



# De la **M**olécule aux **N**ano-objets: **R**éactivité, Interactions et **S**pectroscopies

Director: Pr Christophe Petit  
Deputy Director : Pr Lahouari Krim

CNU 30 et 31, CoCNRS 13, 14 (Chimie ) et 4 (Physique), ED 388 (CAPT), ED 564 (PIF)

*Institut Parisien de Chimie Physique et Théorique, IP2CT*



*UFR DE CHIMIE et UFR DE PHYSIQUE*

# Presentation of MONARIS

## Elaboration, Understanding and Characterization

Focusing on ***the chemical bond into the organization and reactivity*** of the matters from the molecules to the nanostructured materials

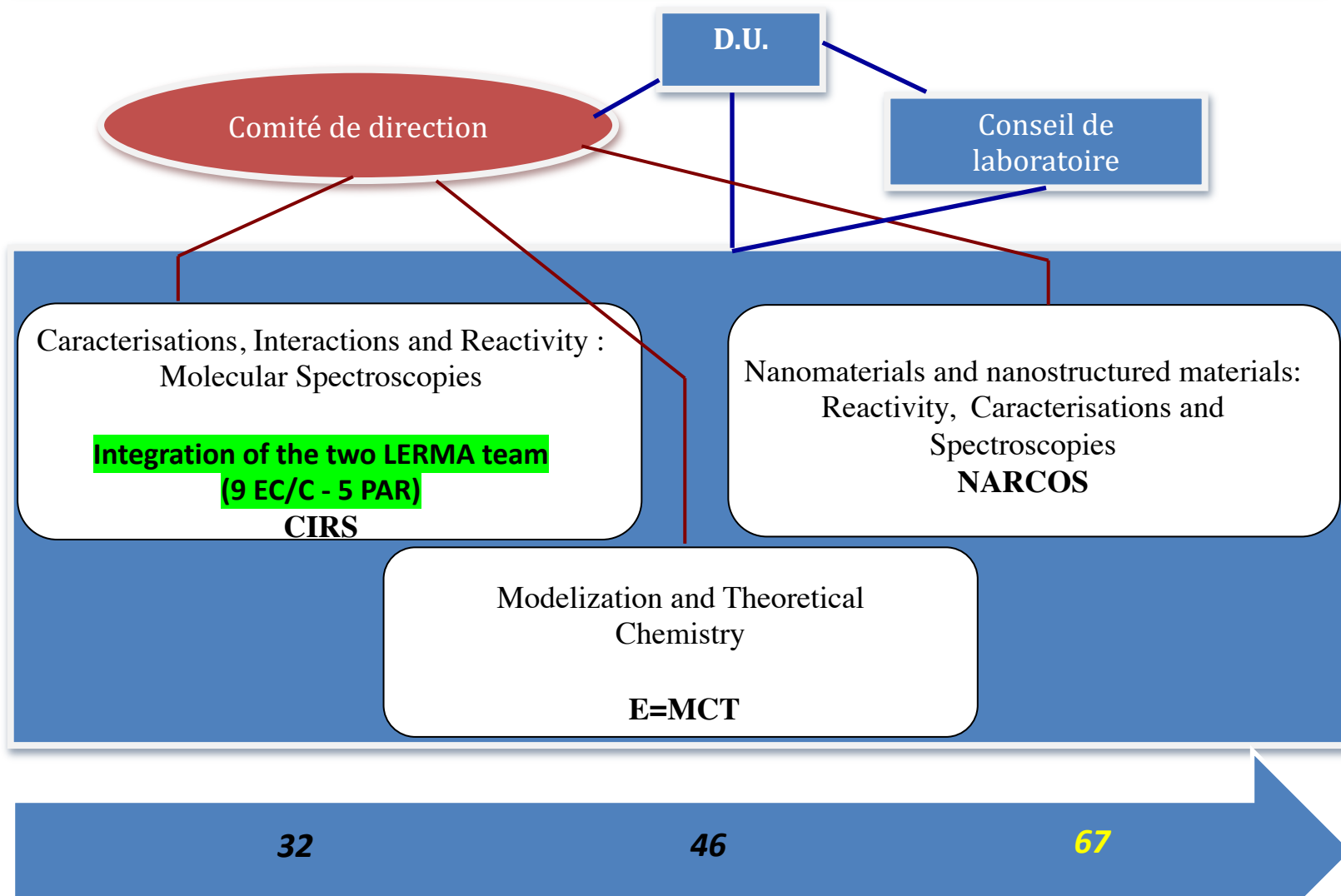
Exploring the fundamental root of chemical reactivity to understand and tailor the physical and chemical properties and allow innovative applications

⇒ Relation structure-reactivity *in situ* and *operando*

⇒ Physical techniques of investigation (spectroscopies and microscopies)

⇒ Modelling from the molecular level to solid

# MONARIS 2024



## Organigramme 2024

### Directeur

Christophe PETIT (PR)

### Directeur Adjoint

Lahouari KRIM (PR)

