Investigación fundamental en materiales: desde aplicaciones en energía a las grandes facilidades en América Latina (Sirius-LAHN)

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Outline

R&D at the Materials Characterization Department

- R&D in SOFC: Solid Oxide Fuel Cells
- Materials in SOC: solid oxides ionic or mixed conductors.
- One example: Cathode/Anode Nano LSTC for symmetric cells

New Latin-American Big Science Facilities

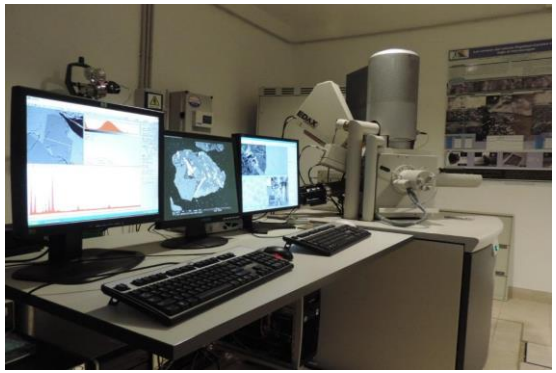
- Why BIG SCIENCE facilities in LA (Latin-America)?
- Big science projects
  - The LAHN Project
  - The SIRIUS Project

Remarks

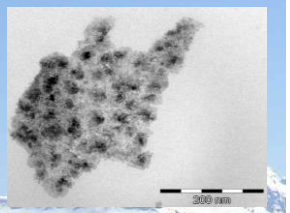
R&D Departamento Caracterización de Materiales

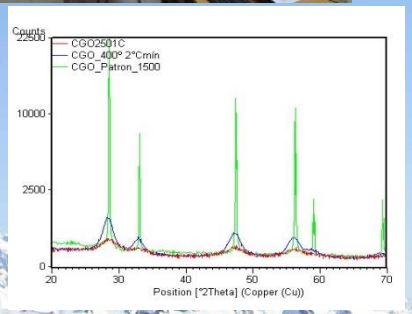
SERVICIOS

SEM Scanning Electron Microscope

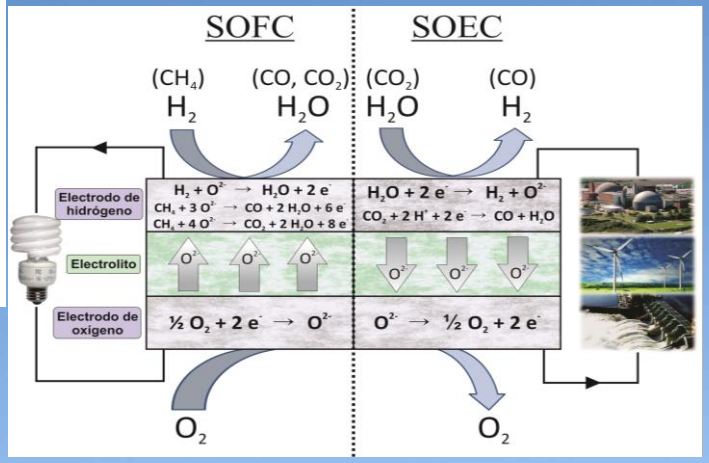


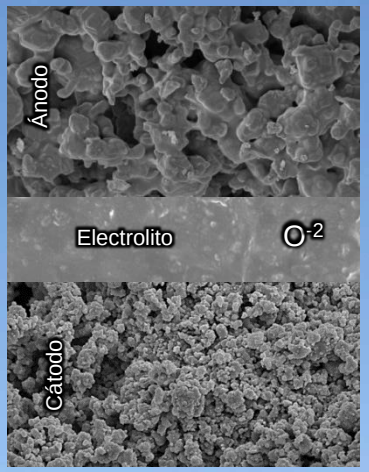
XRD Powder X-ray diffraction



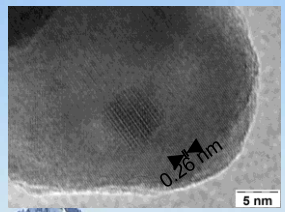


Desarrollo y síntesis de NUEVOS materiales (en particular óxidos cerámicos y composites Me/óxido y óxido/óxido con diferentes micro y nanoestructura porosos, densos)



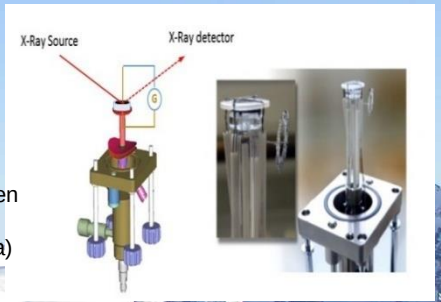


Aplicaciones : energía, producción y almacenamiento



Diseño y construcción de equipos/sistemas de medición

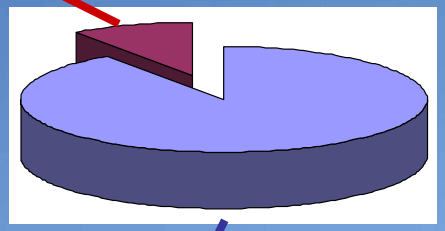
específicos para estudiar propiedades de materiales en condiciones no ambientales (alta temperatura, atmósfera) acoplados con técnicas de sincrotón



Por qué materiales para energías limpias

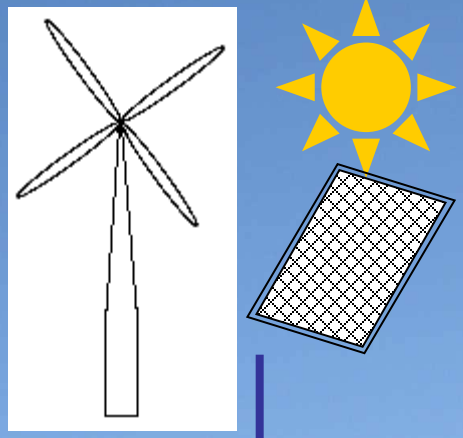
Los combustibles fósiles tienen que ser reemplazados

Generación Argentina*



Petróleo, gas (carbon) 90%

- No - renovables
- Emisión de gases de efecto invernadero



inttermitentes

H_2

- Producción
- Almacenamiento
- Uso
  - Electrolizadores
  - Pilas de combustible

Conversión de energía eficiente

* Fuente Secretaría de Energía Argentina (2015)

Reversible! SOC (Solid Oxide Cell)

MODO COMBUSTIBLE

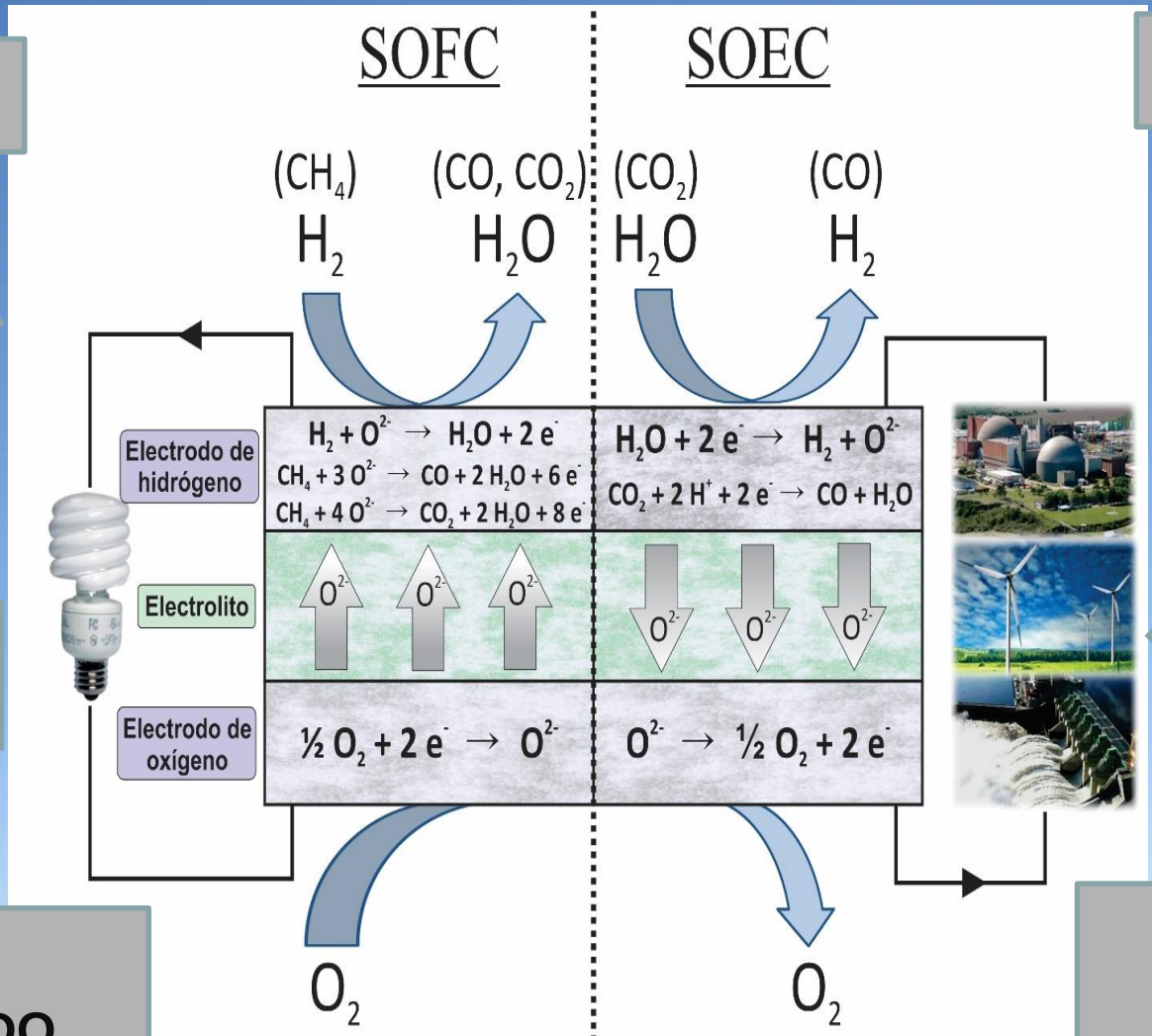
MODO ELECTROLIZADO

COMBUSTIBLES

H_2, CO, CH_4

Electricidad + Calor

CICLO COMBINADO



COMBUSTIBLES

H_2, CO, CH_4

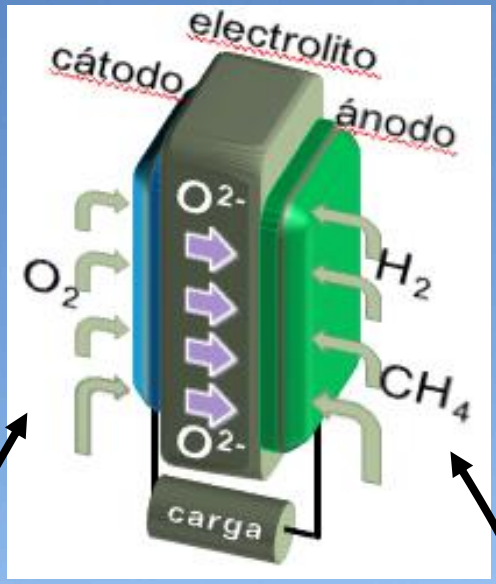
Electricidad + Calor

FUENTE PRIMARIA

Electrodos: SOFC

Cátodo

- Catalizador de reacción de reducción de O2
- Buen conductor electrónico
- Buen conductor iónico



