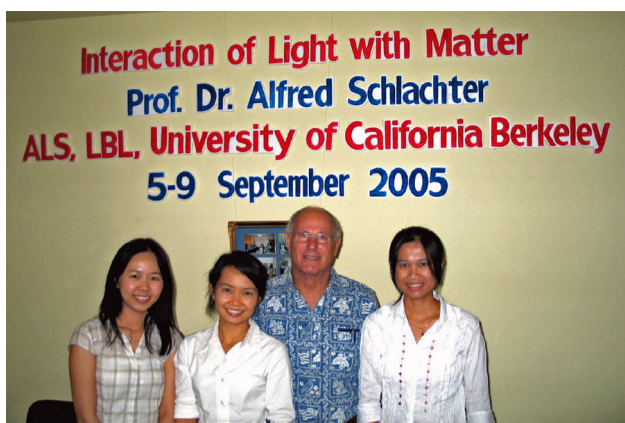
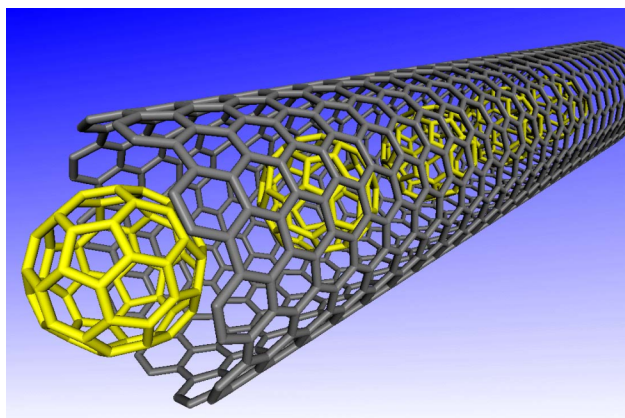
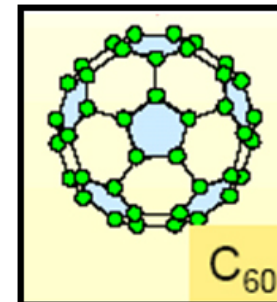


# Making buckyballs ring: collective electron motion in a $C_{60}$ molecule.

Shining light from an ultrabright synchrotron light source on a unique nanomaterial



**Dr. Fred Schlachter**

Lawrence Berkeley National Laboratory

American Physical Society

Chiang Mai University



ดร. เฟรด ชลัคเทอร์

อาจารย์พิเศษ

ภาควิชาฟิสิกส์

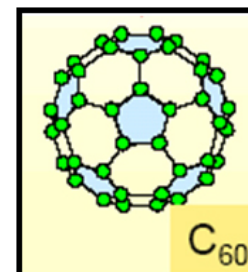
มหาวิทยาลัยเชียงใหม่

ศูนย์ปฏิบัติการวิจัยแห่งชาติ

ลอเรนซ์ เบิร์คเลย์

(Lawrence Berkeley National Laboratory)

## Collective electron motion in C<sub>60</sub>



*Absorption of photons from an ultrabright beam of synchrotron radiation illuminates new excitation and ionization processes in the C<sub>60</sub> molecule*

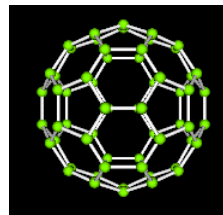
Bridging the gap between atoms and bulk matter.

- Photoionization cross sections are measured for photoionization of C<sub>60</sub><sup>+</sup>.
- Two “plasmon” resonances indicating **collective electron motion** are observed, similar to collective resonances found in nuclear and plasma physics.
- *It is remarkable to find this manifestation of bulk matter in a molecule with only 60 atoms, likely due to the special shape of the C<sub>60</sub> molecule: a hollow conducting sphere.*

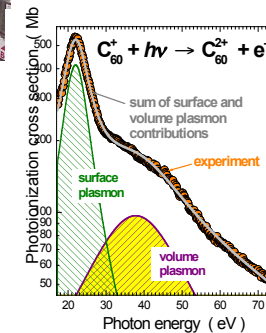
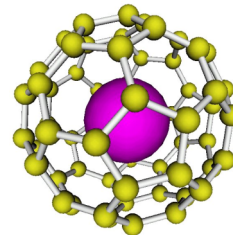
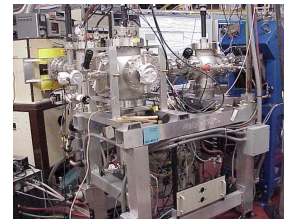
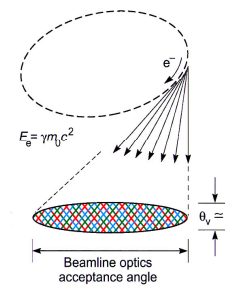


# Collective electron motion in C<sub>60</sub>: outline

- approach
- producing an ultrabright beam of x rays
- carbon in its various forms
- measurement of photoionization of ions
- collective motion of electrons in C<sub>60</sub>
- endohedral atoms
- photoionization of ions...



Bend-Magnet Radiation



Looking for macroscopic (bulk) effects at the nano-level of matter.

## Collective electron motion in $C_{60}$ : approach

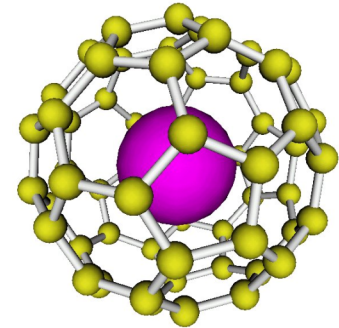
Look for **collective motion of electrons** in a large molecule

Collective motion is usually a characteristic of large systems (plasma, metal)

Example: collective motion of water in a bowl being tipped back and forth -> normal mode of motion

Study by looking for resonances leading to ionization

Perform experiment with **ion beam** rather than with gas target; 239 or 240 valence electrons behave the same.



Water sloshing in bowl: collective motion of water molecules.

# X rays and science

Photons interact selectively with electrons bound in matter.

X rays allow study of the **electronic structure of matter**, seeing inside objects, and determination of spatial structure of small objects. There are uses in many fields of science.

Periodic Table of Elements

Key:

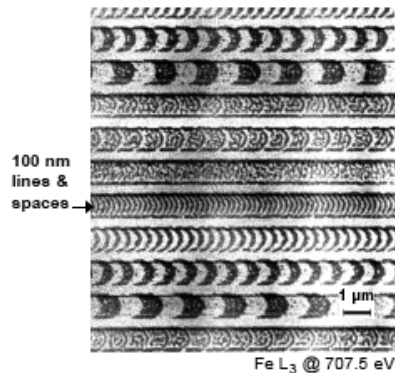
- Atomic number
- Atomic weight
- Symbol
- Electron configuration
- Group
- Period
- Block
- State
- Color
- Radioactivity

References: International Union of Pure and Applied Chemistry (IUPAC), London, 1993 (Ref. 44)

Lanthanide series

Actinide series

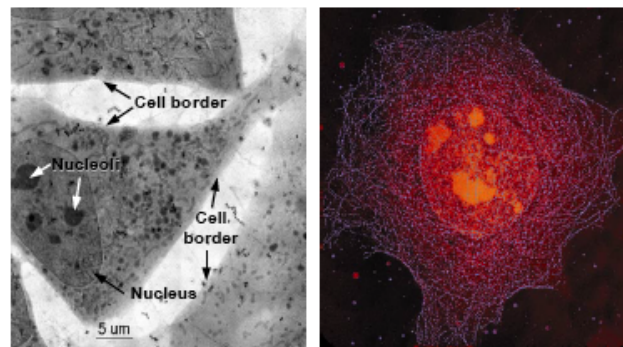
Magnetic Recording Materials



FeTbCo Multilayer with AL Capping Layer

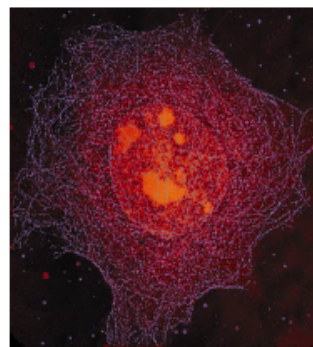
Courtesy of P. Fischer, Wuerzburg and G. Denbeaux, CXRO/LBNL

Cryo Microscopy for the Life Sciences

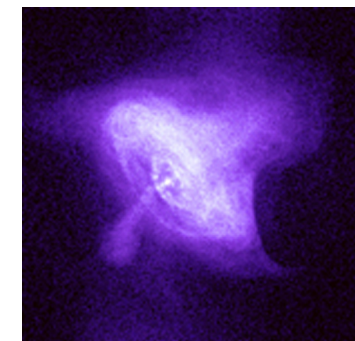
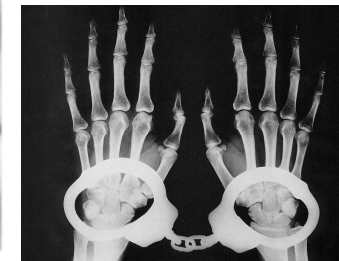


Cryo X-Ray Microscopy of 3T3 Fibroblast Cells

Courtesy of C. Larabell, UCSF and W. Meyer-Illse, CXRO/LBNL



Protein Labeled Microtubule Network



# Spectrum of electromagnetic radiation



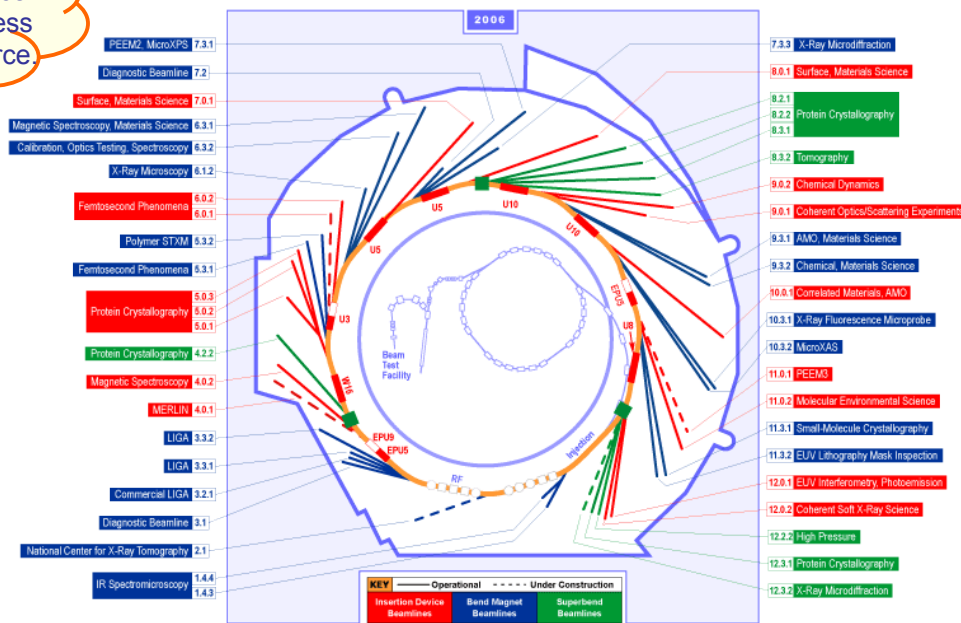
VUV and soft-x-ray regions of the spectrum



# Lawrence Berkeley National Laboratory



Advanced Light Source:  
an ultra-high-brightness  
synchrotron light source.



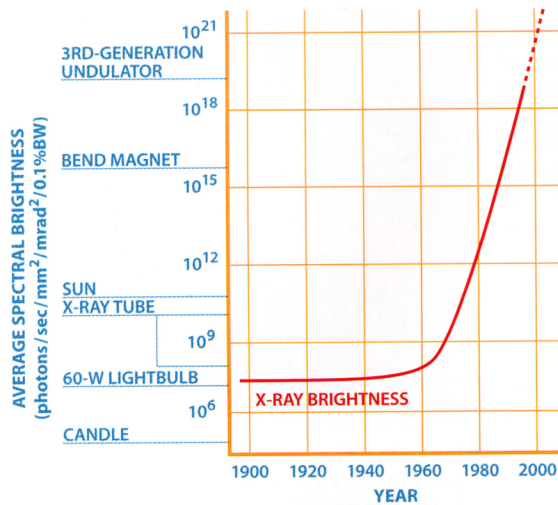
**BERKELEY LAB**

**A PLACE OF WONDER**



# Brightness: photon flux density in phase space

The brightness of x-ray beams has increased even faster than Moore's Law in the past forty years.



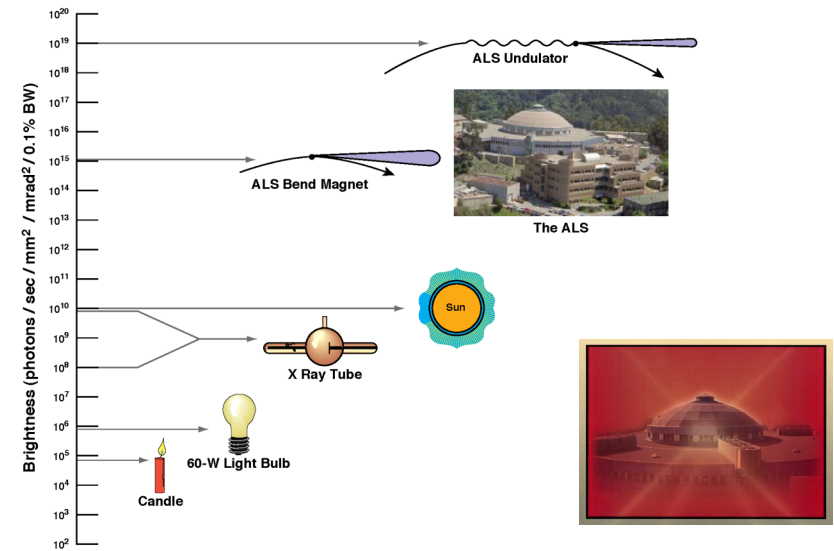
**Brightness:** photons/second/cm<sup>2</sup>/solid angle/bandwidth

*Meaning* lots of photons in a narrow monochromatic beam with small spatial divergence.