### GESTIONNAIRE FINANCIER

Patrice SEBASTIEN (TCE CNRS)

### GESTIONNAIRE ADMINISTRATIF

Mylène COLMAR (ADT, SU)

### 1- Caractérisations, Interactions et Réactivités : Spectroscopie Moléculaires (CIRS)

L. KRIM (PR), P. ASSELIN (CR), M. BERTIN (Mdc), C. BOURSIER (Mdc),  
G. FERAUD (Mdc), J.H. FILLION (PR), M. GUINET (Mdc), D. JACQUEMART (Mdc),  
C. JANSSEN (CR), X. MICHAUT (PR), L. PHILIPPE (Mdc), P. SOULARD (CR),  
Y. TE (Mdc), B. TREMBLAY (Mdc), T. ZANON (Mdc).

Y. BERGER (IE), H. ELANDALOUSSI (IR), A. HESSANI (IE SU 50%), P. JESECK (IR),  
P. MARIE-JEANNE (IE), G. ROSE (IE CNRS 50%), C. ROUILLE (IR),  
T. SEROPIAN (TCE CNRS 50%), N. THEODOSE (TCN SU 50%)

M. IBRAHIM (ATER), K. CARADEC (Doc), H. FU (Doc),  
A. HACQUARD (Doc), M.V. KHAN (Doc), C. MAHOB (Doc),  
M. LEMAITRE (Doc), D. TORRES-DIAZ (Doc ISMO-CIRS),

### 2- NANomatériaux et matériaux nano-structurés : Réactivité, Caractérisation et spectrOscopies (NARCOS)

L. BELLOT-GURLET (PR) & A. COURTY (PR)

P. COLOMBAN (DR Em), G. GOUADEC (Mdc)

A. GIRARD (Mdc) I. LISIECKI (DR), M. GUERRA (DR), A. PERCOT (Mdc),  
C. PETIT (PR), H. PORTALES (Mdc), C. SALZEMANN (Mdc), G. SIMON (Mdc)

I. ARFAOUI (IR CNRS), A.T. NGO (IE, CNRS), C. PARIS (IE CNRS),  
G. ROSE (IE CNRS 50%), N. GOUBET (AI SU), P. MARIE-JEANNE (AI 50%),  
T. SEROPIAN (TCE CNRS 50%), N. THEODOSE (TCN SU 50%),  
A. HESSANI (IE SU 50%).

S.DUCHENE (Doc), M. VALVALI (Doc), N. KHALFAOUI (Doc), Z. SAFAR ZADEH  
KERMANI (Doc), C. VERNIER (Doc), B. ROSELLI (Doc), M. MOHAMMADI (Doc), N.  
REIHANIAN (Doc), S. MEFTA (Doc), M. DELOM (Doc),

### 3- Modélisation et Chimie Théorique

#### E=MCT

B. MADEBENE (Mdc)

E. ALIKHANI (PR Em), V. LABET (Mdc),  
E. ZINS (Mdc).

O. AROUL (Doc)

## Organigramme 2024

### SOUTIEN DE LA RECHERCHE

I. ARFAOUI (IR CNRS) , H. ELANDALOUSSI (IR), A. HESSANI (IE SU) , P. JESECK (IR CNRS)  
P. MARIE-JEANNE (AI), Y. BERGER (IE SU), N. GOUBET (AI) SU, J.L. LINDOR (ADT SU), A.T. NGO (IE CNRS)  
G. ROSE (IE CNRS), C. ROUILLE (IR), T.SEROPIAN (TCE CNRS), N. THEODOSE (TCN SU 50%)  
M.COLMAR (ADT, SU), P.SEBASTIEN (TCS, CNRS), C. MAYOUTE (ATRF SU)