Ánodo

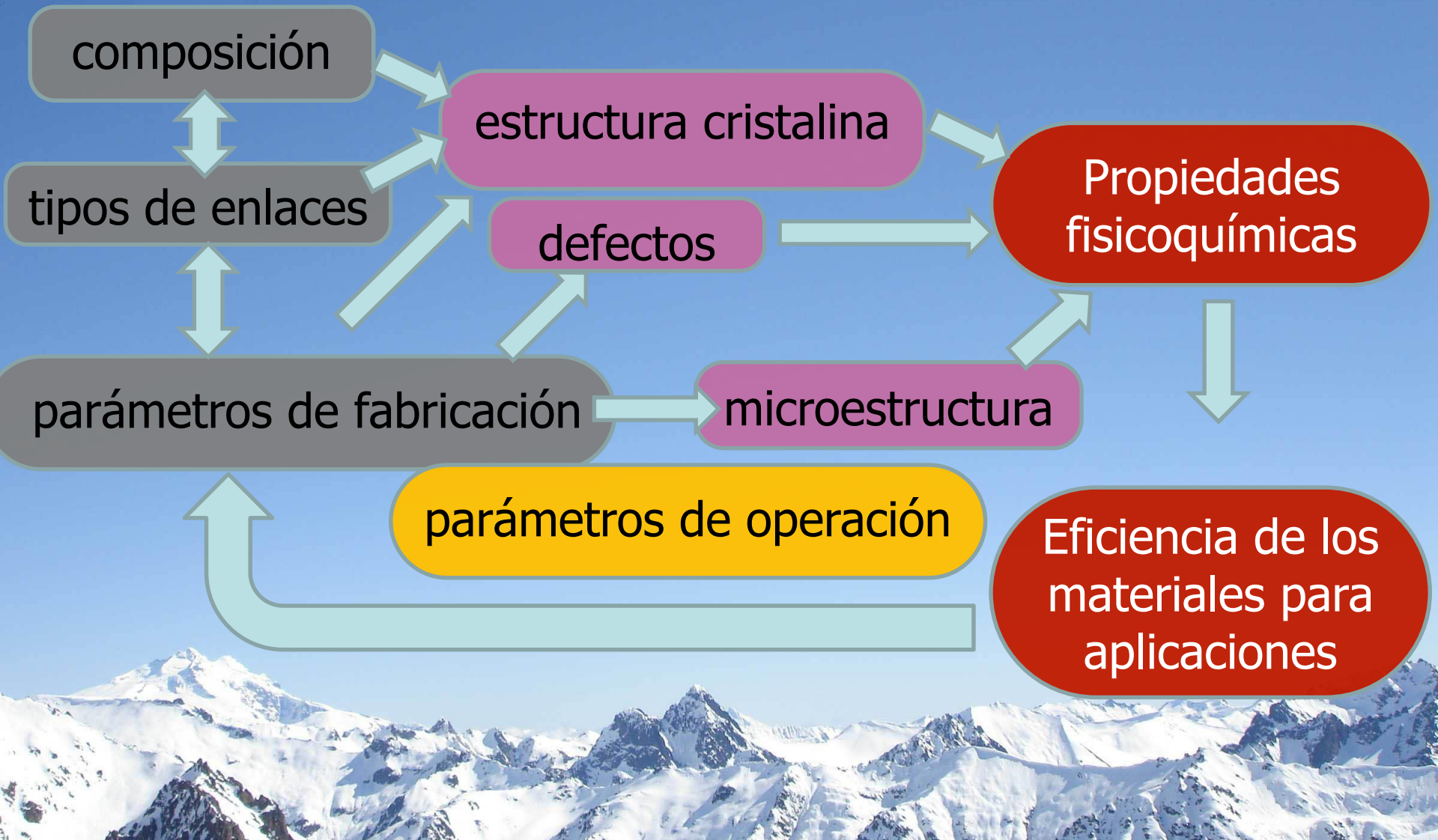
- Catalizador de reacción de oxidación del combustible
- Buen conductor electrónico
- Buen conductor iónico

$$O_2 + 4e^- \rightarrow 2O^{2-}$$

$$2H_2 + 2O^{2-} \rightarrow 2H_2O + 4e^-$$

$$CH_4 + H_2O \rightarrow 3H_2 + CO$$

R&D en materiales



R&D en materiales

Óxidos

- perovskitas
- fluoritas
- Ruddlesden
-Popper

Caracterización cristalográfica

Microscopía electrónica(SEM, TEM)
Difracción de Rayos-X y Neutrones
Métodos de radiación sincrotrón
(XANES, EXAFS, etc)

Propiedades electroquímicas

técnicas in-situ/in-operando

SOC: celdas de óxido sólido

R&D en materiales

Búsqueda
(de nuevos materiales)

Nuevos métodos:

Perovskitas

$(La,Sr)(Fe,Co)O_{3-\delta}$

$SrFe_{0.7}Ti_{0.3}O_{3-\delta}$ with nanoparticles

$(La,Sr)(Cr,Mn)O_{3-\delta}$

Double perovskites

$LnBaCo_2O_{6-d}$ (Ln = La, Nd, Pr)

$SrFe_{0.7}Ti_{0.3}O_{3-\delta}$ (STF)

Sr_2MgMoO_6

Ruddlesden-Popper

Ln_2NiO_{4+d} (Ln = La, Nd,

Fluorites

$Ce_{0.9}Gd_{0.1}O_2$

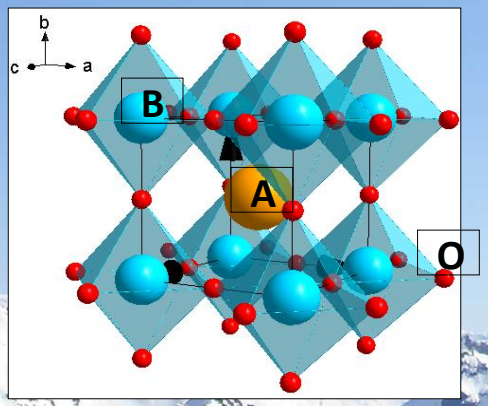
Nuevos compuestos:

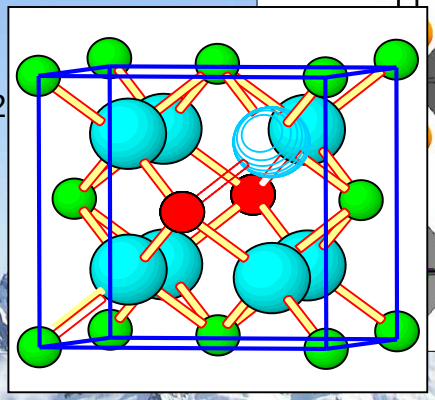
$La_{0.6}Sr_{0.4}Ti_{1-x}Co_xO_{3\pm\delta}$

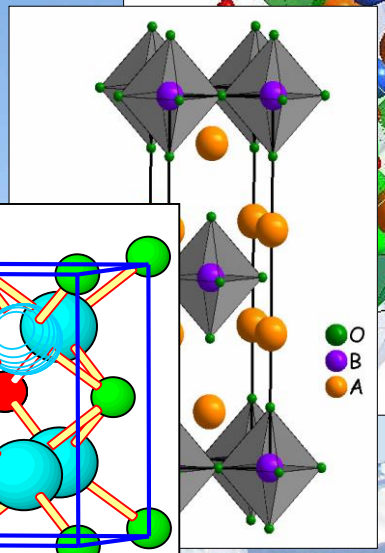
$Sr_2MgMo_{1-x}Co_xO_{6-d}$

$Sr_2MgMo_{1-x}Mn_xO_{6-d}$

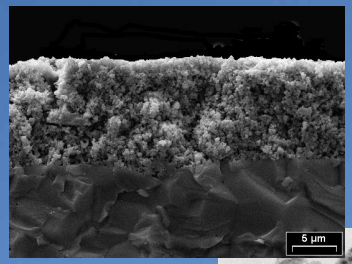
Perovskita ABO_3

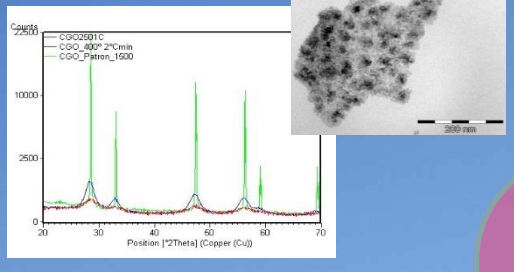






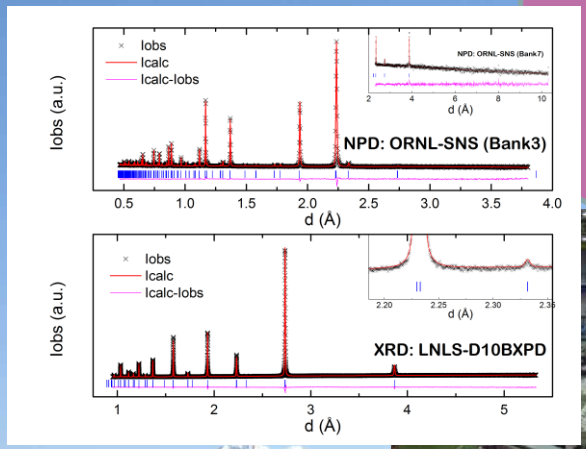
R&D en materiales

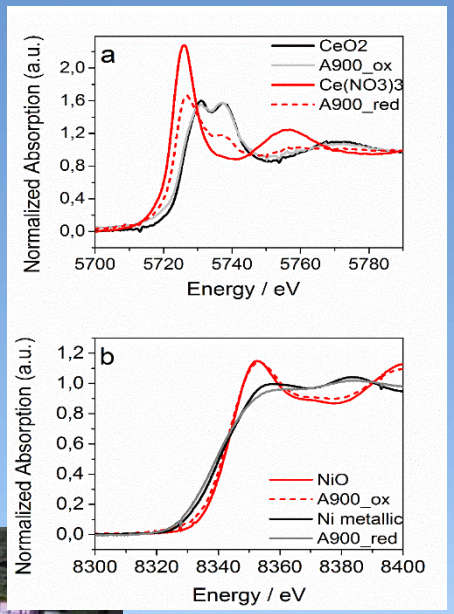




Caracterización cristalográfica

Microscopía electronica (SEM, TEM)
Difracción de RX (XRD)
Difracción de neutrones (NPD)
Métodos de radiación sincrotrón
(XANES, EXAFS, etc)