Altarelli, Schlachter, and Cross  
*Scientific American* December 1998

**Radiation a billion times brighter than the sun's is produced by an undulator at the ALS.**

ALS



dd.fs/how\_bright/3-99

## Making Ultrabright X-rays

*Radiation a billion times brighter than the sun's is illuminating a host of scientific and technical phenomena*

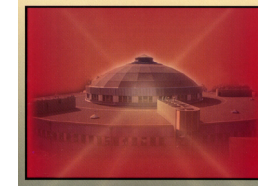
by Massimo Altarelli, Fred Schlachter and Jane Cross

DECEMBER 1998 • VOLUME 279 NO. 6 • PAGES 66 THRU 73

SCIENTIFIC  
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**Brightness:**  
photon flux density in phase space

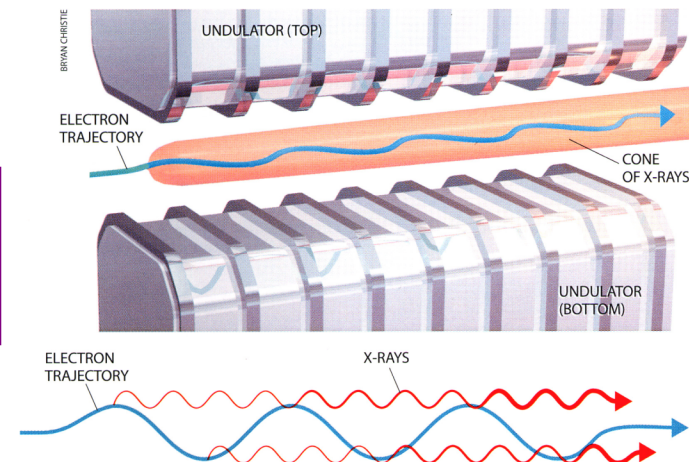


**Brightness:** photons/second/cm<sup>2</sup>/solid angle/bandwidth

*Meaning* lots of photons in a narrow monochromatic beam with small spatial divergence.

Producing a high-brightness photon beam requires a very small source size and small angular divergence of the electron beam....plus an undulator.

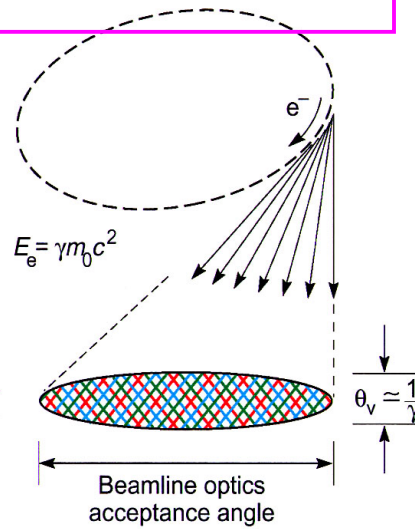
A high-brightness photon beam with tunable photon energy is produced by an undulator: a spatially alternating magnetic array.



# ALS has bend magnets and undulators

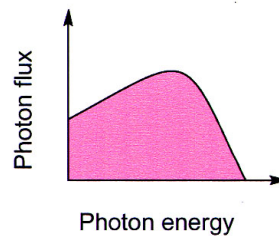


## Bend-Magnet Radiation

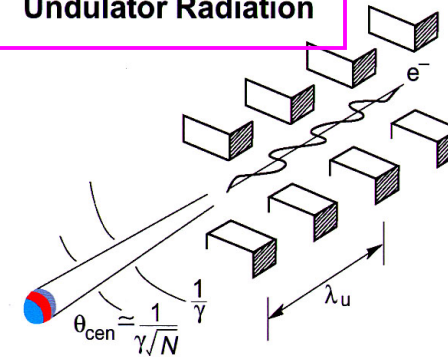


Spatial distribution of radiation

Spectral distribution of radiation



## Undulator Radiation

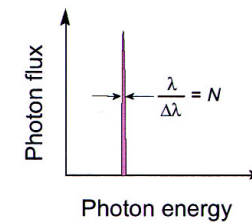


$$\lambda_x = \frac{\lambda_u}{2\gamma^2} \left( 1 + \frac{K^2}{2} + \gamma^2 \theta^2 \right)$$

In the central radiation cone:

$$\frac{\Delta\omega}{\omega} \approx \frac{1}{N}$$

$$\theta_{cen} \approx \frac{1}{\gamma\sqrt{N}}$$



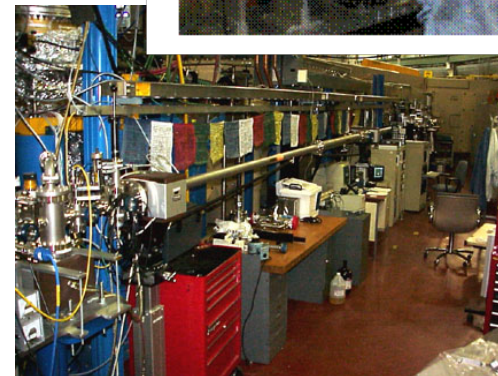
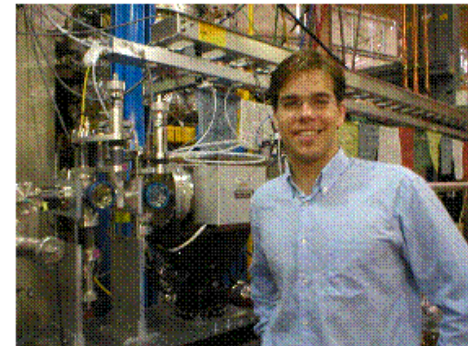
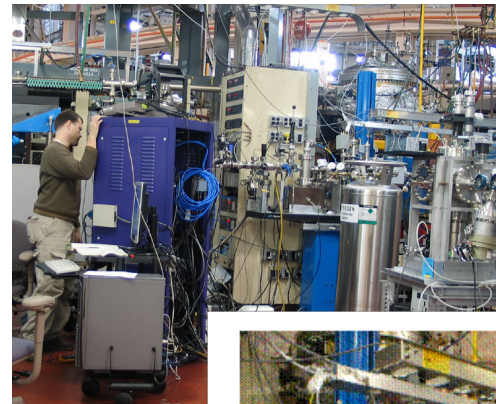
# Properties of synchrotron radiation



## Properties of synchrotron radiation

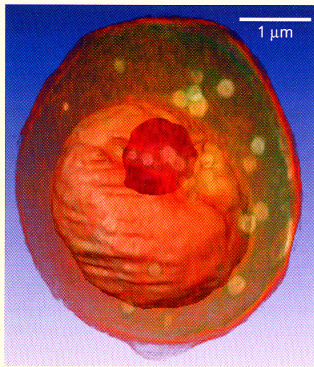
- Continuous spectrum
- Tunable monochromatic radiation
- High brightness (radiation in a narrow cone)
- Polarization control (linear, circular)
- Time-pulse structure
- Partially coherent

**X rays interact selectively with electrons in matter.** This allows elemental and chemical sensitivity. The short wavelength allows seeing small features.



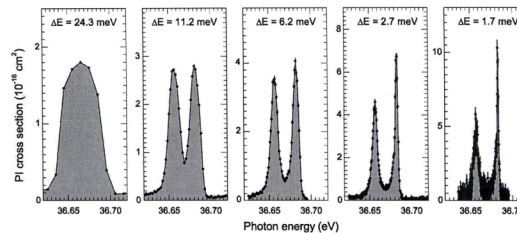
# A high-brightness light source provides small photon spot

Microscopy and  
nanoscience



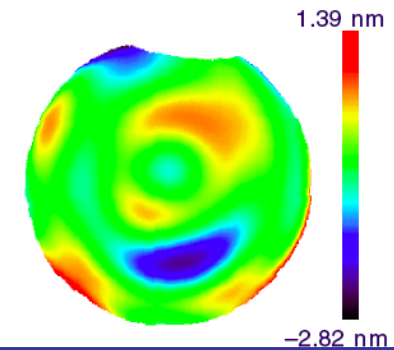
Enabling progress in nanoscience  
and new microscopies

High-resolution  
spectroscopy



Enabling researchers to learn  
in detail about the  
elemental, chemical, and  
magnetic structure of matter

Coherent radiation

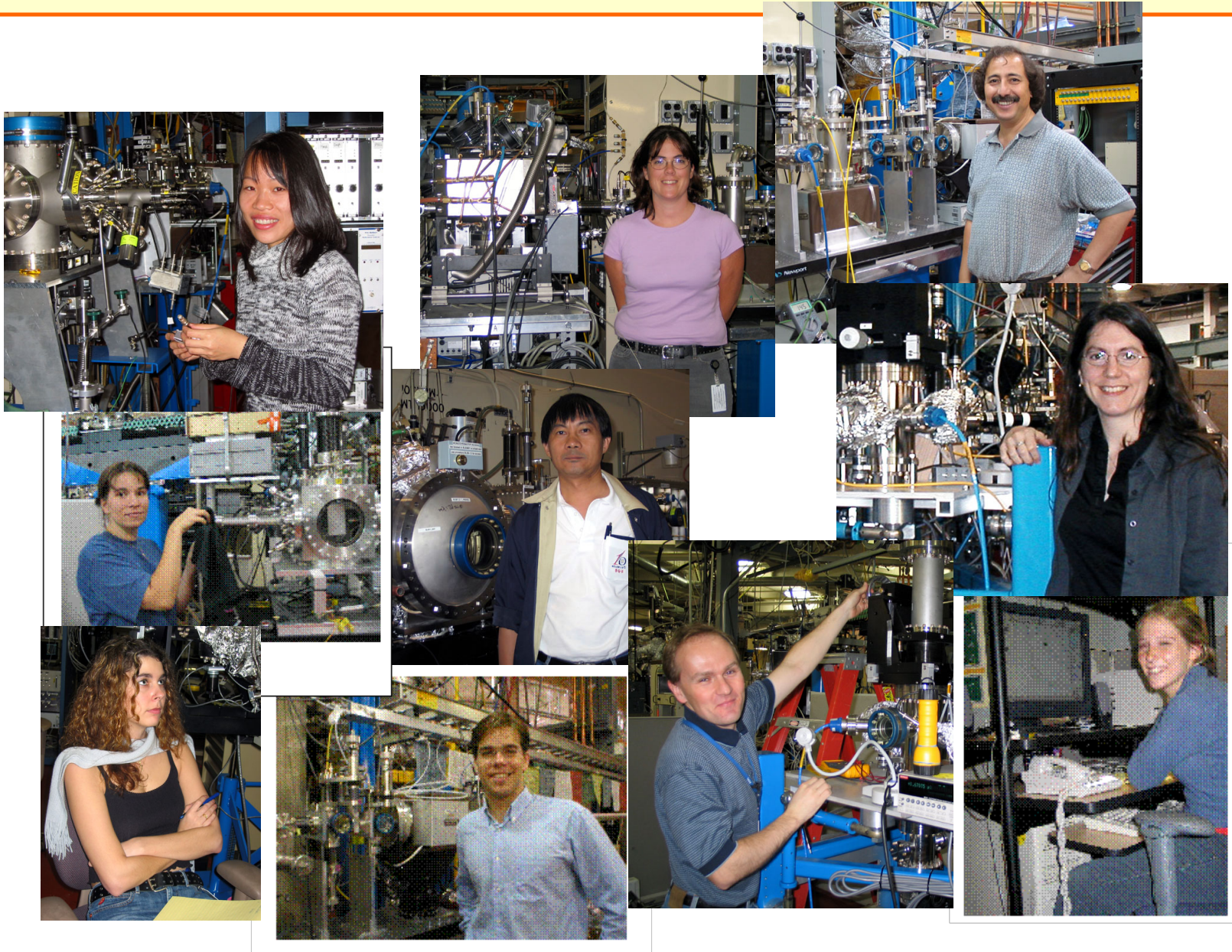


Enabling studies using  
interferometry and speckle  
techniques.

A high-brightness x-ray beam is required to produce a narrow parallel beam of photons.

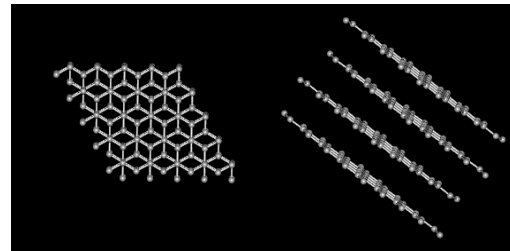


## ALS beamline users: students and visitors from around the world



# Carbon has three forms: graphite, diamond, and buckyballs

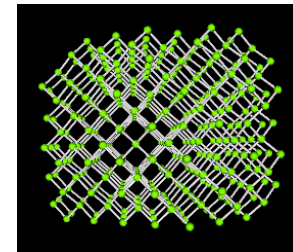
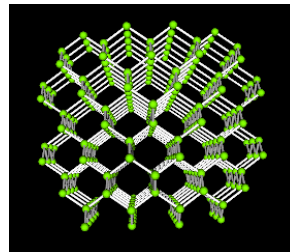
**Graphite.** Soft and slippery. Strong covalent bonds between carbon atoms in each layer: 2-dimensional bonding.



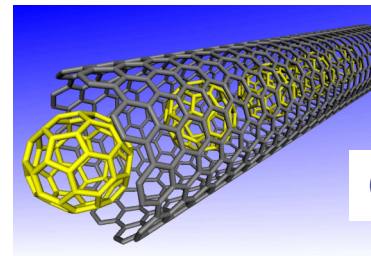
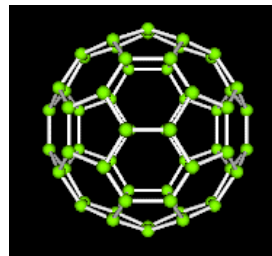
Carbon also has an amorphous form

**Diamond.** Tetrahedral bonds. Very hard. Each carbon atom is the same distance to each neighbor in rigid 3-dimensional framework.

Note: graphite is the stable form of carbon. Diamond undergoes a slow transformation to graphite.



**Buckyball (Fullerene).** Hollow conducting sphere made of 60 (or more) carbon atoms.



**Carbon nanotube....**

Different properties are a consequence of different geometrical structure, leading to different bonding between valence electrons. (Vos et al 1997)



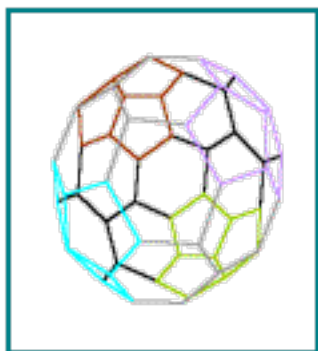
## Fullerene = Buckyball

A  $C_{60}$  molecule consists of 60 carbon atoms bonded to form a hollow conducting sphere.

