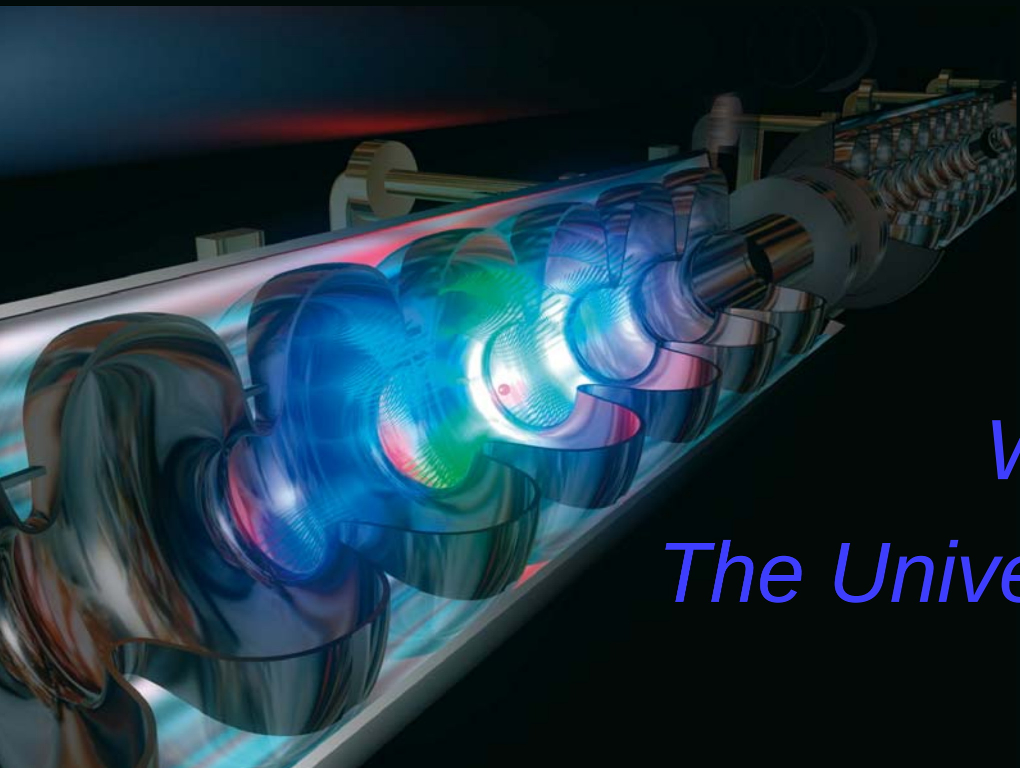
The University of Manchester

MANCHESTER 1824

Next Generation Advanced Light Source Science



Wendy Flavell

The University of Manchester & STFC, UK

Measuring in real time

What if all you saw of a race was this bit? Would you learn anything?

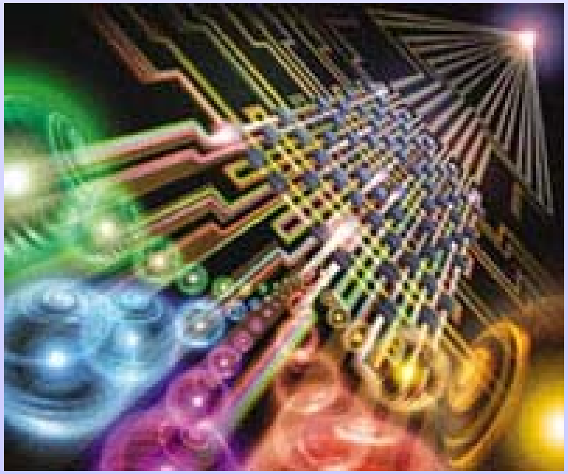
This is our problem with most current SR research - reactions happen so fast we only see the products.

Next generation light sources enable us to watch chemical reactions as they happen (on fs timescales), even in nanoclusters of material

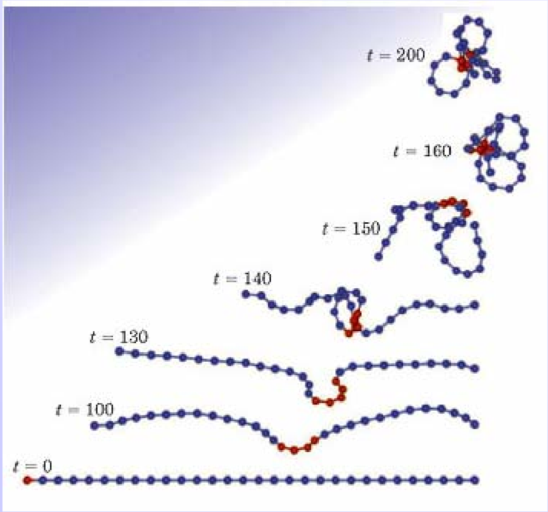
The science need

The fundamental requirement is to understand the *dynamic* behaviour of matter, often in very small (nm) units, on very fast (fs) timescales

We need not just to determine *structure* with high precision, but to understand *how these structures work*

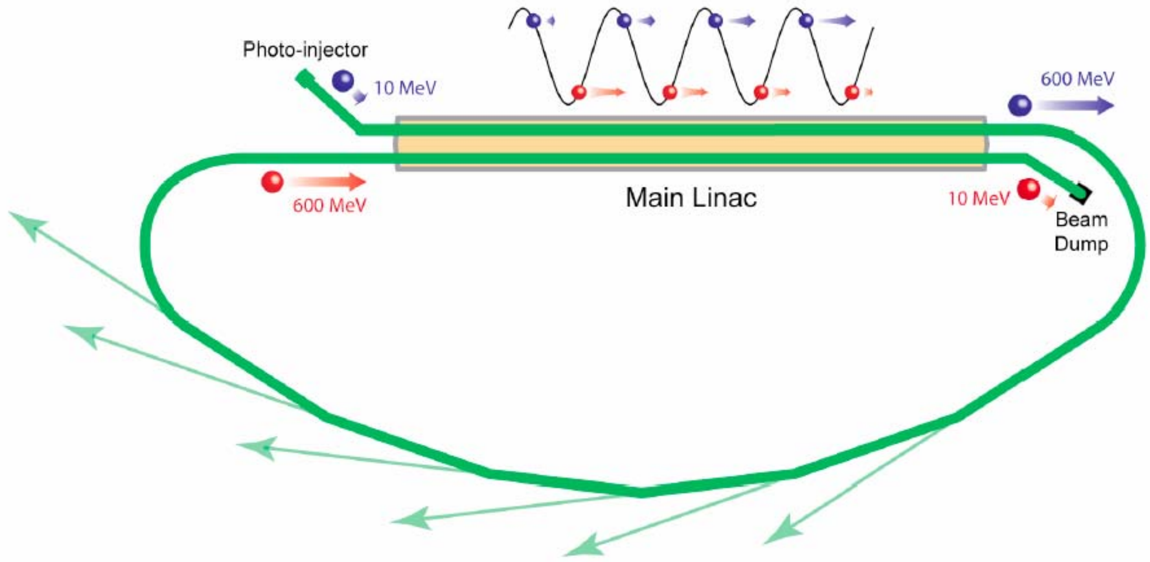


Scientific American Jun 2002



Physics Today Jan 2004

Energy recovery in a linac

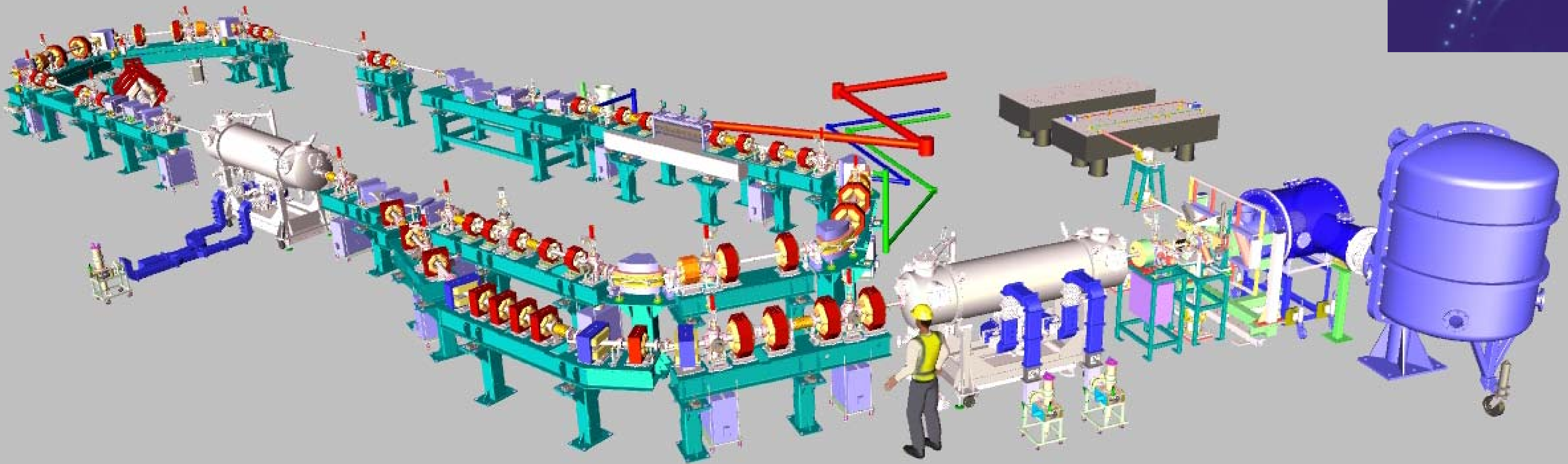


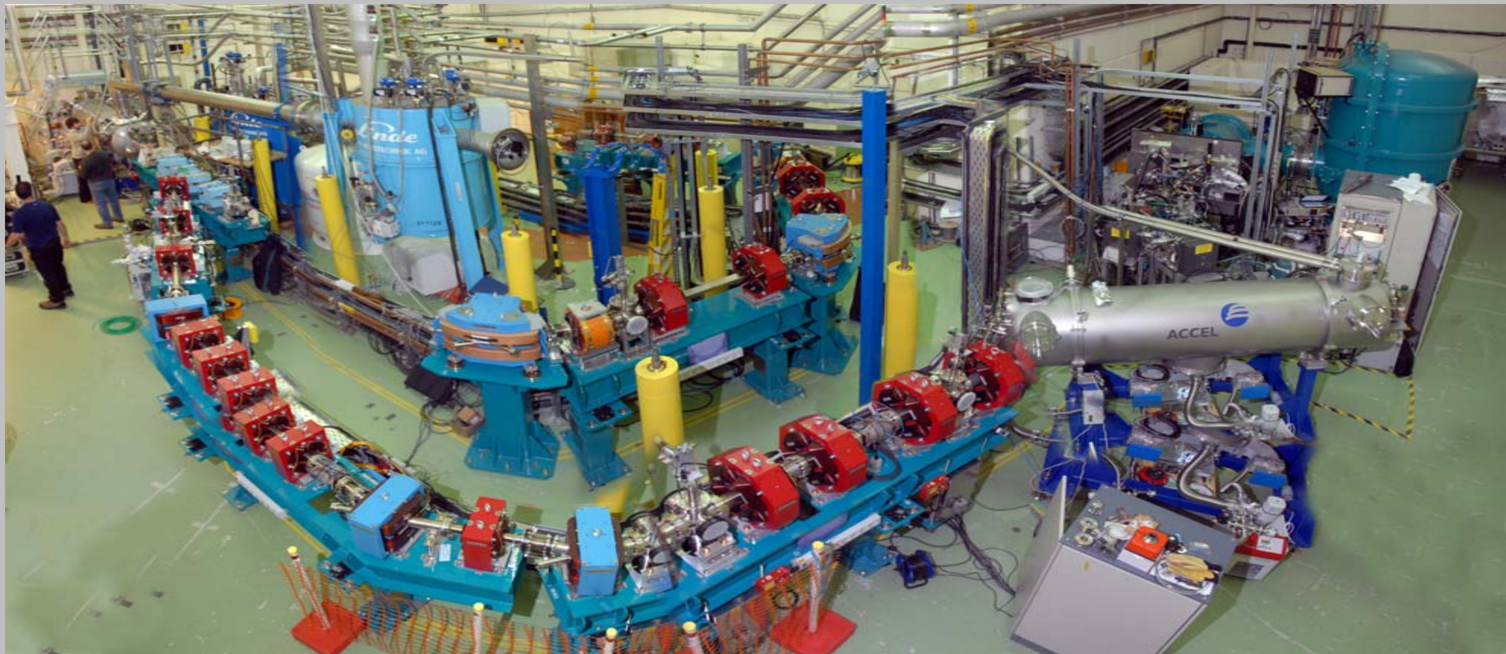
Some world ERL light source projects:

- JLab (US)
- JAEA (Japan)
- BINP(Russia)
- ERLP (UK)
- CHESS(US)
- KEK(Japan)
- 4GLS (UK)
- BNL (US)
- APS? (US)

pulse lengths *ca.* 100 fs
(storage ring *ca. 10's -100 ps)*

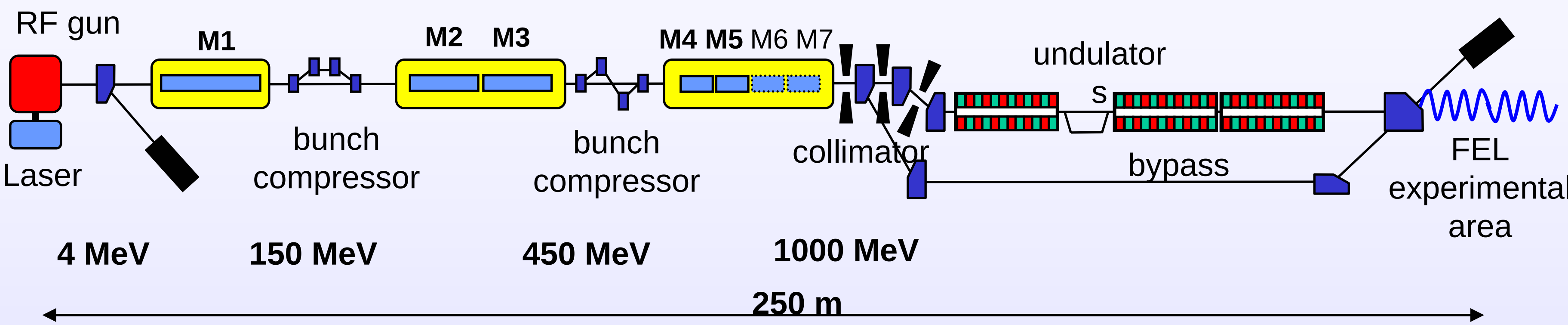
The 4GLS prototype, ERLP takes shape





March
2007

FLASH



status

operational with users

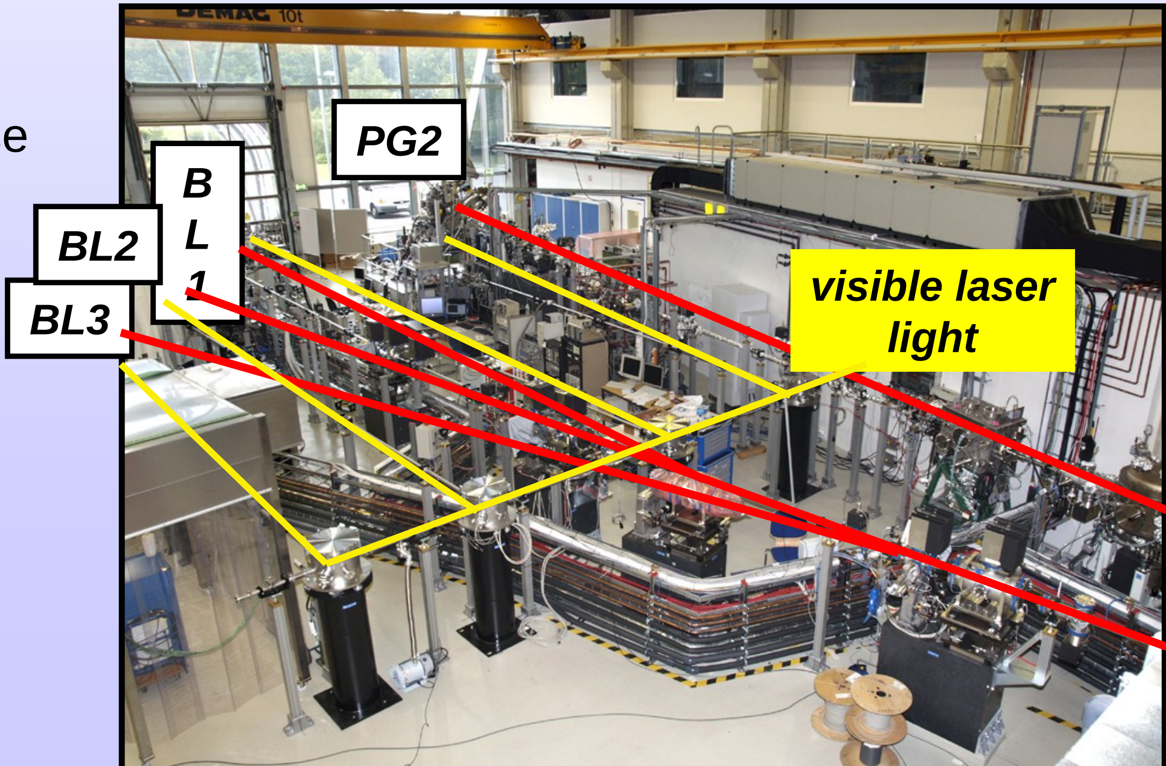
has achieved 13.8nm, 40μJ pulse

Repetition rate up to 150 Hz

Photon range 45-15 nm

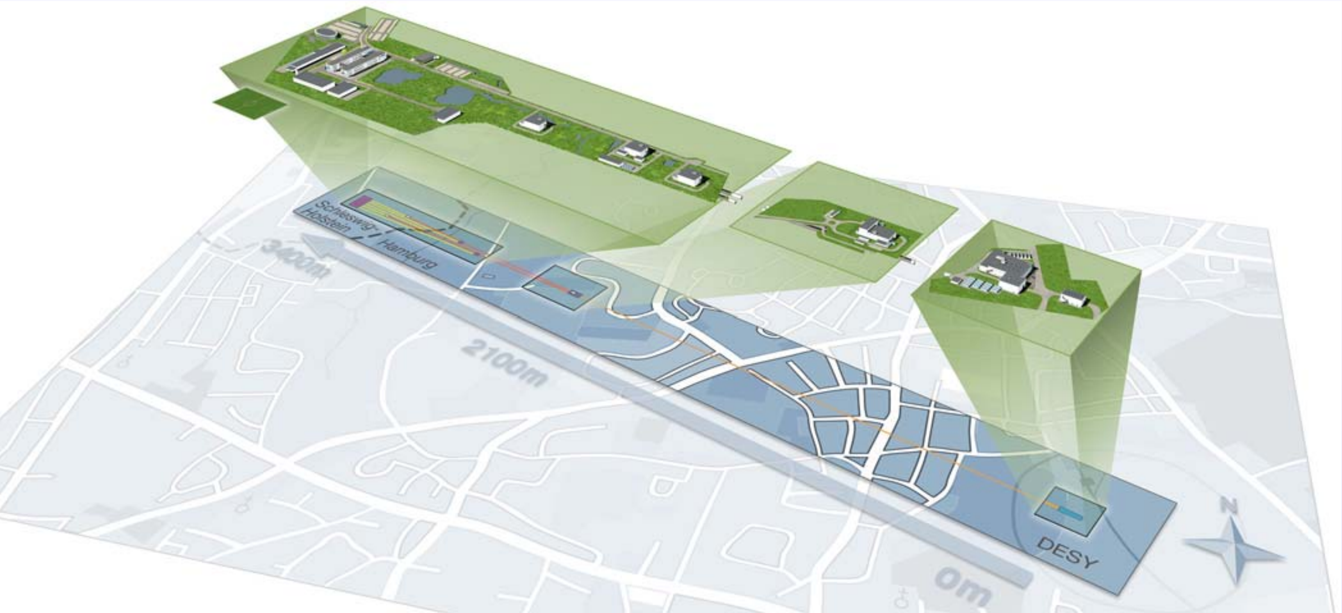
10^{13}-10^{14} ph/pulse

Pulse duration 10-50 fs

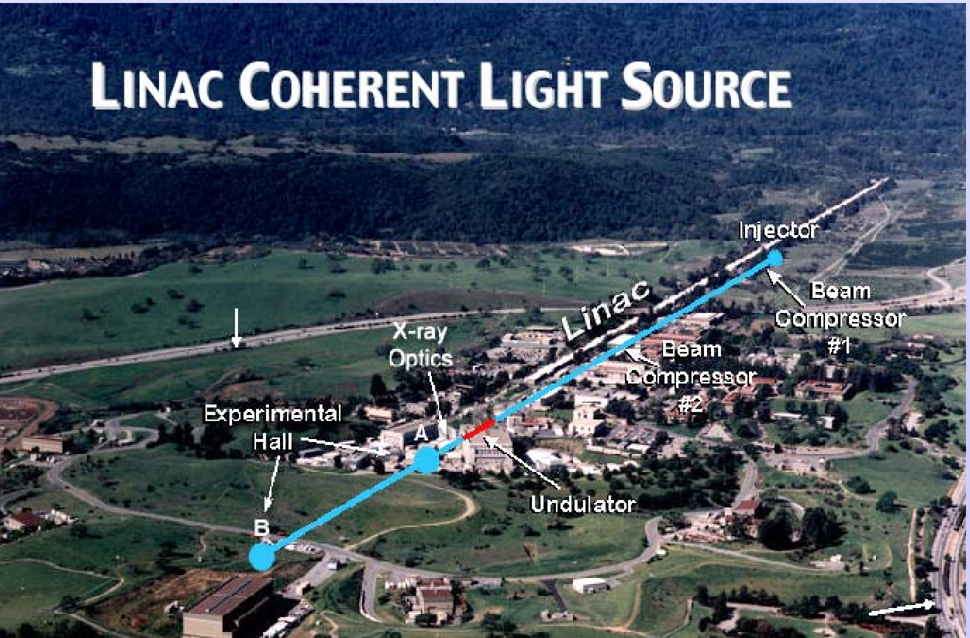


J. Schneider, DESY

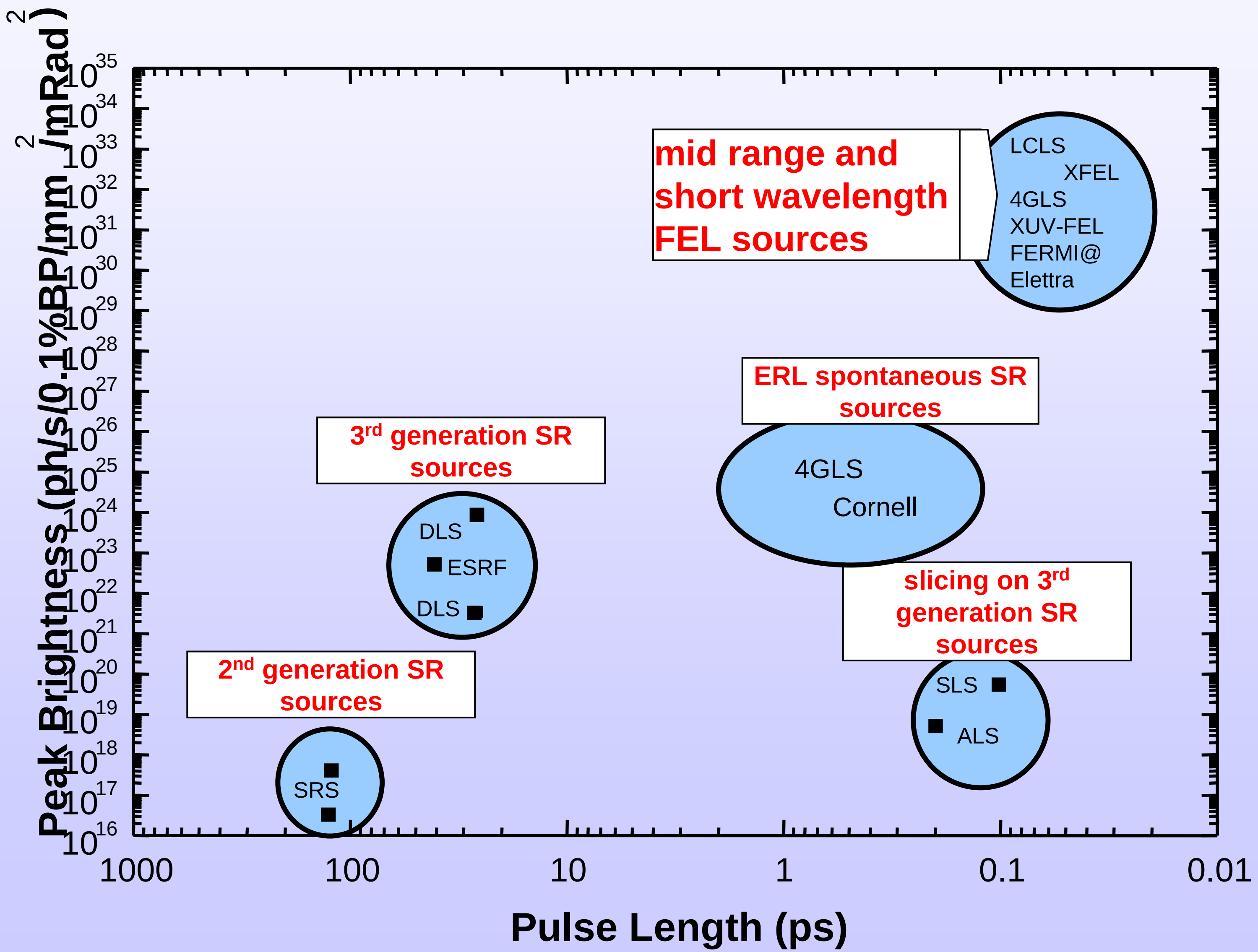
Some planned X-ray FELs

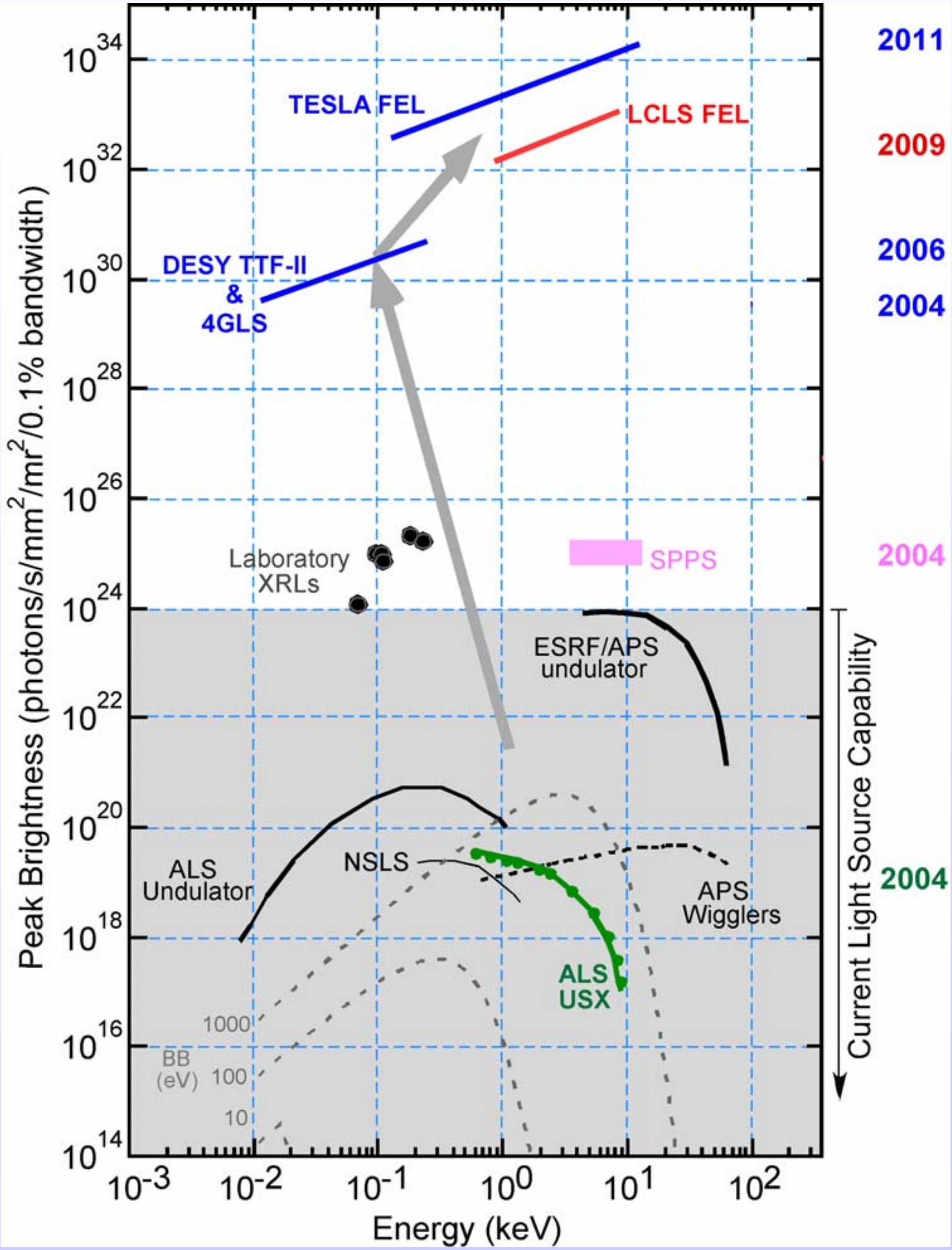


LCLS (SLAC)
XFEL (DESY)
SCSS (SPring-8)



Linac-based light sources





