El Sincrotón ALBA y la Ingeniería Química

Carles Solà

XXIX Jornadas de Ingeniería Química

Universitat Autònoma de Barcelona

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Agradecimiento

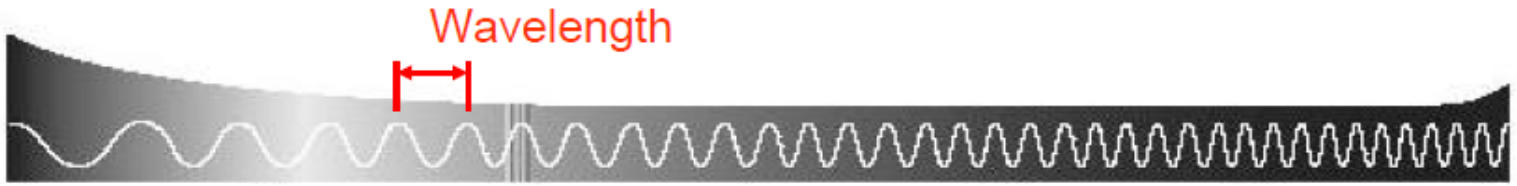
La inmensa mayor parte del material de esta presentación pertenece al Profesor Ramon Pascual de Sans, que ha tenido la amabilidad de proporcionarme.