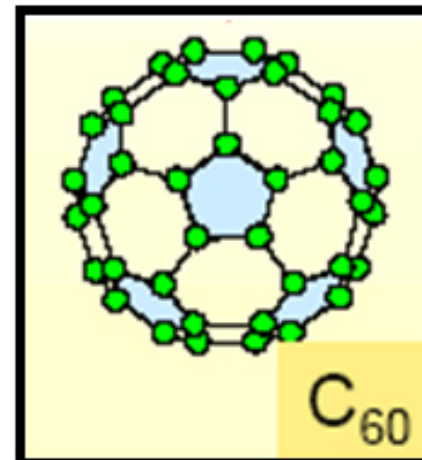
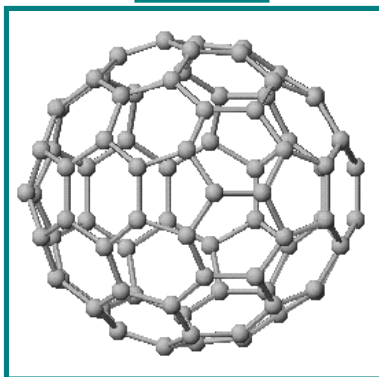
$C_{60}$  is small: diameter 0.7 nm (*less than 5 times the diameter of a hydrogen atom*).

Fullerenes come in many sizes.

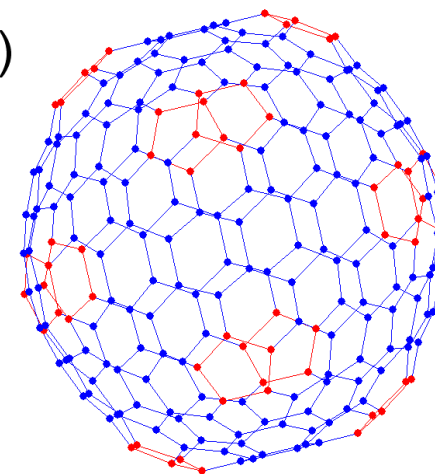
C56



C84

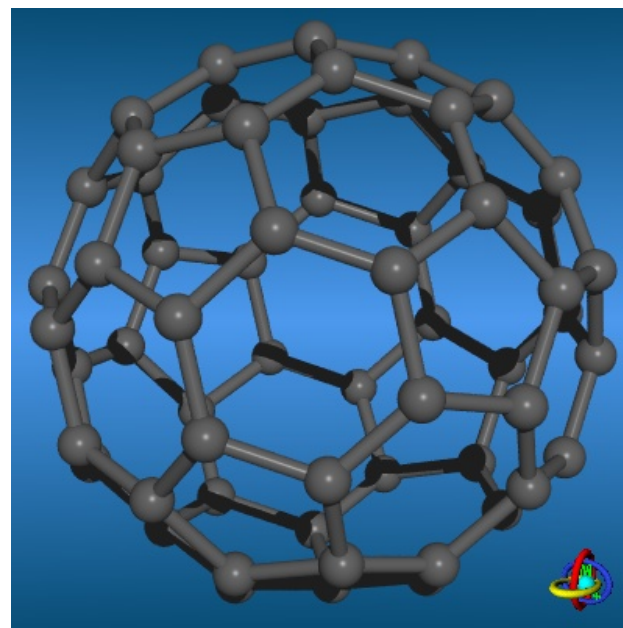


C240 ( $I_h$ )



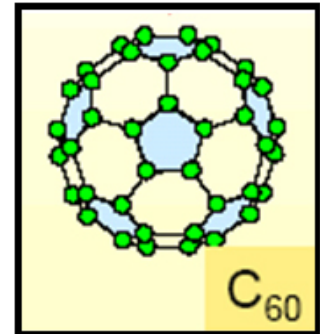
We can study all of these....

Soccer ball: same “bonding” as  $C_{60}$



A soccer ball and  $C_{60}$  both are made of alternating pentagons and hexagons.

## Buckminster Fuller: inventor of geodesic dome

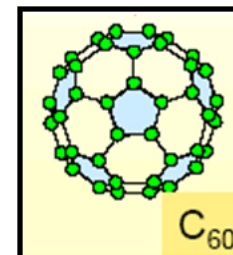


Composed of triangles...

Richard Buckminster “Bucky” Fuller was an American engineer, designer, author, inventor, and futurist. He is most known for the **geodesic dome**.

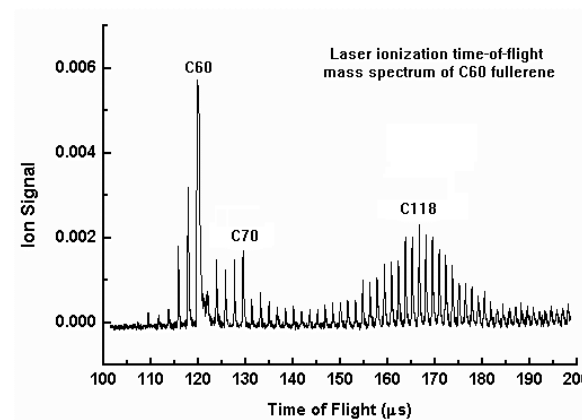
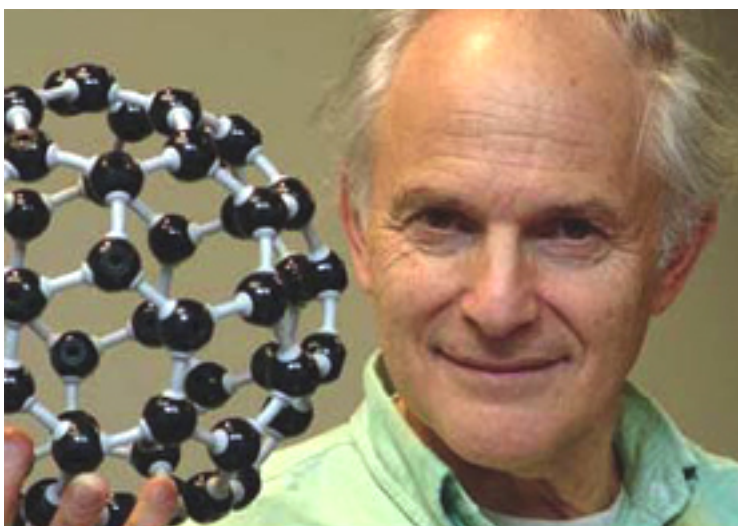


$C_{60}$  was discovered accidentally in 1985.



Mass spectroscopy of laser-produced plasma showed *unexpected* peaks at mass 60, 70, ....

...a serendipitous discovery...


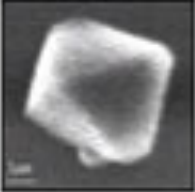





Smalley, Curl, Heath, O'Brien, and Kroto.....1996 Nobel Prize

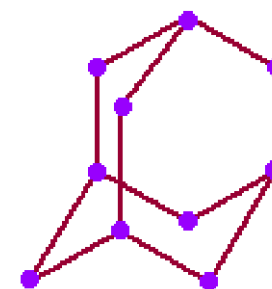


## Other structures: diamondoids and adamantane.

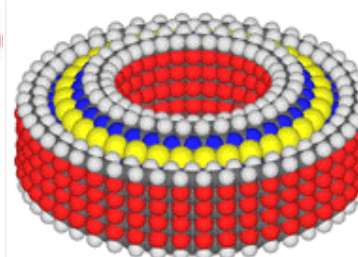
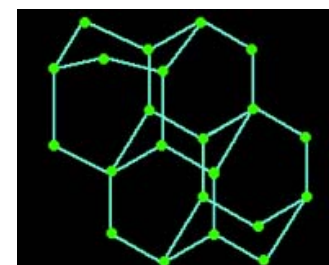
Diamondoids are small molecules with a diamond-like structure.

millimeters	microns	>2 nanometers	1-2 nanometers	< 1 nanometers
				
Natural Macroscopic Diamond, photograph Fixter, U. Nebraska)	CVD Diamond, SEM Sunkara, 1993)	Ultrananocrystalline Diamond, HRTEM (Praver et al. 2000)	Higher Diamondoids <b>Unknown Properties</b>	Lower Diamondoids

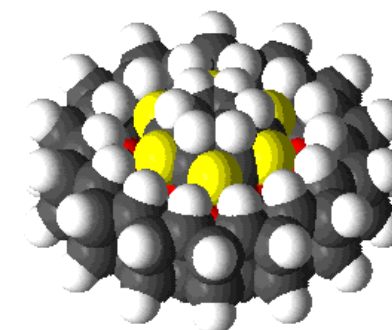
Higher Diamondoids have "knowable" molecular structure



The most common is adamantane,  $C_{10}H_{16}$ :



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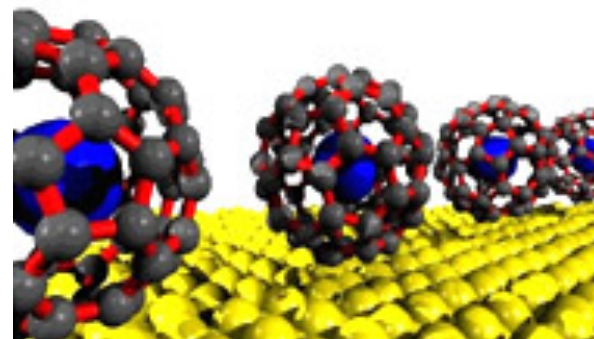
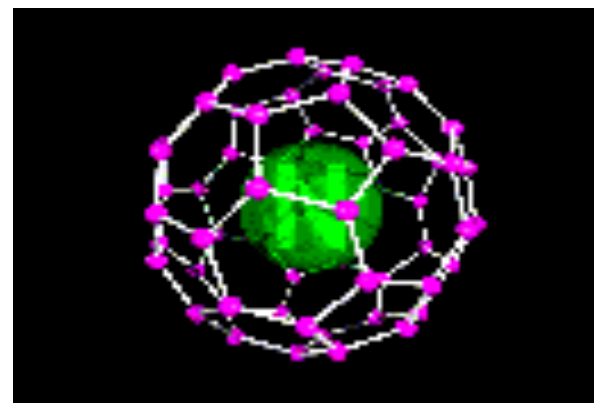
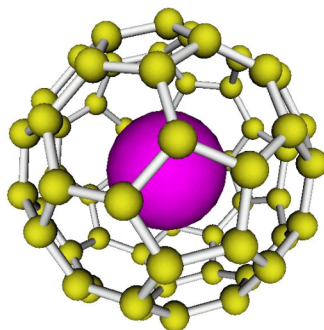


# Endohedral Fullerenes\*

\*another name for buckyballs

Fullerenes are hollow molecules providing space to incorporate atoms inside.

There is a great diversity of complexes  $X@C_n$  meaning species  $X$  is endohedral in the Fullerene  $C_n$  cage.



The *endohedral* atom  $X$  can be a metal (e.g., La, Ca, etc.), a nonmetal (e.g. Ne, P, etc.) or a molecule (e.g.  $N_2$ , CO).

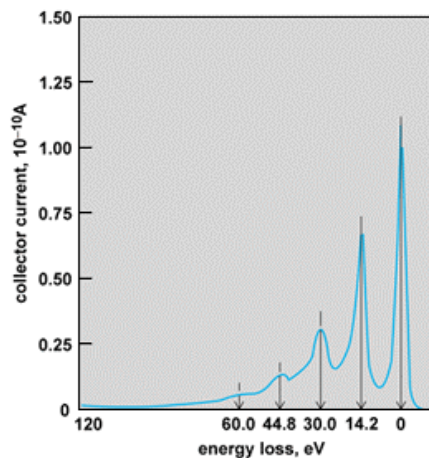
Encapsulating an atom or molecule in a Fullerene structure provides a possibility to alter the atomic or molecular properties of the atom or molecule.

See, for example, Averbukh and Cederbaum, Phys. Rev. Letters 96, 053401 (2006); and references therein.

# Collective resonances in physics: a few examples

- **Plasmon**

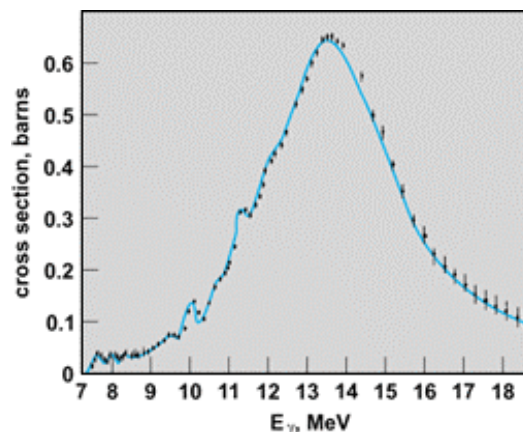
Collective effect of large numbers of electrons in matter when the electrons are disturbed from equilibrium, typically in a metal.



Ferrell et al., Asmer. Sci. **73**, 344 (1985). Electron energy loss in a thin Al foil.

- **Giant nuclear resonance**

Giant nuclear resonance is elementary mode of oscillation of the entire nucleus. Example is E1 resonance in which all the protons and all the neutrons oscillate with opposite phase, producing a time-varying electric dipole moment.



Veyssiere et al., Nucl. Phys.. **A159**, 5612 (1970). Neutron production of  $^{208}\text{Pb}$  and  $^{197}\text{Au}$  by gamma-ray bombardment..

# Interaction of photons with ionized matter

...applications to astrophysics and hot plasmas

## Fundamental:

- Most of the visible matter in the universe exists in the ionized state.
- Vacuum ultraviolet photons are a highly selective probe of the electronic structure of atoms, molecules and ions.

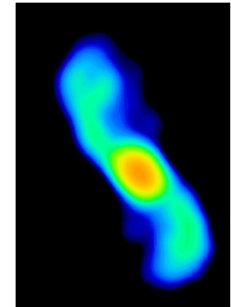
Data on photoionization of ions are needed to interpret satellite measurements.

## Applications:

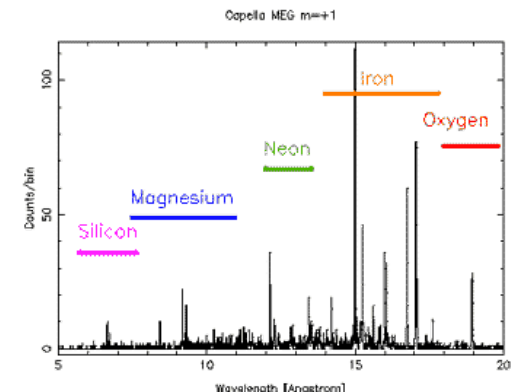
- Photons carry most information that we have about the distant universe.
- Advanced extreme ultraviolet (EUV) lithography light sources are being developed to produce the next generation of semiconductor chips.



