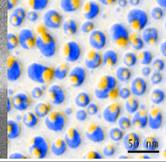
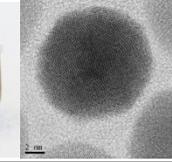
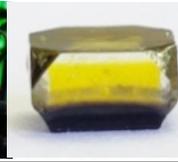
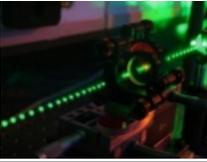
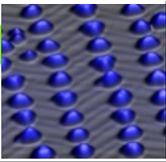
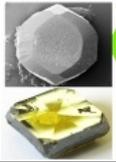
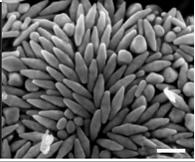
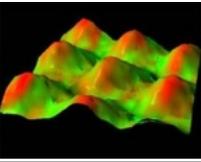
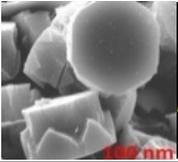


## LABEX SEAM

### Composante modélisation

- Les travaux de modélisation/simulation viennent souvent en appui à des développements expérimentaux
- Nous couvrons un large spectre de savoirs/compétences dans le champ de la modélisation/simulation des matériaux et de leurs procédés d'élaboration
- Le Labex dispose de compétences différentes, mais complémentaires
- Les moyens mis sur la modélisation/simulation sont conséquents
- **Utilisation et production de données : Pertinences ? Qualité ? Cohérence ? etc.**





# LABEX SEAM

## Caractéristique multi-échelle

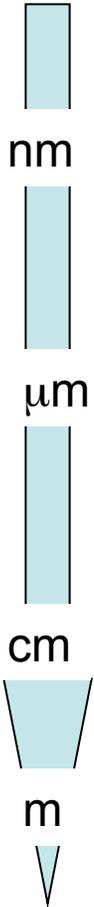
**MPQ** Électrodynamique quantique en cavité →  
conception de fonctionnalité électronique et  
photonique

**LSPM** : Simulation moléculaire MC sur ensemble  
grand canonique  
→ équilibre de systèmes gaz/solide

**MPQ**  
Simulation électromagnétique en microcavité et propriétés  
optiques de systèmes IR

**MSC** : Rhéologie-hydrodynamique de fluides  
complexes.  
→ Comportement collectifs de populations en grand  
nombre à partir de modèles microscopiques

**LSPM** —Modélisation d'écoulements réactifs hors équilibre  
(plasmas), polyphasiques (dispersions)  
→ Procédés d'élaboration



### ITODYS

Modélisation moléculaire et chimie quantique → **prédiction  
de structures et caractéristiques spectro de nanomat  
hybrides**

### LSPM

Calculs Abinitio, DFT sur solide cristallin  
→ **Propriétés élastiques**

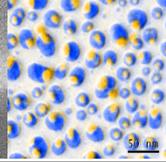
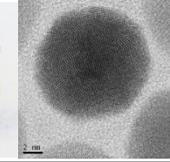
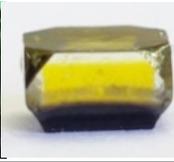
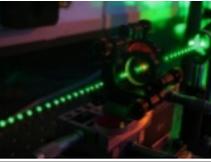
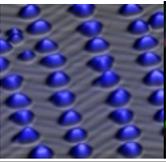
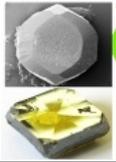
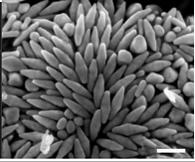
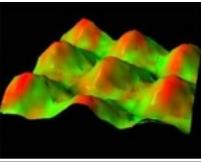
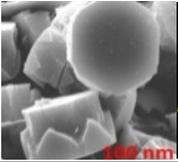
### LSPM :

Approches d'homogénéisation. Modèle micromagnétique  
→ Propriétés mécanique, magnétique, etc. et couplages  
Modèles de croissance cristalline en couche mince  
→ Conditions de textures, etc.