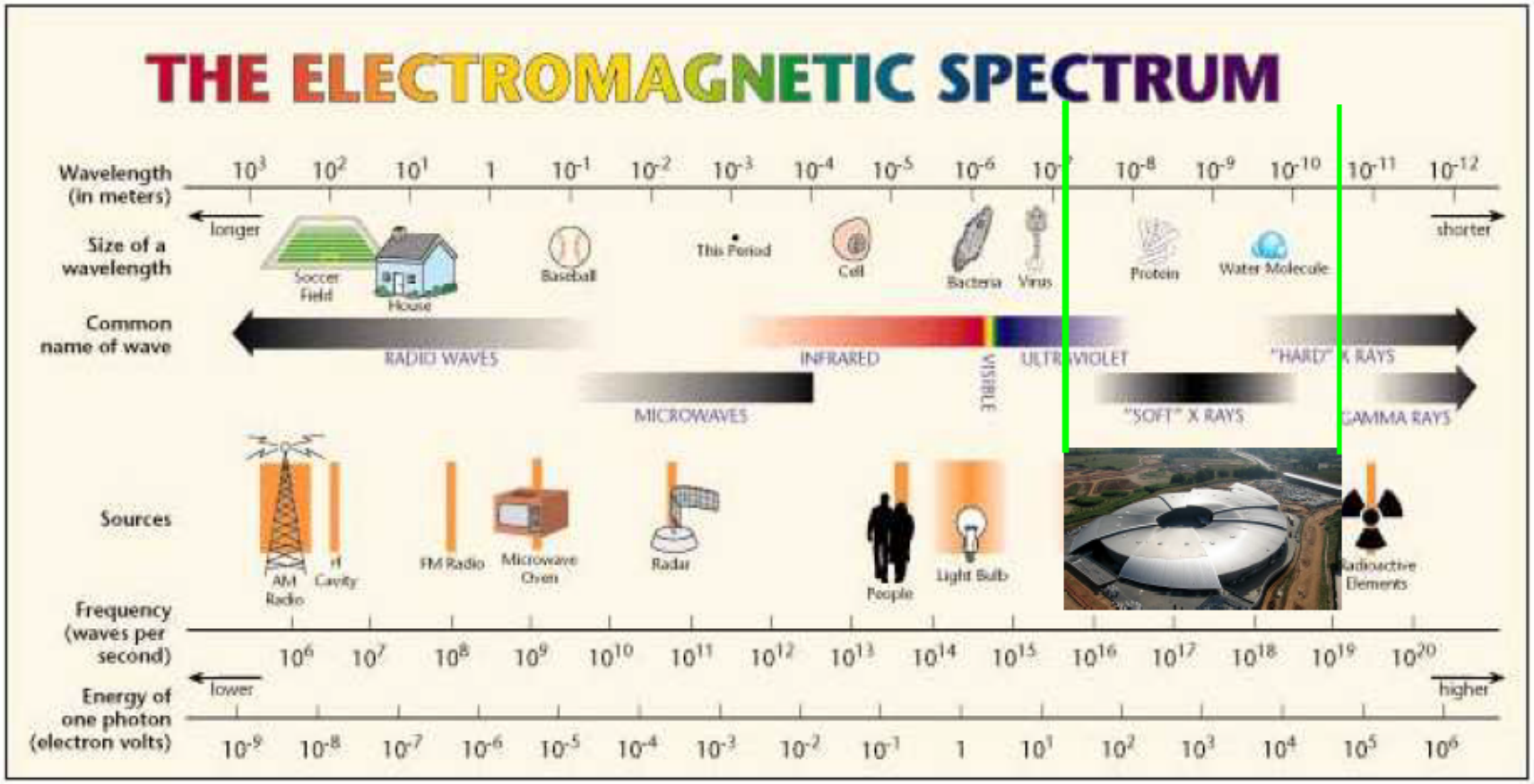
The ALBA Synchrotron Light Facility

R. Pascual
Chairman Executive Commission

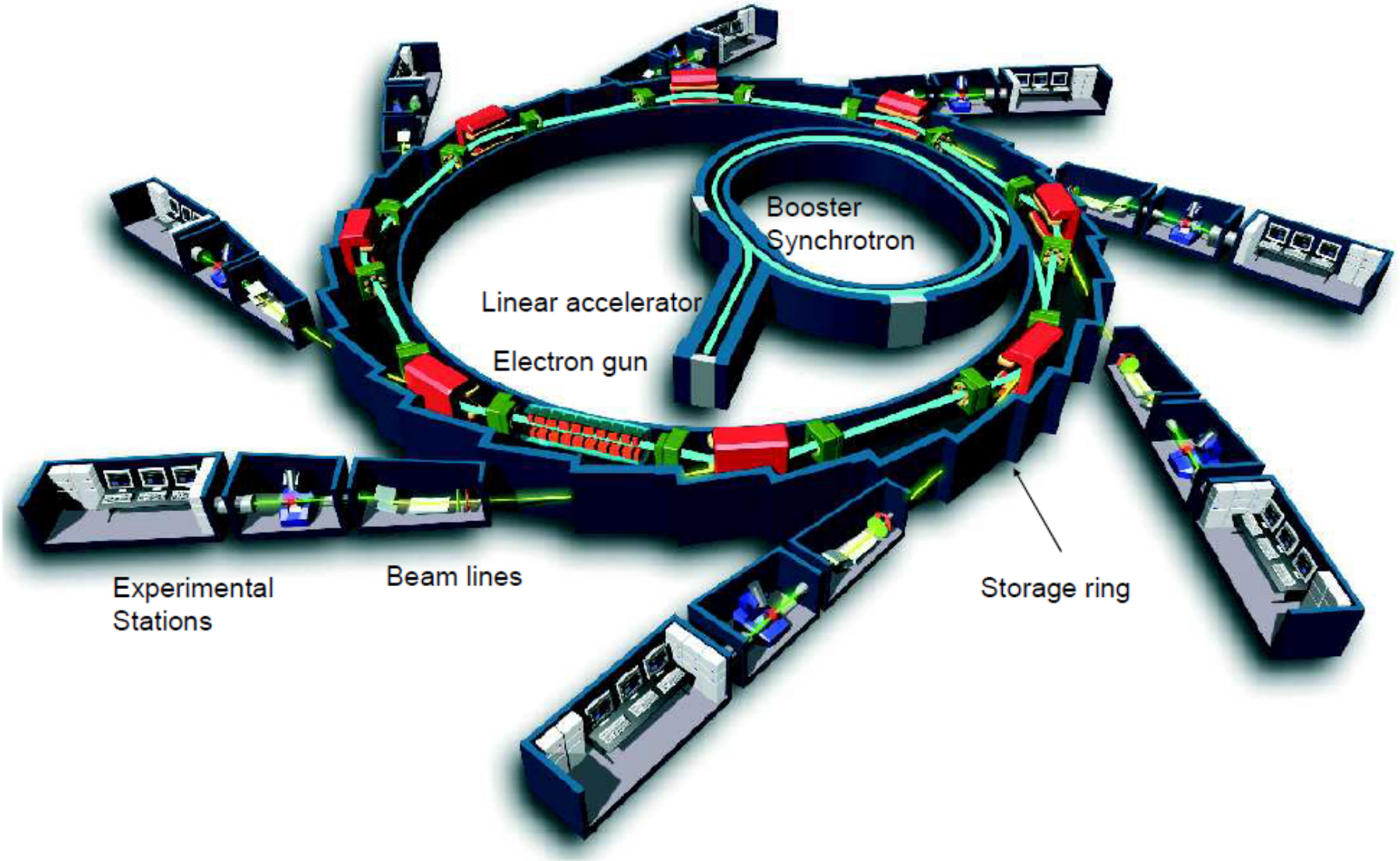
New projects in Spain

- Grantecan
- Synchrotron Light Source ALBA
  - To be operative in 2011
- Buque Oceanográfico SARMIENTO DE GAMBOA
- Centro Nacional de Investigación sobre la Evolución Humana (CENIEH, Burgos)
- Participation in the European Neutron Spallation Source (Bilbao)
- And the new "Instalaciones Científicas y Técnicas Singulares" decided in January 2007:
  - Mouse Clinic and Structural Biology Centre

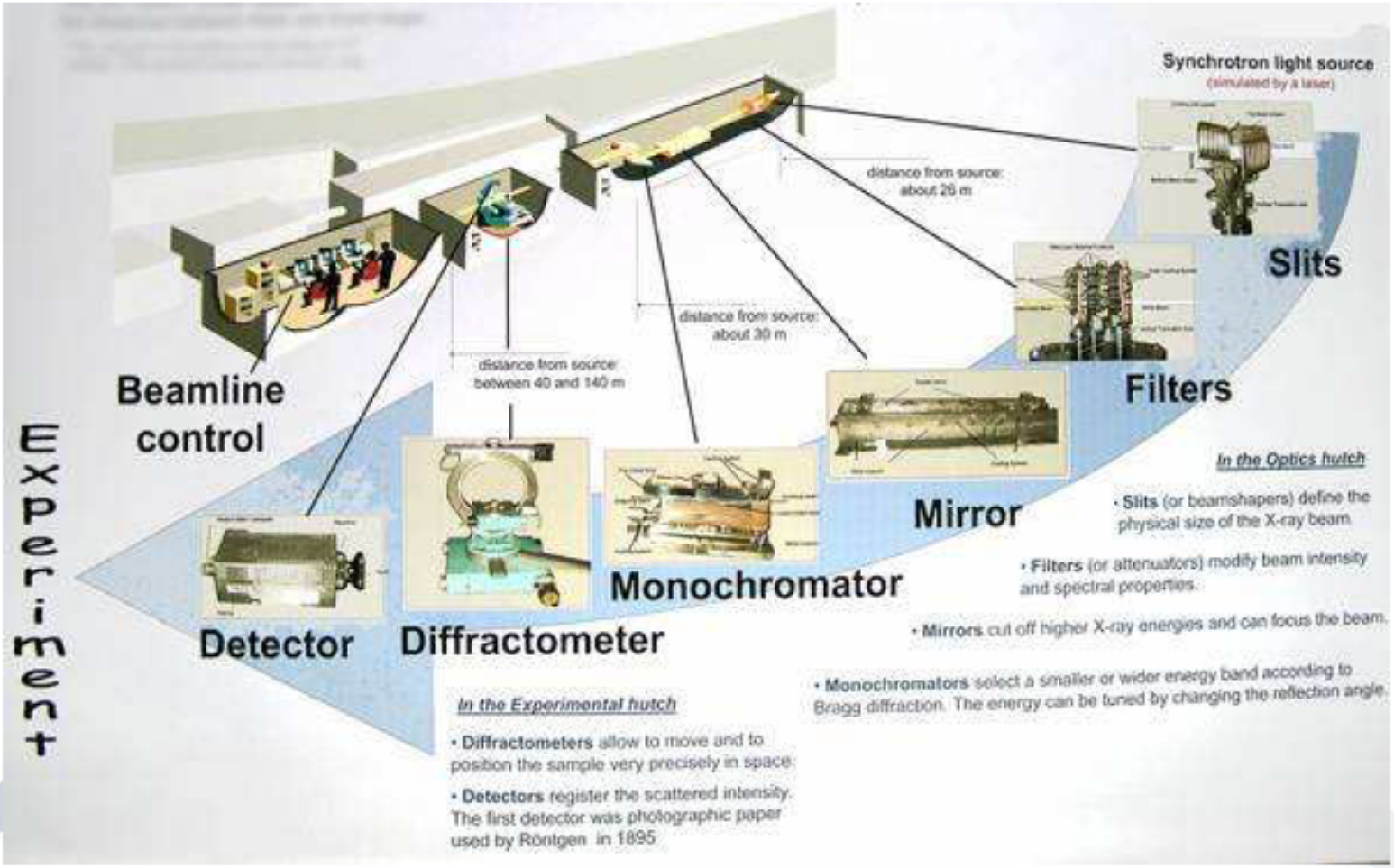

Wavelength


THE ELECTROMAGNETIC SPECTRUM
Wavelength (in meters)
longer
shorter
Size of a wavelength
Soccer Field
House
Baseball
This Period
Cell
Bacteria
Virus
Protein
Water Molecule
Common name of wave
RADIO WAVES
MICROWAVES
INFRARED
VISIBLE
ULTRAVIOLET
"SOFT" X RAYS
"HARD" X RAYS
GAMMA RAYS
Sources
AM Radio
rf Cavity
FM Radio
Microwave Oven
Radar
People
Light Bulb
Radioactive Elements
Frequency (waves per second)
lower
higher
Energy of one photon (electron volts)