#### **PLATEFORME INSTRUMENTALE** **MICROSCOPIES ELECTRONIQUES**

A.T. NGO – N. GOUBET

#### **MICROSCOPIES CHAMP PROCHE**

I. ARFAOUI

#### **LABORATOIRE NANOMATERIAUX**

N. GOUBET

#### **MESURE MAGNETIQUE**

A.T. NGO

#### **SPECTROSCOPIE IR**

Y.BERGER, A. HESSANI, P. JESECK, C. PARIS

#### **SPECTROSCOPIE RAMAN**

A. HESSANI

#### **INFORMATIQUE (Matériels et logiciels)**

B. MADEBENE - G.ROSE - T. SEROPIAN

#### **MECANIQUE-ELECTRONIQUE**

T. SEROPIAN, G. ROSE, Y. BERGER, P. MARIE-JEANNE (IE),  
N THEODOSE (50%),

#### **OPTIQUE ET MICRO SPECTROMETRE**

A.HESSANI

#### **ENTRETIEN/LOGISTIQUE**

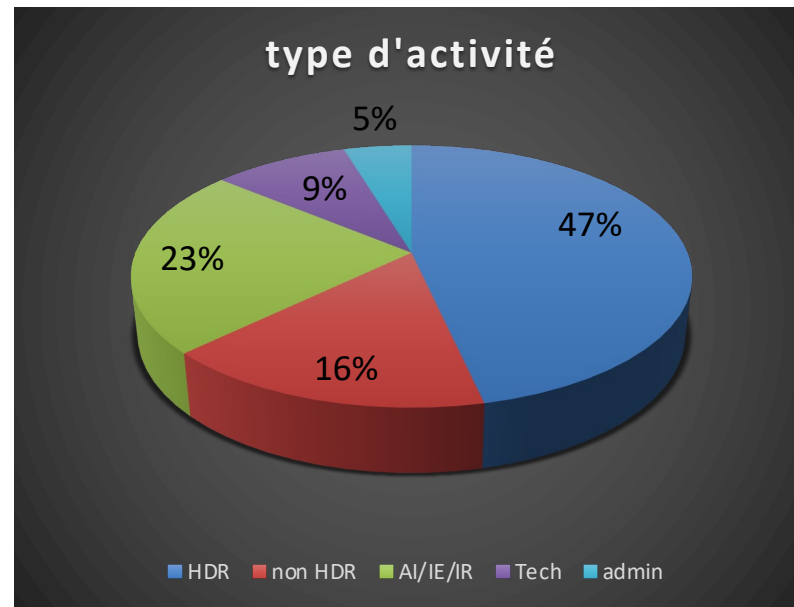
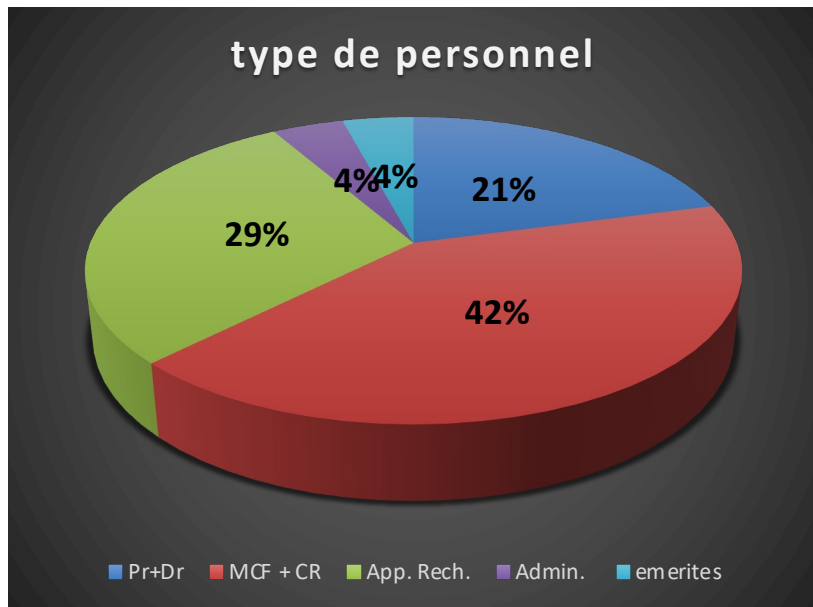
J.L LINDOR, C. MAYOUTE

#### **SST**

Y.BERGER, E.ZINS, M. COLMAR

#### **APS**

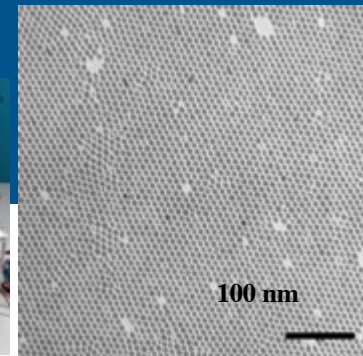
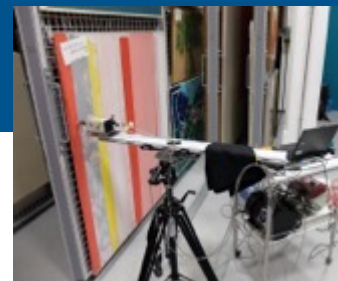
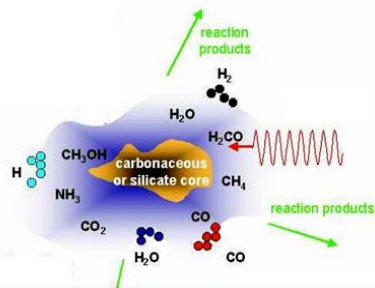
A.T. NGO, T. SEROPIAN, A. HESSANI, L. PHILIPPE  
(PCR A. HESSANI, RSL Y. BERGER et G. FERAUD)



8 Professeurs et 2 Directeurs de Recherche  
 17 Maîtres de Conférence et 3 Chargés de Recherche  
 16 Ingénieurs et Techniciens (8 CNRS, 8 SU)  
 1 DR Emérite, 1 Pr Emérite