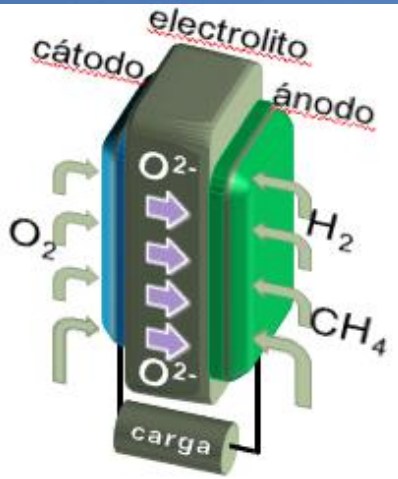


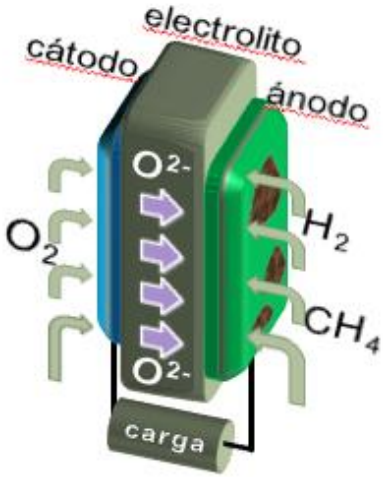


D10B-XPD
D08B-XAFS2

Un ejemplo: SOFC Simétricas

SOFC





Las SFC tienen la capacidad inherente de invertir la función de los electrodos

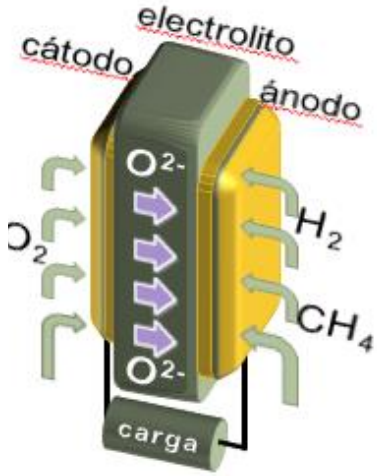
ánodo ⟷ cátodo

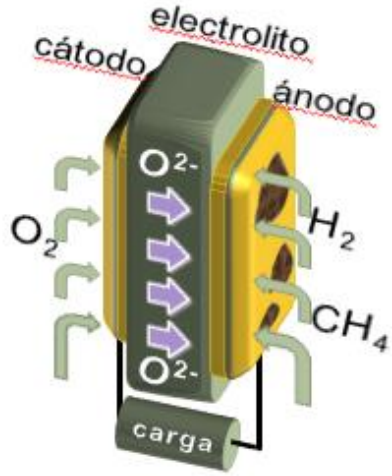
Lo cual permite remover el C depositado en el ánodo durante la operación