Satellite observation of multiply charged ions...

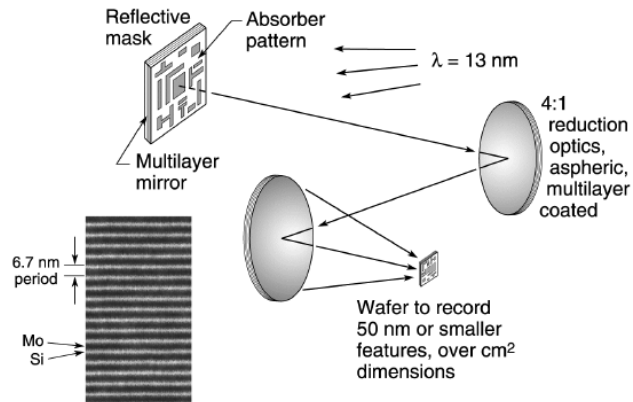


Radio-telescope image of an old star transforming into a planetary nebula.





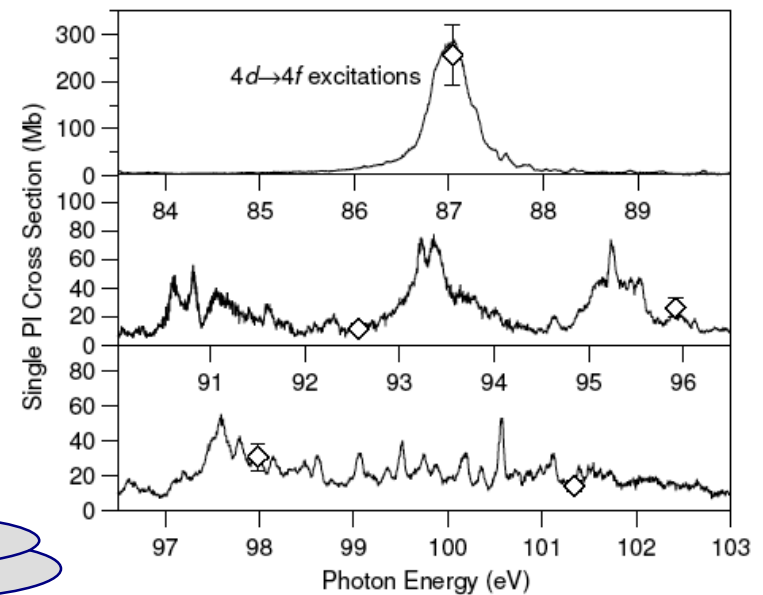
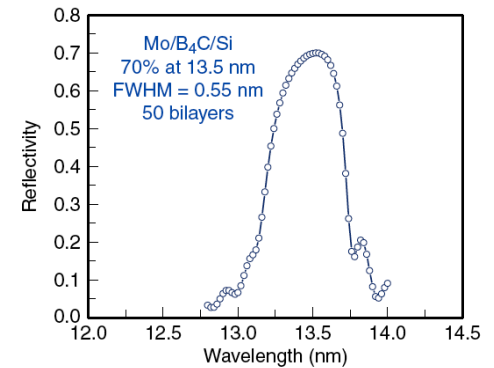
# EUV lithography: photoionization of $\text{Xe}^{3+}$



Photoionization measurements at ALS indicate that  $4d - nf$  excitation of  $\text{Xe}^{3+}$  results in photoabsorption within the EUV lithography light-source window.

Data on interaction of photons with multiply charged ions will aid modeling of plasmas for sources of short-wavelength radiation.

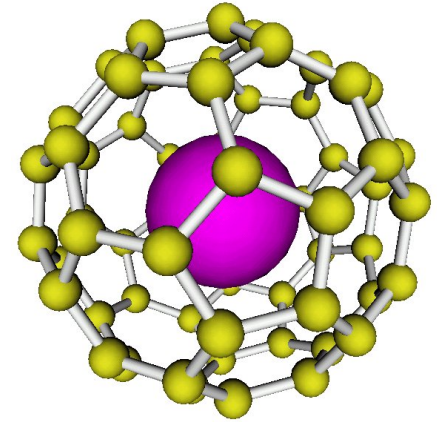
Multilayer Mirrors Have Achieved 70% Reflectivity



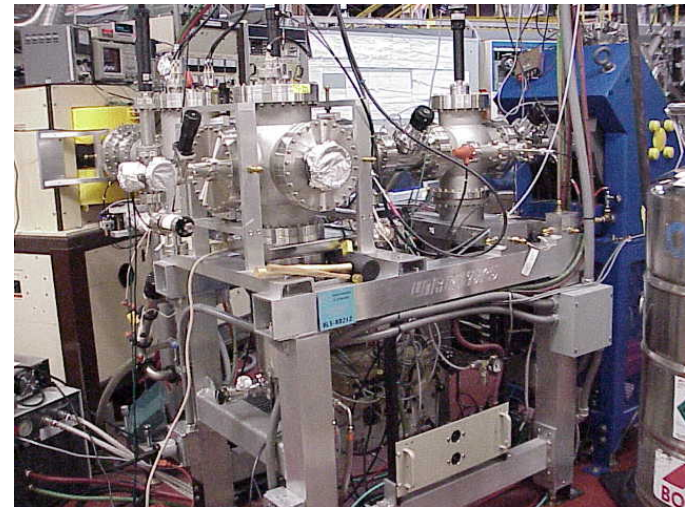
Emmons et al., Phys. Rev. A **71**, 042704 (2005)

## Interaction of photons with $C_{60}$ ions

We expect the *same physics* for  $C_{60}$  or  $C_{60}^+$  ions, because of the very large number of valence electrons (240 or 239 or 238, depending on ion charge state).

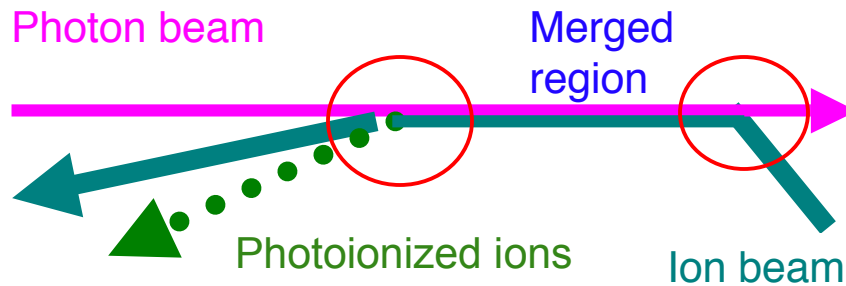


Measurements performed with  $C_{60}^+$  ions rather than  $C_{60}$  neutral atoms because an experiment with an ion beam eliminates background and allows clear elucidation of the electronic structure of  $C_{60}$ .

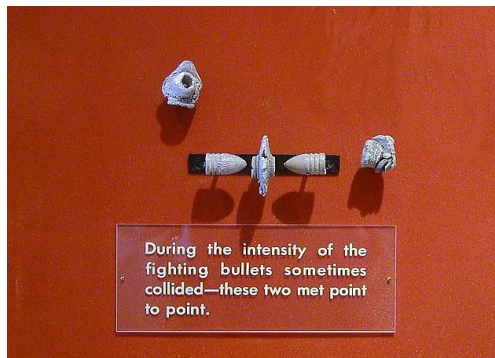
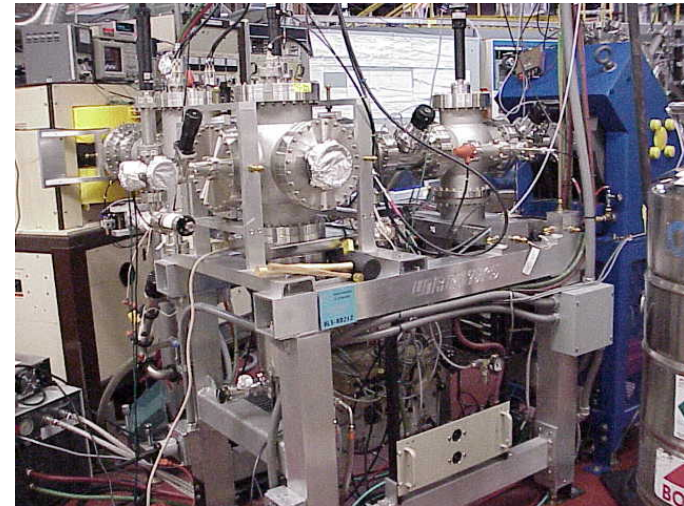


# A Merged Photon-Beam Ion-Beam Apparatus

Apparatus to measure interaction of photons with ions



A merged-beams experiment is like guns being fired and the bullets collide.

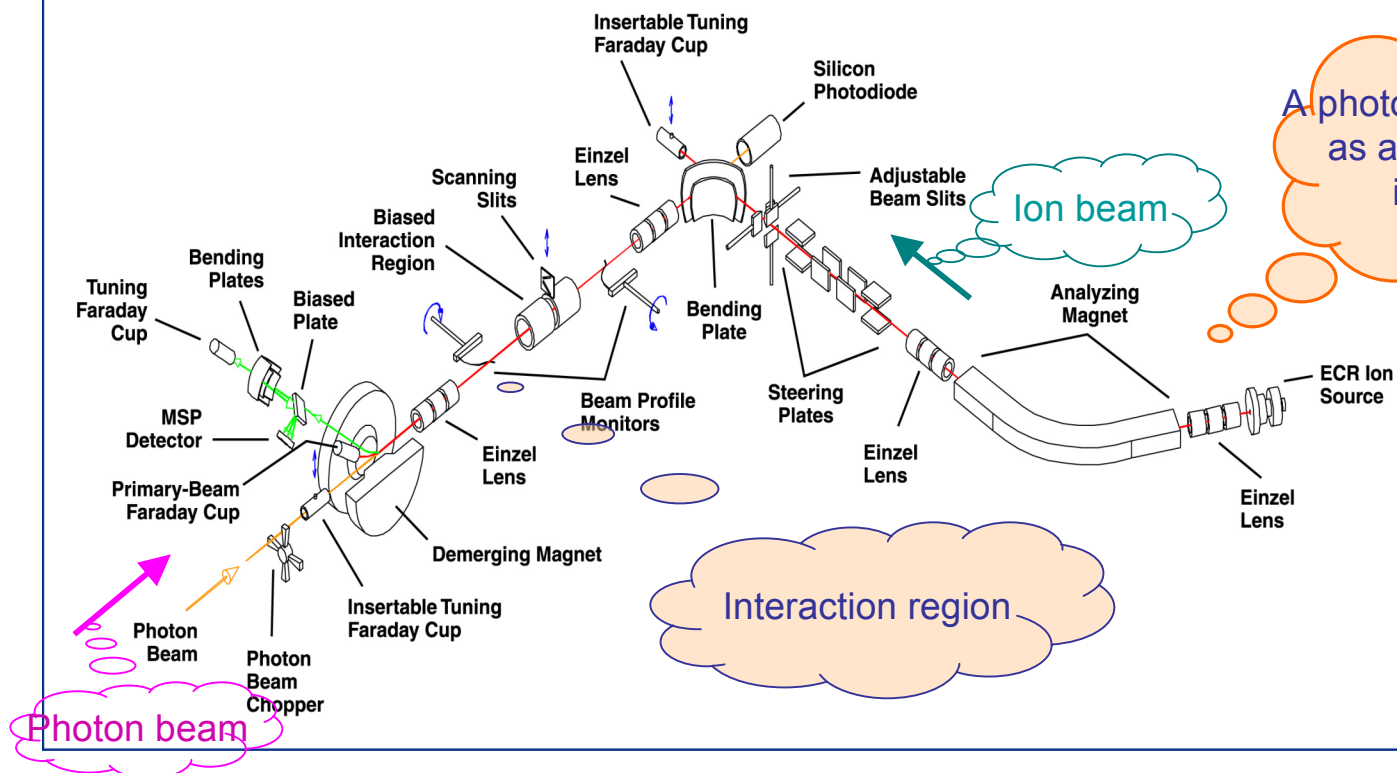


# A Merged Photon-Beam Ion-Beam Apparatus



## Beamline 10.0.1

### • Merged photon and ion beams





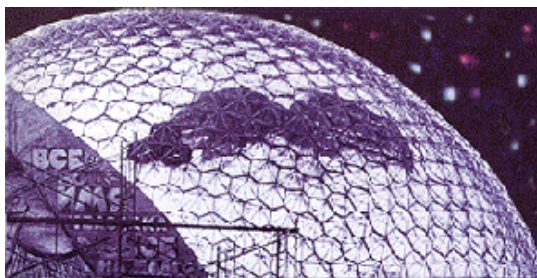
# Photoionization of Fullerene Ions: $C_{60}^+$

## Bridging the gap between molecules and solids: photoionization of buckyball ions.

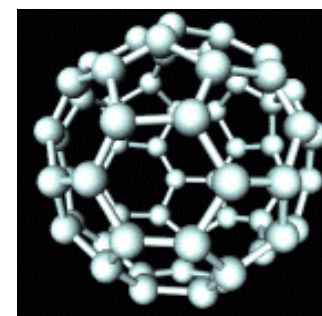
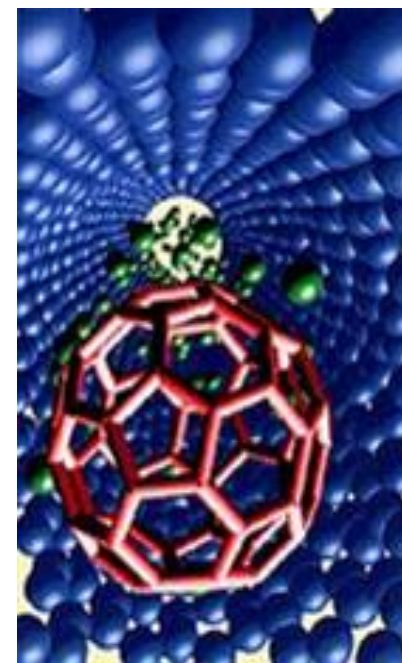
Buckyball (Fullerene) molecules consist of 60 carbon atoms arranged in a hollow, spherical cage-like structure. The carbon atoms form 20 pentagons and 12 hexagons, like the facets of a football. *Other Fullerenes are possible.*

Experiment is to look for behavior characteristic of a solid in a large molecule where such behavior is unexpected: observe collective motion of the electrons (“plasmon”).