19 HDR (ED PIF et CPCA)

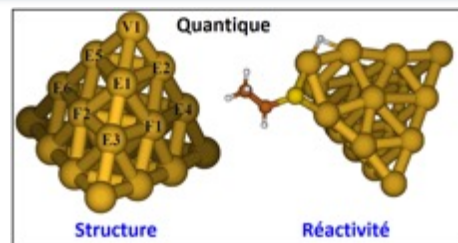
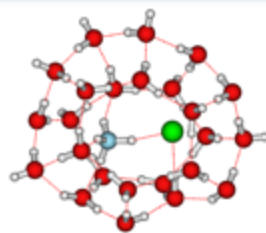
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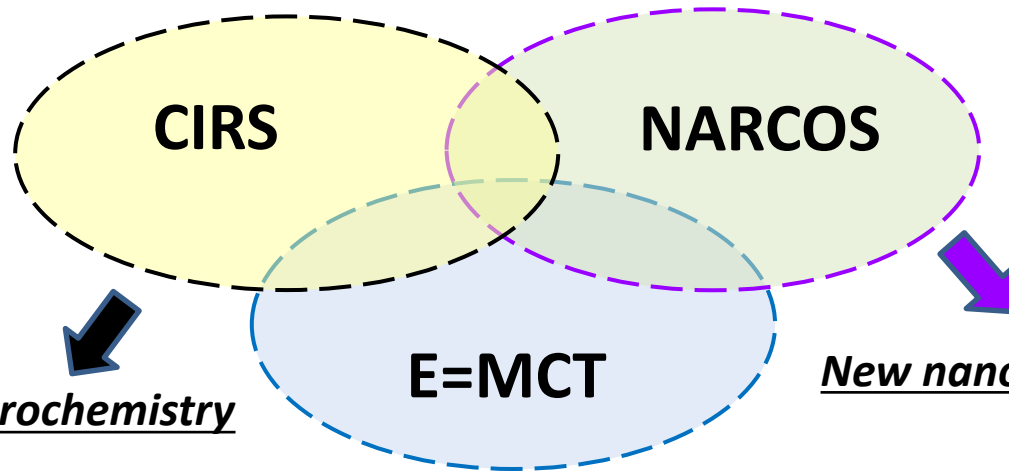
Characterisations, Interactions and  
Reactivity : Molecular Spectroscopies  
**CIRS**

Nanomaterials and nanostructured materials:  
Reactivity, Characterisations and  
Spectroscopies  
**NARCOS**

Modelization and Theoretical  
Chemistry  
**E=MCT**



# The MONARIS Project



**CIRS**

**NARCOS**

**E=MCT**

*Astrophysics & Astrochemistry*

*New nanotechnology innovations*

Cometary and Planetary atmospheres  
Chemistry of the ISM  
Prebiotic chemistry and Origins of life  
Climate change and air Pollution

*healthcare sector*  
*nanocomputing and data storage*  
*green hydrogen and energy storage*  
*Decarbonization and Pollution Control*  
Heritage Materials and Objects  
Durability of materials

Modelling stress-affected chemical reactions



- CIRS -

# Characterizations, Interactions and Reactivity: molecular Spectroscopy

CIRS 2024

**CIRS**  
2024

*The current CIRS team*

*Chemistry Department*

*SMILE & SPICES teams*  
*/LERMA*

*Physics Department*



**Physical Chemistry, Astrophysics, Astrochemistry, Atmospheric sciences**

- **CIRS** -

# Characterizations, Interactions and Reactivity: molecular Spectroscopy

## 15 Chercheurs, Chercheuses, enseignant-chercheur, enseignantes-chercheures

CNU Section 31 - UFR de Chimie et Section 30 - UFR de Physique - sections 04 et 13 CNRS

## 7 Personnels d'Appui à la Recherche - développements instrumentaux

2 IE de l'UFR de Chimie - 1 IE et 1 IR UFR de Physique - 2 IR CNRS - 1 IR CDD

## 7 Doctorants et doctorantes

2 ED 388 - Chimie / 1 ED 127 - Astrophysique / 4 ED 564 : Physique

## Collaborations anciennes à l'interface physique et chimie



Mission  
Interdisciplinarité  
MITI

Programmes  
Nationaux  
CSAA  
INSU



## Activités scientifiques au sein de l'équipe CIRS

2 axes thématiques en lien avec la physico-chimie de l'atmosphère terrestres, les atmosphères planétaires et cométaires et les milieux astrophysiques

# CIRS in 2024

*Physical Chemistry, Astrophysics,  
Astrochemistry, Atmospheric sciences*

Characterization of molecular species of  
atmospheric and astrophysical interest.