A step change

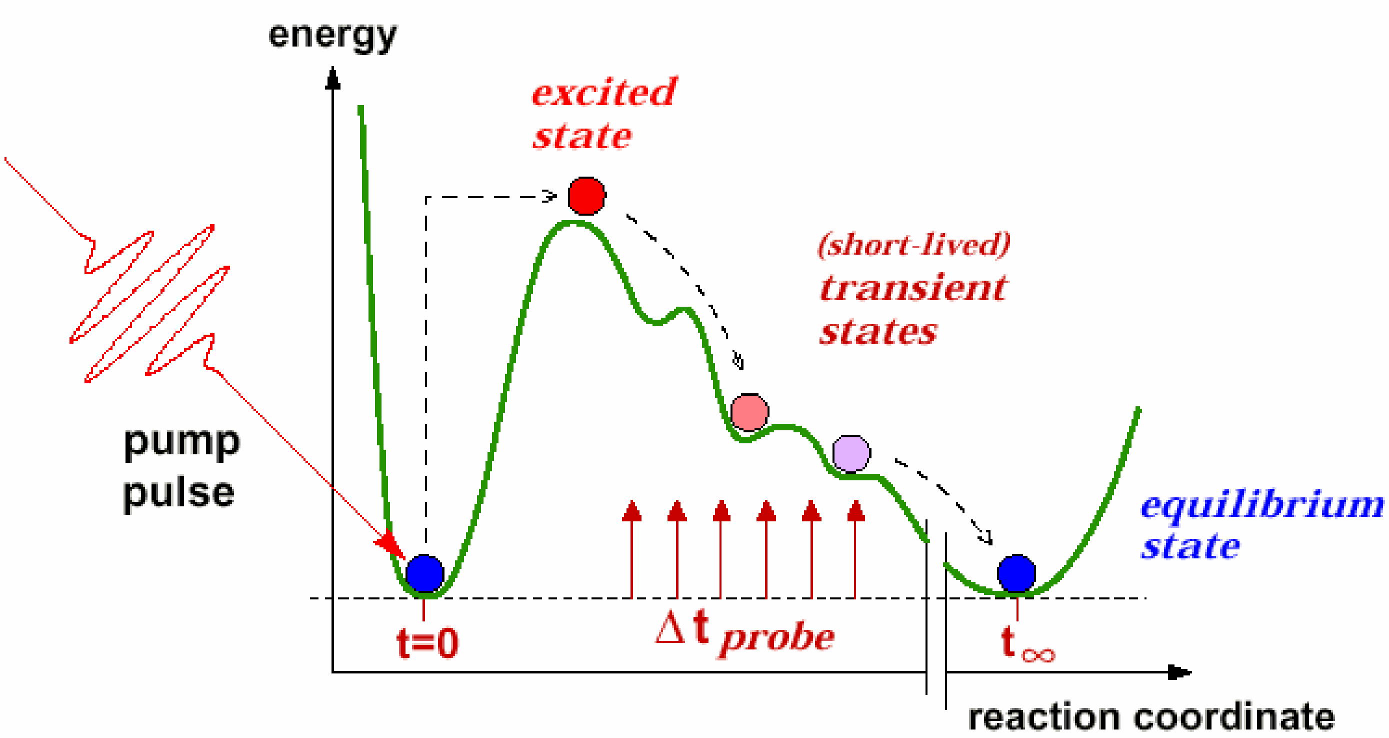
The advent of world 4th generation sources will bring a step change in brightness in the VUV/XUV and X-ray regimes (and THz too!)

…..and the pulse lengths are similar to the time it takes to break a chemical bond

Dynamics and kinetics

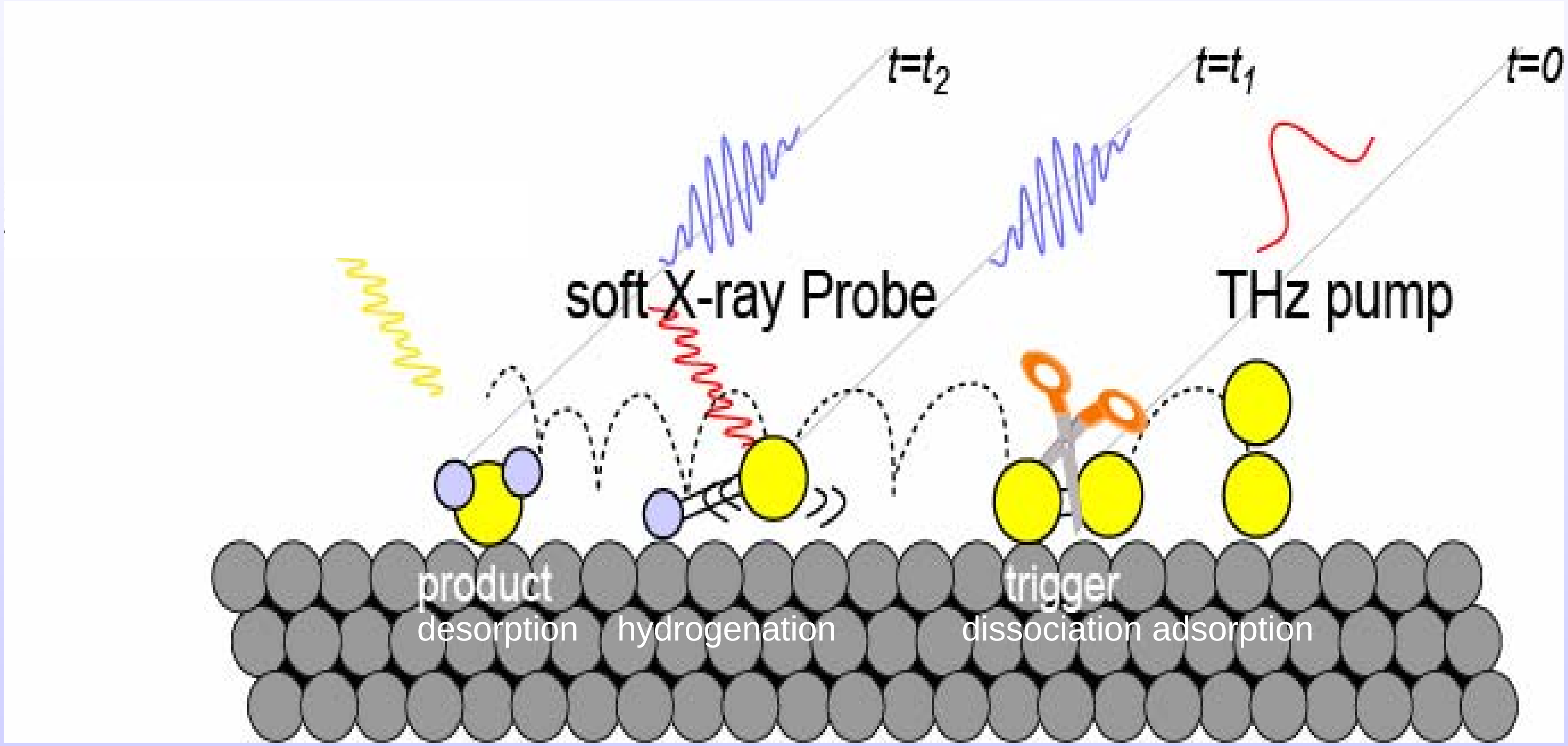
- pulse lengths down to sub-100 fs,
- naturally synchronised sources
- real time monitoring of chemical reactions,

bond breaking and making



TESLA technical design report, March 2001

Pump-probe:
understanding reaction pathways

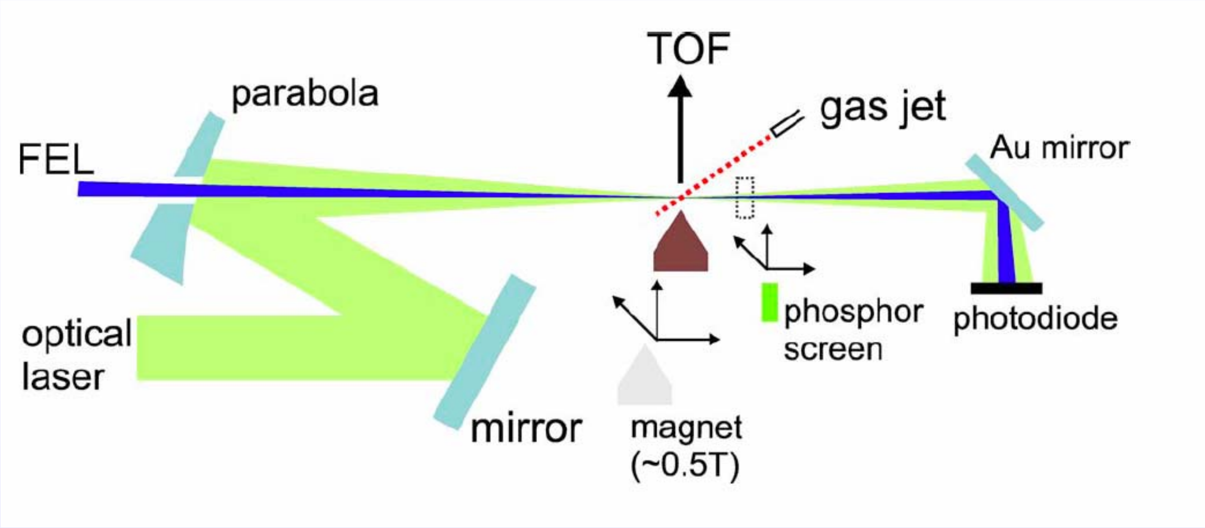


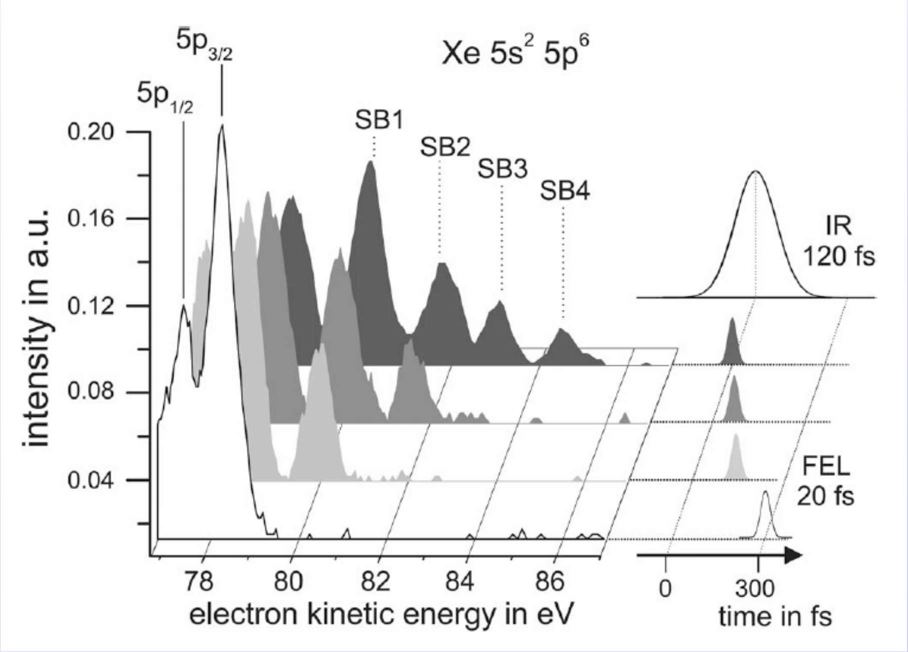
- real-time catalytic reaction monitorring
- we can study dilute, rare or shortlived species and their reactions