Accelerator complex to produce SR



Beam Lines


Synchrotron light source
(simulated by a laser)
distance from source:
about 26 m
Slits
distance from source:
about 30 m
distance from source:
between 40 and 140 m
Beamline
control
Filters
Mirror
Monochromator
Detector
Diffractometer
Experiment
In the Optics hutch
• Slits (or beamshapers) define the physical size of the X-ray beam.
• Filters (or attenuators) modify beam intensity and spectral properties.
• Mirrors cut off higher X-ray energies and can focus the beam.
• Monochromators select a smaller or wider energy band according to Bragg diffraction. The energy can be tuned by changing the reflection angle.
In the Experimental hutch
• Diffractometers allow to move and to position the sample very precisely in space.
• Detectors register the scattered intensity. The first detector was photographic paper used by Röntgen in 1895

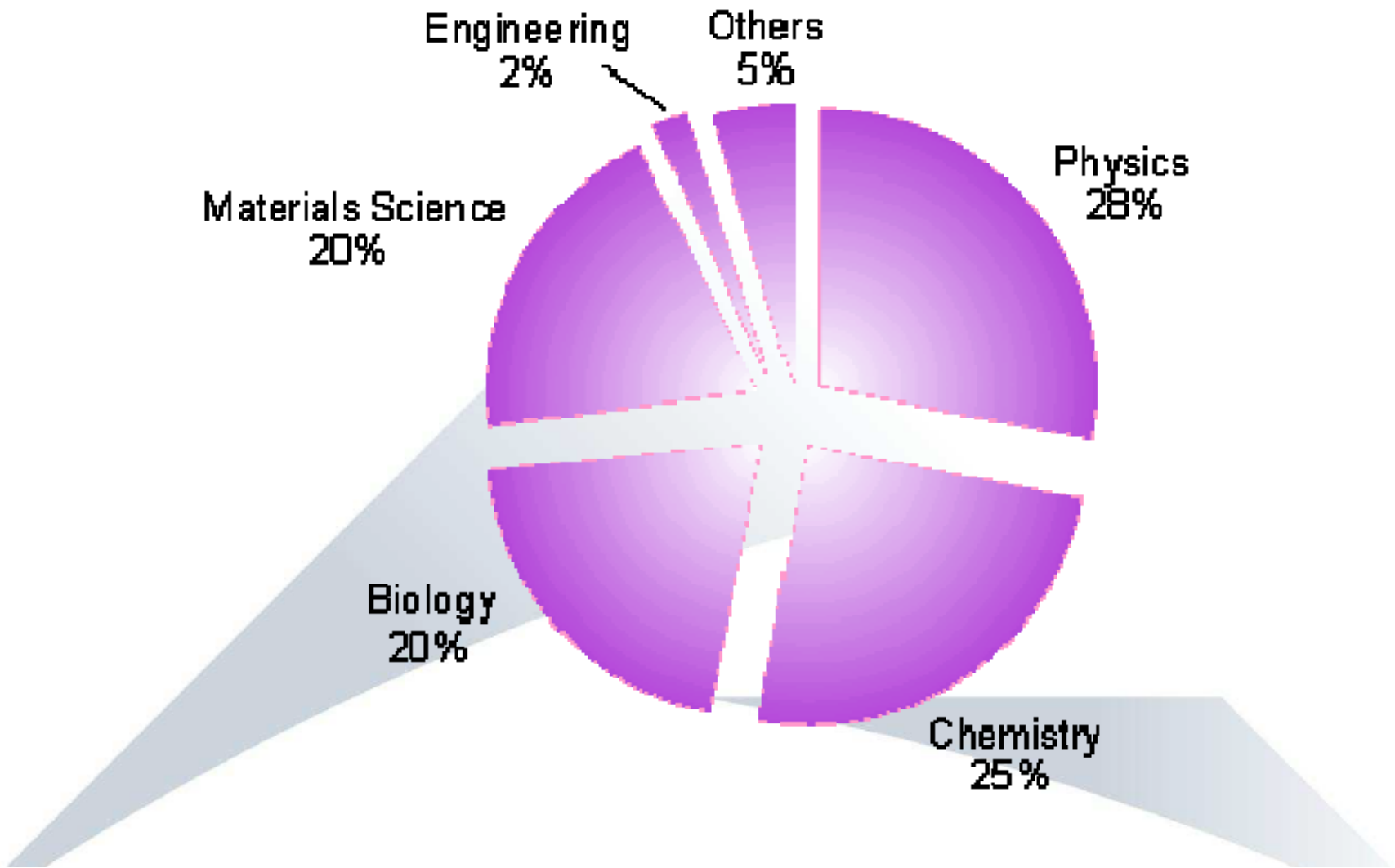
Fields of application

- **Basic Science**

- Physics
- Chemistry
- Material sciences
- Surfaces
- Life sciences
- Medicine
- Lithography & Microfabrication
- Metrology
- Cultural heritage
- Paleontology

- **Applied Science**

- Pharmacy and Health
- Alimentation
- Plastics
- Microelectronic
- Environment
- Metallurgy
- Cosmetics
- Textile and paper
- Construction


Engineering
2%
Others
5%
Physics
28%
Materials Science
20%
Biology
20%
Chemistry
25%

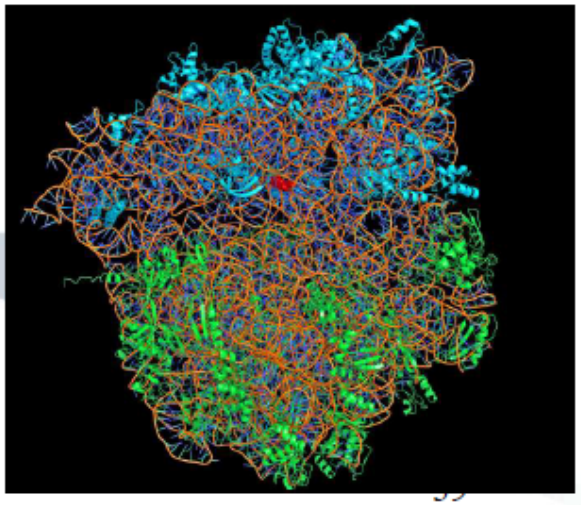
Venkatraman Ramakrishnan

Thomas A. Steitz

Ada E. Yonath

The Nobel Prize in Chemistry 2009

"for studies of the structure and function of the ribosome"



An X-ray structure of a bacterium ribosome. The rRNA-molecules are colored orange, the proteins of the small subunit are blue and the proteins of the large subunit are green. An antibiotic molecule (red) is bound to the small subunit. Scientists study these structures in order to design new and more effective antibiotics.