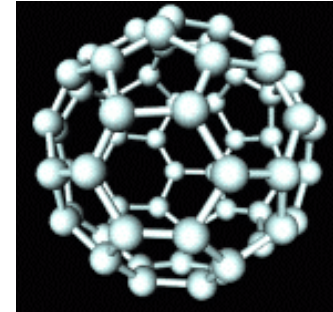
Curl, Kroto and Smalley won the Nobel Prize in 1996 for their 1985 discovery of Fullerenes.



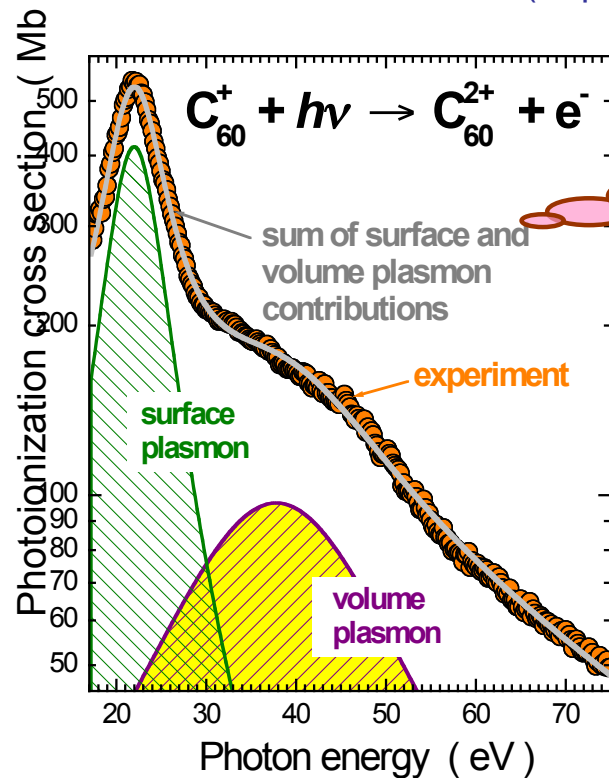
Dome of 1967 World Exhibition in Montreal by the architect R. Buckminster Fuller.



# Setting 240 valence electrons in motion: $C_{60}^+$



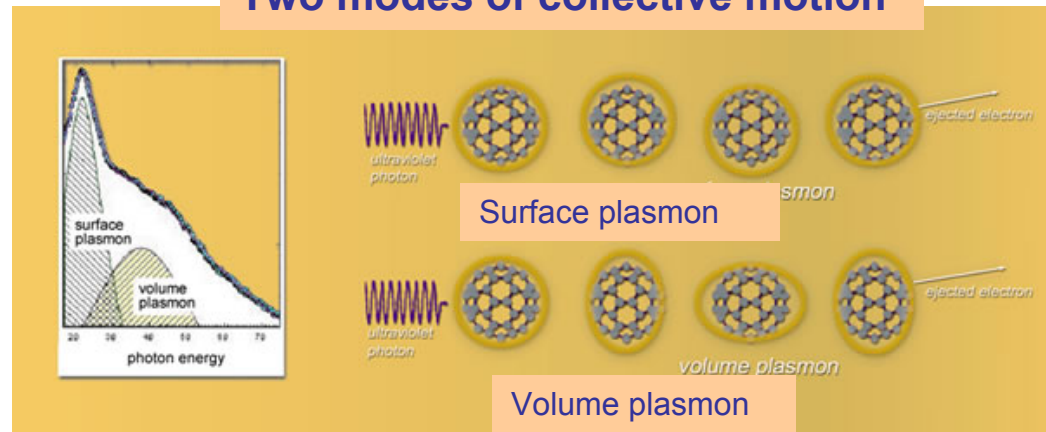
Absorption of a soft-x-ray photon from the Advanced Light Source: the energy of the photon is converted into a collective movement of the electrons (a “plasmon”).



S.W.J. Scully et al., Phys. Rev. Lett. 94, 065503 (2005).

Two resonances are observed: these resonances are attributed by theory to collective motion of the 240 valence electrons.

## Two modes of collective motion



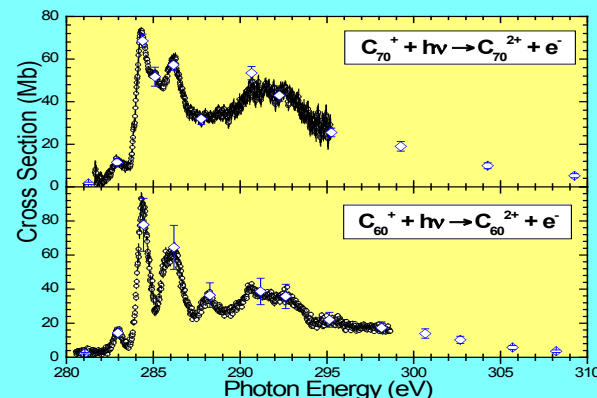
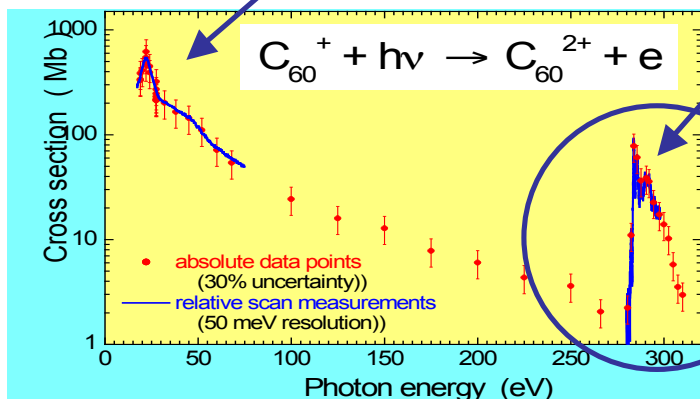
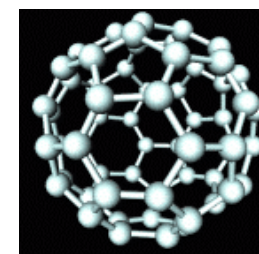
M. Ya Amusia and J-P Connerade Rep. Prog. Phys. 63, 41 (2000).

# K-shell Excitation of $C_{60}^+$ and $C_{70}^+$ Ions: collective and localized effects

Collective Plasmon Excitations

Localized Molecular Excitations

$C_{60}^+$

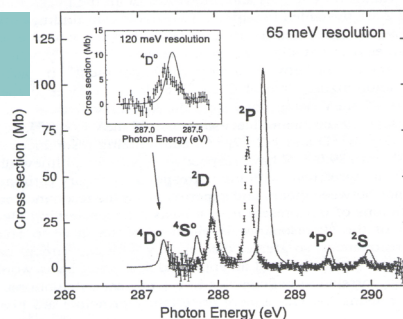


L-shell excitation

K-shell excitation

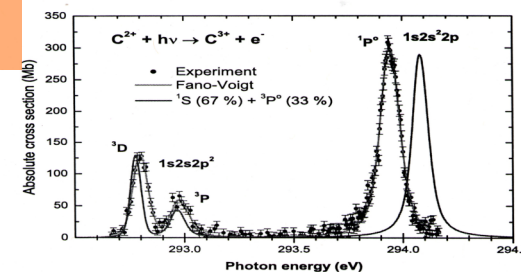
Comparison: K-shell excitation  
of  $C^+$  and  $C^{2+}$  ions.

$C^+$



Schlachter et al, J. Phys. B **37**,  
L103 (2004)

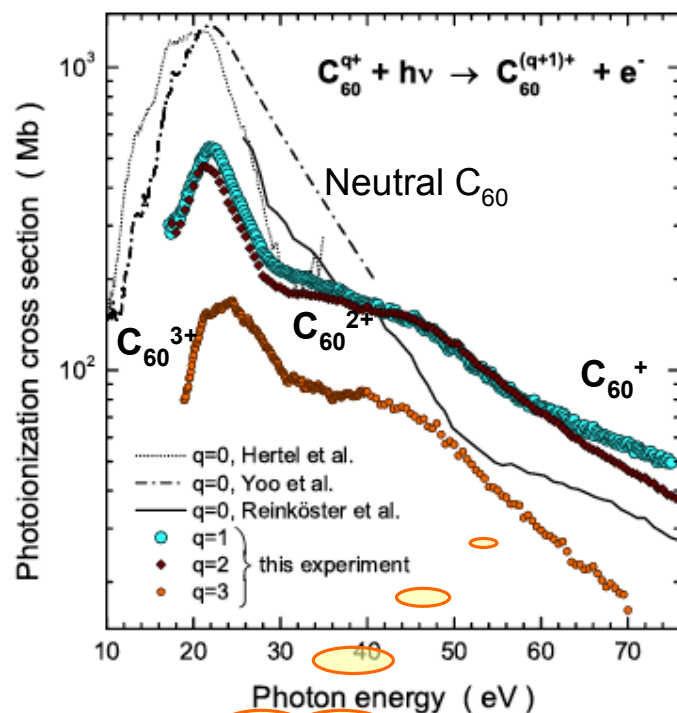
$C^{2+}$



Scully et al, J. Phys. B **38**,  
1967 (2005)

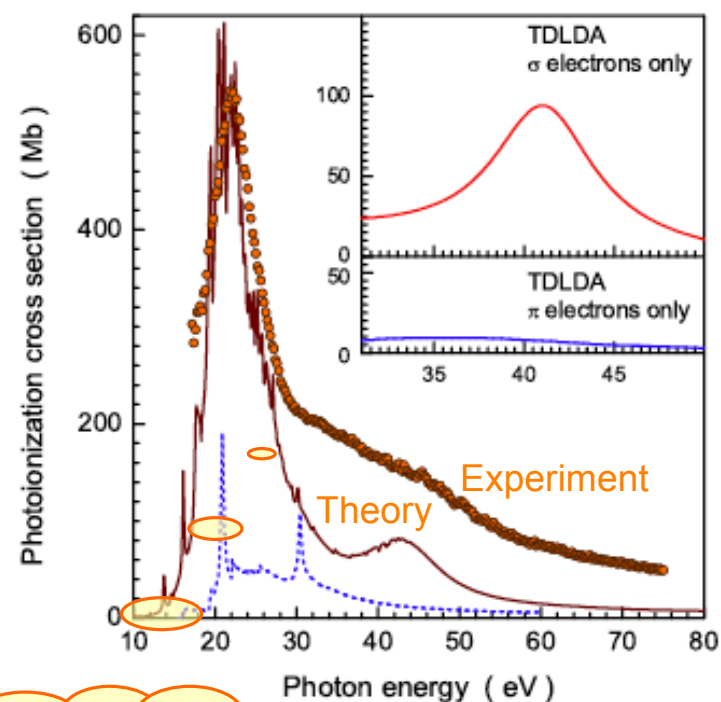
# More physics of $C_{60}^+$ and $C_{70}^+$ Ions

Single photoionization of  $C_{60}^{q+}$ :  
as function of ion charge state and  
comparison with neutrals



Absolute photoionization  
cross sections for  $C_{60}$  ions

Single photoionization of  $C_{60}^{q+}$ :  
Comparison with theory (Time-  
Dependent Local-Density Approximation)

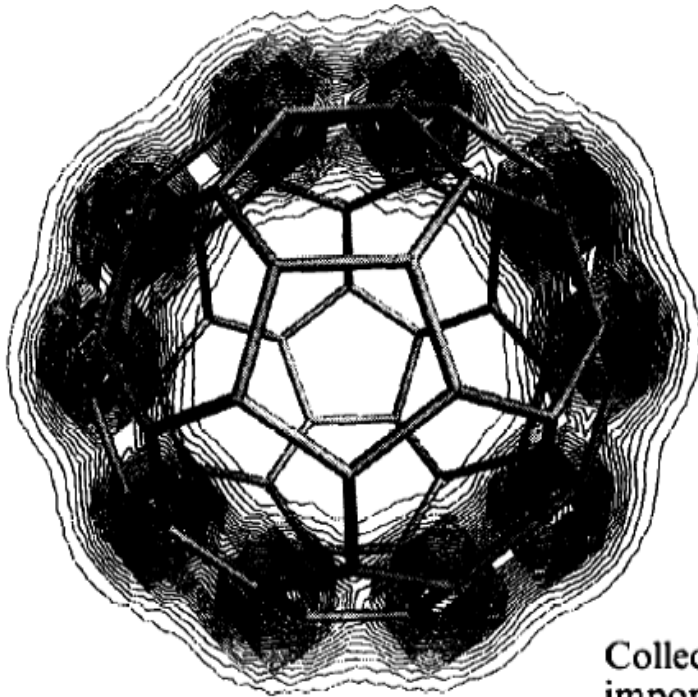


Theory scaled to experiment  
at 22 eV. Note that theory shows  
both resonances

Scully et al., Physical Review  
Letters **94**, 065503 (2005)



There is considerable theoretical literature...



Two-dimensional cross section along the plane parallel to the pentagonal face of the  $C_{60}$  molecule showing the total density of valence electrons.

Michalewicz and Das, Solid State Communications **84**, 1121 (1992)

Collective electronic excitations on the novel fullerenes play an important role in cohesion of  $C_{60}$  crystal. We use the dispersive hydrodynamic model for the collective electronic excitations to study surface plasmons on a model of the  $C_{60}$  molecule. This simple model consists of a spherical metallic jellium shell of finite thickness. We find four molecular surface plasmons of energy between  $15\text{ eV} < \omega < 32\text{ eV}$  for the shell thickness corresponding to our quantum chemical calculations. Our results are compared with the electron-energy-loss spectroscopy studies and with other complementary theoretical calculations.

## Endohedral atoms: Ce in $C_{82}^+$

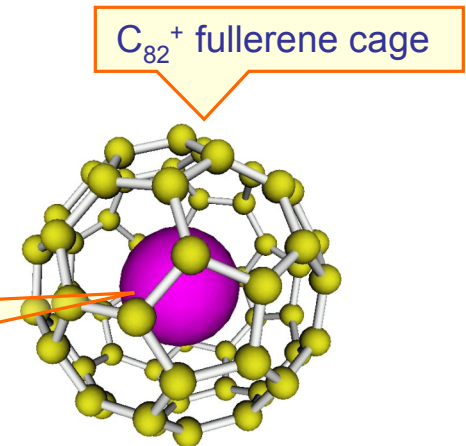
Encapsulating an atom or molecule in a Fullerene structure provides a possibility to alter the atomic or molecular properties of the atom or molecule: **creating new forms of matter with new applications.**

New possibilities for applications in nanostructure science and technology are being vigorously explored....

