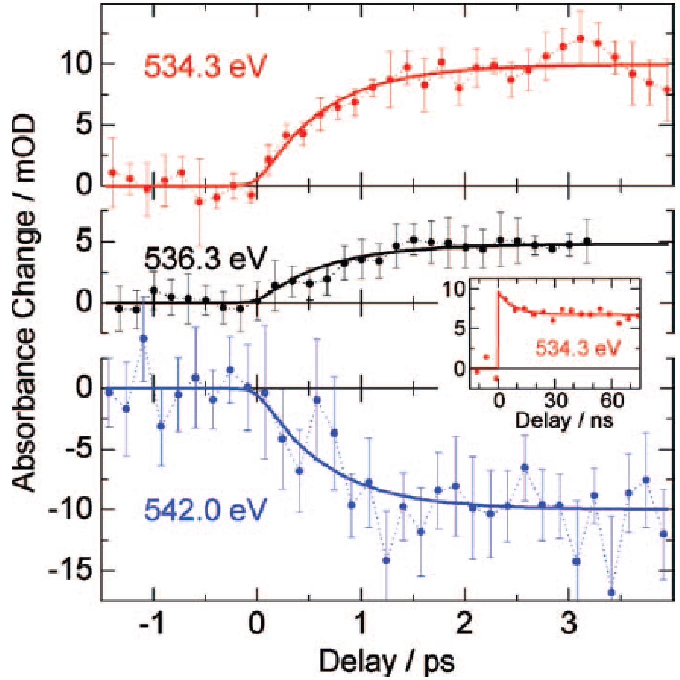


Figure 21. *Absorbance change as a function of time delay between the infrared pump pulses and the X-ray probe pulses at three characteristic spectral positions in the O K-edge: 534.3 eV (red), 536.3 eV (black), and 542.0 eV (blue). Solid lines are single exponential fits to the data with a time constant of 0.7 ps. The inset shows a time transients on nanosecond time scales. Taken from ref. 8, Wen et al., J Chem. Phys.* ***131****, 234505 (2009).*

Full agreement with literature:
S. A. Trushin, W. Fuss, K. L. Kompa, W. E. Schmid.
Femtosecond Dynamics of Fe(CO)5 Photodissociation at 267 nm Studied by Transient Ionization.
J. Phys. Chem. **A 104**, 1997 (2000).

Short pulses to beat radiation damage? Light harvesting Cycles

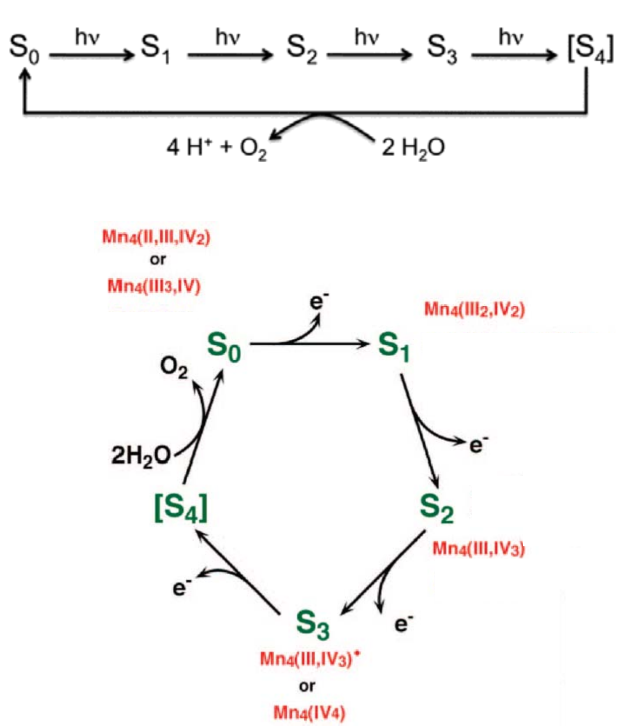


Figure 23. *Reaction cycle for water oxidation in PSII with the four states S_0-S_4 reached by consecutive absorption of four photons [top, taken from J. Kern et al., Science, 14 February 2013 DOI: 10.1126/science.1234273 (2013)] and with the corresponding proposed oxidation states of the Mn cluster [bottom, adapted from ref. 1, J. Yano, V. Yachandra, Inorg. Chem.* ***47****, 1711 (2008)].*