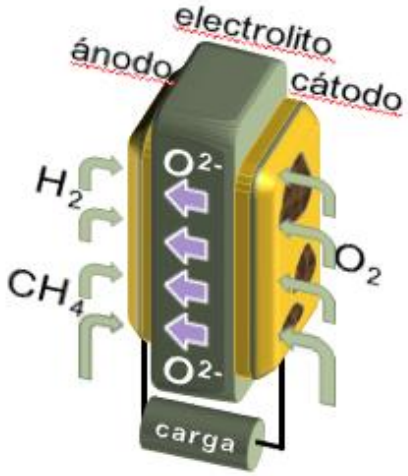
$(La,Sr)TiO_3$ $(La,Sr)CoO_3$

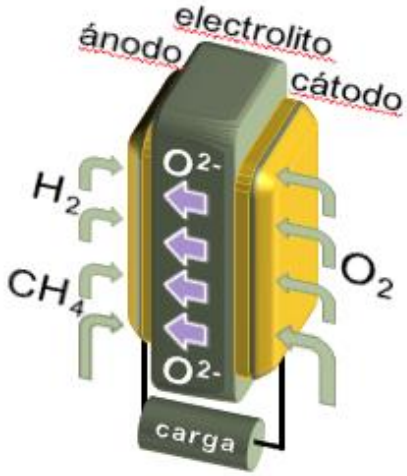
Tiempo de operación

SSOFC



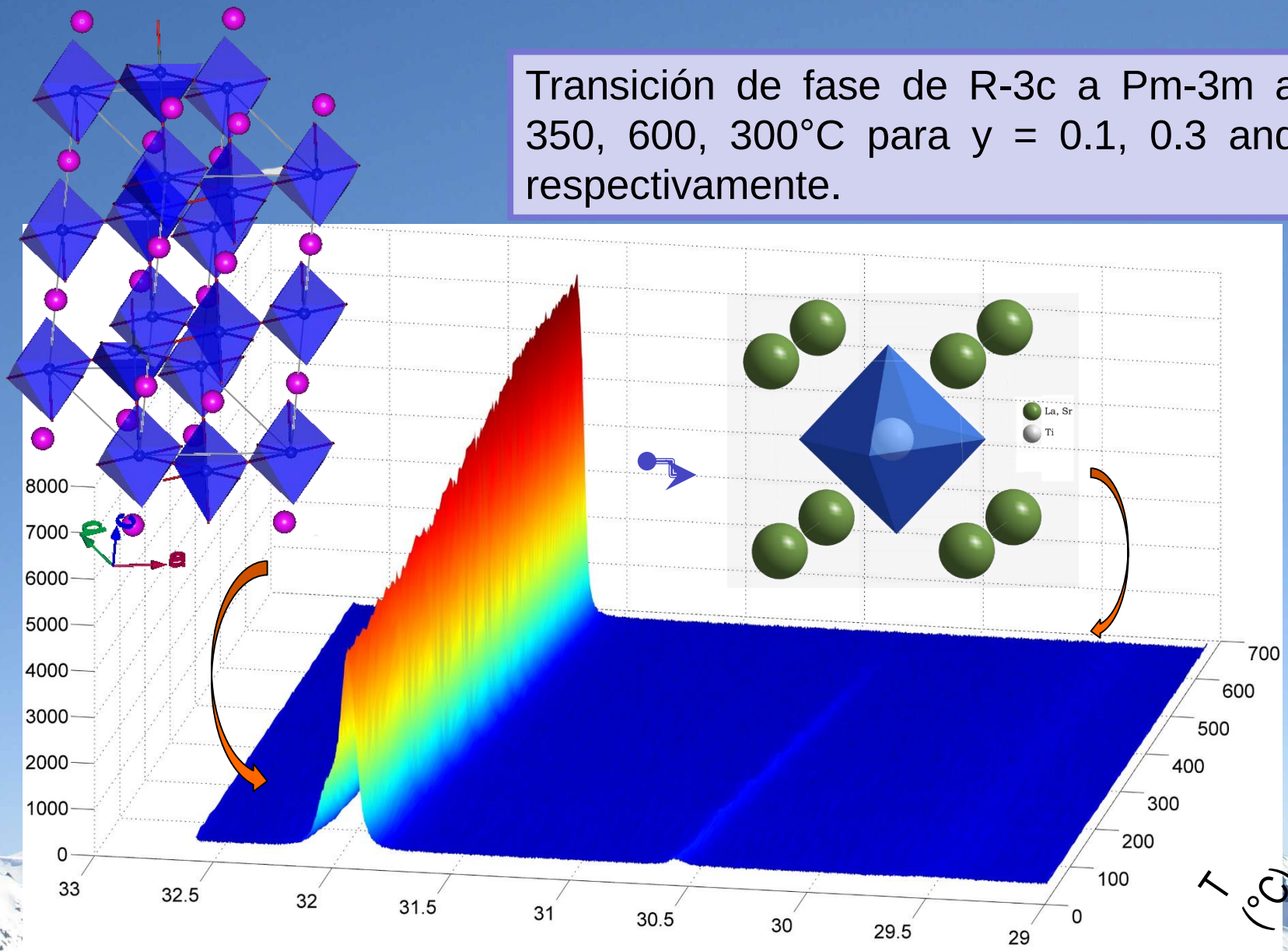




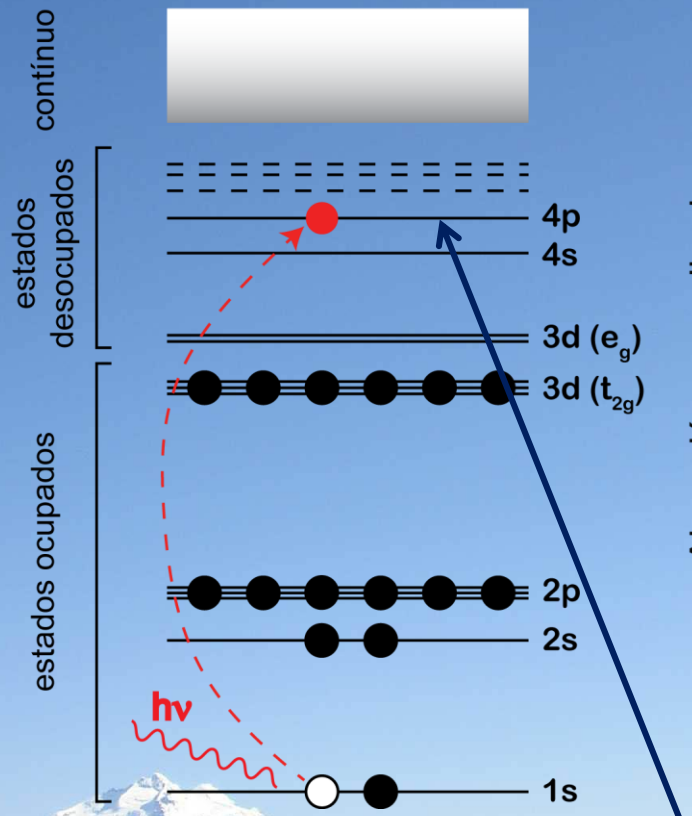


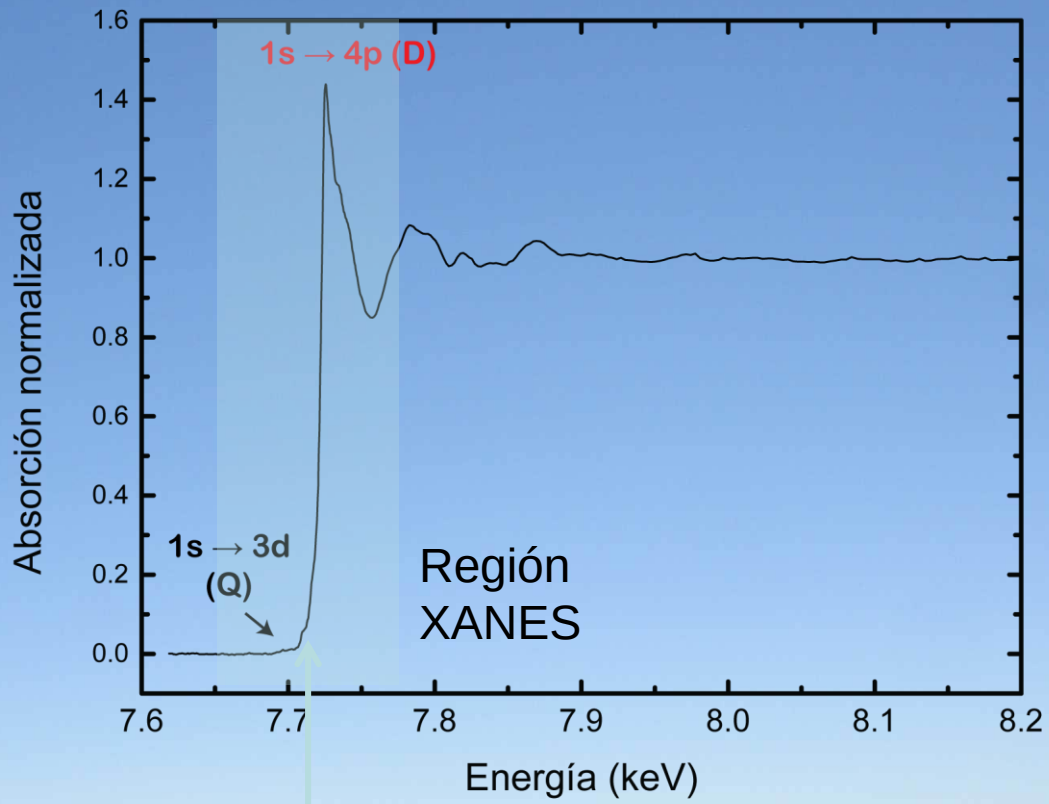
Determinación de estructura

Transición de fase de R-3c a Pm-3m a T ~ 350, 600, 300°C para y = 0.1, 0.3 and 0.5, respectivamente.



Espectroscopía de Absorción (XANES)

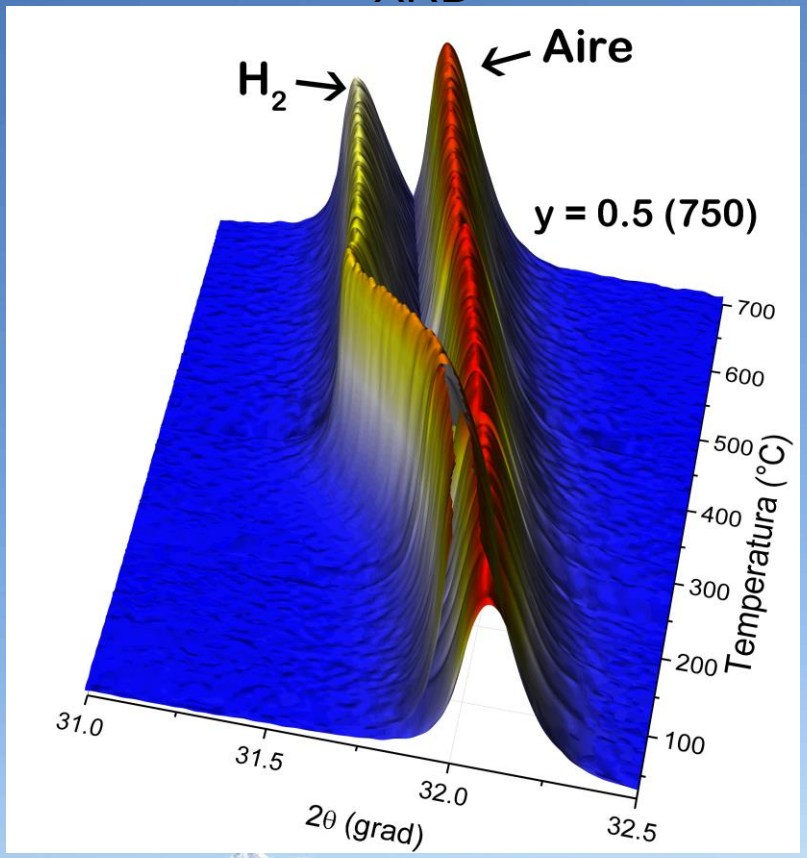




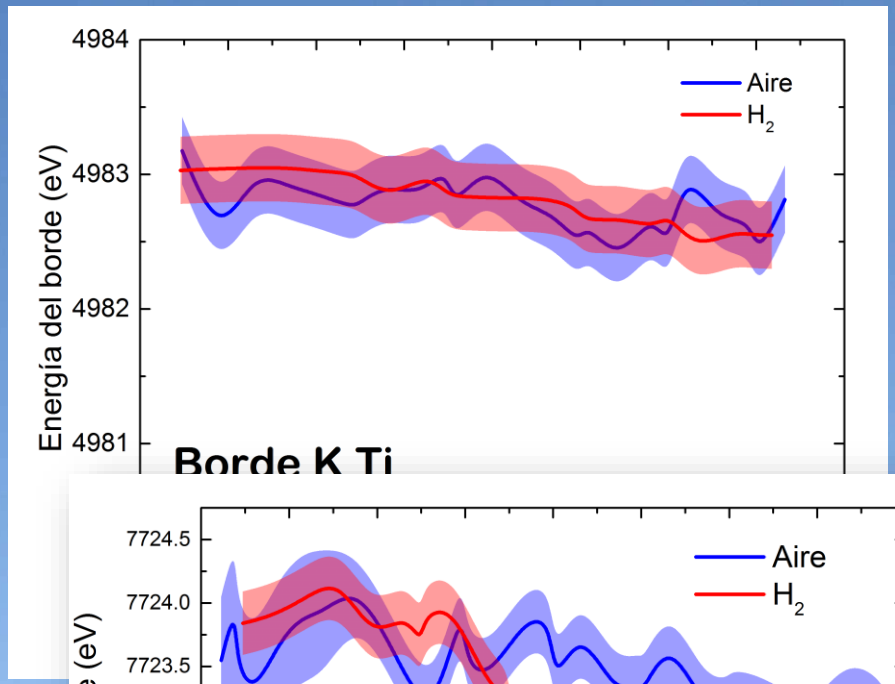
Depende del entorno local del átomo absorbente