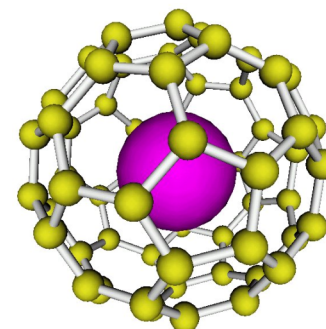
*Potential applications:*

- isolating an atom from its environment thus applications as q-bit for quantum computing.
- Chemical isolation of reactive or poisonous atoms may open new possibilities in medical imaging and cancer therapy.

How are the energy levels of a *cerium atom* changed by being in the unique environment of a fullerene cage?



# Endohedral atoms: Ce in $C_{82}^+$

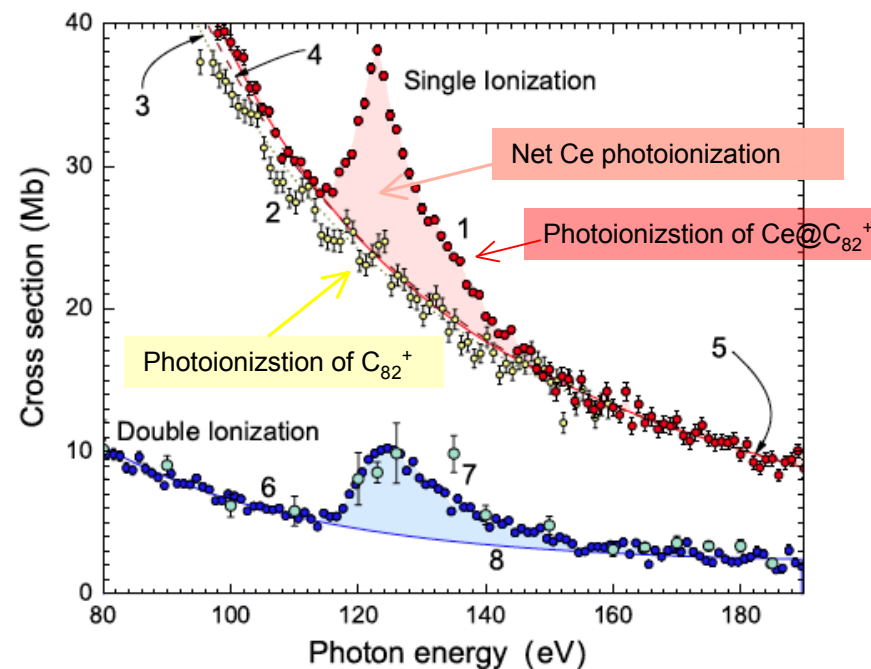
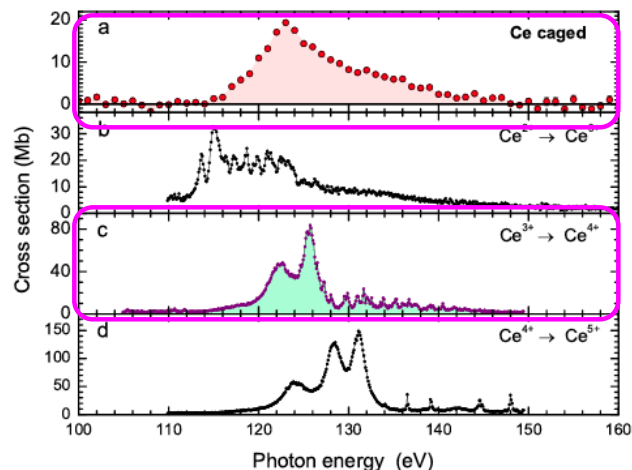


**Objective:** determine how the electronic structure of a cerium atom is altered by being enclosed in a  $C_{82}^+$  fullerene cage.

**Experiment:** measure photoionization of:

$Ce^{3+}$  (isolated cerium ion),  $C_{82}^+$  (empty fullerene cage), and  $Ce@C_{82}^+$  (endohedral cerium atom in fullerene cage).

Caged Ce atom looks like  $Ce^{3+}$  with energy levels blurred by hybridization.



Mueller et al, Phys Rev Letts **101**, 133001 (2008) and references therein; Amusia, J. Electron Spectrosc. Relat. Phenom. **161** 112 (2007).

## Discussion about nature of plasmon resonances... ongoing in Physical Review Letters

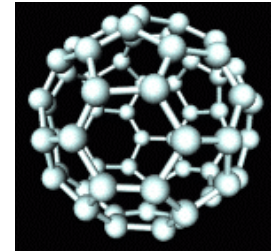
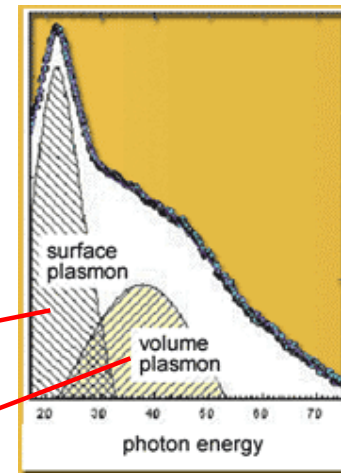
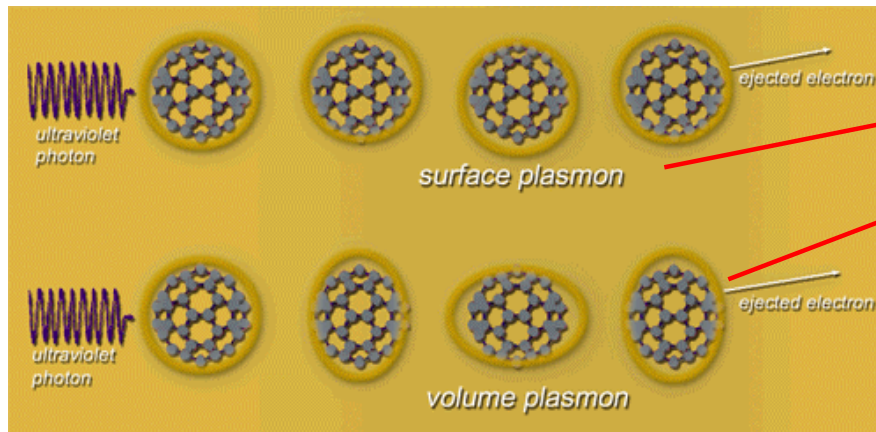
Korol and Solov'yov—Phys. Rev. Letters 98, 179601 (2007)—contend that observed volume plasmon can be interpreted in terms of coupled surface plasmons.

Scully et al.—Phys. Rev. Letters 98, 179602 (2007)—respond that a volume plasmon is associated with a spatial modulation of electron density, rather than a collective excitation with constant electron density.

*Theorists* are continuing this discussion on the pages of Physical Review Letters. Meanwhile we experimentalists are pleased with our observation of the second (volume plasmon) resonance, which had been overlooked in experiments on neutral C<sub>60</sub>.



## Plasmons: historical view



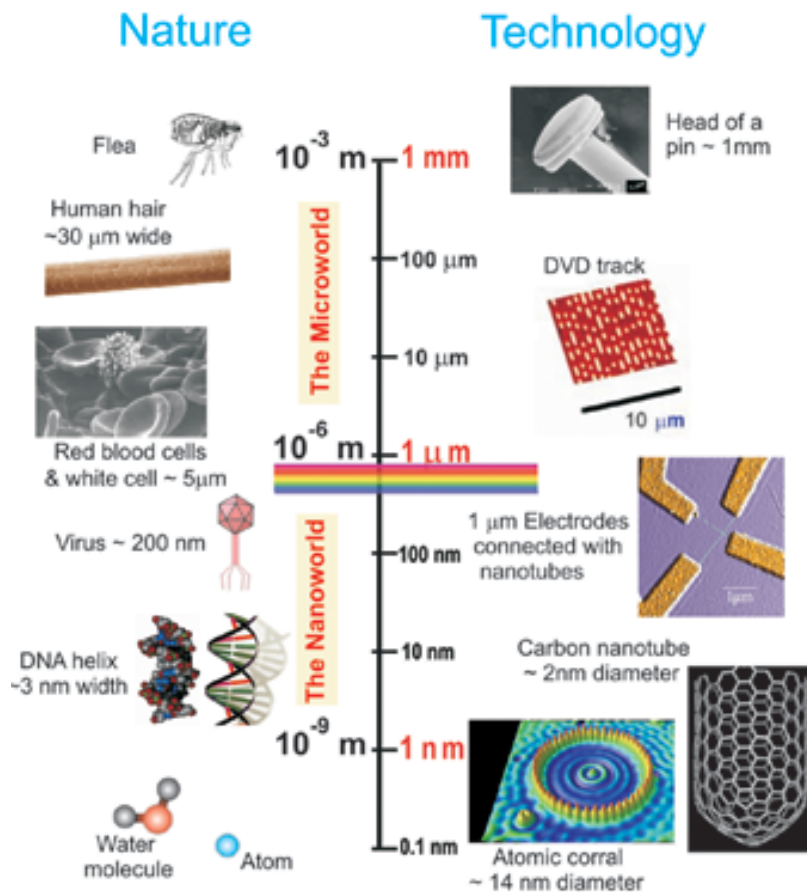
Plasmons confined to the surface of a material can produce obvious effects. **The deep red color in medieval stained-glass windows is actually produced by nanoparticles of gold:** "Electrons at the surface of the nanoparticles slosh back and forth in unison, absorbing blue and yellow light. But longer-wavelength red light reflects off the particles." **The New York Times calls the stained-glass artisans "the first nanotechnologists."**

Stained-glass window makers in the Middle Ages achieved deep reds by dissolving gold in the molten glass. Surface plasmons on the nanosized particles of metal cause them to reflect red light selectively.

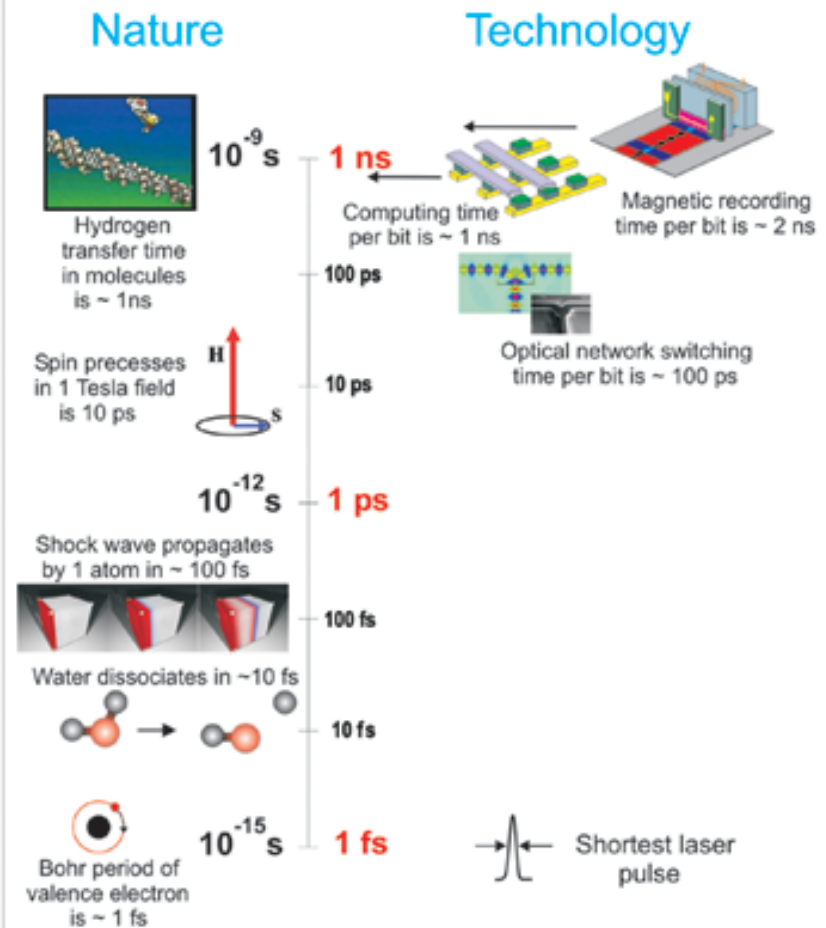


# Frontiers in physics

## Ultra-Small



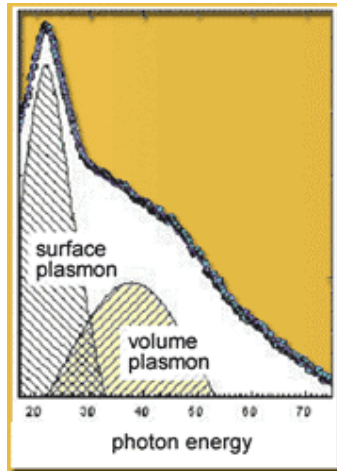
## Ultra-Fast



## Further references

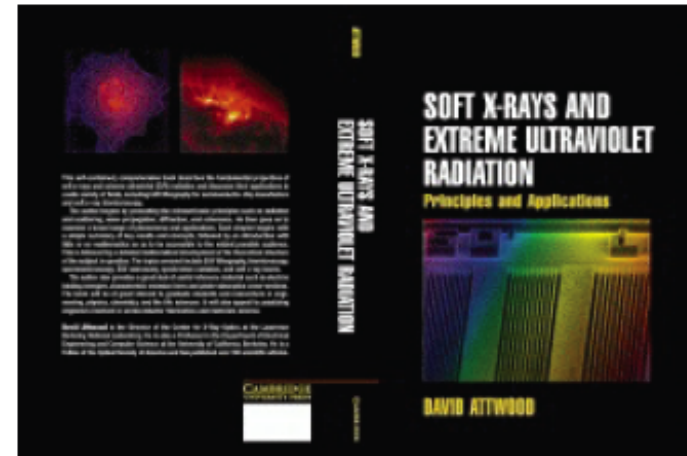
Soft x-rays and extreme ultraviolet radiation: principles and applications, David Attwood, Cambridge University Press

([www.coe.berkeley.edu/AST/sxreuv](http://www.coe.berkeley.edu/AST/sxreuv))



[http://www-als.lbl.gov/als/science/sci\\_archive/103plasmon.html](http://www-als.lbl.gov/als/science/sci_archive/103plasmon.html)

<http://www.lbl.gov/Science-Articles/Archive/sabl/2005/May/06-buckyballs.html>



APS NEWS

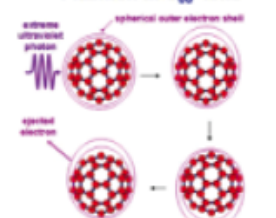
February 2005 5

## Physics News in 2005

A Supplement to APS News

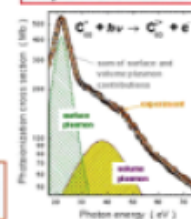
Edited by Phillip F. Schewe, Ben Stein and Ernie Tretkoff

### Photoexcitation of a Volume Plasmon in $C_{60}^+$ Ions



After approximately one period of oscillation of the outer electron shell, one electron may be ejected, resulting in photoionization.