OTHER RELEVANT EXAMPLES OF DISCOVERIES WHERE SYNCHROTRON WORK WAS ESSENTIAL

- **1. ATP synthase**

In 1999, Sir John Walker was awarded the Nobel price for his studies of the ATP synthase (molecular biology.

- **2. Water and ion channels in cells and membranes**

In 2003, Peter Agre and Rodenick MacKinnon, were awarded the Nobel prize in Chem. for their studies of water flow on membranes and how cells communicate; this is important for a better understanding of the molecular pathways of disease.

- **3. Gene transcription, RNA**

In 2006, Roger Kornberg was awarded the Nobel Prize in Chem. for revealing the molecular basis of eukaryotic (gene) transcription

- **4. Foot and mouth virus**

In 2001, the "foot and mouth" disease cost UK 8 million pounds. Scientist of Oxford, Porton Down and company Wellcome Biotech used SR to study the 3D structure of this virus. That was very important for the development of vaccines.

- **5. Influenza drugs**

Dr. Peter Doherty, medical researcher and Nobel prize winner, recently comment that

"synchrotron light technology is currently central to about 80% of drug discovery and development".

The anti-influenza drug Relenza (trade mark) is the world's first structure-based anti-viral drug and an early example of rationally based drug design methodologies. RelenzaTM was developed in the mid-1990s by a CSIRO team led by Peter Coleman and Jose Varghese, using synchrotron protein crystallography.

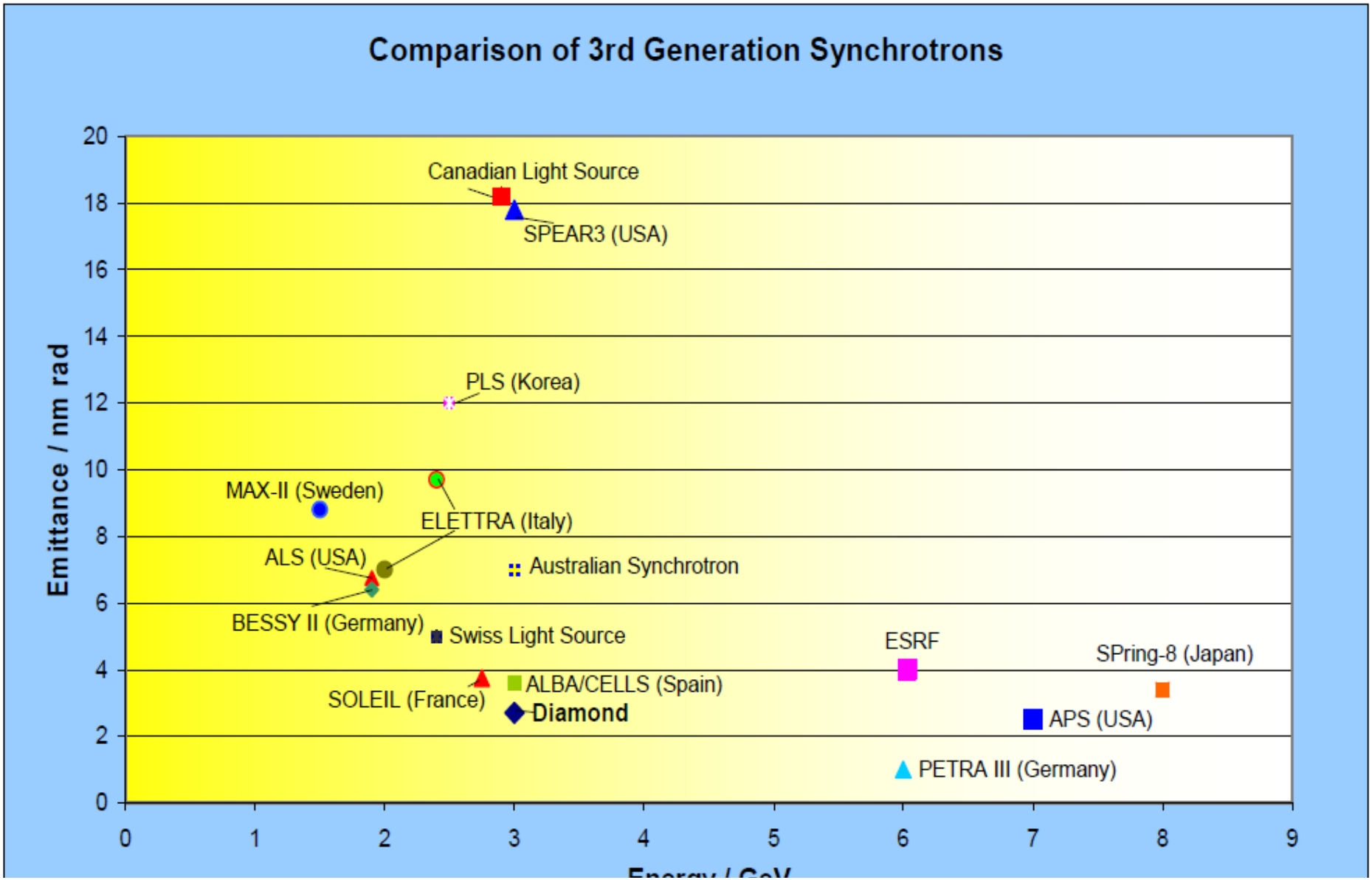
- **6. Flat liquid crystal displays**

Today's laptop computers utilize flat panel displays where the light transmission from the back to the front of the display is modulated by orientation changes in liquid crystal (LC) molecules (a $10 billion/year industry). Synchrotron studies guided development of new process for manufacture flat panel displays.