Pierre Asselin	CNRS
Mickael Guinet	SU
David Jacquemart	SU

*Research Support 50%: Y. Berger (IE), A. HESSANI (IE), T. Seropian  
(Tech), G. Rose (IE), N. Theodose (Tech)*

*3 PhD students: K. CARADEC, M. LEMAITRE, M.V. KHAN, T. Gaillot.*

*1 Post-Doc: M. IBRAHIM (ATER)*

Molecular Spectroscopy and Laser  
Instrumentation for Environment

Corinne Boursier	SU
Christof Janssen	CNRS
Yao-Veng Té	SU
Thomas Zanon	SU

*Research Support H. Elandaloussi (IR), P. Jeseck, (IR), P. Marie-  
Jeanne (IE), C. ROUILLE (IR)*

*5 PhD students: H. FU, A. HACQUARD, C. MAHOB, D. Torres-  
Diaz, J. MICHOU.*

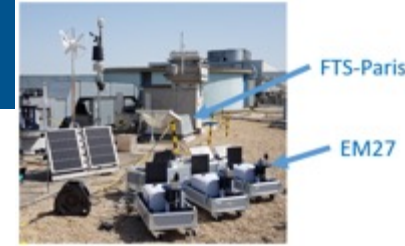
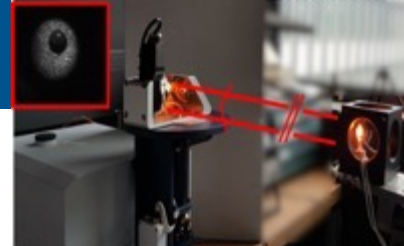
Reactivity under extreme conditions and in  
controlled environments.

Lahouari Krim	SU
Benoît Tremblay	SU
Pascale Soulard	CNRS

Spin, photons and astrophysical ices

Mathieu Bertin	SU
Géraldine Féraud	SU
Jean-Hugues Fillion	SU
Xavier Michaut	SU
Laurent Philippe	SU

# CIRS



Theme 1

Molecular Spectroscopy for Atmospheres and Remote sensing

Theme 2

Low Temperature Molecular Sciences for Astrophysics and Astrochemistry

Spectroscopy, Reactivity, Interstellar Media, Air Quality, Environmental Transition, Origin of life  
Interferometry, Metrology...



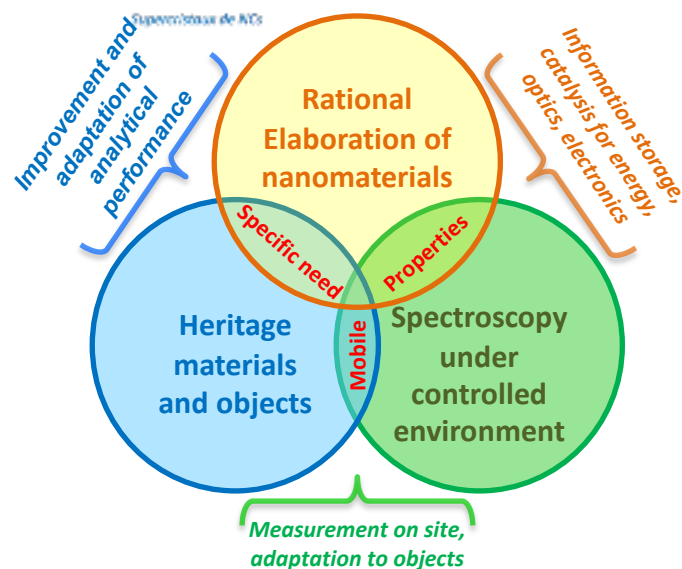
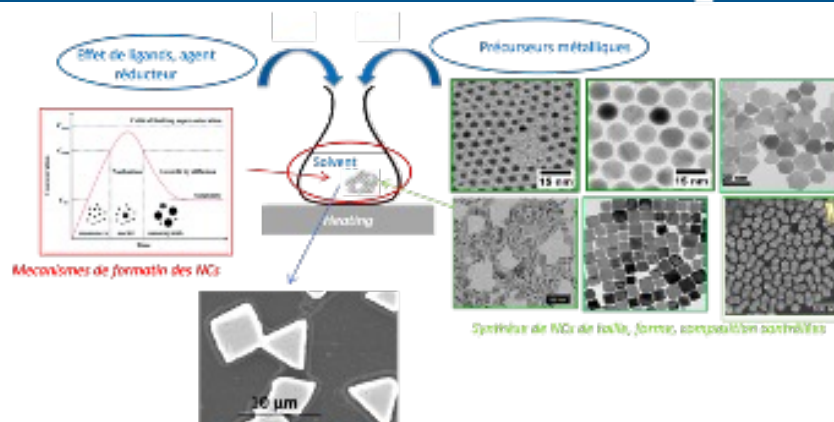
*UFR de physique*

