Energy@Stanford & SLAC:

Photon Science 101

Tom Devereaux, Director
We face an energy crisis

• In the short term, technologies/viewpoints need to be changed/improved.

• History is replete with examples where basic research produced results that greatly impacted our world (transistor, internet, etc).

“...I might have claimed that I had come to the conclusion... that valuable anti-microbial substances were made by moulds, and that I set out to investigate the problem. That would have been untrue, and I preferred to tell the truth that penicillin started as a chance observation. My only merit is that I did not neglect the observation and that I pursued the subject...” ~ Alexander Fleming, accepting the 1945 Nobel Prize for his discovery of penicillin.

Whenever you find yourself on the side of the majority, it is time to pause and reflect.
~Mark Twain
Last Weekend, Half of Germany Was Running on Solar Power

Brian Merchant
Energy/Energy Policy
May 28, 2012

Solarstromanlagen seit 2006 rund 65% günstiger

Sustainable Energy Enabling Technologies: The Grid

breakthroughs needed
long distance reliable, efficient delivery of electricity
Energy density: apply new paradigms
We face an energy crisis

In the long term, we will solve this crisis by inventing new technologies. SIMES conducts the basic materials science research needed to discover technological solutions to today’s energy generation, storage, and transmission problems.

• **Superconductivity**: carry electricity at without resistance for $10^3$ kilometers.

• **Nano-design**: increase battery storage beyond doubling current Li-ion technologies.

• **Photon harvesting**: construct cheap and environmentally-friendly solar cells to be economically competitive with coal.
What is Photon Science?

How light interacts with matter to answer questions of what things are and how and why they work.

Photon science drives discoveries across a diverse range of fields including biology, chemistry, communications, medicine, physics, astronomy, engineering and materials science.

Examples:
* **Medicine**: shining a laser beam into a finger to detect the amount of blood sugar in a patient's blood without having to take a blood sample.

* **Manufacturing**: discovering faults in the structure of an aircraft well before the plane becomes unsafe.
Impact of x-rays on science

X-rays were discovered by Wilhelm Conrad Röntgen in 1895.

Nobel Prizes Based on X-ray Work

**CHEMISTRY:**
- 1930: Peter Debye
- 1962: Max Perutz & Sir John Kendrew
- 1964: Dorothy Hodgkin
- 1976: William Lipscomb
- 1985: Herbert Hauptman & Jerome Karle
- 1988: Johann Deisenhofer, Robert Huber & Hartmut Michel

**PHYSICS:**
- 1910: Wilhelm Röntgen
- 1917: Charles Barkla
- 1924: Karl Manne Siegbahn
- 1927: Arthur Compton
- 1931: Kai Siegbahn

**MEDICINE:**
- 1946: Hermann Joseph Muller
- 1962: Francis Crick, James Watson & Maurice Wilkins
- 1979: Allan Macnab & Sir Geoffrey N. Hounsfield
Where are the atoms? What is the structure?

Electron Diffraction:

\[ 2d \sin(\theta) = n\lambda \]

Von Laue developed a law that connects the scattering angles and the size and orientation of the unit-cell spacings in the crystal, for which he was awarded the Nobel Prize in Physics in 1914.

Can locate every atom
X-ray crystallography: workhorse

The three-dimensional structure of penicillin, for which Dorothy Crowfoot Hodgkin was awarded the Nobel Prize in Chemistry in 1964.

The green, white, red, yellow and blue spheres represent atoms of carbon, hydrogen, oxygen, sulfur and nitrogen, respectively.
X-ray crystallography: proteins
Many Photon Spectroscopies: where are the electrons, what happens during photoexcitations?

Photoemission (PES, XPS) – measures occupied density of states

Absorption (XAS) – measures unoccupied density of states

X-ray Light Scattering – measures order, excitations & dynamics

Technique

(A) $h\nu_i \Psi_N \rightarrow h\nu_i + \Psi_{N+1} + e$

(B) $h\nu_i \Psi_N \rightarrow h\nu_i + \Psi_N$

(C) $h\nu_i \Psi_N \rightarrow h\nu_i + h\nu_s$
Developing high-performance batteries with the aid of soft x-ray spectroscopy

- **Synthesis/Manufacture**

  - Low-cost Anode: 7X energy capacity than currently used graphite anodes
  - **Soft X-ray spectroscopy** shows WHY the material works and HOW to optimize
  - Patent (US2010/035120) licensing towards 3 major US companies already

Theoretical Simulations

- **PFFO**
  - Anode Capacity (mAh/g)
  - Battery Cycle Number

- **State-of-the-art Graphite Anode**

- **Soft X-ray Spectroscopy**

  - Key Function Group
  - Key Electron State!
As the crystal's repeating unit, its unit cell, becomes larger and more complex, the atomic-level picture provided by X-ray crystallography becomes less well-resolved (more "fuzzy") for a given number of observed reflections.