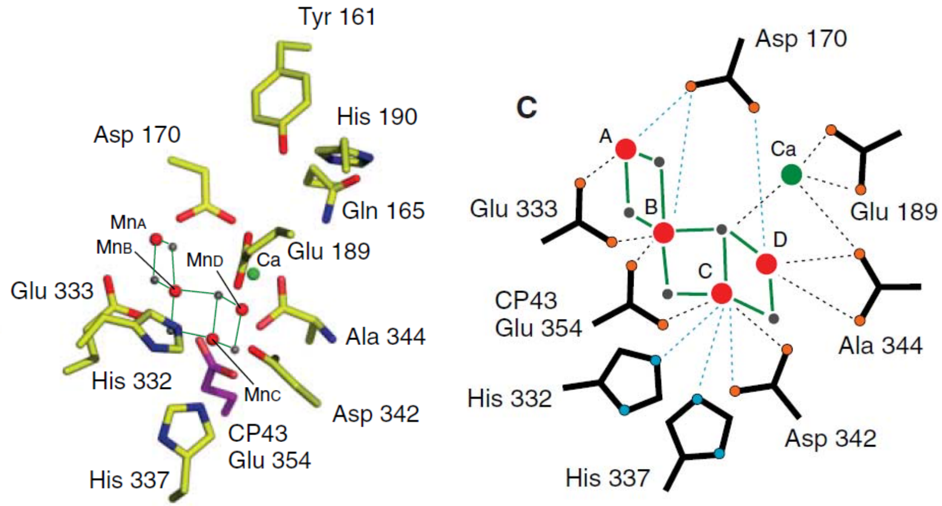


Figure 24. *Two representations of a model representing the immediate vicinity of the Mn_4CaO_5 cluster in PSII. The assignment of ligands is tentative because it is based on the electron density of the cluster, and its immediate environment may be altered by x-ray damage. Bonds in the representation on the right between Mn and the bridging oxo are shown as solid green lines. Bonds to proposed ligand amino acid groups and to Ca atoms are shown as dotted lines (black, less than 3.0 Å; blue, more than 3.0 Å). Taken from ref. 2, J. Yano et al., Science* ***314****, 824 (2006).*