(Anders Nilsson and colleagues, SLAC)

Pump-probe at FLASH

2-colour ionisation of Xe and He;
20 fs XUV (45.8, 89.9 eV), 5 Hz;
120 fs 800 nm Ti:sapph

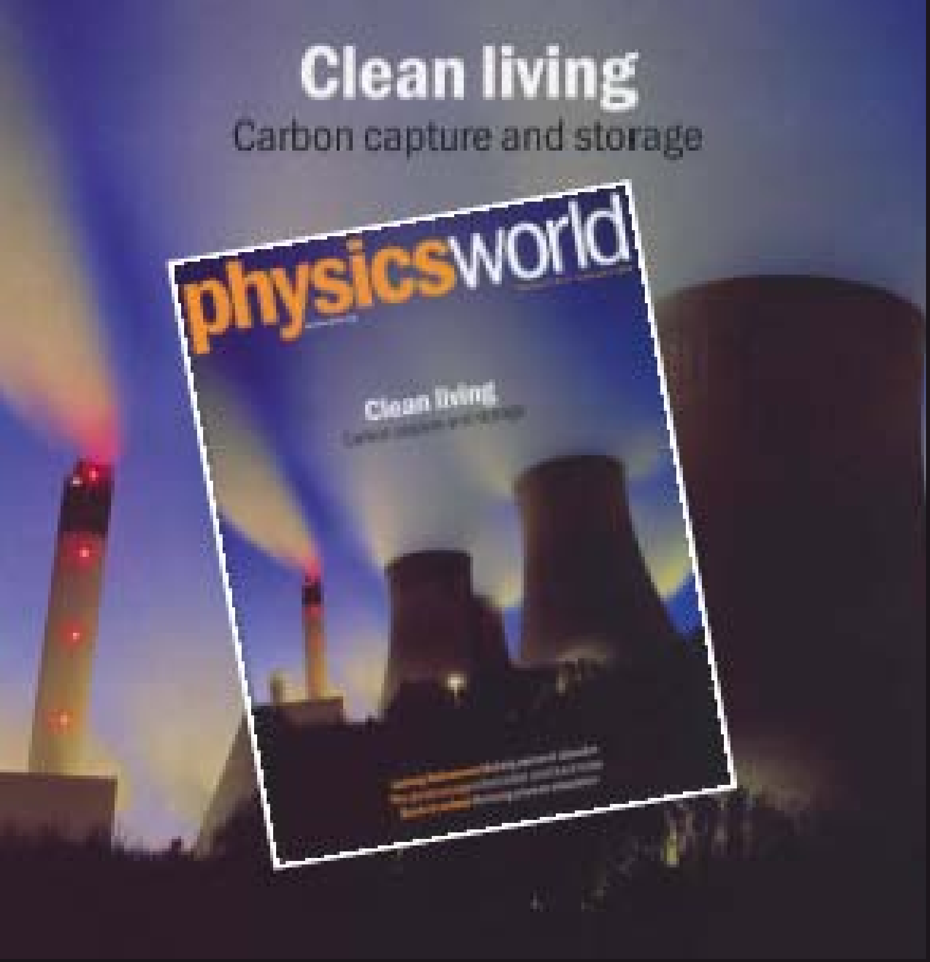




Single-shot spectra

Photoemission sidebands as a pulse diagnostic

Meyer *et al.*, Physical Review A, 74, 011401(R), (2006); Radcliffe *et al.*, Appl. Phys. Lett., 90, 131108, (2007).



Energy and climate change

How do we combust hydrocarbons more efficiently?

Taatjes et al., Science, **308**, 1887, (2005)

Our environment

Reactions and processes in the biosphere

How do we clean up our environment?

What are the reaction pathways of the free radicals and ions contributing to atmospheric pollution?

pollutant creation & removal

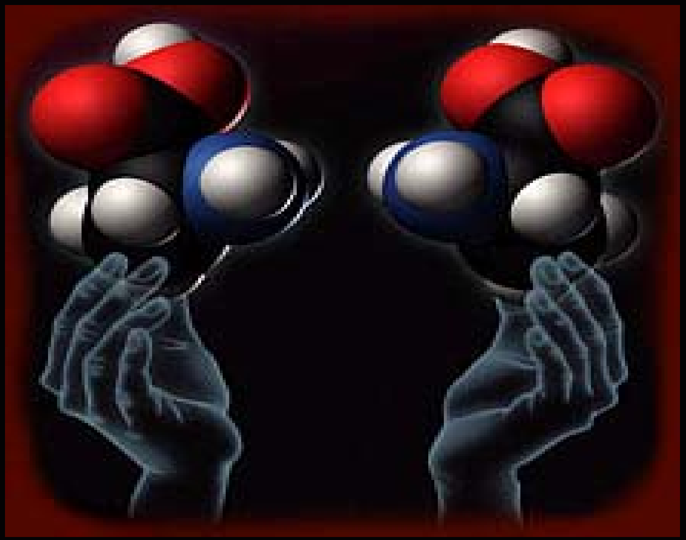
What are the mechanisms of bioremediation?

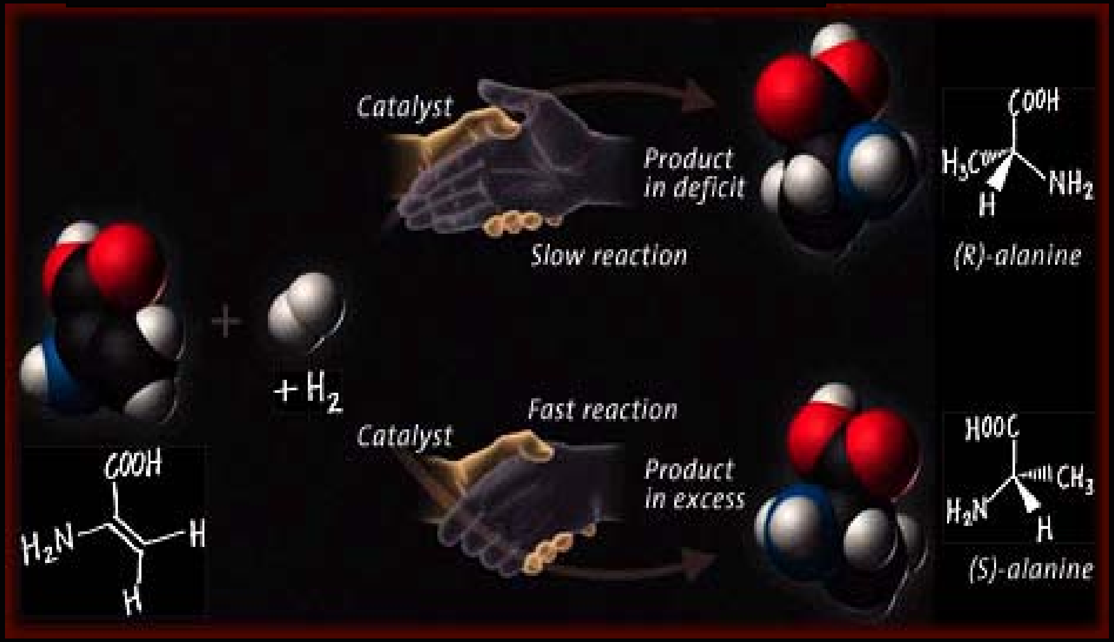
environmental effects of toxins (atmospheric, inorganic, fungal) on photosynthetic systems

Cleaner catalysts by design

How do we design cleaner, more efficient catalysts?

Can we understand and optimise the synthesis of chiral pharmaceuticals?





- Studies of enantiomer-selective chemistry
- Need to understand asymmetric reaction pathways: key to improving turnover number

Asymmetric hydrogenation

Courtesy William Hems,Johnson Matthey Catalysts -Chiral Technologies

Fundamental reactions in the interstellar medium

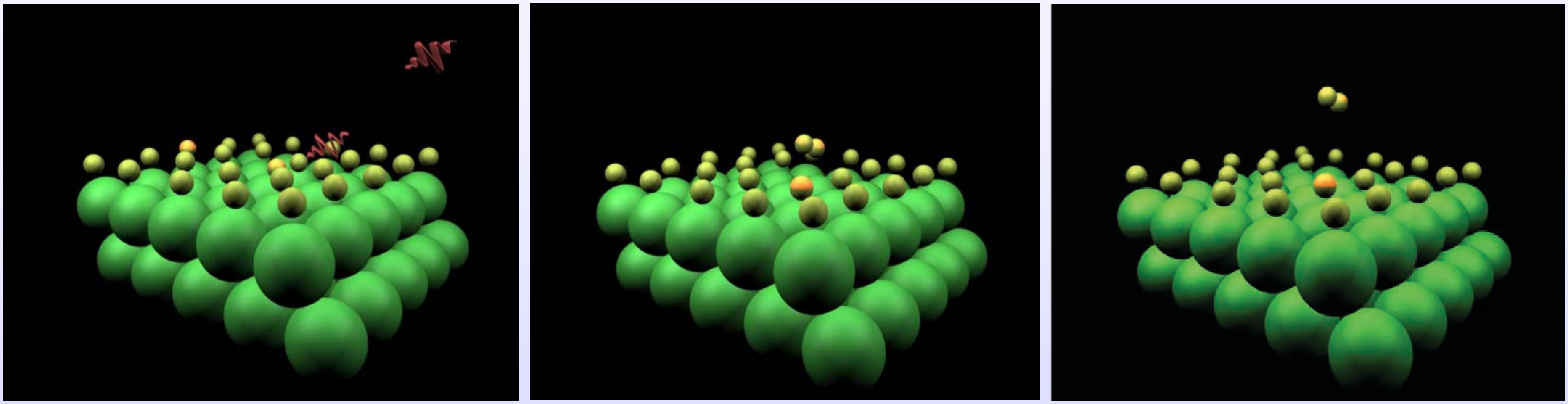
How do stars form and work?

How did life originate?

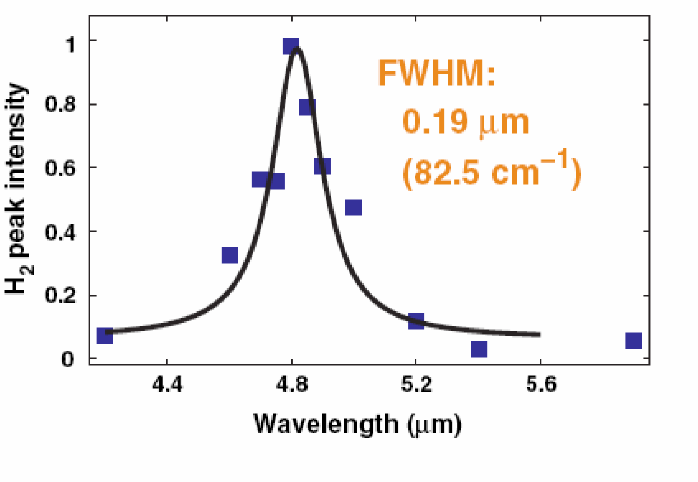
- key fundamental measurements on multiply charged species - remove reliance on computed parameters
- chemistry of the interstellar medium - ion-surface and gas phase interactions, formation of complex ions and molecules, molecular interactions on ultracold surfaces
- Interactions of biomolecules with intense CP VUV light; homochirality of life
- improving our understanding of the origins of the universe