ISA
MAX LAB
DIAMOND
SRS
DESY
BESSY
FELIX
DELTA
ANKA
SOLEIL
SLS
ESRF
ELETTRA
ALBA

Parameters of the recent or European sources

Name and place	E GeV	Cells	Circumf.	Emit. H. nmrad
ANKA (Karlsruhe, GeV	2.5	8	110.4 m	80
SLS (Villengen, CH)	2.4	12	288.0 m	5
DIAMOND (Chilton, UK)	3.0	24	561.6 m	2.7
SOLEIL (Saint-Aubain, F)	2.5	24	354.0 m	3
ALBA (Cerdanyola)	3.0	16	268.8 m	<4


Comparison of 3rd Generation Synchrotrons
Emittance / nm rad
Energy / GeV
0
2
4
6
8
10
12
14
16
18
20
0
1
2
3
4
5
6
7
8
9
Canadian Light Source
SPEAR3 (USA)
PLS (Korea)
MAX-II (Sweden)
ELETTRA (Italy)
ALS (USA)
Australian Synchrotron
BESSY II (Germany)
Swiss Light Source
ESRF
SPring-8 (Japan)
SOLEIL (France)
ALBA/CELLS (Spain)
Diamond
APS (USA)
PETRA III (Germany)

Main steps of ALBA

- ✓ 1992: A Committee of the Generalitat (regional administration) order a viability study
- ✓ 1993: A Steering Committee is nominated and a training program is established
- ✓ 1995: Agreement between Spanish and Catalan governments to make a detailed study (within the IFAE)
- ✓ March 2002: Formal agreement between governments
- ✓ March 2003: A consortium CELLS is created
- ✓ June 2003: First meeting of the CELLS Council
- ✓ October 2003: Starts the activity

Main Steps in ALBA

- Geological studies of a possible site
- Socio-economic study
- Decision on the site and design of the executive project
- Establishment of the Advisory Boards (MAC and SAC)
- Selection of personnel and establishment of provisional headquarters (UAB)
- Final Detailed Design and contacts with technological companies
- Starting of civil works (May 2006, fast track method)
- Installation and commissioning of the linac (summer 2008)
- Final of civil works (end 2008)
- Starting of booster and SR installation (December 2008)
- First light production: end 2009
- Routine activities: end 2010

- (1+ 1 years latter than initially expected, with some 5% more than the expected budget)

Some figures about ALBA

- The electrons are accelerated in the booster in 150 ms, turning about tens of thousand turns
- The final velocity of the electrons of 3 GeV is 0,999 999 99 c
- The Lorentz factor (γ) is 6000
- At this velocity, the travel time of the electrons from the nearest by star Sirius (4 light years away) will be only 2 seconds shorter than its light
- Each bunch of electrons (of about 2 cm long and 1 μm wide) have a time length of the order of a few ps, separated by about 20 ns

Building requirements

- Very high mechanical stability to differential movements
- Very high electrical stability:
  - Redundant supply:
    - Connection to a 220 kV electric line through a dedicated transformer
    - Connection to a natural gas cogeneration plant for electrical and thermal energies
- Air conditioning with a variation of ±0.5ºC and ± 1ºC (depending of the zone)
- Static and dynamic (flying inertial wheels) continuity systems for the supply to the critical parts
- Very strict conditions to the deionised refrigeration water
- Controls by the “Consejo de Seguridad Nuclear”

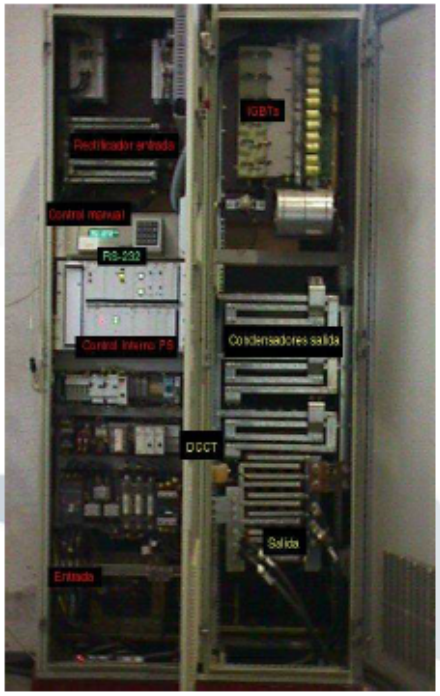
ALBA

CABLING (experimental stations excluded):

Booster and Storage ring:	**1200 cables - 30 Km.**
Cabling of the "timing" network:	**550 cables - 13 Km.**
Cabling of the network:	**4500 cables - 66 Km.**
Instrumentation cabling:	**7500 cables - 143 Km.**
Total:	**13750 cables - 252 Km.**
False floor:	**1000 m^2**

Implied Technologies

- Civil Engineering and security system
- Electromagnets
  - Power supplies
  - Refrigeration
  - Electrical Materials
  - Precision Mechanics
- Electronics and Radiofrequency
- Ultra-High Vacuum Techniques
- Instrumentation
  - Accelerator
  - Beam Lines
  - Insertion Devices (Wigglers and Undulators)
- Computation and control
  - Software
  - Hardware
- Diagnostic Systems
- Optical Systems
- Services
- Cryogenics



Budget and Characteristics

- Total budget: 201 M€ (including personnel and running costs from 2003 to 2009)
- Annual starting budget since 2010: 16 M€
- Personnel: 138
- Around 1000 users per year (for the first phase beam lines)
- Atraction of companies and new investments: (XFEL, Centro de Biología Estructural,…)