Basic Energy Science: Catalysis, Electrophotochemistry/Solar fuels

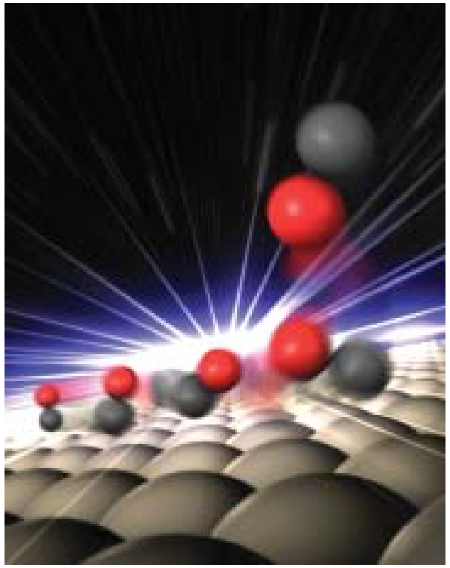
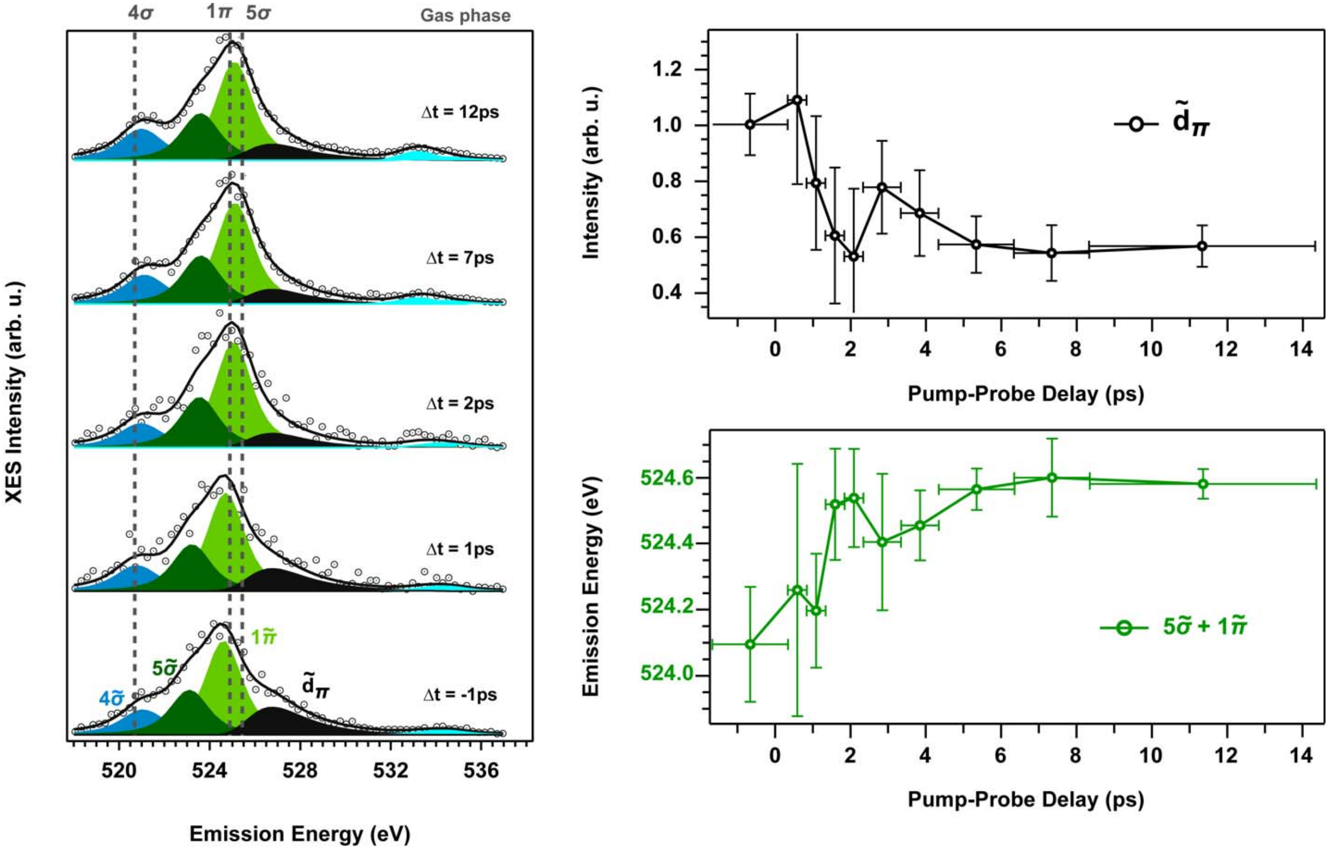


__Figure 26.__ . The role of transient states on catalytic surfaces can be investigated with the selectivity of X-ray methods on a fast picosecond time scale available at BESSY^{VSR}. The important initial step of CO oxidation in the presence of a suitable catalyst has been observed recently, ref. 1, Dell'Angela et al., Science __339__, 1302 (2013). Artwork by Gregory Stewart at SLAC National Accelerator Laboratory.

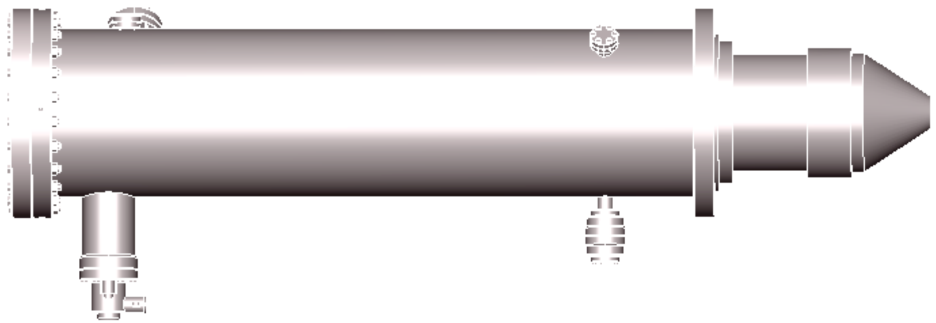
Martina Dell´Angela et al.; Science, 2013; DOI: 10.1126/science.1231711
Martin Beye et al.; PRL 2013