Mode-selective control of chemical reactions

Desorption of hydrogen by resonant excitation of the Si-H vibrational stretch



Liu, Feldman, Tolk, Zhang and Cohen, Science **312** 1024, 2006



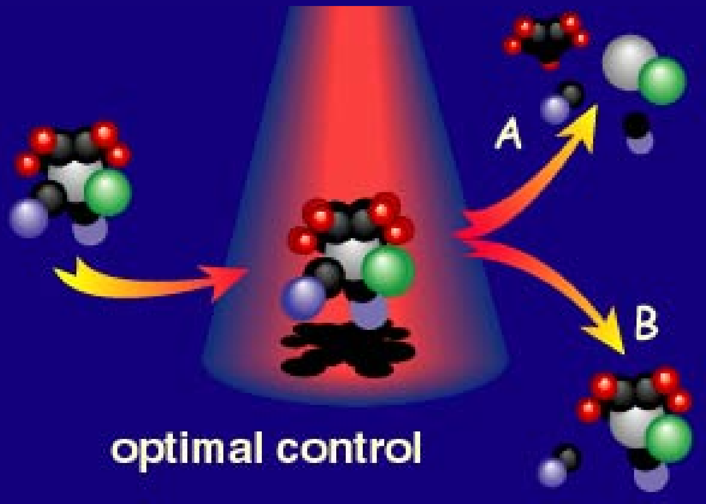
Reaction diverted from thermal pathway

Potential impact on:

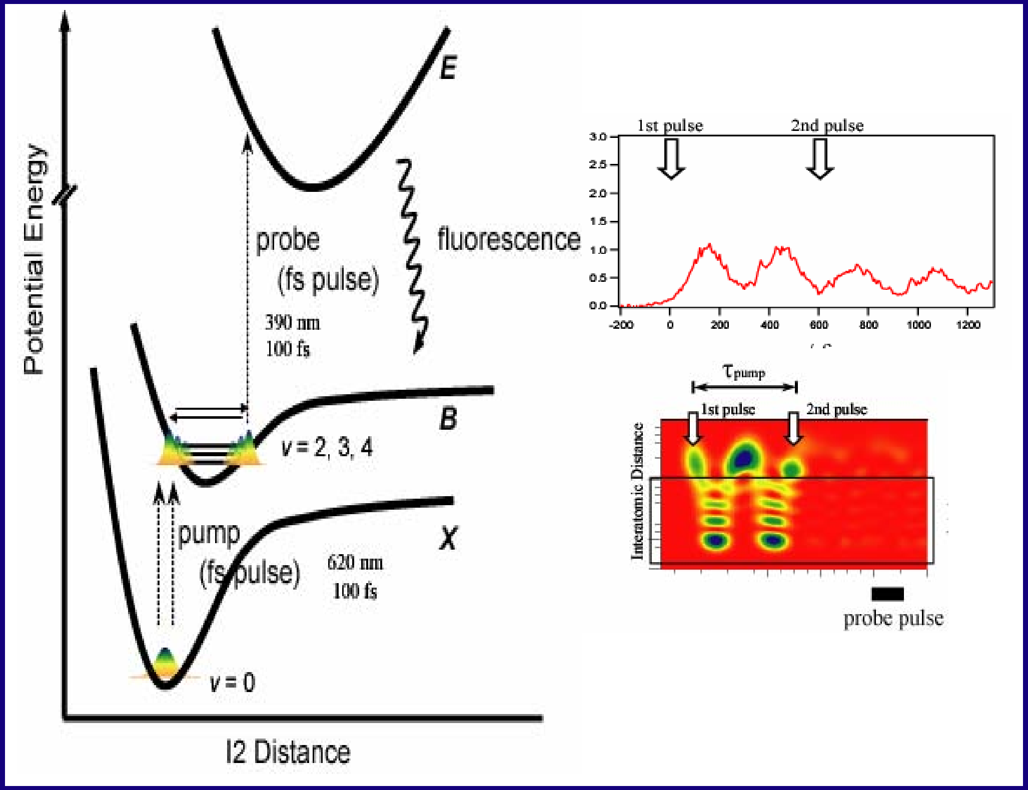
- the storage, transport and delivery of hydrogen for the hydrogen economy
- reactive chemistry on surfaces

Quantum chemical control

Quantum chemical control- using phase coherent double pulse sequences

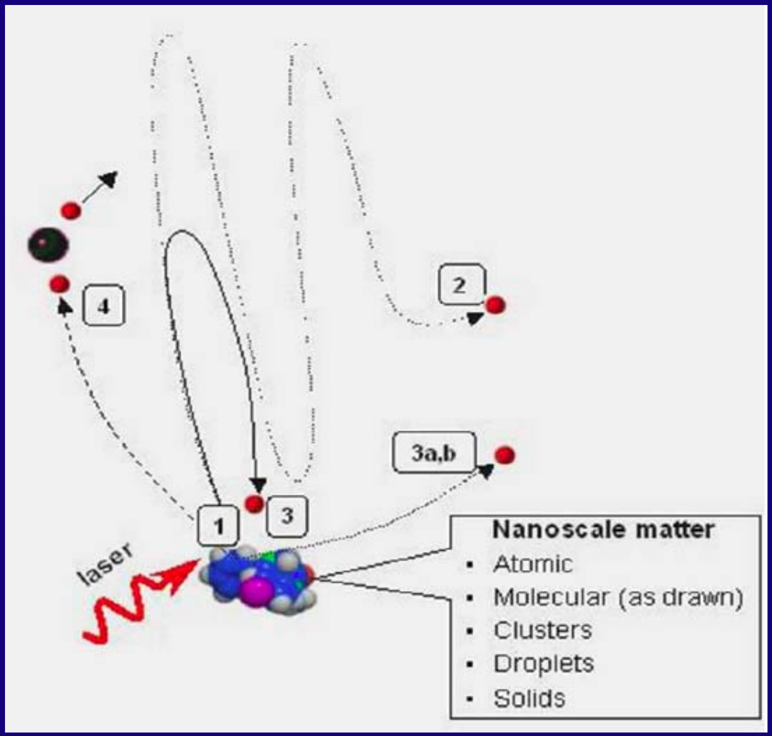


Can we ***control*** the direction of a chemical reaction?



First observation of real-time vibrational wavepacket interference Kiyoshi Ueda *et al.*,*PRL* **96** 093002 (2006)

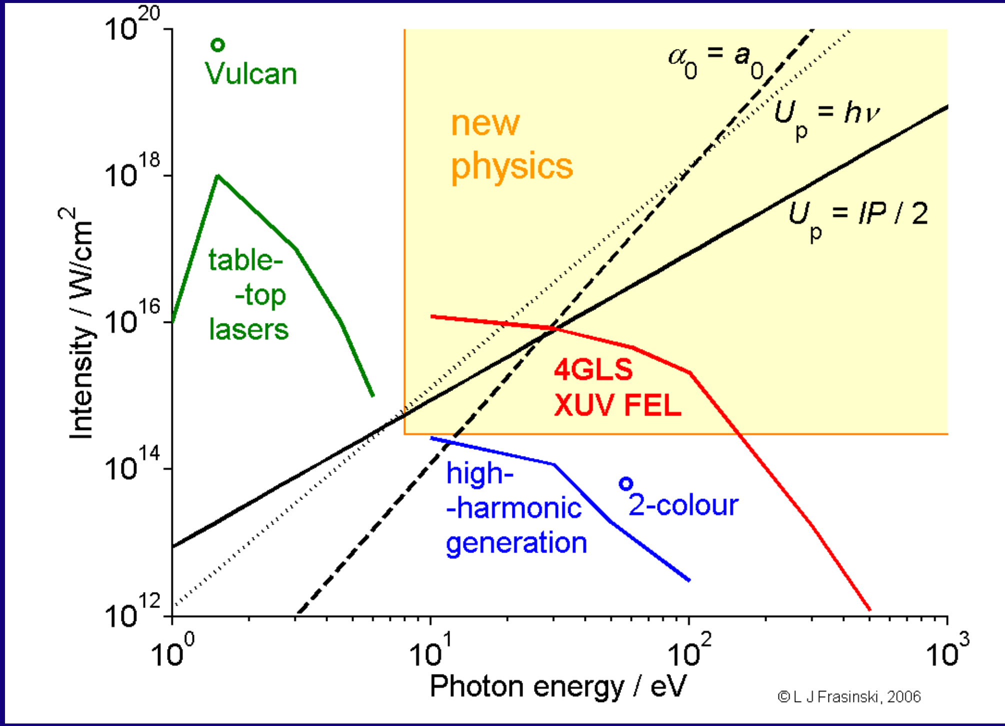
Atomic and molecular dynamics in uncharted territory………



Exploring the behaviour of atoms and molecules in high intensity, high frequency field regimes

XUV field intensities 10^{16} - 10^{17} Wcm^{-2}

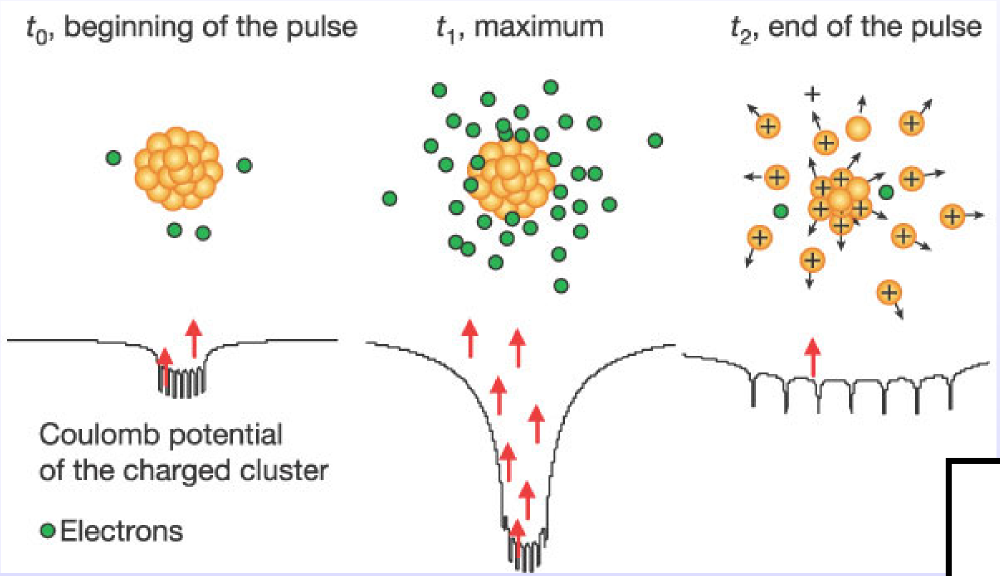
Providing data for new theory development



Can we understand electron correlation?