80 M€

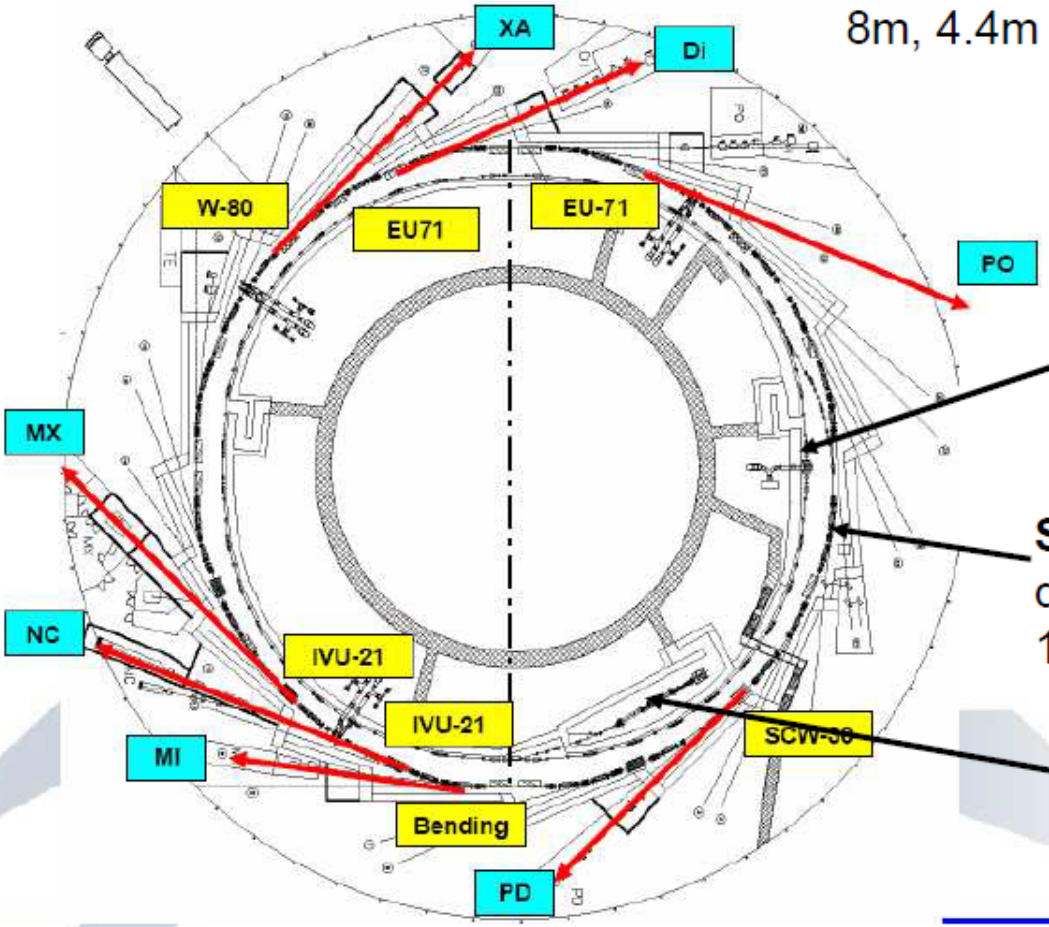
65 M€

La Vanguardia,
20 June 2010

75 M€

55 M€

16 straight sections of
8m, 4.4m and 2.6 m long



Booster: 3 GeV, 250 m
4 fold symmetry
emittance smaller **20 nm·rad**

Storage ring: 268 m
double bend achromat lattice
16 cells with 4 fold symmetry

Linac: 100 MeV
At 3 GHz
Repetition rate of 3Hz

First phase of beamlines: operative in second half of 2011

Port	Beam-line	Experimental techniques	Scientific applications
4	**MSPD** (SCW-30)	Materials Science and Powder Diffraction	Structure of Materials, Time resolved diffraction
9	**MISTRAL** (BM)	X-ray microscopy.	Cryogenic tomography of biological objects. Spatially resolved spectroscopy
11	**NCD** (IVU-21)	Non-Crystalline Diffraction	Structure and phase transformations of biological fibers, polymers, solutions. Time resolved X-ray studies
13	**XALOC** (IVU-21)	Macromolecular Crystallography	Protein crystallography, with particular emphasis on large unit cell crystals
22	**CLÆSS** (MPW-80)	Core Level Absorption & Emission Spectroscopies	Material Science, Chemistry, Time resolved studies
24	**CIRCE** (EU-62)	Photoemission Spectroscopy and Microscopy Photoemission microscopy (PEEM) Near atmospheric pres. Photoem. (NAPP)	Nano-science and magnetic domain imaging (PEEM). Surface chemistry (NAPP)
29	**BOREAS** (EU-71)	Resonant Absorption and Scattering	Magnetism, surface magnetism and magnetic structure

Indicators of the Financial Analysis in the baseline scenario *

Indicators	
VAN** (5%)	30,7 Mil. €
VAN (4%)	**58,5 Mil. €**
VAN (2,5%)	114,8 Mil. €
B/C***	1,14
TIR****	6,5%

*The basic scenario considers an inflation rate of 2.5%, a discount rate of 4%, 230 days of annual operation of the facility and 5 years until saturation

** Valor Actualizado Neto (Net Actualized Value)

***Benefit/Cost

***Tasa Interna de Rentabilidad (Internal Rate of Return)

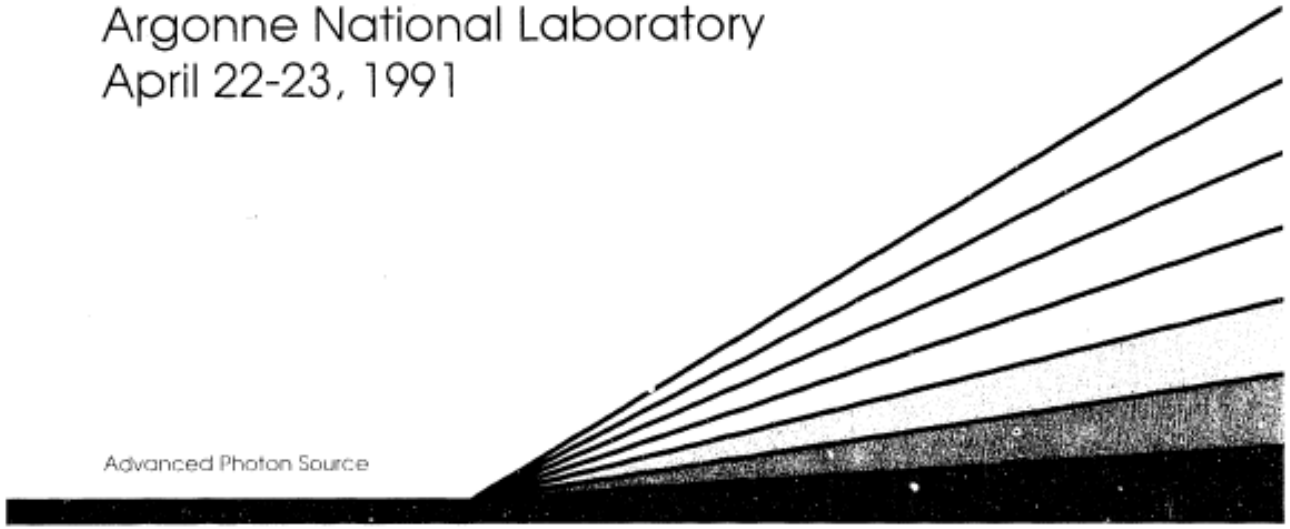
The Economical Impact of ALBA. España
Milions of 2003 euros

	Investment (2003-08)	Operation (2009-33)	Total (2003-33)
Gross Production	266	735	1.001
Added Value	140	417	557
Employment	463	257	720

- From these (and other) studies we can say that, in numbers, the returns from the collaborations with “big science” centres present average multiplier factors in the range from 2.7 (ESA) to 3.7 (CERN)

Applications of Synchrotron Radiation to Chemical Engineering Science: Workshop Report

Proceedings of a workshop held at
Argonne National Laboratory
April 22-23, 1991



Argonne National Laboratory
operated by The University of Chicago for the U.S. Department of Energy under Contract W-31-109-Eng-38