*UFR de chimie*





# NAnomaterials and nanostructured materials : Reactivity, Caracterisation and spectrOscopies



# NARCOS

Theme 1

Nanomaterials : From rational elaboration to applications

Theme 2

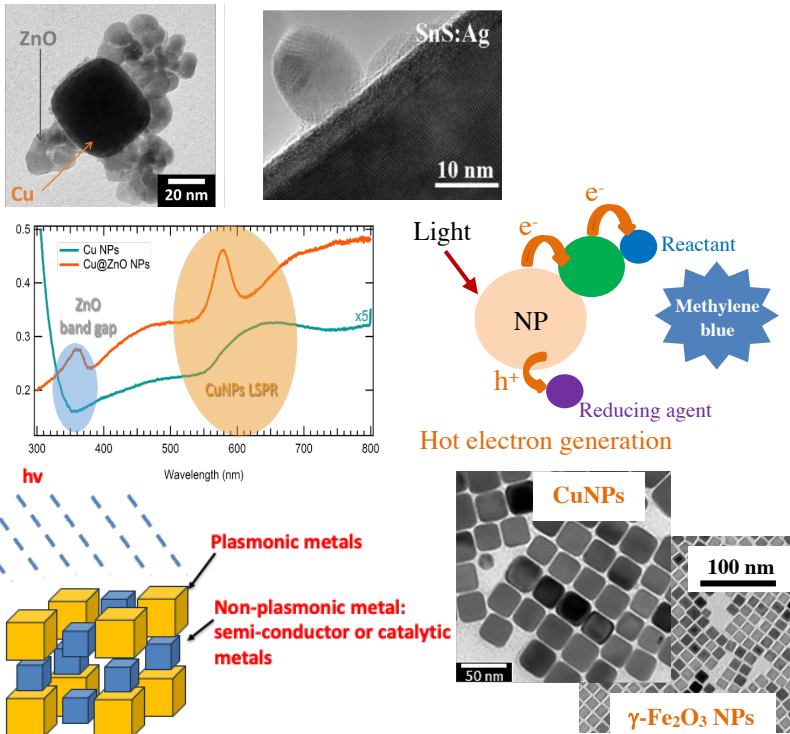
Spectroscopy for physical chemistry under controlled environments

Spectroscopies, Microscopies, Reactivity, Energy, Environmental transition, Origin of life

# NARCOS

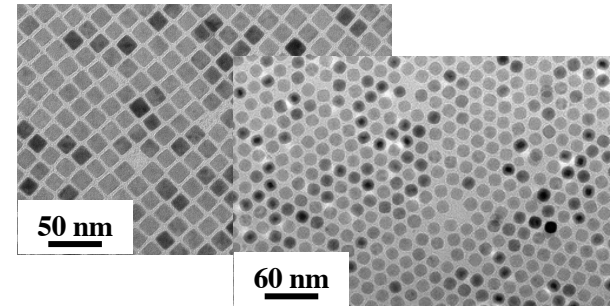
## Nanomaterials : From rational elaboration to applications

### Plasmonic and (photo)catalysis



### Study of magnetic hyperthermia processes in assemblies of magnetic NPs

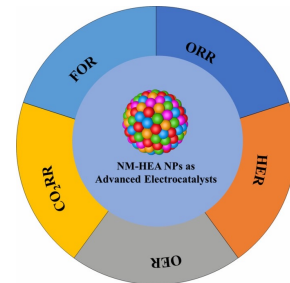
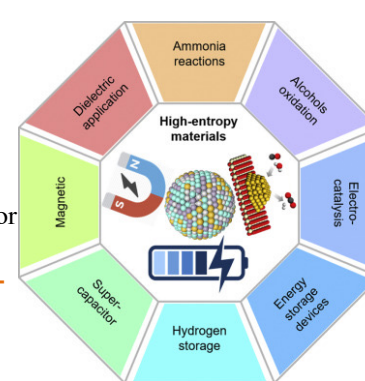
Assemblies of cubic and spherical magnetic NPs ( $\text{Co}$ ,  $\gamma\text{-Fe}_2\text{O}_3$ ) with tunable dipolar interactions



### Chemical synthesis of multicomponents NPs for new properties

- Co
- Ni
- Pt
- Pd
- Cu
- Zn
- Ag
- Au
- CoP
- NiP

Magnetic and/or plasmonic multicomponents and/or High-entropy-alloy nanoparticles (HEA-NPs)