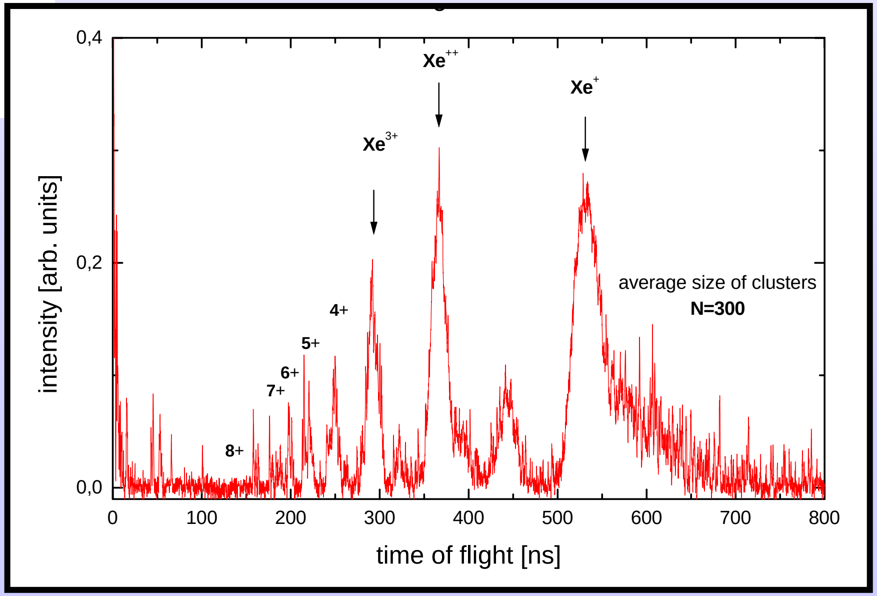
Leszek Frasinski, 2006

Multiphoton excitations of atoms, molecules, clusters…



- Coulomb explosions
- Tests of theory

Single shot time-of-flight spectrum

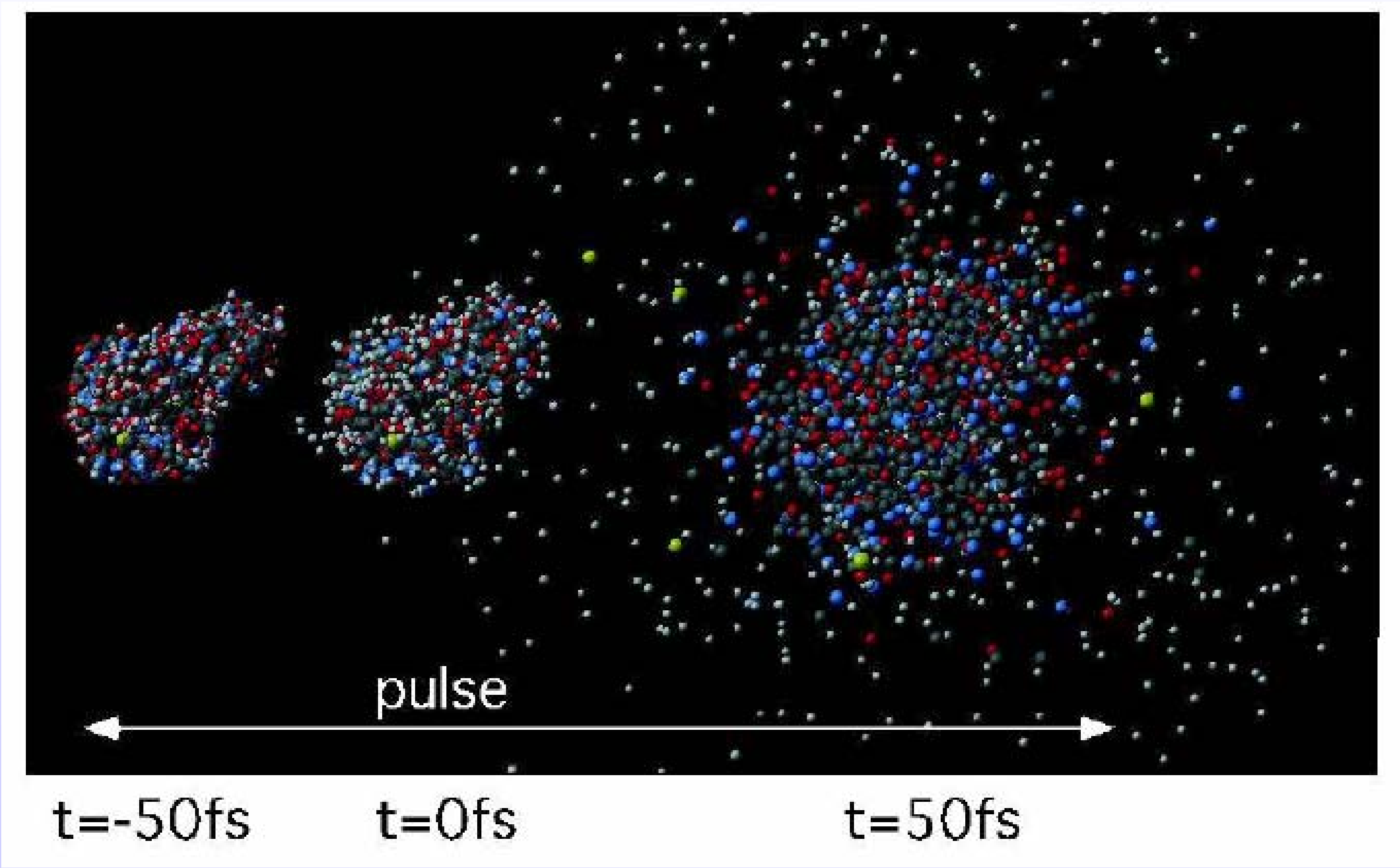


First results from FLASH show Xe clusters undergo a Coulomb explosion in the VUV at field intensities 10x lower than predicted by existing models

(H Wabnitz et al., *Nature*, **420**, 467, (2002), T Laarmann et al., *PRL*, **95**, 063402 (2005))

DESY: J Feldhaus

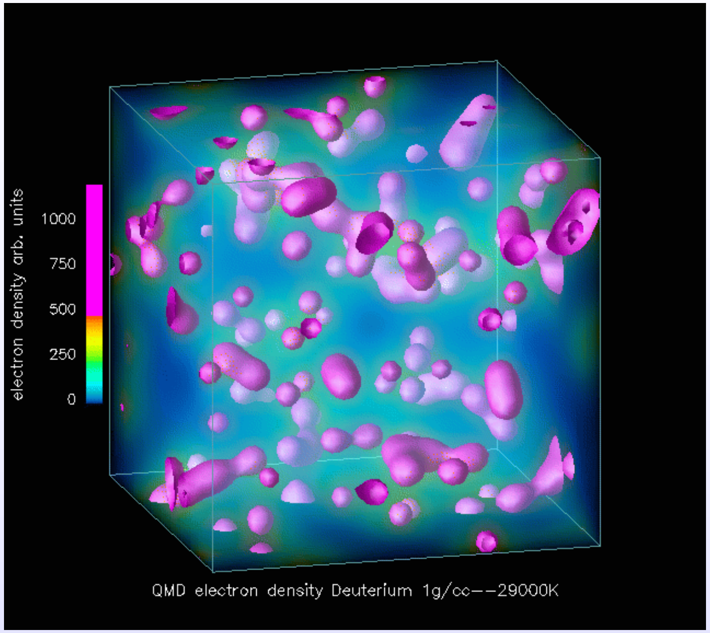
One-shot experiments!



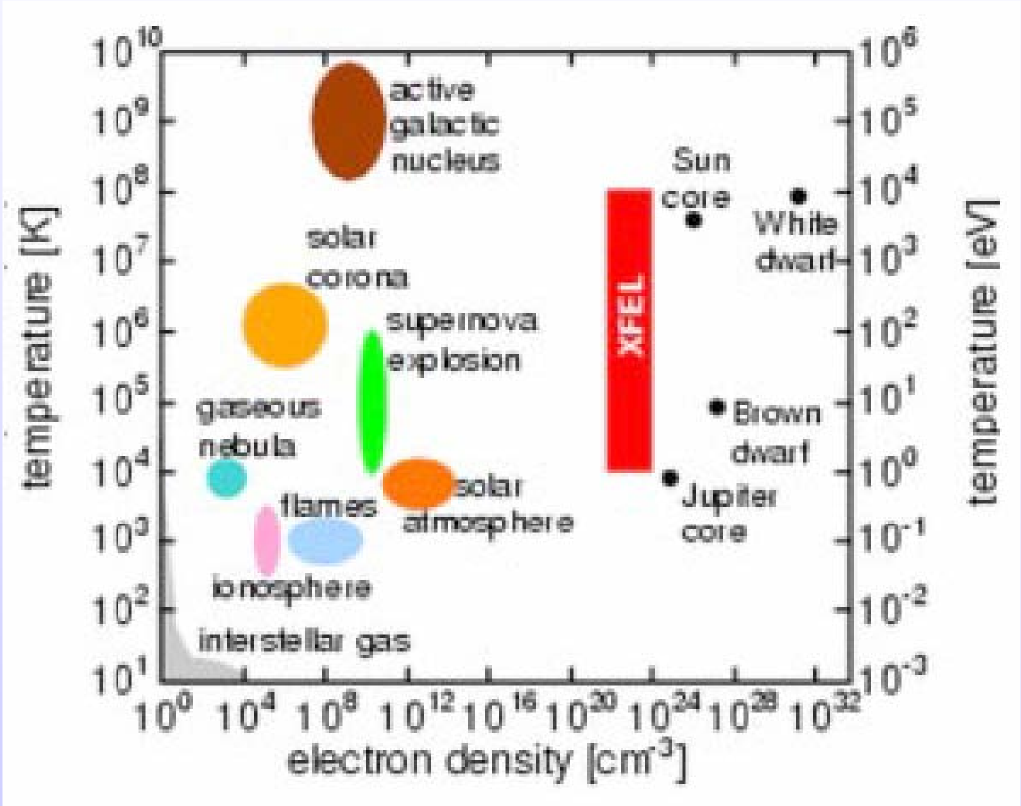
Simulated coulomb explosion of a T4 lysozyme molecule caused by a $3x10^{12}$ photon per $(0.1mm)^2$ pulse of X-rays

(Hajdu et al., *Nature*, **406,** 752, (2000), XFEL TDR 2nd draft 2006)

A tool for plasma physics



http://www.t4.lanl.gov/CECAM/

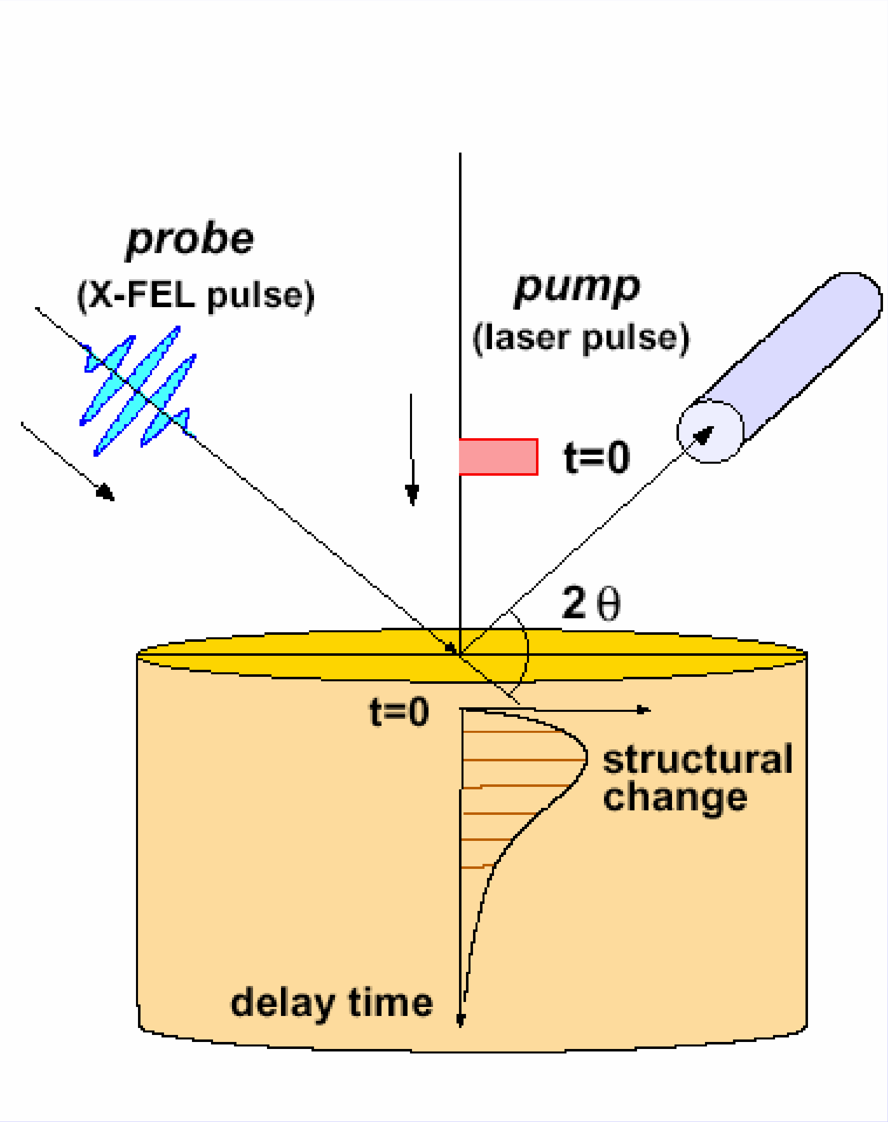


Density-temperature diagram for astrophysical objects

TESLA technical design report, March 2001

- Generation and study of extreme states of matter
- Temperatures up to 10^7 K
- Pressures up to Gbar
- Improved models of stellar formation
- Generation of dense plasmas
- Studies of warm dense matter

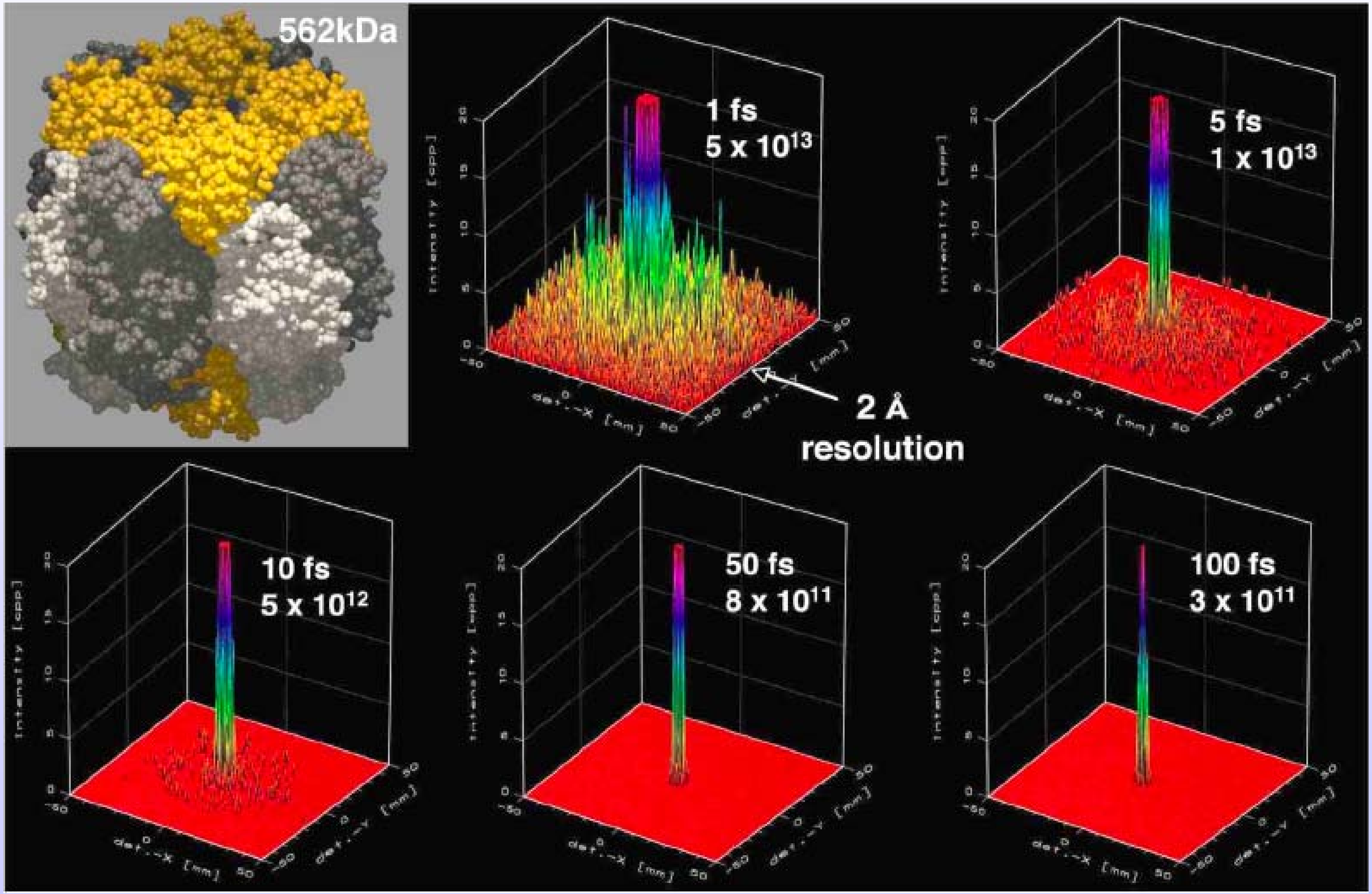
Time-resolved diffraction



TESLA technical design report, March 2001

- structural changes, phase transitions, irreversible changes, cluster vibrations
- via pump-probe approach
- e.g. surface melting transitions
- study the disorder emerging within 100 fs timescale