CONTENTS

User Facilities

Basic Energy Sciences

Advanced Scientific Computing Research

Basic Energy Sciences

Biological and Environmental Research

Fusion Energy Sciences

High Energy Physics

Nuclear Physics

Frequently Asked Questions

CONTACT US

Office of Science
U.S. Department of Energy
1000 Independence Ave., SW

The Basic Energy Sciences program supports the operation of the following User Facilities:

Synchrotron Radiation Light Sources

- National Synchrotron Light Source (NSLS):
  The NSLS at Brookhaven National Laboratory, commissioned in 1982, consists of two distinct electron storage rings. The x-ray storage ring is 170 meters in circumference and can accommodate 60 beamlines or experimental stations, and the vacuum-ultraviolet (VUV) storage ring can provide 25 additional beamlines around its circumference of 51 meters. Synchrotron light from the x-ray ring is used to determine the atomic structure of materials using diffraction, absorption, and imaging techniques. Experiments at the VUV ring help solve the atomic and electronic structure as well as the magnetic properties of a wide array of materials. These data are fundamentally important to virtually all of the physical and life sciences as well as providing immensely useful information for practical applications.

- Stanford Synchrotron Radiation Lightsource (SSRL):
  The SSRL at SLAC National Accelerator Laboratory was built in 1974 to take and use for synchrotron studies the intense x-ray beams from the SPEAR storage ring that was originally built for particle. The facility is used by researchers from industry, government laboratories, and universities. These include astronomers, biologists, chemical engineers, chemists, electrical engineers, environmental scientists, geologists, materials scientists, and physicists. A research program is conducted at SSRL with emphasis in both the x-ray and ultraviolet regions of the spectrum. SSRL scientists are experts in photoemission studies of high-temperature superconductors and in x-ray scattering. The SPEAR 3 upgrade at SSRL provided major improvements that increase the brightness of the ring for all experimental stations.

Catalysis Science

Portfolio Description

This activity develops the fundamental scientific principles enabling rational catalyst design and chemical transformation control. Research includes the identification of the elementary steps of catalytic reaction mechanisms and their kinetics; construction of catalytic sites at the atomic level; synthesis of ligands, metal clusters, and bio-inspired reaction centers designed to tune molecular-level catalytic activity and selectivity; the study of structure-reactivity relationships of inorganic, organic, or hybrid catalytic materials in solution or supported on solids; the dynamics of catalyst structure relevant to catalyst stability; the experimental determination of potential energy landscapes for catalytic reactions; the development of novel spectroscopic techniques and structural probes for *in situ* characterization of catalytic processes; and the development of theory, modeling, and simulation of catalytic pathways. Capital equipment funding is provided for items such as ultrahigh vacuum equipment with various probes of interfacial structure, spectroscopic analytical instrumentation, and specialized cells for *in situ* synchrotron-based experiments, and computational resources.

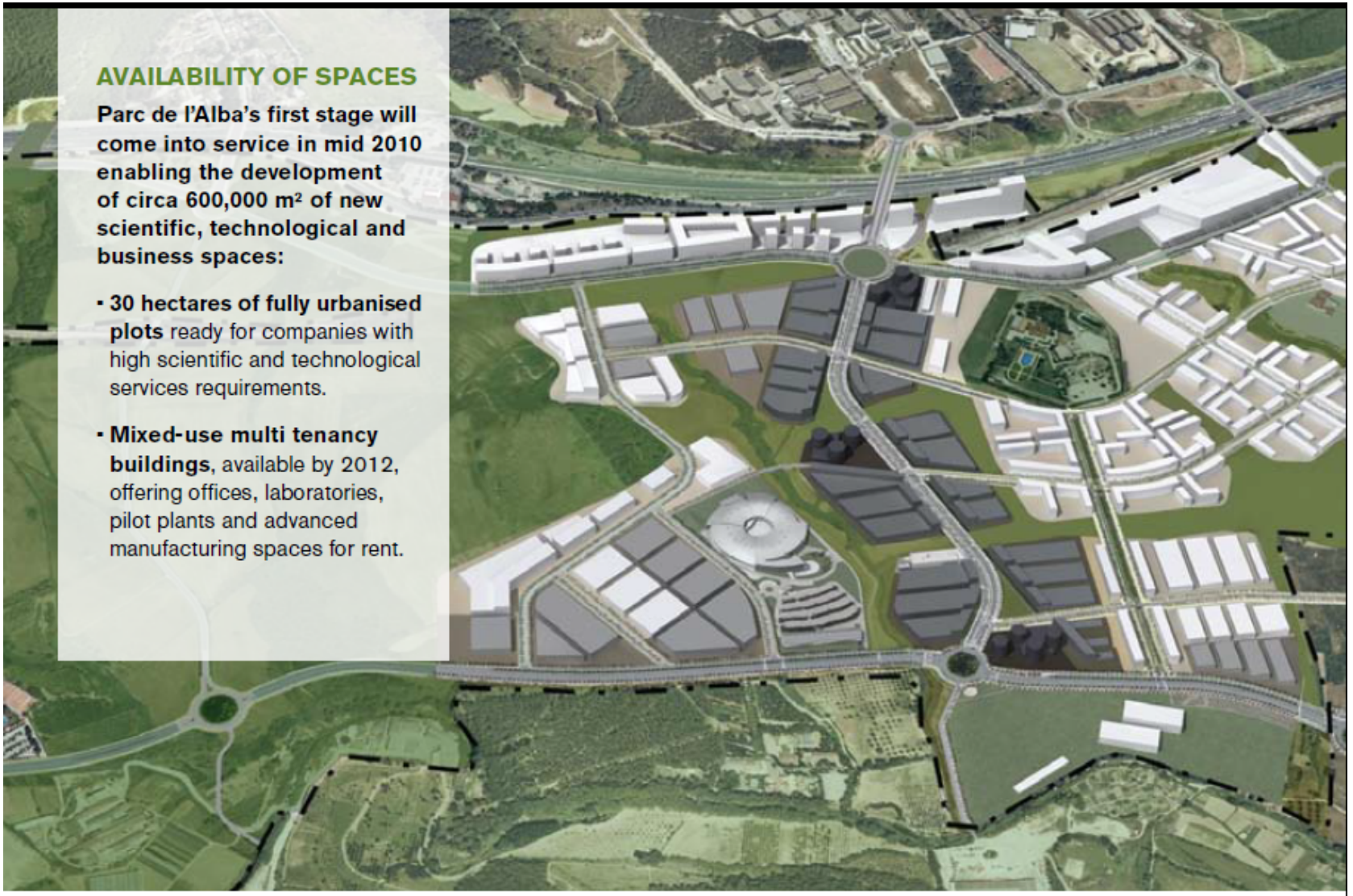
Unique Aspects

This activity funds the largest fraction of basic research in catalysis in the Federal government. It seeks to cross the barriers between heterogeneous, homogeneous, and bio catalysis. The integration promotes synergism among disciplines and innovation in fundamental approaches as well as applications. Multidisciplinary approaches are encouraged by means of multi-PI grants. This program encourages the use of large-scale facilities at DOE national laboratories to significantly advance catalysis research.