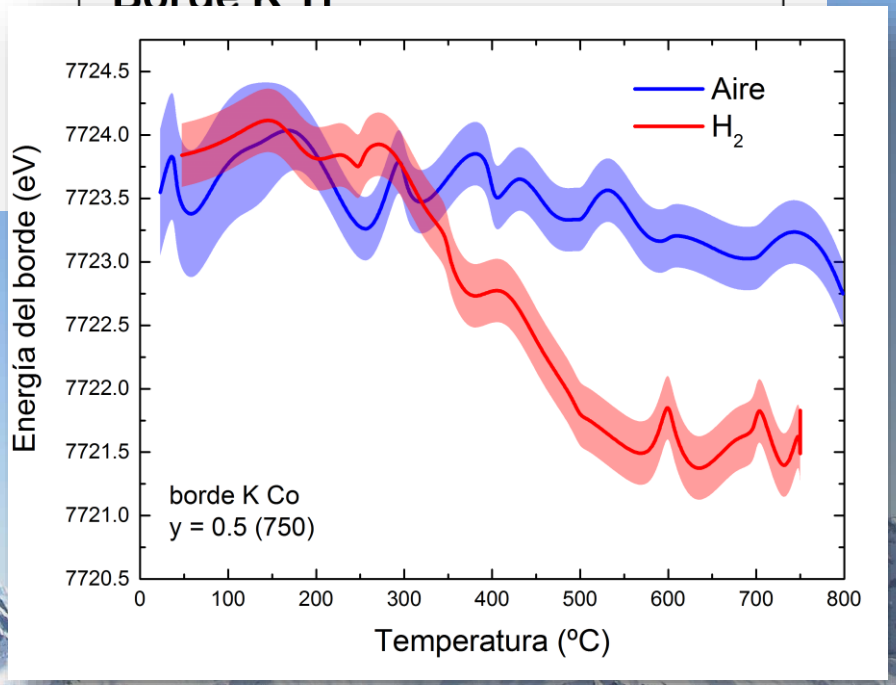
XRD y XANES *in-situ*

XRD



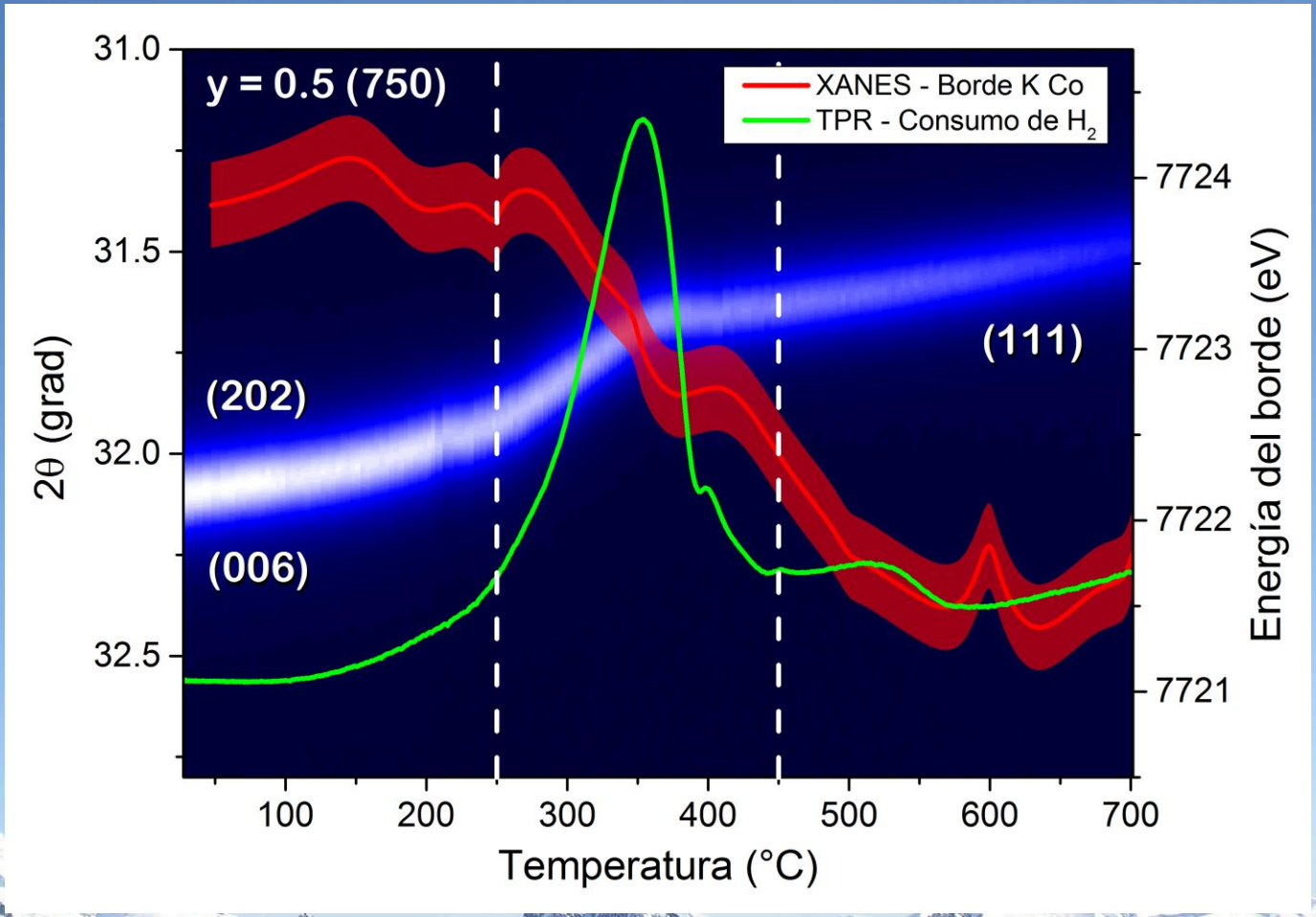
XANES





$La_{0.6}Sr_{0.4}Ti_{0.5}Co_{0.5}O_{3\pm\delta}$

Correlación resultados XRD – XANES – TPR

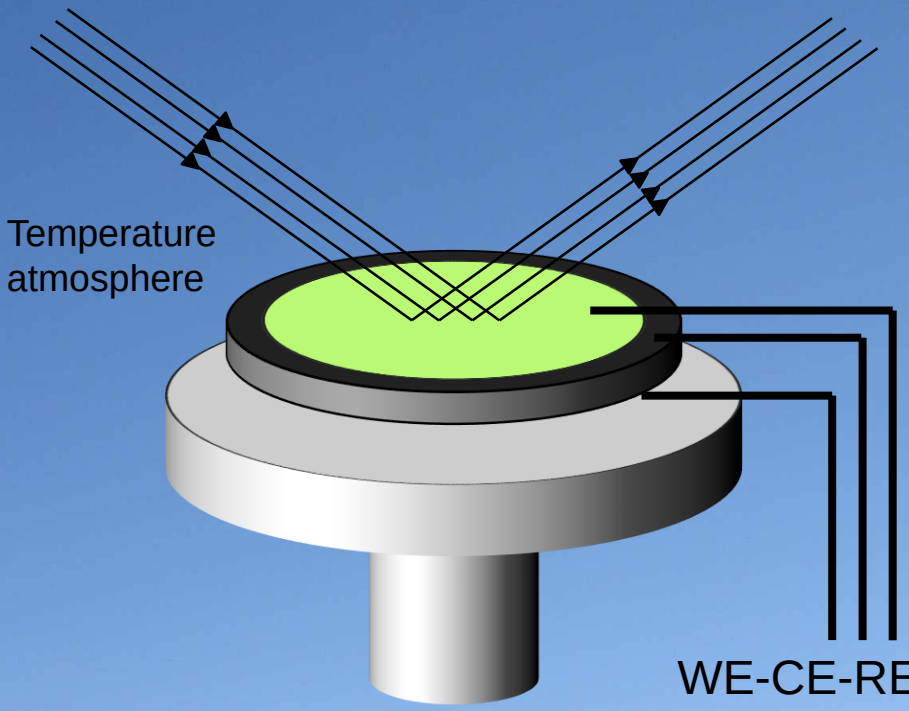


GOAL

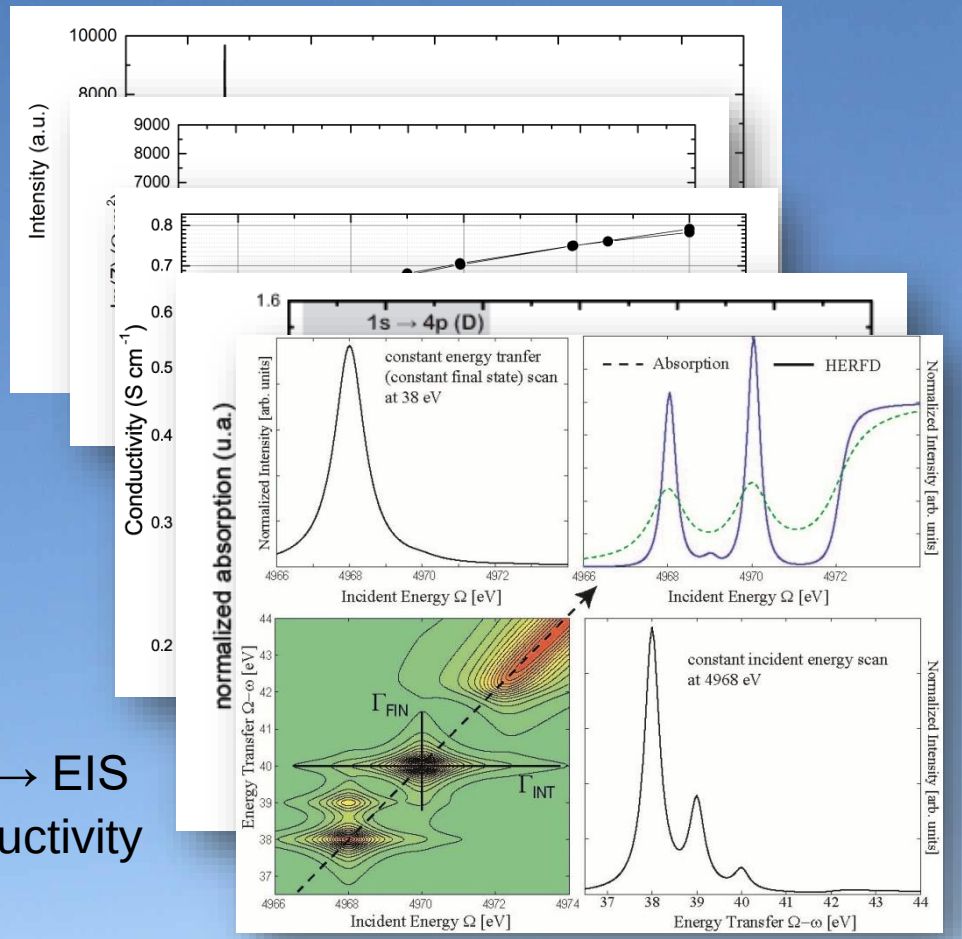
From *in-situ* measurements **to** *in-operando*

$E(t) = h\nu(t)$

XRD



WE-CE-RE → EIS
2W/4W conductivity



- **XRD**: Volume averaged crystallography
- **XAS**: element specificity (electronic structure, local environment)
- **IXS**: electronic structure, DOS

- **EIS**: Electrochemical characterization
- **Electrical conductivity**: transport properties, charge carrier identification
- Full cell measurements

Federico Napolitano

2do lugar concurso de planes de negocios

SÉPTIMA EDICIÓN IB50K 2017

SOFC

GENERADORES ELÉCTRICOS PARA APLICACIONES REMOTAS

2do lugar concurso de pla

21/11/2017 | IB50K - CONCURSO DE PLANES DE NEGOCIO DEL INSTITUTO BALSEIRO

Investigadores y becarios del CONICET premiados en el IB50K

Un dispositivo láser para "escribir" a escala microscópica y el desarrollo de un generador eléctrico recibieron el primer y segundo premio, respectivamente.

A modo de resumen…

- Las celdas de combustible son dispositivos que permiten transformar energía química en eléctrica de manera muy eficiente
- El desarrollo de nano materiales deberá permitir resolver los desafíos planteados para su comercialización masiva:
  - Costo
  - Confiabilidad
  - Durabilidad
- Para comprender los efectos es necesario una variedad de técnicas de caracterización **in-situ e in-operando** tanto estructural (XRD, microscopías) como su correlación con propiedades electrónicas y de transporte (EIS, XANES, etc)

New Latin-American Big Science Facilities (*)

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Argentina

LAHN: The Argentinean Neutron Beams Laboratory

Brazil

Laboratório Nacional de Luz Síncrotron

(*)Presented at the IBSP (International Basic Science Program) Unesco, Marzo 2018

Why BIG SCIENCE?

BIG SCIENCE FACILITIES

- (according to DOE) were changing from high-energy and nuclear physics to BASIC ENERGY and LIFE SCIENCES,
- may be defined as fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy, life and environment technologies

Today, in an world ever more competitive scientifically and technologically, deep knowledge of materials properties is fundamental