Experiments show evidence for photoexcitation of two distinct modes of collective oscillation of the 239 valence electrons that bind the  $C_{60}^+$  molecular ion. Both modes may result in the ejection of an electron.



<http://www.aps.org/apsnews/0206/>



# Acknowledgments

International team working at ALS

Shane Scully, Erik Emmons, Mohamed Gharaibeh, and Ron Phaneuf, University of Nevada Reno  
Stefan Schippers and Alfred Müller, Justus-Liebig-Universität Giessen  
Himadri Chakraborty, Mohamed Madjet, and Jean-Michel Rost, Max Planck Institute, Dresden



“Photoexcitation of a Volume Plasmon in  $C_{60}$  Ions,” Scully et al, Physical Review Letters **94**, 065503 (2005)



## Conclusion: collective motion of electrons in $C_{60}$

**Collective motion** (plasmons) are observed in  $C_{60}$ , which is intermediate between an atom and a solid. *Behavior characteristic of bulk matter is observed in a molecule with only 240 valence electrons.*

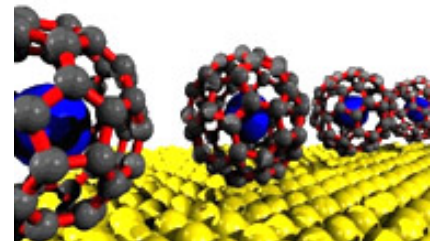
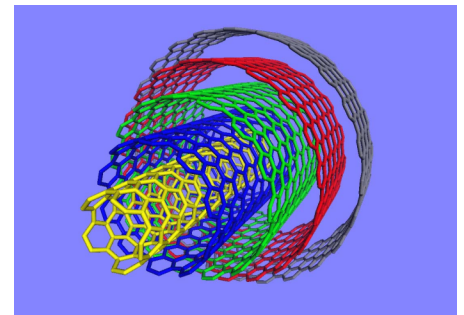
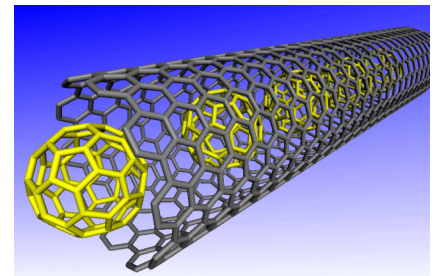
Exciting new science is possible with **nanomaterials**.

A synchrotron light source is a powerful tool for the exploration of the **electronic structure of matter**.

**Theory and experiment** work together to understand the electronic structure of matter.



[fsschlachter@lbl.gov](mailto:fsschlachter@lbl.gov)



## Fred: diving in Thailand

<http://www.lbl.gov/Publications/Currents/archive/>  
February 16, 2007

### From Buckyballs to Manta Rays: The Diving Adventures of an ALS Beamline Scientist

BY LYN HUNTER

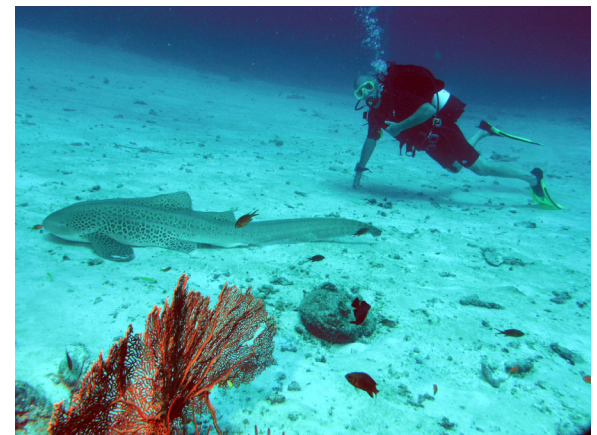
There sat Fred Schlachter on the dark ocean floor, 36 feet below the surface. Just an arm's length away swam a manta ray. Though elated at the sight of this magnificent creature, visions of Steve Irwin — the Australian TV show host who died last fall from a stingray's stab — flashed before him.

**Schlachter heads out to the Similan Islands near Thailand for a dive.**

Schlachter is on the faculty at Chiang Mai University, where he lectures in the physics department and mentors a Ph.D student.

**Schlachter is careful to leave plenty of distance between himself and a leopard shark in the Andaman Sea.**

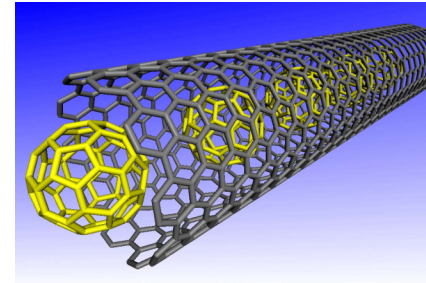
When he's not diving, the 31-year Lab veteran is assisting ALS users. He researches "how electrons give atoms and molecules their properties, and how big an atom has to be to begin to behave classically, as opposed to quantum mechanically." He was also involved with the search for quantum chaos and collective oscillation of electrons in buckyballs.



Thanks for your attention.....

**Additional lecture topics:**

- Light: a user's guide to the universe (lay audiences)
- Synchrotron radiation: a tool for exploring the electronic structure of matter (multi-hour seminar series)
- Lasers in science and industry: economic impact ([www.laserfest.org](http://www.laserfest.org))
- Over a barrel: revolutionizing the way we power our cars (lay or professional audiences) (RevModPhys 2008)
- The search for quantum chaos.



ขอบคุณครับ



[fsschlachter@lbl.gov](mailto:fsschlachter@lbl.gov)



Chulalongkorn University, September 27, 2010

“Lasers in science and industry: economic impact.”





## LCLS: x-ray laser



LCLS (Stanford)



$\nu = 10^{17} \text{ Hz}$   
 $\lambda \sim 2 \text{ \AA}$   
 $L = 3.5 \text{ km}$   
 $P = 30 \text{ MW}$

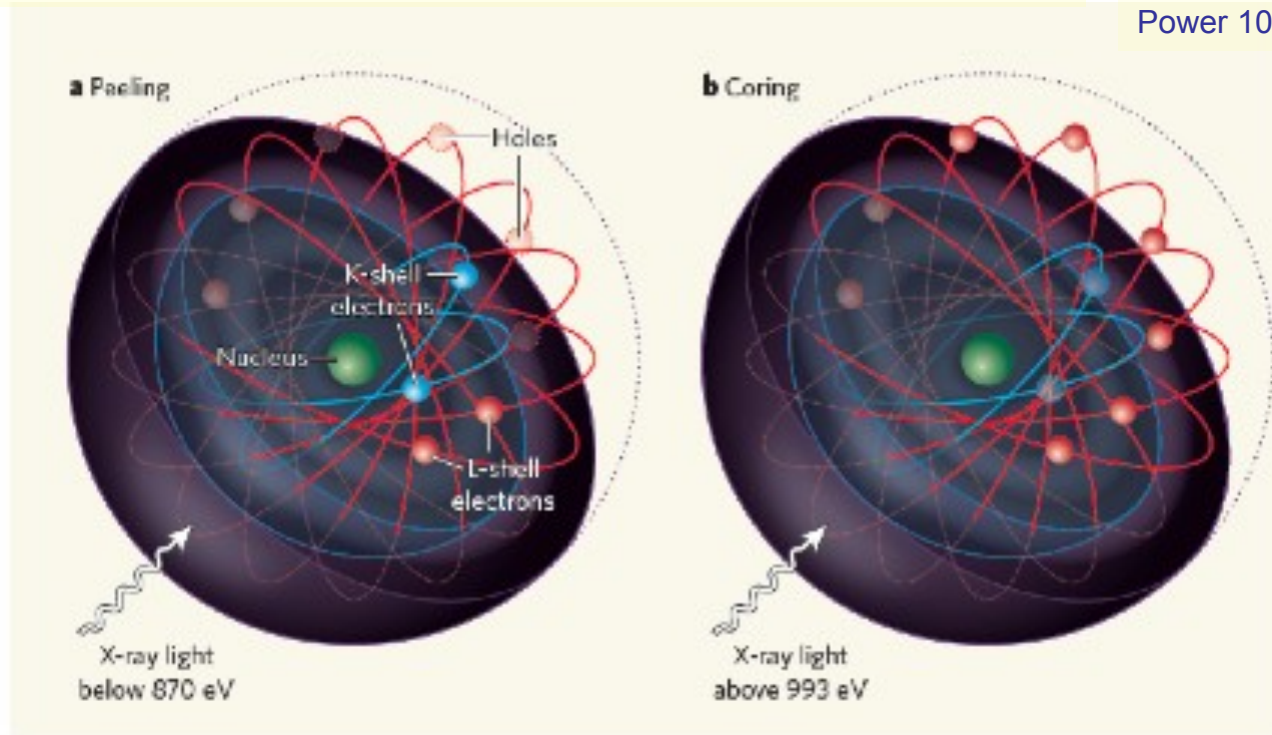
X-ray lasers photograph  
molecular bonds breaking

## X-ray laser: producing hollow atoms

Removing inner-shell electrons from neon atom.

**LCLS** pulse: tens of femtoseconds

Power  $10^{18}$  watts/cm<sup>2</sup>.



Nature vol. **466** July 1, 2010

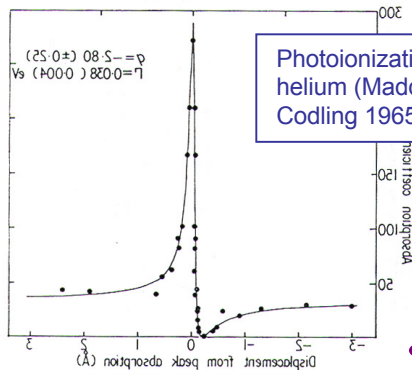
**Hollow atoms: Advanced Light Source 1996-2002:**

**hollow helium:** Physical Review Letters **86**, 3747 (2001). Search for quantum chaos in doubly excited atoms of helium.

**hollow lithium:** Physical Review Letters **79**, 1241 (1997). Hollow lithium atomic states.

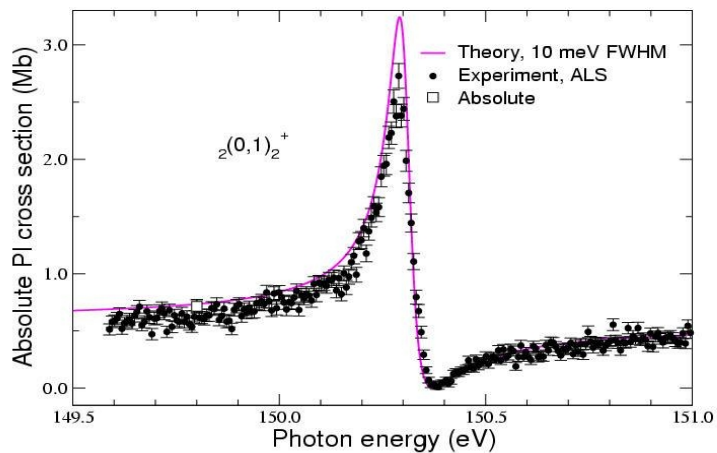
# Photoionization of helium-like $\text{Li}^+$

Photoionization of both electrons in He neutrals and  $\text{Li}^+$  ions: the search for quantum chaos



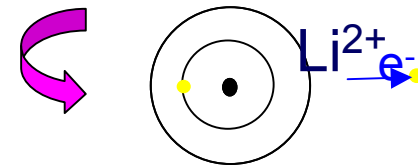
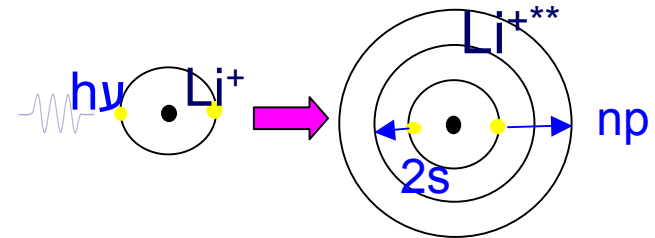
The two electrons are left in excited states, resulting in autoionization

Photoionization of  $\text{Li}^+$   
Theory: R-matrix, RMPS (65CC), Experiment, ALS

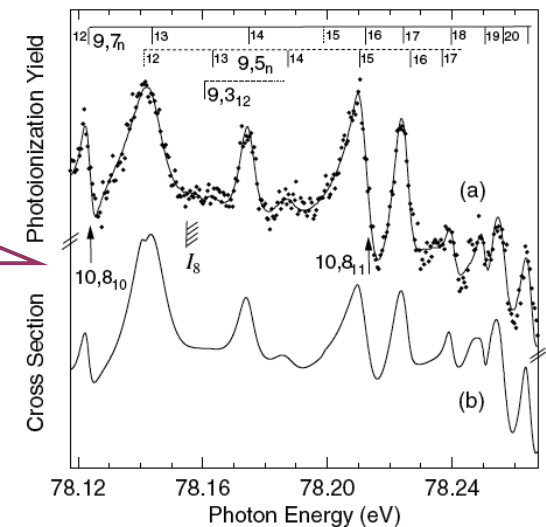


Scully et al, J. Phys. B **39** 3957 (2006)

Loss of quantum states in the spectrum of doubly excited helium atoms



Ultrahigh spectral resolution measurements of absorption in helium atoms -> quantum chaos