PARC DE L'ALBA
SCIENCE AND TECHNOLOGY PARK

BARCELONA SYNCHROTRON PARK

Parc de l'Alba Science and Technology Park sets your business in the right environment to build alliances with top research and technology centres, prestigious universities and business schools, and market leading companies.



AVAILABILITY OF SPACES

Parc de l'Alba's first stage will come into service in mid 2010 enabling the development of circa 600,000 m² of new scientific, technological and business spaces:

- **30 hectares of fully urbanised plots** ready for companies with high scientific and technological services requirements.
- **Mixed-use multi tenancy buildings**, available by 2012, offering offices, laboratories, pilot plants and advanced manufacturing spaces for rent.

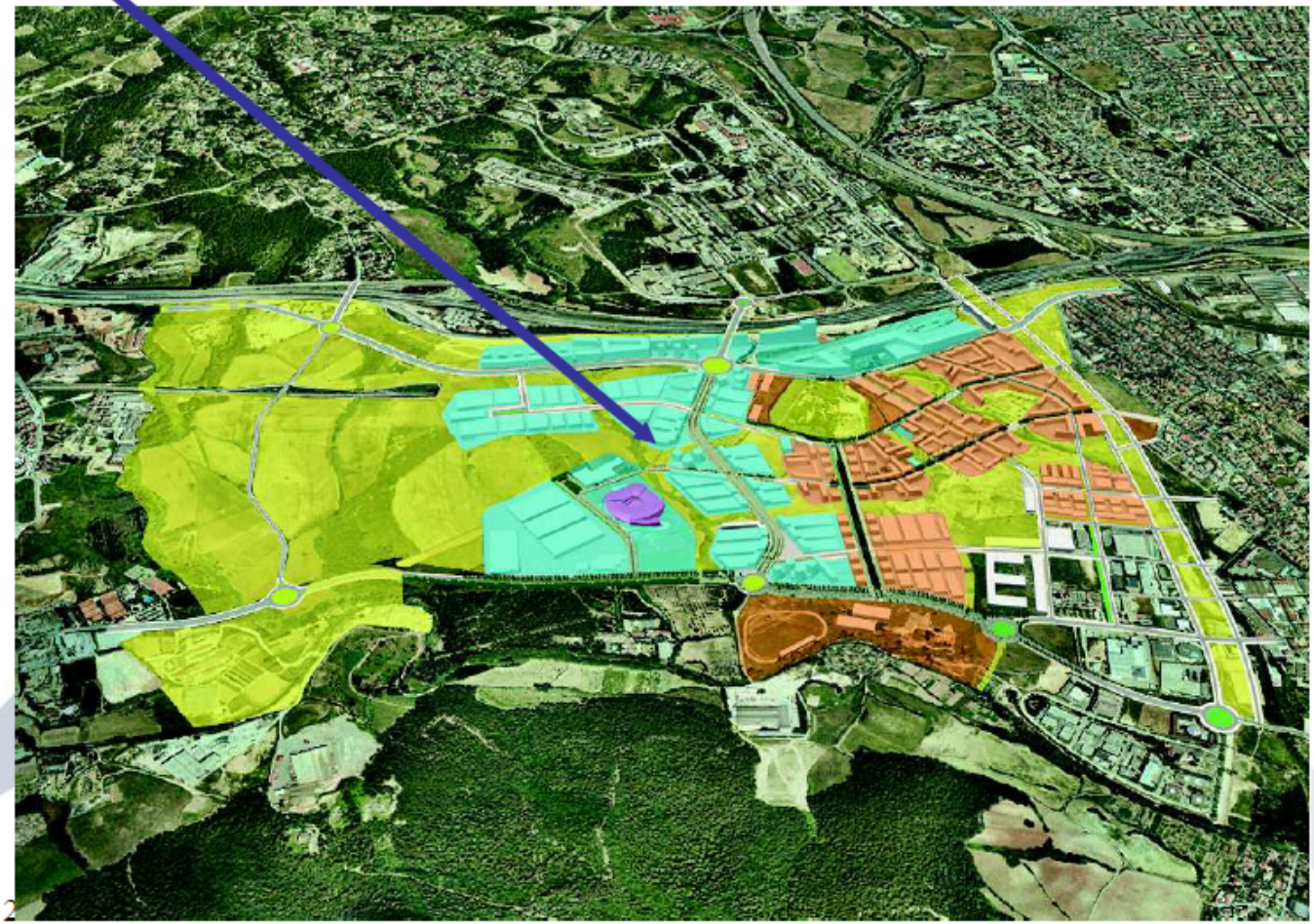
PARC DE L'ALBA'S 1ST STAGE

Science avenue	Total building area	Plot size area	Buildable floor space	Built spaces (2012)
Science & technology transfer centres	80,000 m²	7,000 - 11,000 m²	22,000 - 30,000 m²	200 - 10,000 m²
Knowledge-based companies	300,000 m²	4,000 - 10,000 m²	9,000 - 19,000 m²	200 - 10,000 m²

ALBA

Parc de l'ALBA

ALBA
2 technical buildings of La Caixa
Centre de Biologia Estructural



PARCDEL'ALBA

CONSORCI URBANÍSTIC
DEL CENTRE DIRECCIONAL
DE CERDANYOLA DEL VALLÈS

Ajuntament de Cerdanyola del Vallès

INCASÒL Institut Català del Sòl

CASTELLANO ◆ CATALÀ

1st PHASE: UNIVERSITY CAMPUS

2nd PHASE: TECHNOLOGY PARK

3rd PHASE: SYNCHROTRON
SCIENCE AND TECHNOLOGY PARK
RESIDENTIAL NEIGHBOURHOOD
GREEN AREAS

PARCDEL'ALBA

CONSORCI URBANÍSTIC
DEL CENTRE DIRECCIONAL
DE CERDANYOLA DEL VALLÈS

Ajuntament de Cerdanyola del Vallès

INCASÒL
Institut Català del Sòl

Bloqueja...

SCIENCE AVENUE

CONSORCI URBANÍSTIC
DEL CENTRE DIRECCIONAL
DE CERDANYOLA DEL VALLÈS

Ajuntament de Cerdanyola del Vallès

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CASTELLANO ◆ CATALÀ

PARCDEL'ALBA

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- AVENUES AND STREETS
- URBAN SERVICES
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- HOUSING
- NATURAL SPACES

POLY-GENERATION PLANT

1 2 3 4 5