If we want to have a closer look at smaller objects, or if we want to find out what the electrons are doing in operando, we need more photons!
Some Stanford History:

E. A. Muybridge
LCLS – a new era of science

- coherent x-ray imaging, pump-probe, femto-chemistry...
- "First light", April 2009
LCLS – a perspective of scales

• it's bright (8 orders of magnitude)
LCLS – a perspective of scales

• it’s bright (8 orders of magnitude)
• it’s small (1.5 Angstroms)

STM image of NaCl (3.9 nm x 3.9 nm) Omicron

Capture dynamics at these small lengthscales
LCLS – a perspective of scales

• it’s bright (8 orders of magnitude)
• it’s small (1.5 Angstroms)
• it’s fast (10 femtoseconds or less)

Time for light to travel to the moon and back –
LCLS – a perspective of scales

- it’s bright (8 orders of magnitude)
- it’s small (1.5 Angstroms)
- it’s fast (10 femtoseconds or less)

Time for light to travel to the moon and back – 2.4 seconds.

Distance light travels in 100 femtoseconds
LCLS – a perspective of scales

- it’s bright (8 orders of magnitude)
- it’s small (1.5 Angstroms)
- it’s fast (10 femtoseconds or less)

Time for light to travel to the moon and back – 2.4 seconds.

Distance light travels in 100 femtoseconds – width of a human hair.

Capture dynamics at these small timescales.
LCLS – a perspective of scales

- it’s bright (8 orders of magnitude)
- it’s small (1.5 Angstroms)
- it’s fast (10 femtoseconds or less)
- it’s powerful (mJ/pulse = 10 Gwatts)
LCLS – a perspective of scales

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LCLS – Probing the ultrasmall & ultrafast

**Ultra-Fast**
- **Nature**: Hydrogen Transfer Time in Molecules is $\sim 1$ ns
- **Technology**: Magnetic Recording Time per Bit is $\sim 2$ ns
- **LCLS Operating Range**: Shortest Laser Pulse is $\leq 1$ fs

**Ultra-Small**
- **Nature**: Flea, Red Blood Cells, Virus, Water Molecule
- **Technology**: Pin Head, Micro Gears, DVD Tracks, Carbon Nanotube

**Time Scale**:
- $10^{-15}$ s to $10^{-9}$ s
- $10^{-3}$ m to $10^{-6}$ m
LCLS: Results

Protein Structure for Photosystem 1 used during photosynthesis

Imaging a Mimivirus

Creating 2,000,000 °C plasma

Molecular structure of proteins as measured by X-ray Patterns
Extending RXS into the time domain

Resonant Ni L-edge doped nickelates
Soft x-ray beamline at the Linac Coherent Light Source @
Energy Research: examine paradigms

Stanford-SLAC team uses X-ray imaging to observe running batteries in real time

Scientists at Stanford and SLAC are using X-ray technology to observe lithium-sulfur batteries in action. Their findings could lead to improvements in this promising power source for electric vehicles.

BY MARK SHWARTZ

Most electric cars, from the Tesla Model S to the Nissan Leaf, run on rechargeable lithium-ion batteries – a pricey technology that accounts for more than half of the vehicle's total cost. One promising alternative is the lithium-sulfur battery, which can theoretically store five times more energy at a much lower cost.

But lithium-sulfur technology has a major drawback: After a few dozen cycles of charging and discharging, the battery stops working.

"The cycle life of lithium-sulfur batteries is very short," said Johanna Nelson, a postdoctoral scholar at the SLAC National Accelerator Laboratory at Stanford University. "Typically, after a few tens of cycles the battery will die, so it isn't viable for electric vehicles, which require many thousands of cycles over a 10- or 20-year lifetime."
Ultrafast Materials Science

Research to expand our understanding of chemistry and materials sciences by allowing stroboscopic investigations of the earliest stages of dynamic phenomena.

~10-100 fs pulses are short enough to resolve processes at the fundamental timescales of electronic and nuclear motion allowing for the discrimination of different dynamics.

Understanding the interplay between atomic and electronic structure
- Beyond single-electron band structure model: correlated systems (charge, spin, orbit, lattice)
- Beyond simple adiabatic potential energy surfaces
- Competing order parameters

Understanding the nature of quasiparticles
- Formation dynamics, scattering processes, relaxation channels and dynamics

Creating new states of matter
- Photoinduced phase transitions—fast switching, probing dynamics where the order parameter has been perturbed, creating nonthermally accessible phases.

Source: D. Basov
Energy Research: apply new paradigms

Organic Solar Cells
- Low-cost, high-volume production

- 1D channels for electrons
- Insulating side chains
- 2D sheets for holes

Photon Enhanced Thermionic Emission for Solar Concentrators
- Use entire solar spectrum: PV + thermal

High-capacity batteries
- Use Si nanowires as anode material to yield 10-fold increase over carbon

Efficient 1D electron transport
Good contact with current collector
Facile strain relaxation
Thank you.
Some Stanford History:

SSRL (1973) – first GeV storage ring


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