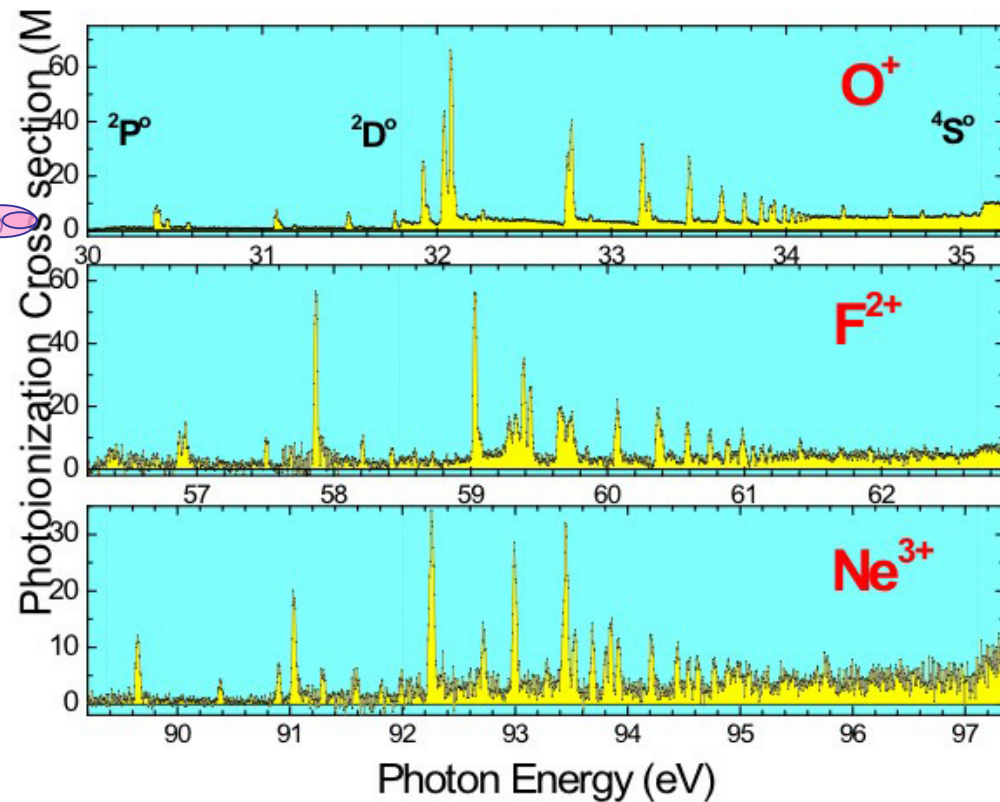


Püttner al, Phys. Rev. Letts. **86**, 3747 (2001)

## ...photoionization measurements...

### Photoionization of ions of the nitrogen isoelectronic sequence

Measurements of photoionization along an isoelectronic (ions with same number of electrons) sequence can reveal systematics in atomic structure.



Aguilar et al, J. Phys. B 38, 343 (2005)



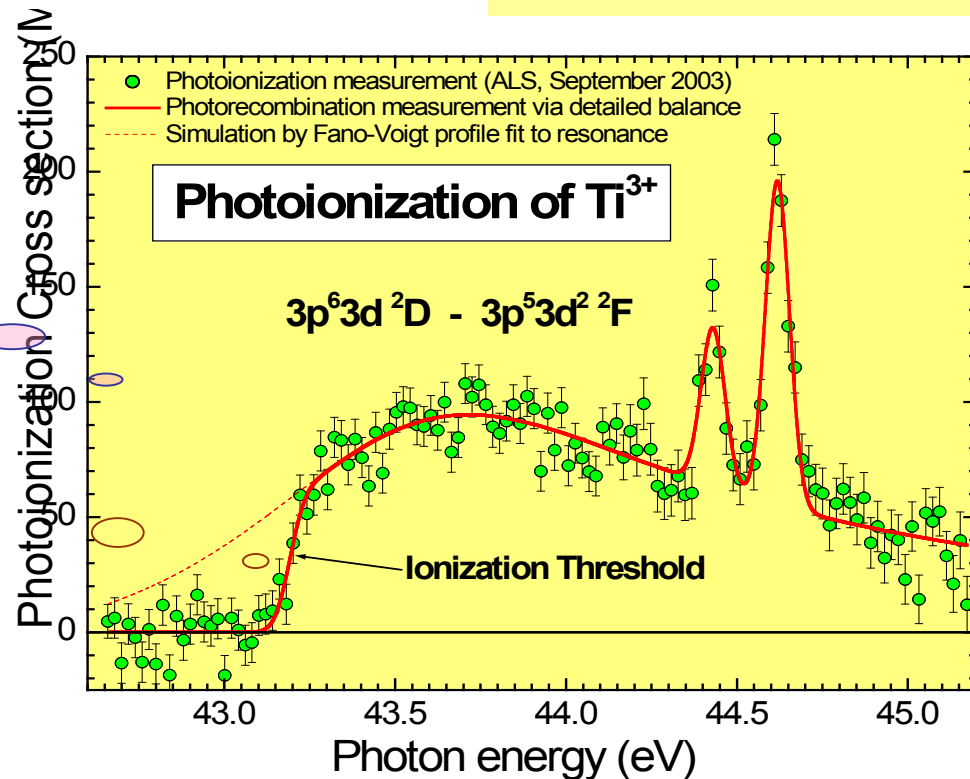
## ...photoionization measurements...

$\text{Ti}^{3+}$  photoionization: a broad resonance lying just above an ionization threshold

A giant dipole resonance 1.5 eV wide lies only 0.2 eV above the ionization threshold, and is therefore truncated.

Truncation of a giant dipole resonance in photoionization of  $\text{Ti}^{3+}$  ions.

Curve:  
photorecombination measurement at TSR in Heidelberg inverted using principle of detailed balance



Time-reversal symmetry

Photoionization of  $\text{Sc}^{2+}$

S. Schippers et al.  
Phys Rev. Lett. **89**, 193002 (2002).

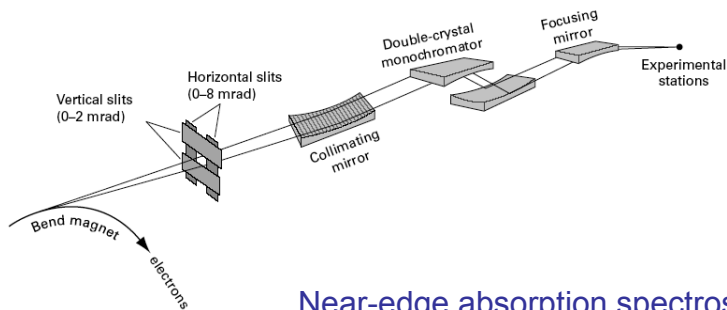
Schippers et al, J. Phys. B **73**, L209 (2004)

# Soft x-ray beamline at ALS

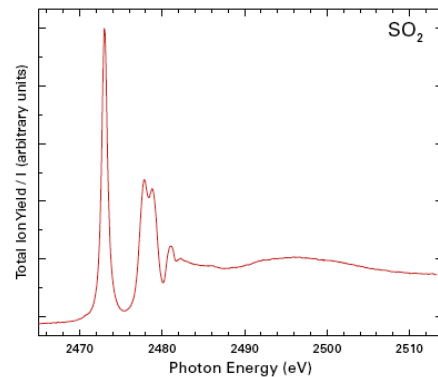
## Beamline Specifications

Photon Energy Range (keV)	Photon Flux (photons/s)	Spectral Resolution (E/ $\Delta$ E)	Spot Size (mm)	Availability
2.2–6.0 [with Si(111) crystals]	$>10^{11}$	3000–8000	$<0.5$	NOW

Electron beam 1.9 GeV: 1-T bend magnet. Photon energy range 2.3–5.5 keV with  $10^{11}$  photons/s and a resolving power up to 8000.



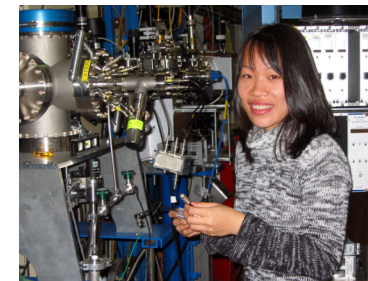
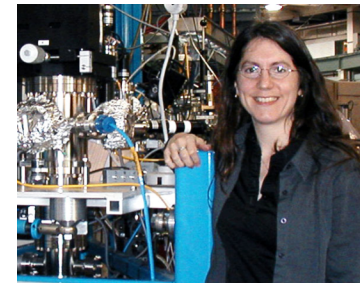
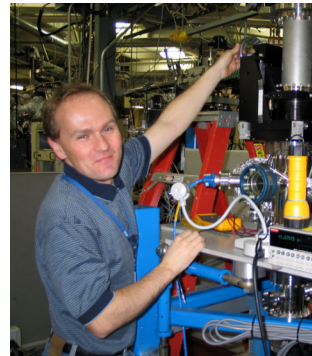
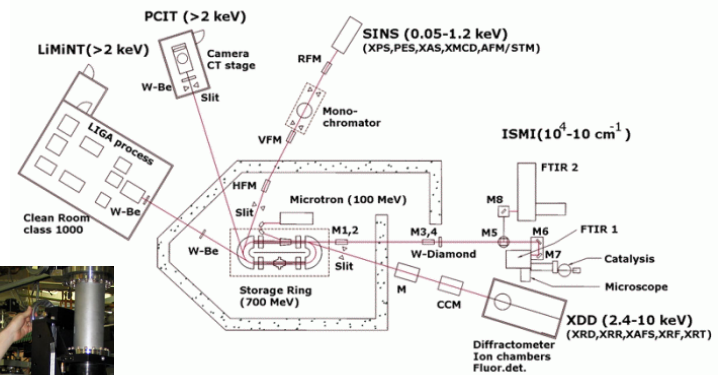
## Near-edge absorption spectroscopy



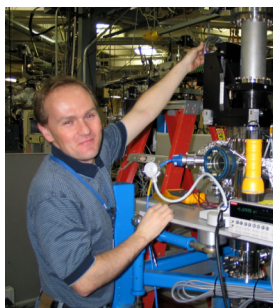
Electron beam 700 MeV

Dipole field 4.5 T

Characteristic energy 1.47 keV

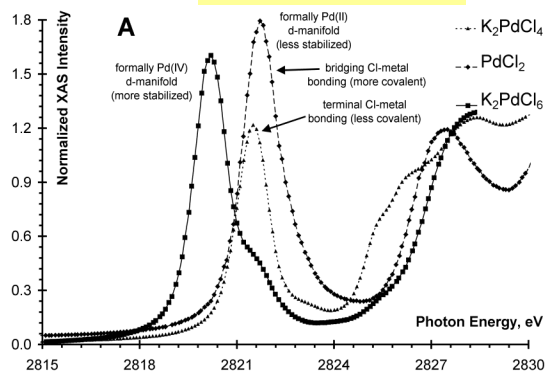


# Soft x-ray beamline at ALS: spectroscopy ...

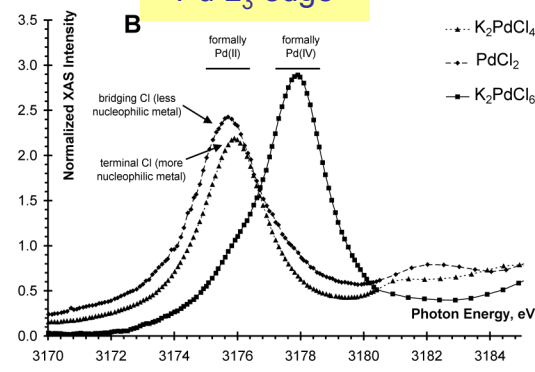


## Spectroscopy of Palladium Complexes

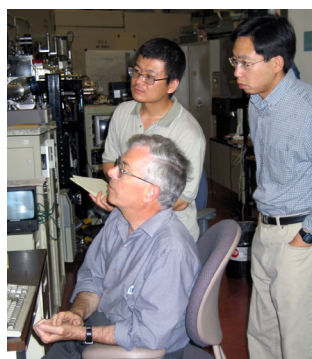
### Cl K edge



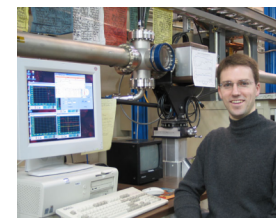
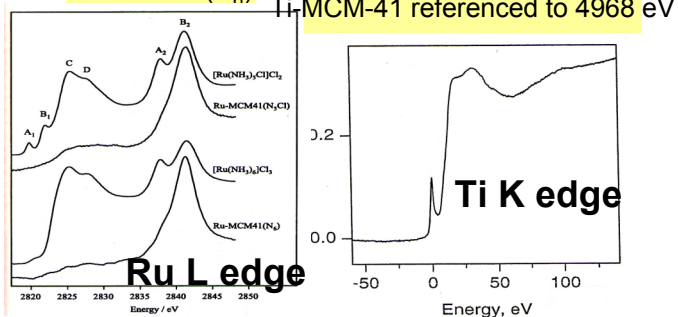
### Pd L<sub>3</sub> edge



## Catalysts: absorption studies of molecular sieves and zeolites



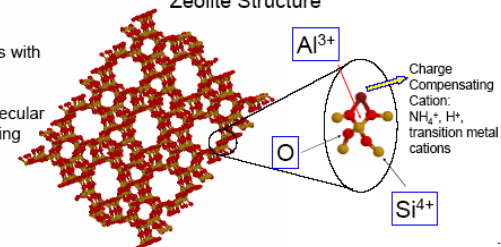
### Ru-MCM41(N<sub>6</sub>)



### Zeolites

- Crystalline aluminosilicates with interconnecting pores for diffusion of molecules
- Industrial Significance: Molecular sieve, Petrochemical cracking catalyst

### Zeolite Structure



# Synchrotron light sources are worldwide

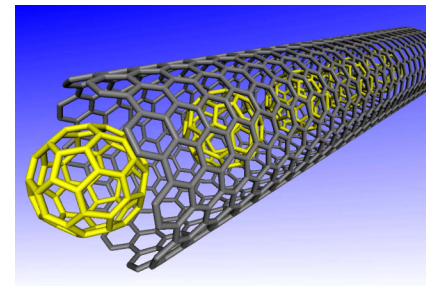
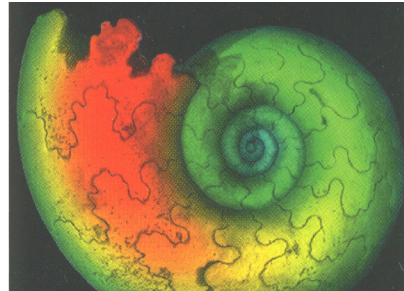


## Synchrotron Radiation Laboratories





Thanks....



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