NANOTECHNOLOGY

ENERGY

CHEMICAL INDUSTRY

NEW MATERIALS

BIOTECHNOLOGY

CIVIL CONSTRUCTION

AUTOMOTIVE INDUSTRY

HEALTH

ENVIRONMENT

AGRICULTURE

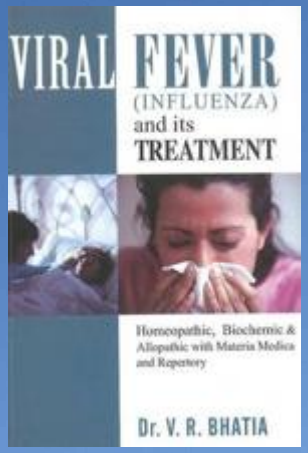
AEROSPACE INDUSTRY

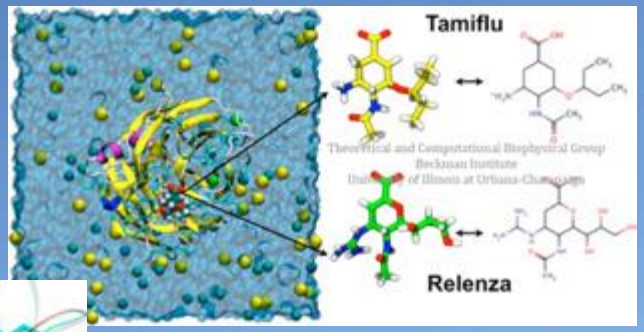
TEXTILE INDUSTRY

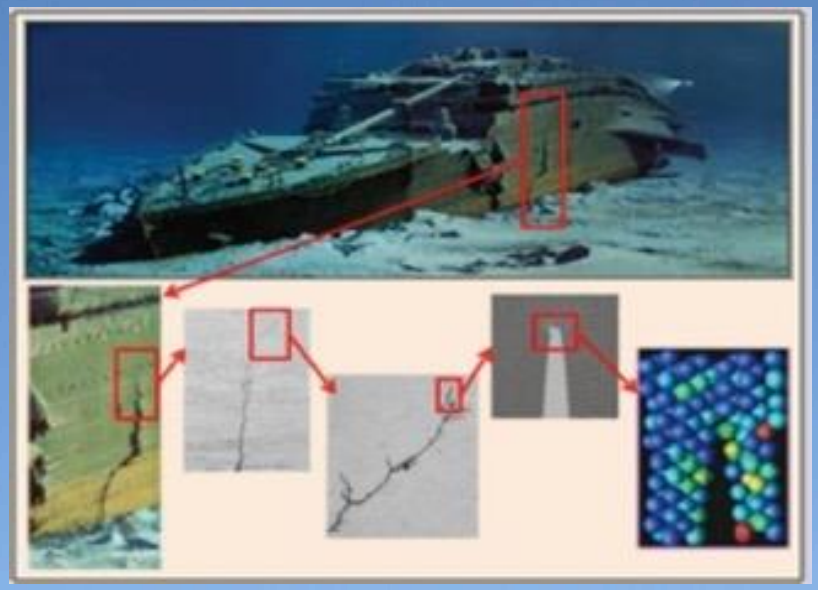
SECURITY

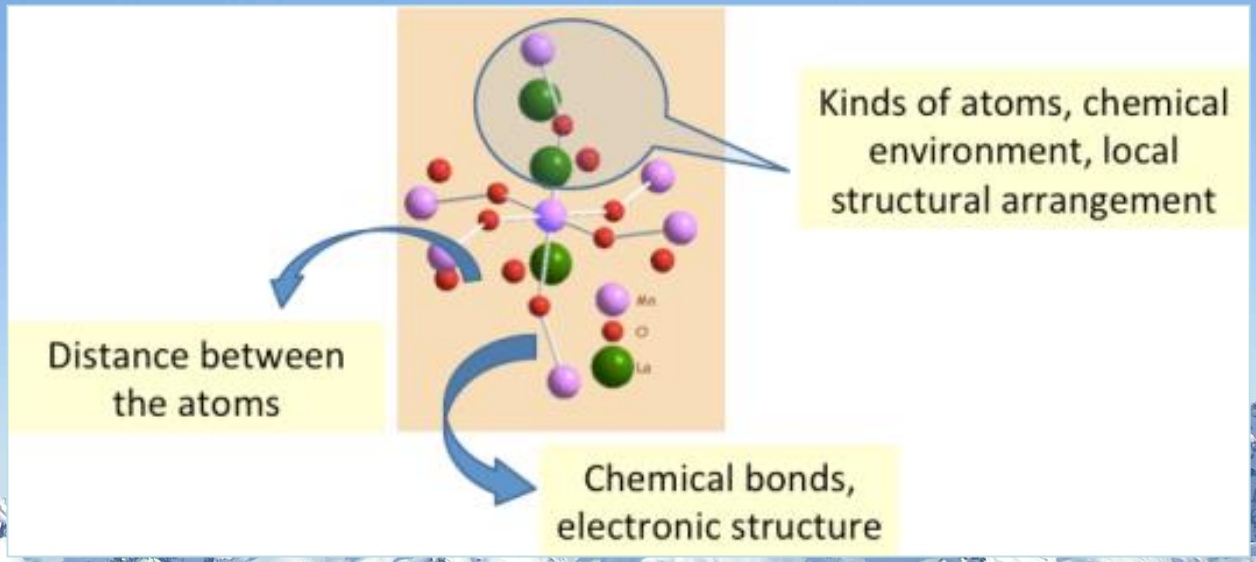
DEFENSE

We need to obtain information about materials and processes at the atomic level, and in real conditions ⇨ special tools are needed





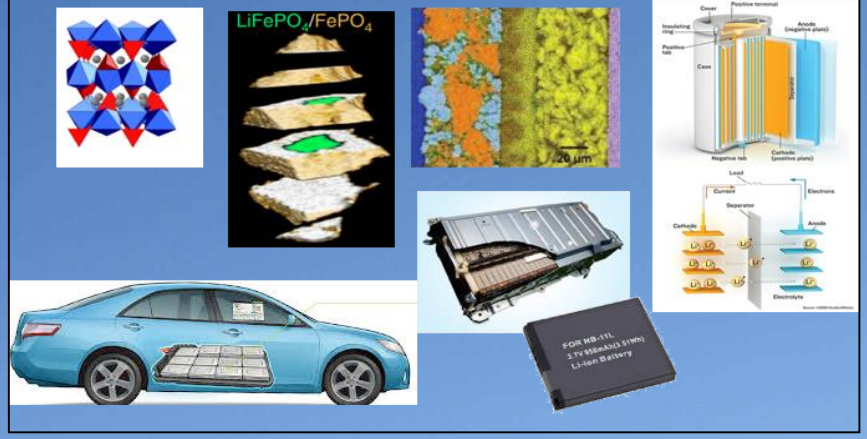




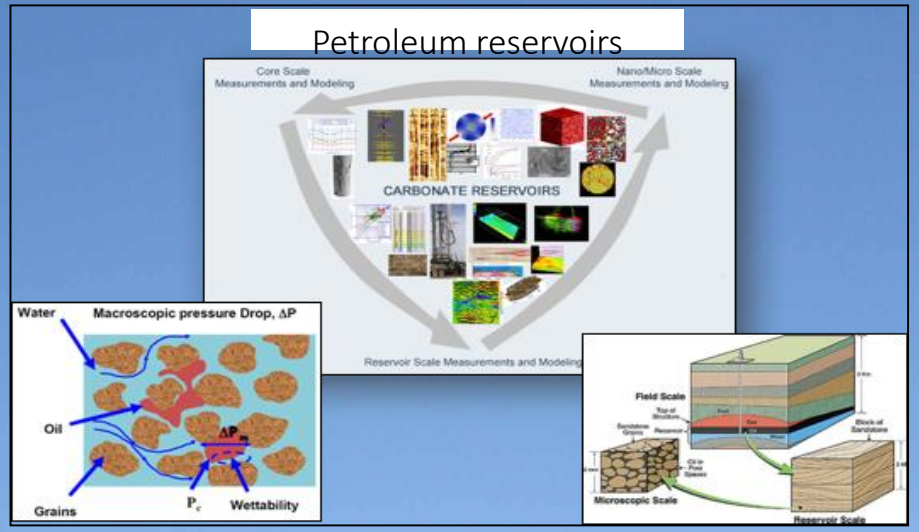
GREAT CHALLENGES OF TODAY AND THE FUTURE

Important and challenging materials and systems are Inhomogeneous, Hierarchic, Composites with distinct spatial and time scales

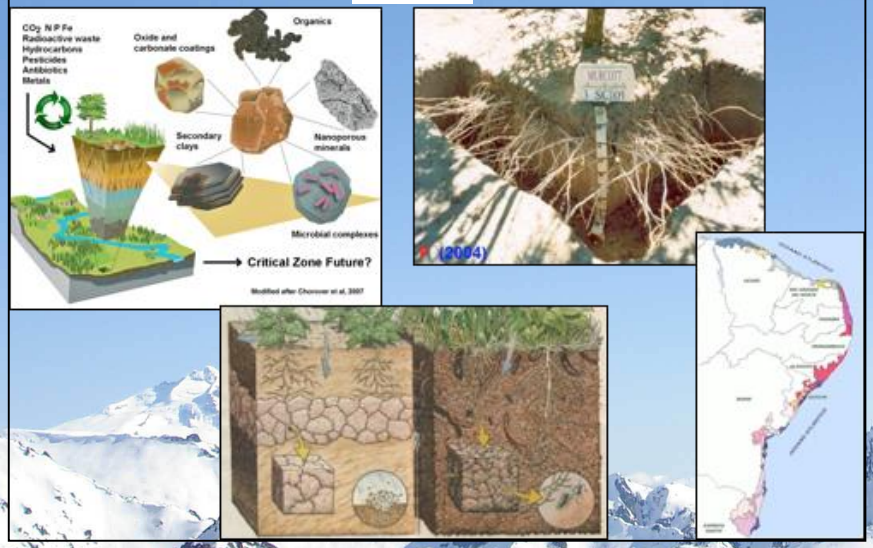
Li-ion Batteries



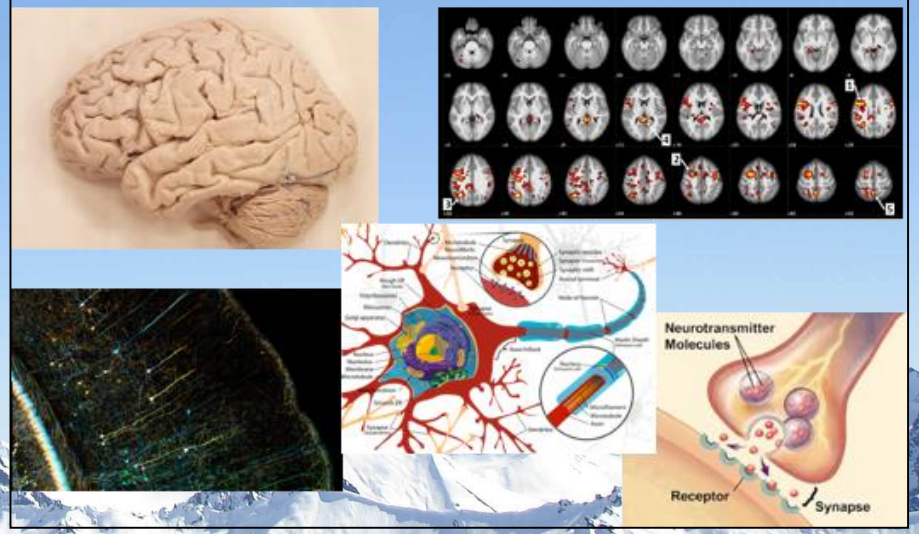
Petroleum reservoirs



Soil



Brain

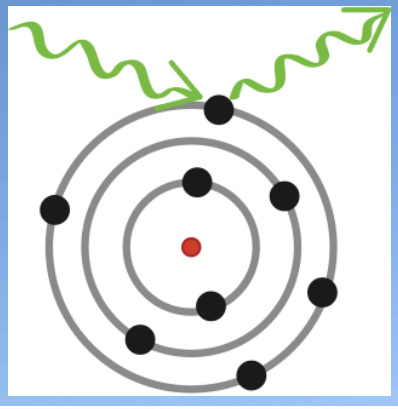


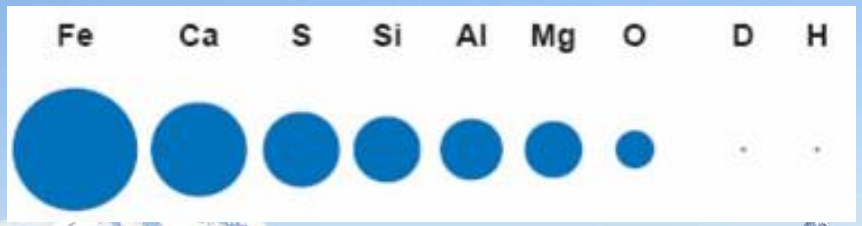
Deep knowledge of materials properties through Photons and Neutrons

PHOTONS (Light Sources)

Particles without charge or magnetic moment Electromagnetic waves (associated electric and magnetic field)

E ≈10 10^4 eV, λ = 0.01-10 nm





NEUTRONS

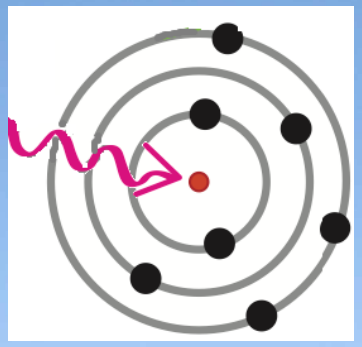
-Particles without charge with spin ½

-Nuclear and magnetic interaction

- wavelength depends on its kinetic energy (Ec).