# NARCOS TEAM Historical Artifact

## Development of analytical strategies for on site studies

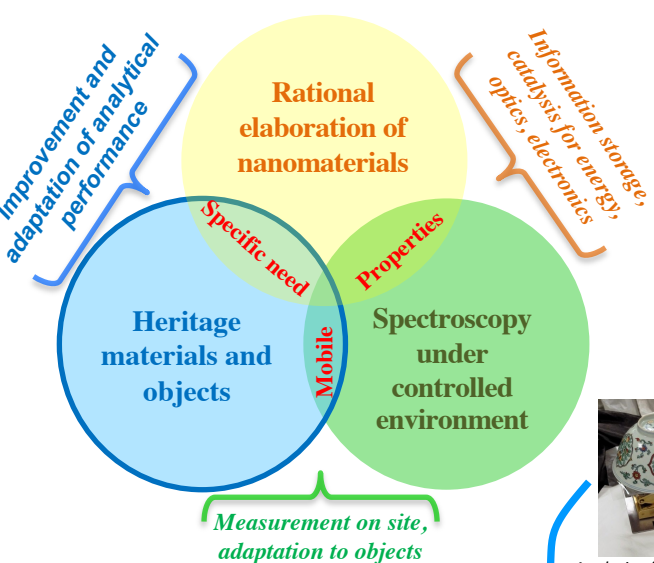
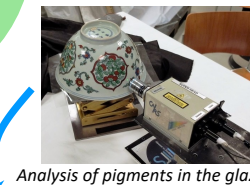
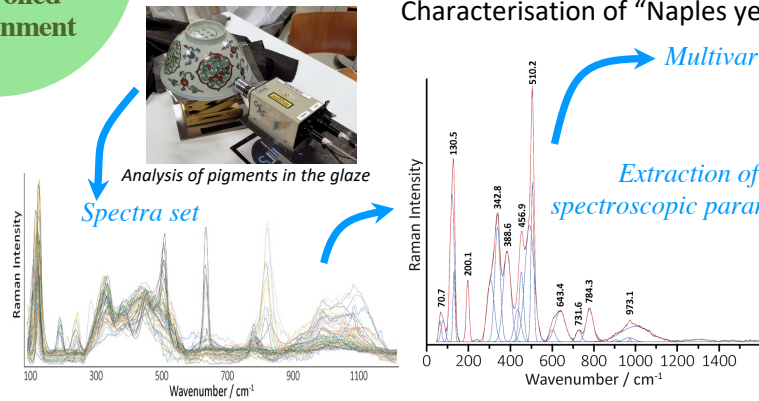
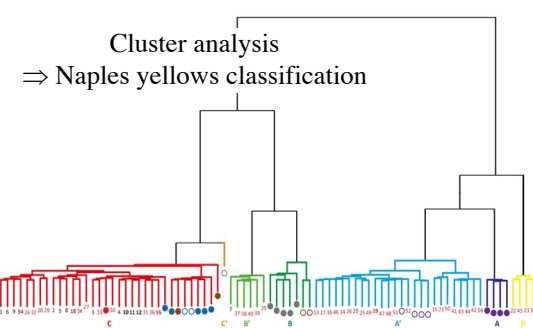


## Study of ceramic technology transfer between Europe and China in the 18<sup>th</sup> century

Characterisation of "Naples yellows" pyrochlores family ( $Pb_2Sb_{2-x-y}Sn_xM_yO_7$ )

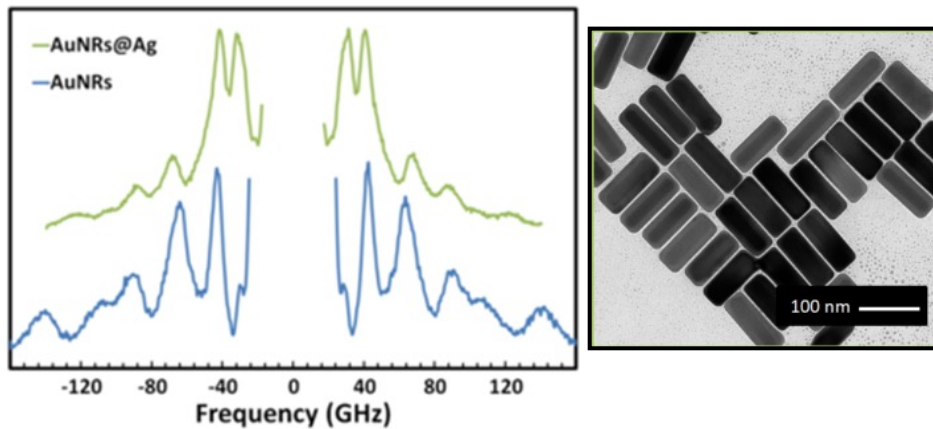
Multivariate analysis of extracted parameters (cluster analysis)

Extraction of spectroscopic parameters



## Spectroscopy for physical chemistry under controlled environment

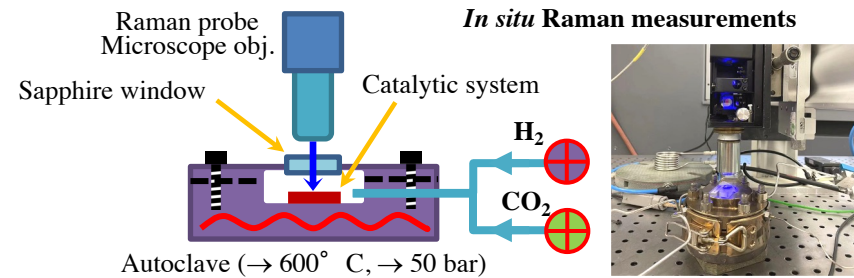
*Properties of nanocrystals with controlled composition & shape*



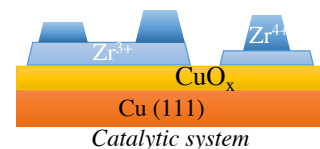
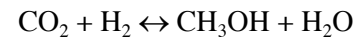
Focus on original controlled non-spherical nanocrystals and their organisation  
Brillouin scattering studies at several wavelengths