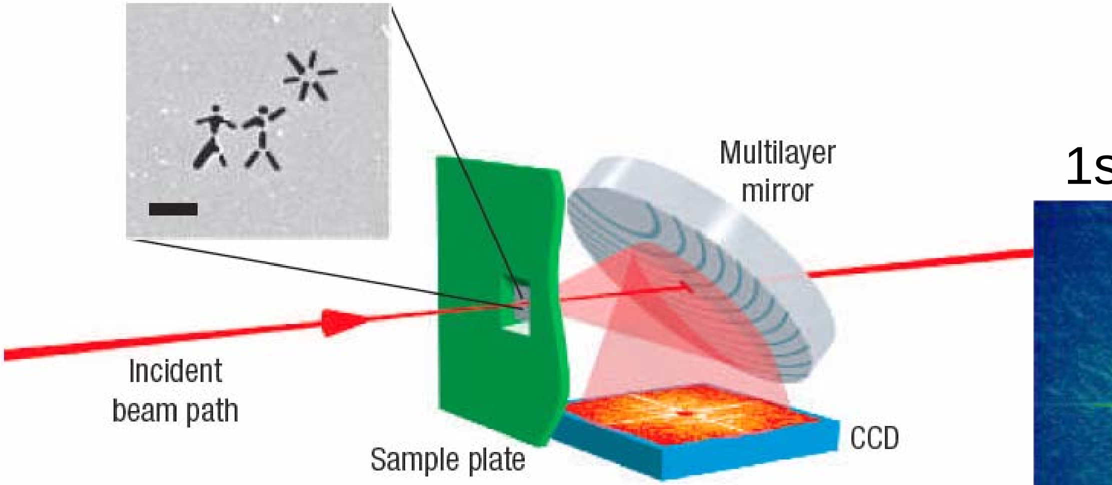
Single molecule diffraction



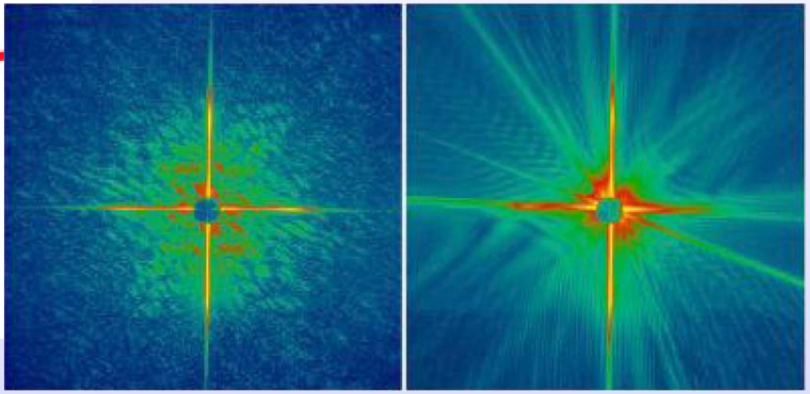
Calculated scattering patterns of a single large biomolecule, Rubisco, with 15% damage-induced errors

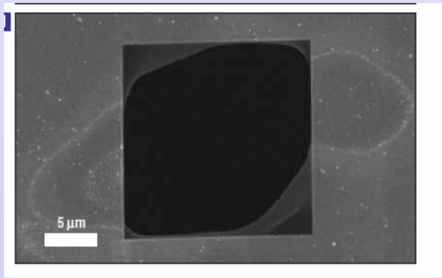
XFEL technical design report 2nd draft 2006

Diffractive imaging at FLASH

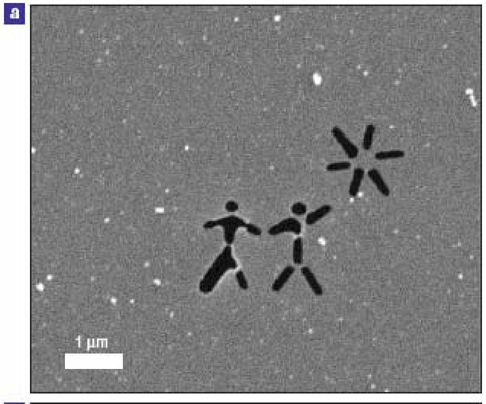


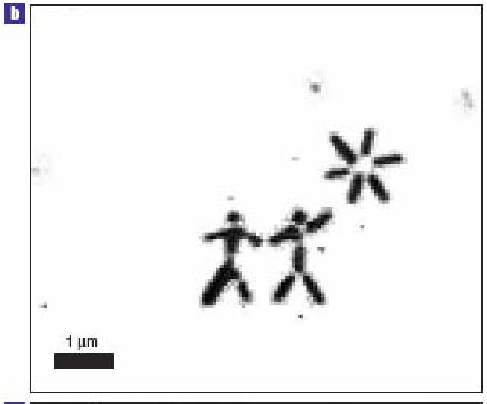
1st shot 2nd shot (20 s later)





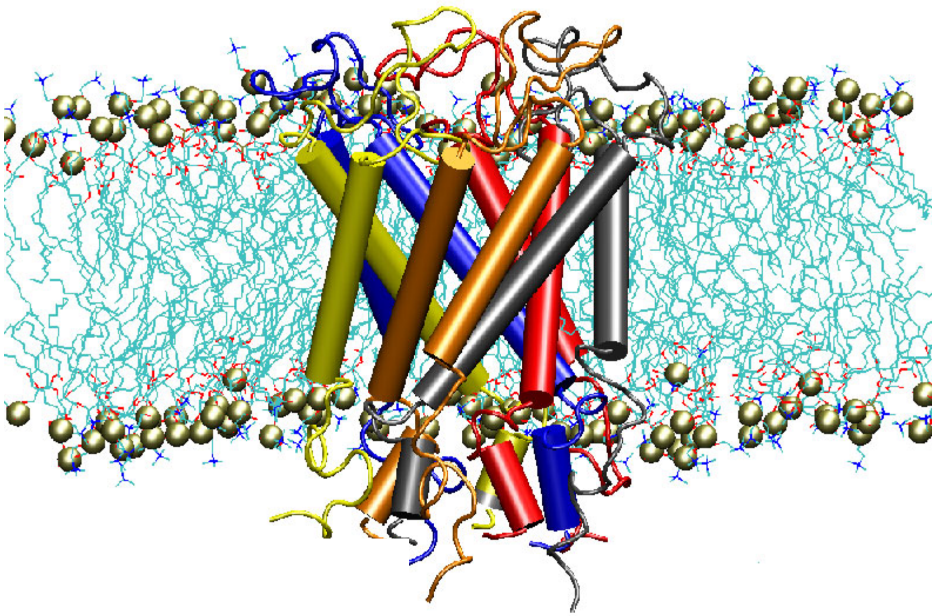
FLASH 32 nm, 25 fs, 4×10^{14} Wcm^{-2}, single shots, 3 µm structure on 20 nm-thick SiN film

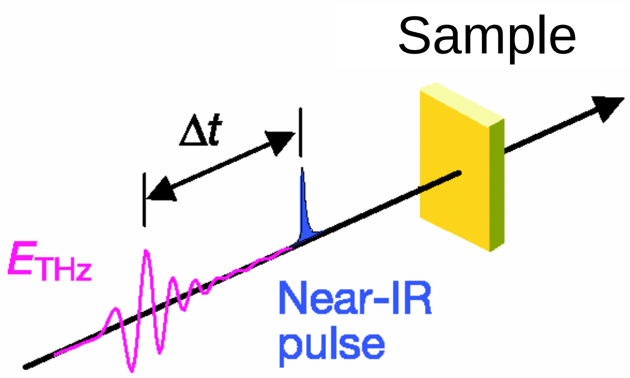




Chapman *et al.*, Nature Phys., 2, 839, (2006)

Function of biomolecules -membrane proteins



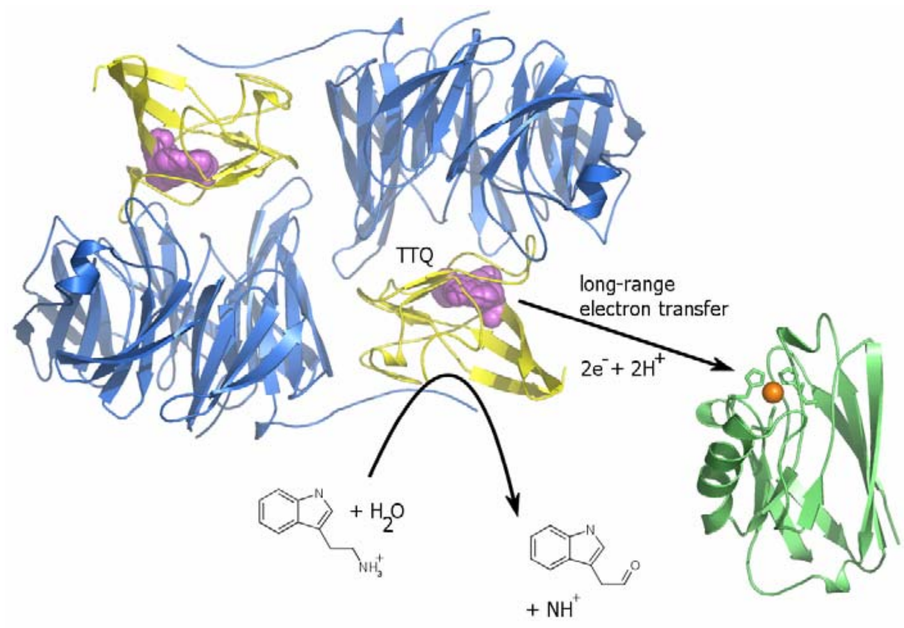


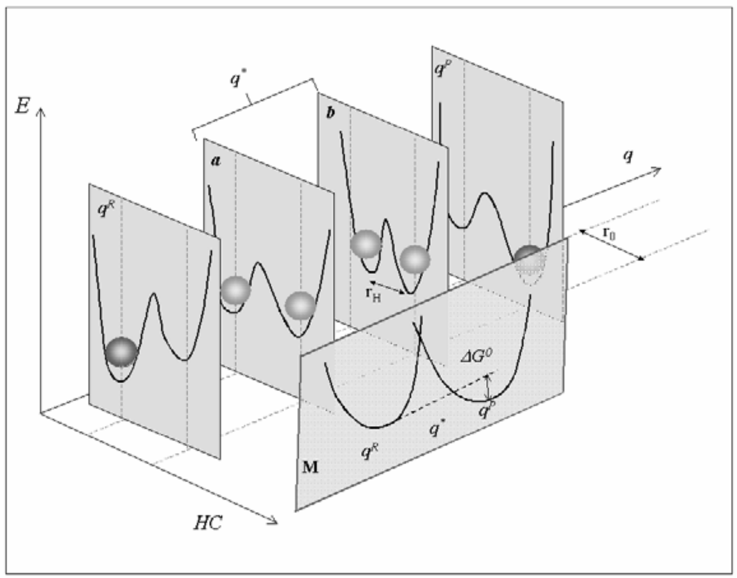
Can we measure the mechanisms of energy, electron, proton and chemical transport at the cell membrane ***in real time***?

How does energy transfer around a biomolecule and between a biomolecule and a substrate?

How do enzymes achieve high catalytic rates?

H-transfers can happen 10^{15} times faster than available theory predicts!





L Masgrau *et al*, Science, **321**, 237, (2006), Arch Biochem Biophys, **428**, 41, 2004)

Small-scale promoting vibrations/motions may promote H- and electron transfer by quantum tunnelling mechanisms.