Thermal Neutrons

~300K, Ec ≈2.5 10^{-2} eV, λ ≈ 0.2nm.

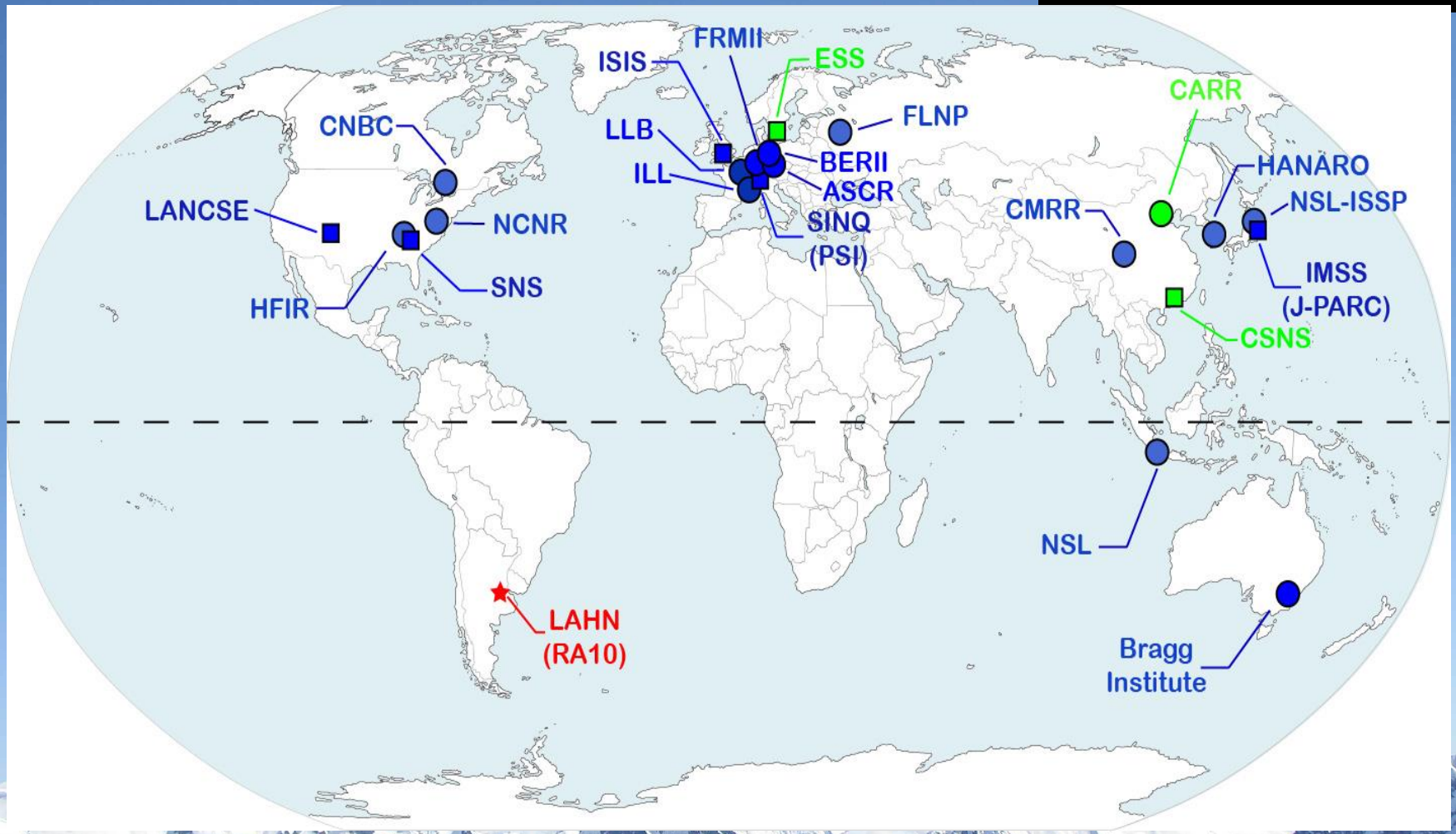


Why in LA?

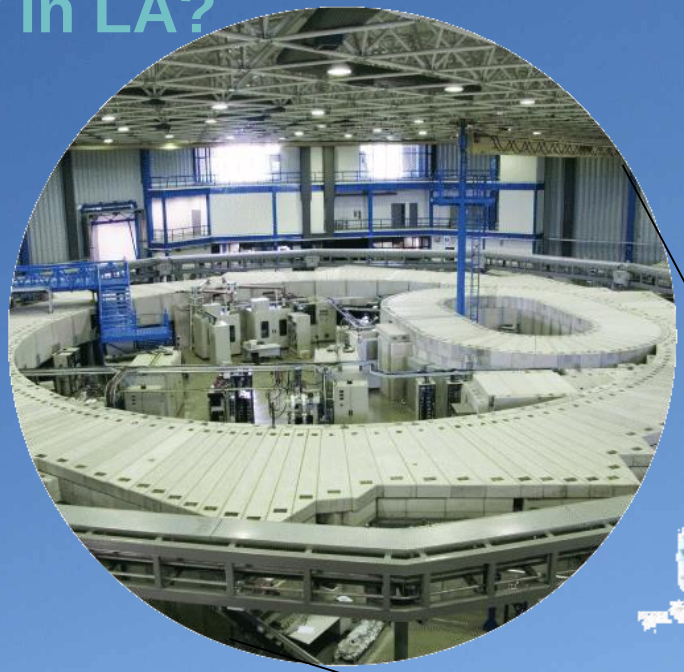
Neutron sources around the world

Third neutron source in the southern hemisphere

None in Latin America



Why in LA?



LNLS – A pioneering lab in Brazil

First synchrotron light source in the southern hemisphere

Still the only one in Latin America

Built between 1987-1997

Around 85% built in house

Training of human resources

Why in LA?

In **Ezeiza, Argentina**, the construction of a (RA-10) nuclear reactor will be completed 2019, and available as a neutron source open to users 2021.

In **Campinas, Brazil**, the operation of the 3GeV fourth generation sncrotron source Sirius will start by 2019.

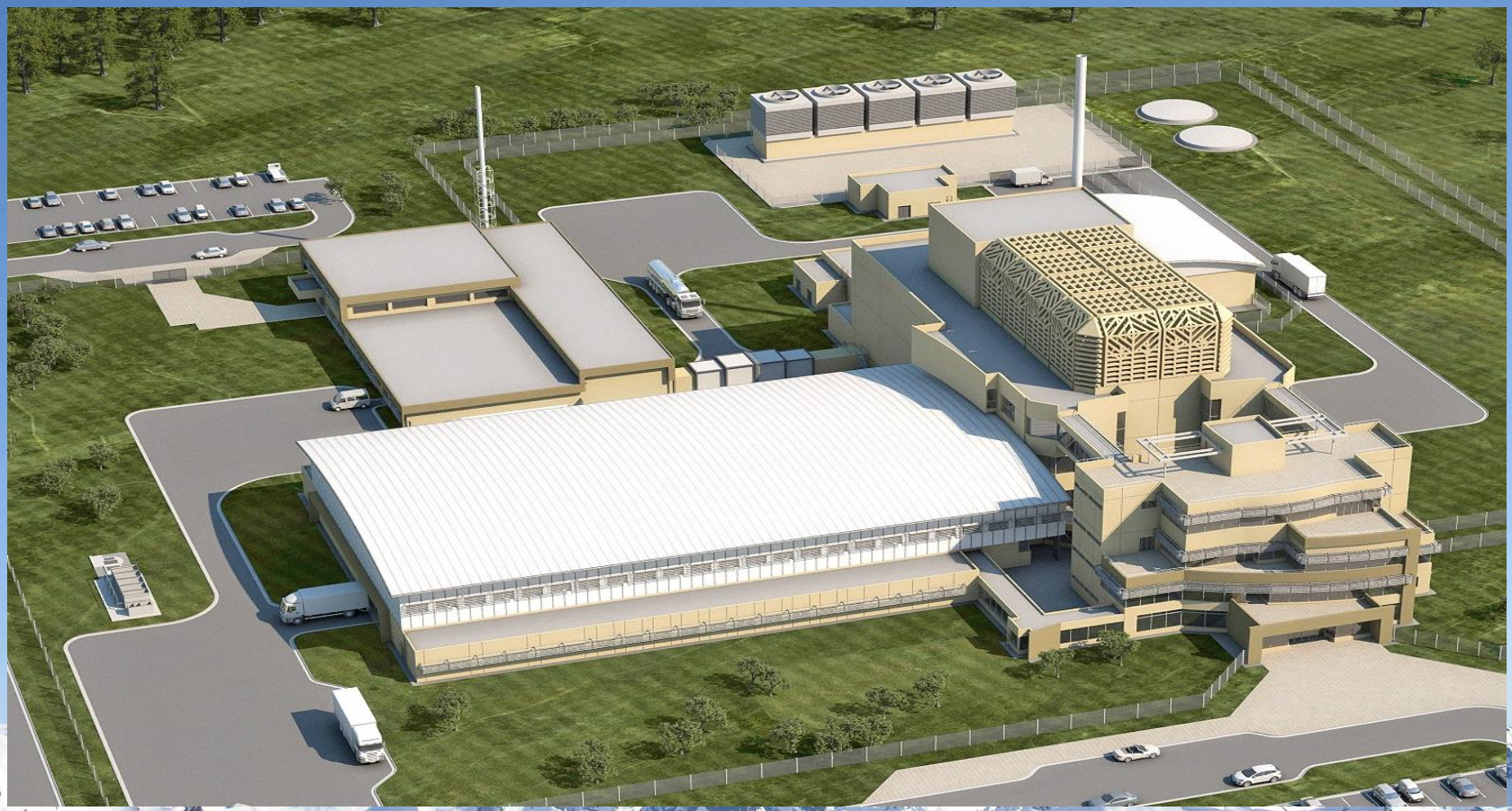
REGIONAL COLLABORATION OPPORTUNITY

"Both new (light and neutron) sources will be open to Latin-American users and also to those from other countries. It is expected that the operation of these two new and modern facilities will enhance de already strong collaboration between scientists form Brasil and Argentina, and also with scientists from other Latin-American countries."

Aldo Craievich- 2017 IUCr Meeting

The RA-10 Reactor

- Novel multipurpose research reactor under construction
- Located at Centro Atómico Ezeiza (close to Buenos Aires international airport)
- Will provide high fluxes of thermal and cold neutrons.