- Modulate compositions, shapes and self-organisations
- Investigation of plasmon-vibration coupling
- Studying shape effects on optical properties
- Control of measurement environments and self-organisations
- Checking numerical model predictions

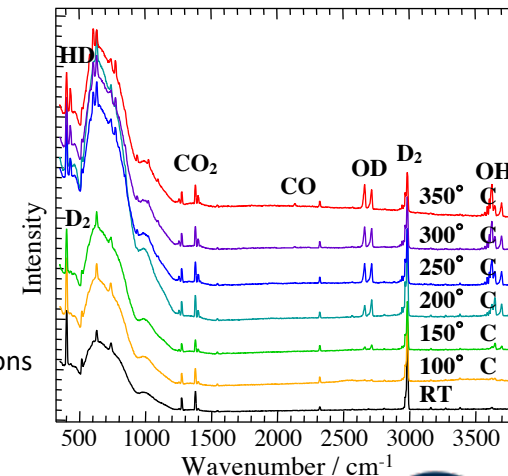
*Study of the reactivity under operating conditions*



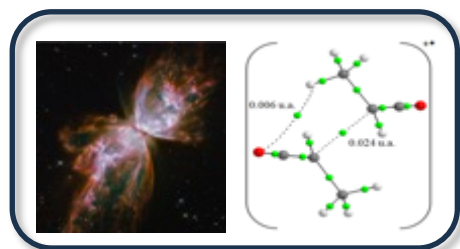
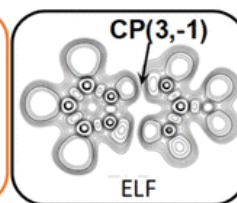
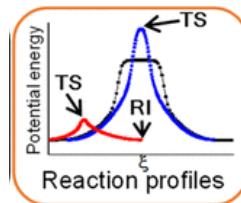
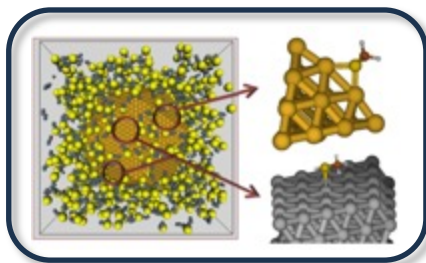
**CO<sub>2</sub> hydrogenation mechanism on ZrO<sub>2</sub> ultrathin film**



- Imposed thermodynamic conditions
- Study of reaction mechanisms
- Assessment of catalysts
- Optimum operating conditions



# Modeling and Theoretical Chemistry: E = MCT



**E=MCT**

Material organization  
at different scales

Evolution of chemical bonding  
and reactivity under stress

**CIRS**

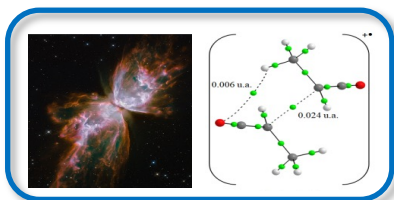
Non Covalent interactions   Metal ligand interactions   Astrochemistry

**NARCOS**

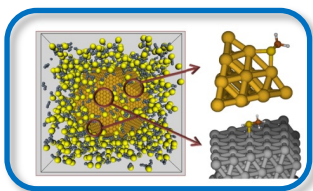
Rational Elaboration of nanomaterials   Spectroscopy under controlled environment

The theoretical team has developed specific know-how that is recognized within SU and by our partners.  
=> specific interaction with experimentalist

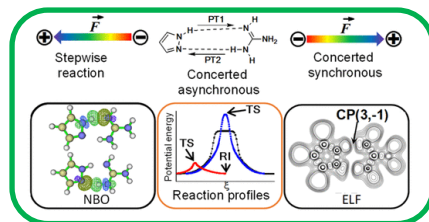
# Modeling and Theoretical Chemistry: E = MCT



Peptidic bond formation:  
medium effect



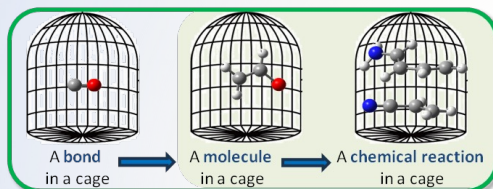
Nanocrystal ↔ Molecular cluster



Electric field:  
Proton-Coupled Electron Transfer

Material organization  
at different scales

Evolution of  
chemical bond and reactivity  
under stress

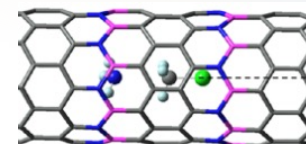


Conceptual Bond evolution  
DFT theory

To be explored for the cage treatment:  
QM/QM: Density functional tight binding



J. Pilmé



Anisotropic stress



G. Hoffmann  
C. Morell

C. Desroches  
S. Forel

CTIA Team  
(Chimie Théorique et I. A.)



## Conclusion

MONARIS is a real opportunity  
for the theoretical and physical chemistry in Paris

It is a living project still in progress

A common challenge shared by a motivated team

=> To be continued