UBjL: Uppsala – Berlin joint Lab on next Generation Electron Spectroscopy: Power application at BESSY VSR

- MHz repetition rate with controlled peak brillance required

- Angle resolved Time of Flight ArTOF (+ derivatives: (Angle, Space, Spin) Gain in transmission >200 over hemisphere



PHYSICAL REVIEW B **79**, 035402 (2009)

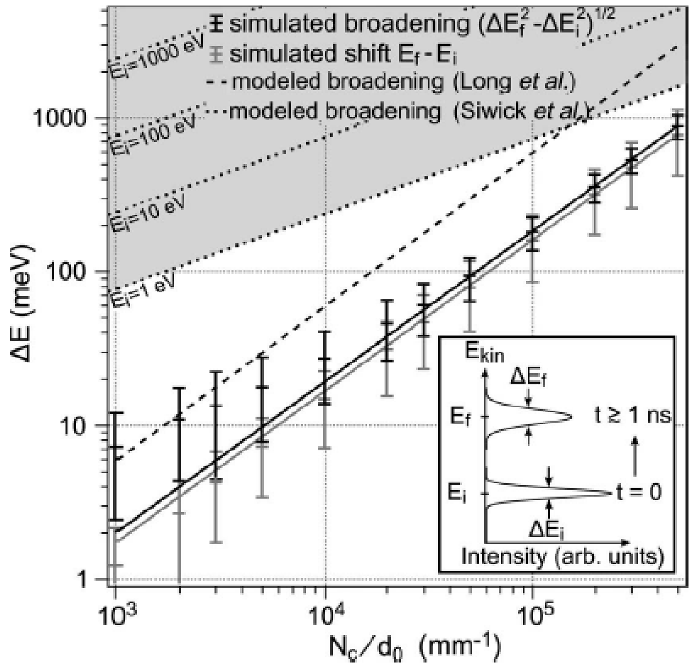


FIG. 6. Simulated energy shift (gray data points) and energy broadening (black data points) as functions of the cloud electron density N_c/d_0 for a situation similar to core-level photoemission spectroscopy. The error bars result from a systematic variation of the light spot diameter d_0 (0.1, 0.4, and 1 mm), mean energy E_i (1, 10, 100, and 1000 eV), and pulse duration τ_0 (20 fs, 1 ps, and 50

Static and dynamic electronic structure down to the sub-ps

- Shift space charge resolution limit to 150 μeV
- Low dose photoemission
- Orbital selective structure from photo electron diffraction: access the ps and sub-ps dynamics in a molecular movie
- Chemical dynamics form ps and sub-ps ESCA
- Sub-natural linewidth information on matter from Coincidence
- (low energy ARPES/PEEM will go to HHG)

BESSY ^{VSR} will be best in class…

Static and dynamics down to the sub-ps

- Ideal for charged particle spectroscopy and microscopy
- Electron Spectroscopy and PEEM
- Absorption Spectroscopies
- Resonant elastic and inelastic Scattering
- Diffraction on big Crystals

… as long as we have no multi-user
seeded MHz Rep-Rate
tuneable X-ray laser

Summary

Up-grade of BESSY II to BESSY^{VSR}:

- Unique Storage ring for combined sub-ps and ps dynamics and static information at high rep rate for spectroscopy, scattering, imaging / microscopy.
- Individual users switch freely between average flux and time resolved mode at MHz repetition rates with BESSY II type brillance and partial coherence.
- The missing link between FEL and Storage rings.

Science goals central to Helmholtz-Mission

- Quantum materials for energy: Superconductivity, Photovoltaics, Topological insulators, Nanoscale materials
- Future information technologies: Magnetism dynamics, Phase transitions, Molecular electronics, Spintronics
- Basic energy science: Photochemistry, Photosynthesis, Catalysis, Solar fuels, beat radiation damage in photosystems

Next Steps

- The Users Workshop 2013 to further improve the BESSY-VSR Scientific Case (How hard shall we push to short timescales / average brillance / compromise)
- Get it funded in POF III (2015 – 2020)
- BESSY III: A future Next generation Light Source in Berlin: Multi-User, Coherence, time-structure, rep-rate, Unique to USR, SASE-FEL, Ideal addition to BESSY-VSR.

Thank you for your attention!