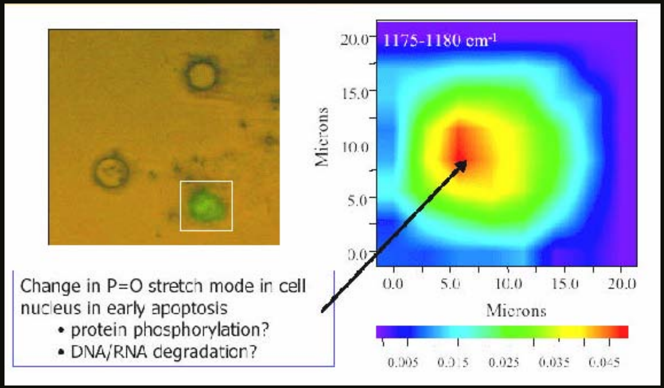
N Scrutton, M Sutcliffe, P Gardner, G Williams
EPSRC Life Science Interface funding

Human health

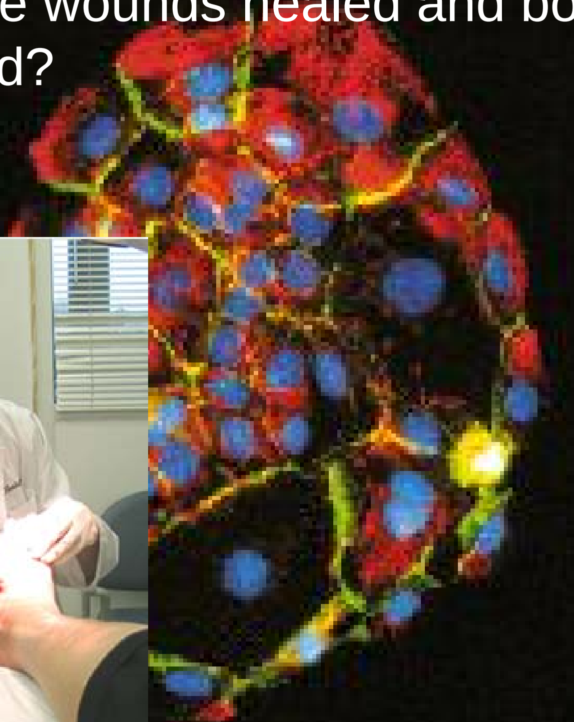
How do we diagnose disease (such as skin cancer) earlier and improve treatment?

How are cells damaged and repaired? How do cells signal in the extracellular matrix? What is the action of a drug?

How are wounds healed and bones repaired?

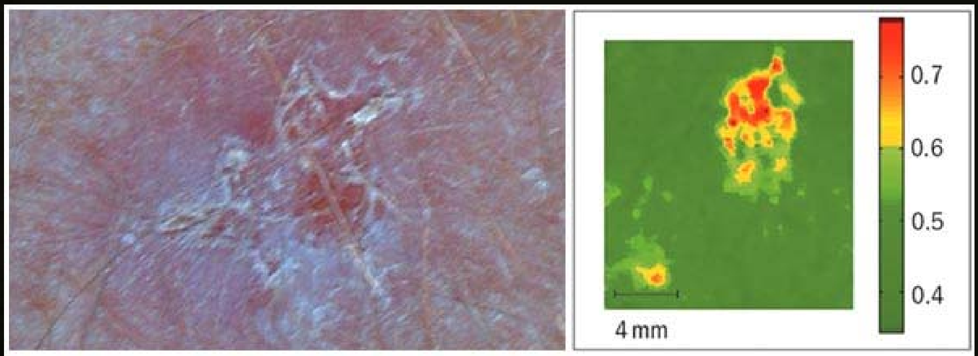


Cell changes during apoptosis (P Dumas, SR IR, LURE)



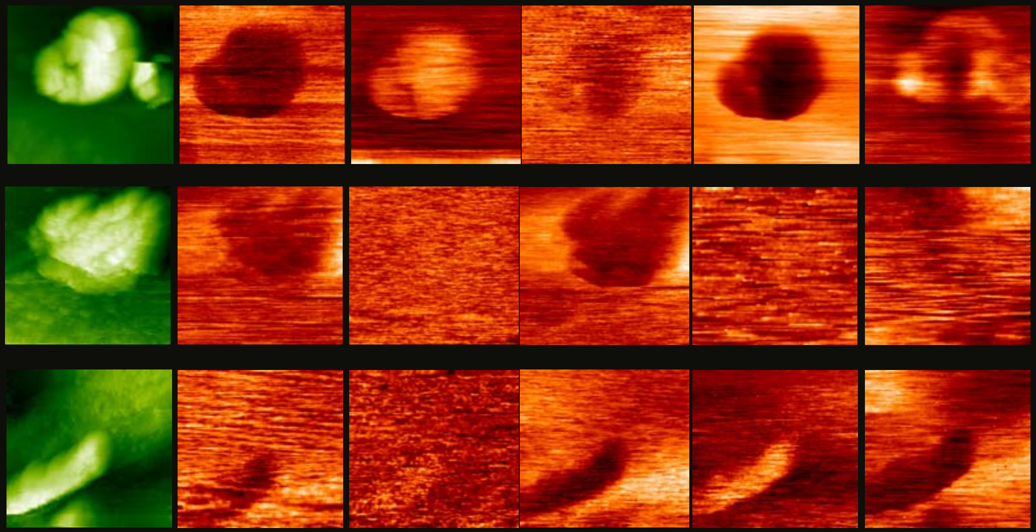
- Overcome diffraction limit using near-field imaging/IR FEL: 30-50 nm resolution

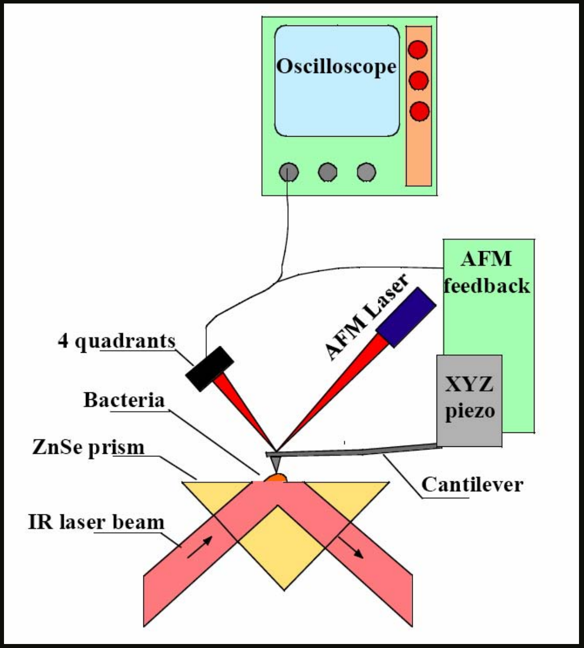
- ERLs are the world's most intense THz sources (10's W output)



THz diagnosis of basal cell carcinoma, Teraview

Breaking the diffraction limit; imaging at subcellular resolution with an IR FEL





Distribution of functional groups in a single cell
IR SNOM: resolution = $\lambda/30$

AFMIR: resolution = $\lambda/100$

A Dazzi *et al.*, Optics Letters, 30, 2388 (2005)

λ= **6.1 µm** amide C=O stretch band

λ= **6.45 µm** reflection of sulphur, key component of amino acids

λ= **6.95 µm** sulfide cell growth medium stretch band

λ= **7.6 µm** $-CH_3$ stretch band

λ= **8.05 µm** phosphorus stretch band, component of DNA and RNA

A Cricenti, Biophysical J., 85, 2705 (2003), Vanderbilt FEL

Understanding carrier dynamics - developing new nanodevices

What happens after CMOS?

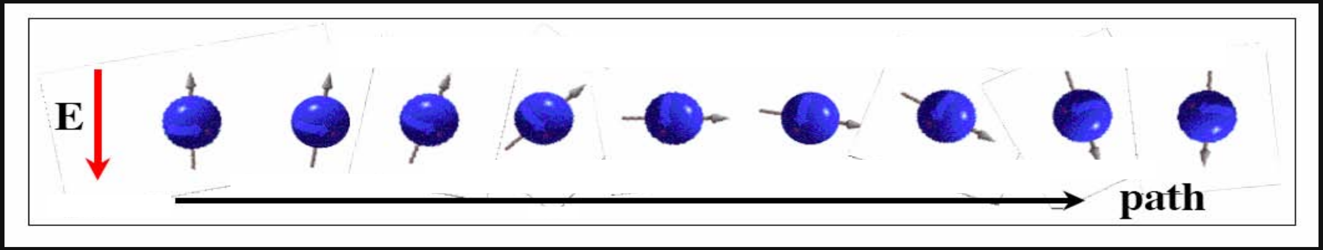
> *by 2010, there will be 21 atoms in the gate legs of a transistor*

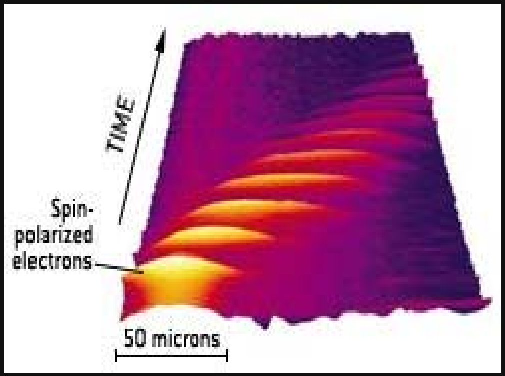
How do carriers ***move*** in devices?

> *we can no longer easily predict where they are*

How do we make more efficient optoelectronic nanomaterials, photovoltaics, high k dielectrics?

Understanding spin dynamics - spintronics





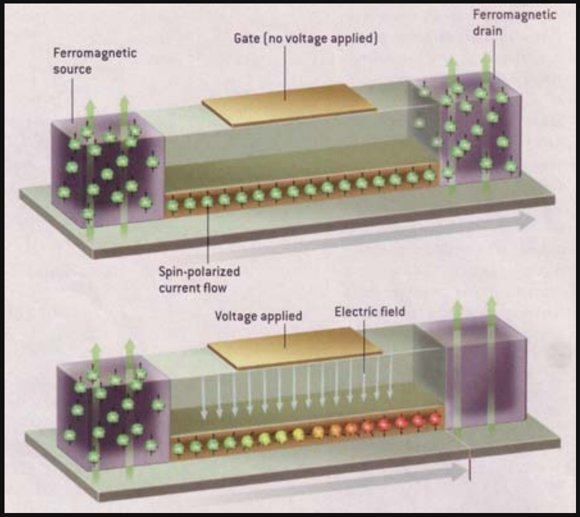
How do we combine semiconductor technology and magnetism?

How does electron spin transport across a boundary?

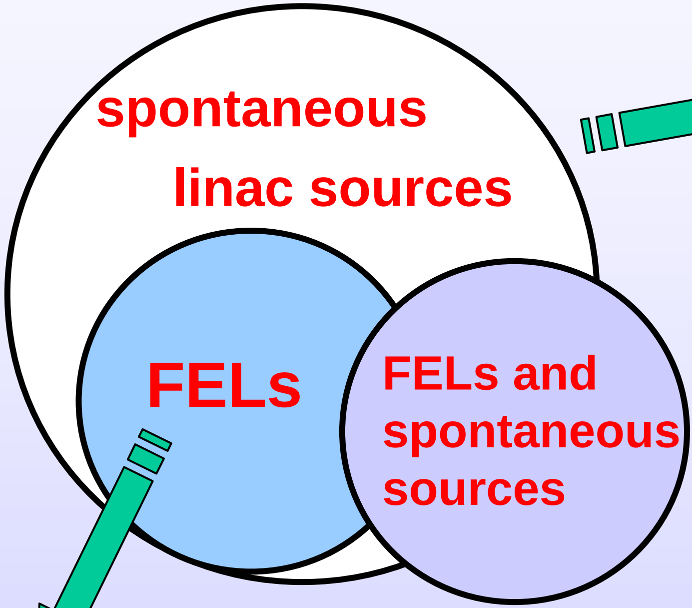
Can we manipulate spin on fast timescales?

Pools of spin polarised electrons in GaAs probed using 100 fs pulses of 1.5 eV CP light
(D D Awschalom *et al.*, *Scientific American*, **286**, 53, (2002))

Spin FET



SR&FEL: more than the sum of the parts



- dynamics of adsorbates, films & interfaces
- nondestructive biosystem dynamics
- ultra-high spectral resolution

+

- pump-probe
  FEL+ spontaneous SR (THz>)
- dynamics in nanoparticles and microdevices, spintronics
- energy transfer in biomolecules

+

- bio and chemical fs dynamics
- materials under extreme conditions
- nonlinear processes
- plasma physics
- nano spectromicroscopy
- nano electronic structure and magnetism

Summary

- **4th generation sources open up completely new science vistas**
  - *with huge potential for dynamics and imaging of nanoscale objects*

- **complementary to 3rd generation SR sources**
  - *primarily giving dynamic information, much higher brightness and shorter pulse length*

- **complementary to tabletop laser sources**
  - *superb coverage in THz, VUV, planned extensions to XUV and X-ray*

- **they bring together the SR and laser communities**
  - *resulting in a ferment of scientific excitement!*

- **we need talented accelerator scientists to deliver them**

Acknowledgments

- Elaine Seddon and other members of the 4GLS team
- Gwyn Williams, George Neil and colleagues at JLab
- Josef Feldhaus and colleagues at DESY
- Kiyoshi Ueda, Tohoku University
- Paul Dumas, SOLEIL
- Musa Ahmed, LBNL
- Anders Nilsson, SSRL
- Norman Tolk, Vanderbilt
- Nigel Scrutton, University of Manchester
- Antonio Cricenti, ISM-CNR Roma
- Jean-Michel Ortega, CLIO
- Michael Meyer, LIXAM/CNRS

4GLS: New Science with Next Generation Light
Friday 6th July 2007
STFC Daresbury Laboratory

Further information
http://www.4gls.ac.uk