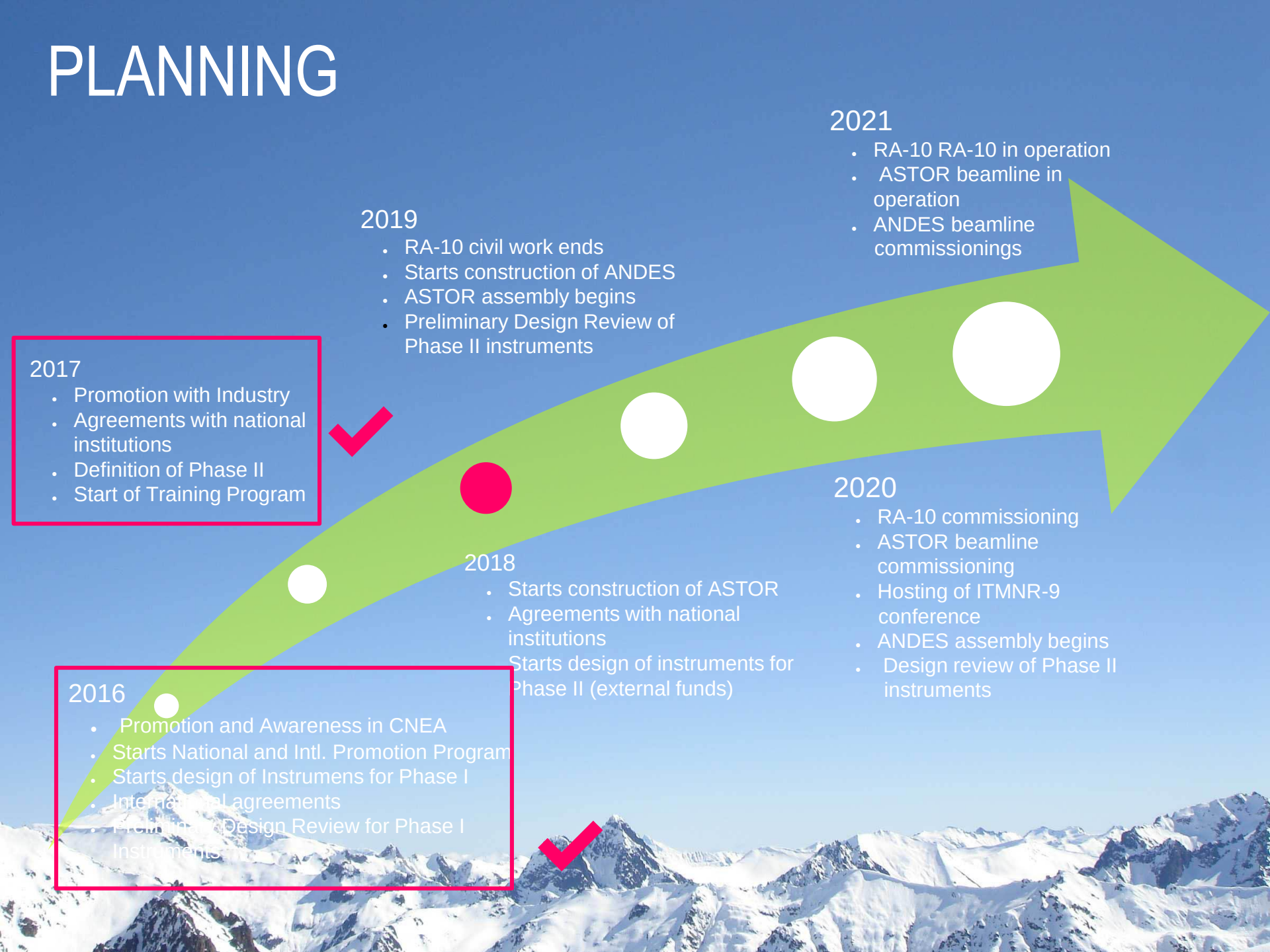
Artistic view of RA-10 building

THE LAHN PROJECT

GOAL:

To become a **National Laboratory** providing state-of-the art neutron techniques to the academy, to technological users and industry from Argentina and Latin-American region.

PLANNING



2016
- Promotion and Awareness in CNEA
- Starts National and Intl. Promotion Program
- Starts design of Instrumens for Phase I
- Inte[illegible]l agreements
- [illegible] Design Review for Phase I Instruments

2017
- Promotion with Industry
- Agreements with national institutions
- Definition of Phase II
- Start of Training Program

2018
- Starts construction of ASTOR
- Agreements with national institutions
- Starts design of instruments for Phase II (external funds)

2019
- RA-10 civil work ends
- Starts construction of ANDES
- ASTOR assembly begins
- Preliminary Design Review of Phase II instruments

2020
- RA-10 commissioning
- ASTOR beamline commissioning
- Hosting of ITMNR-9 conference
- ANDES assembly begins
- Design review of Phase II instruments

2021
- RA-10 RA-10 in operation
- ASTOR beamline in operation
- ANDES beamline commissionings

SCIENTIFIC CASES FOR PHASE II

6 ADDITIONAL INSTRUMENTS WERE PROPOSED DURING A WORKSHOP JOINTLY ORGANISED WITH THE NATIONAL MINISTRY OF SCIENCE AND TECHNOLOGY

Next instruments will result as outcome from user community interests and will be externally funded. So far, six scientific cases
have been proposed, for:

- Dedicated powder diffractometer
- Reflectometer (with polarized neutrons)
- SANS
- Quasi-Laue diffractometer
- Triple-axes spectrometer
- Cancer research (BNCT) instrument

FOR SCIENTIFIC CASES INFO

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LAHN Project
Comisión Nacional de Energía Atómica

www.lahn.cnea.gov.ar

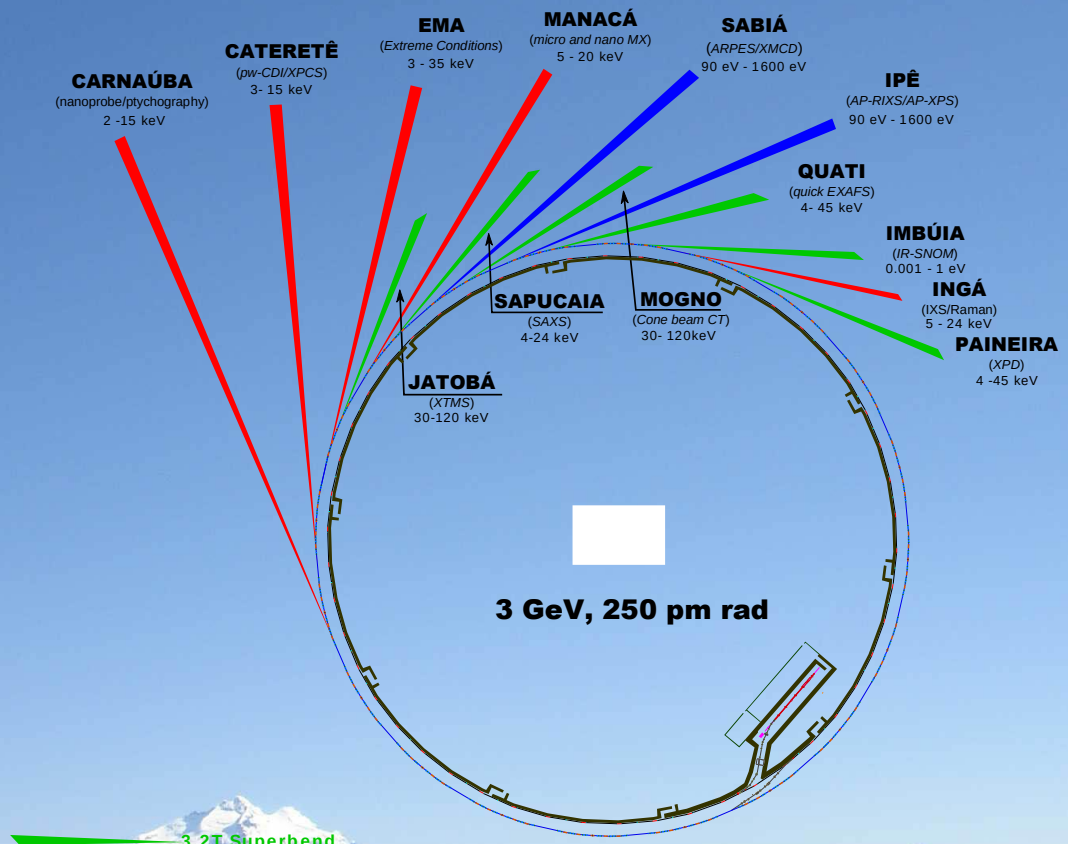
lahn@cnea.gov.ar

A HUGE OPPORTUNITY FOR LATINAMERICAN REGION

- LAHN will be the first and unique large-scale neutron beams facility in Latinamerica
- It will complement perfectly with the novel 4th generation synchrotron SIRIUS in Sao Pablo, Brazil
- Together they may become the most multidisciplinary hub in the region; similar to ILL+ESRF in France, J-Parc in Japan, PSI in Switzerland, ISIS+Diamond in UK, MAXIV + ESS in Sweden, Argonne in USA.

~84% EXECUTED

Sirius: 13 initial phase beamlines (2018-2020)



– Experimental Programs

- Tender nano-probe for spectro-ptychography
- Large FOV (30 μm) Coherent Diffraction Imaging
- Bragg CDI/XRD/XAFS under extreme conditions
- Serial micro and nano MX
- Tender x-ray RIXS
- AP-RIXS/XPS
- ARPES/PEEM
- Cone beam High Energy Tomography
- Quick-EXAFS
- 3D X-Ray Diffraction Microscopy
- High-Throughput SAXS
- Time Resolved Powder Diffraction
- nano-FTIR

REMARKS

- ✓ Two new BIG SCIENCE facilities in LA (Latin-America)
  - ✓ Neutrons: LAHN (Argentina)
  - ✓ Light source: SIRIUS (Brazil)
- ✓ These facilities are within the best in the world
- ✓ UNESCO support is needed to encourage the local governments to improve and continue this unique opportunity
  - ✓ for scientists from latin america to increase collaborations and develop basic science
  - ✓ training human resources are invaluable

"HOW CAN A COUNTRY RAPIDLY IMPROVE ITS CAPACITY IN SCIENCE, TECHNOLOGY, AND INNOVATION?
Invest in people, as Latin America is doing."

Latin America must continue to strengthen the internationalization of its science, as well as exploit its local excellence through intracontinental collaborations, positioning the continent to become a global leader in science, technology, and innovation. Indeed, every nation can benefit by growing a capable and knowledgeable workforce.

– Celia R. S. Garcia, Armando J. Parodi, Glaucius Oliva

www.sciencemag.org SCIENCE VOL 338 30 NOVEMBER 2012

GRACIAS

Argentina

LAHN: The Argentinean Neutron Beams Laboratory

Brazil

Laboratório Nacional de Luz Síncrotron

Gracias