### LSPM

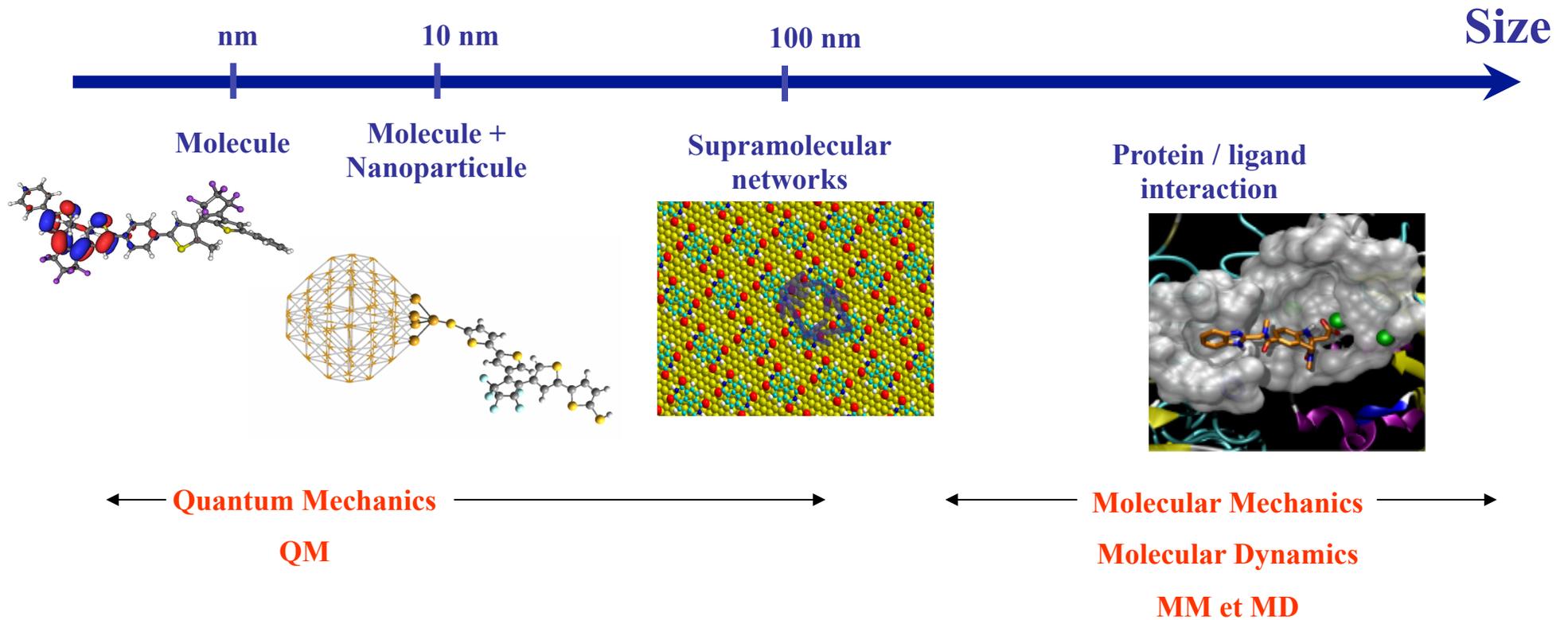
Mécanique des milieux continus  
Modèles de déformation, endommagement et rupture  
dans les matériaux

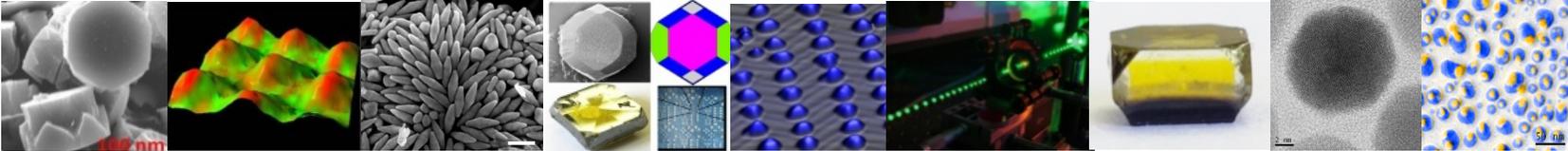




# LABEX SEAM

## Molecular Modelling Team - ITODYS



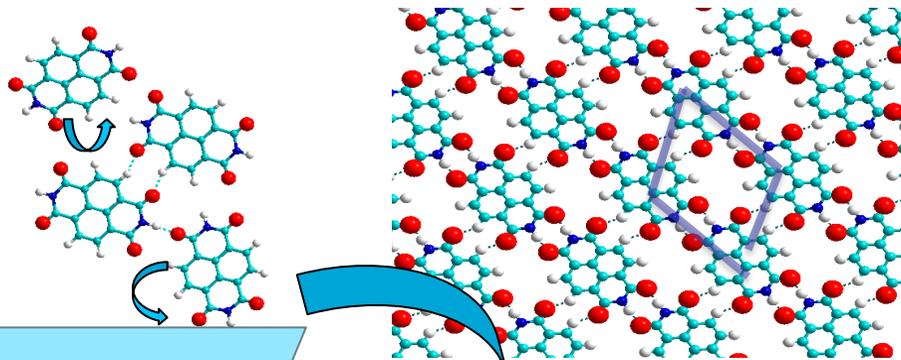


## LABEX SEAM

### *Theoretical study of the organization of supramolecular networks on metallic surface*

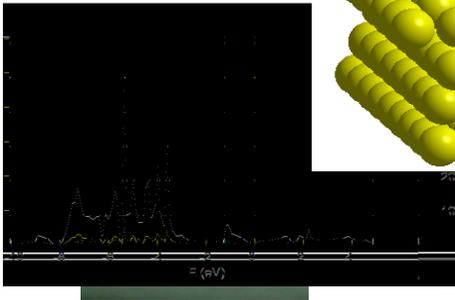
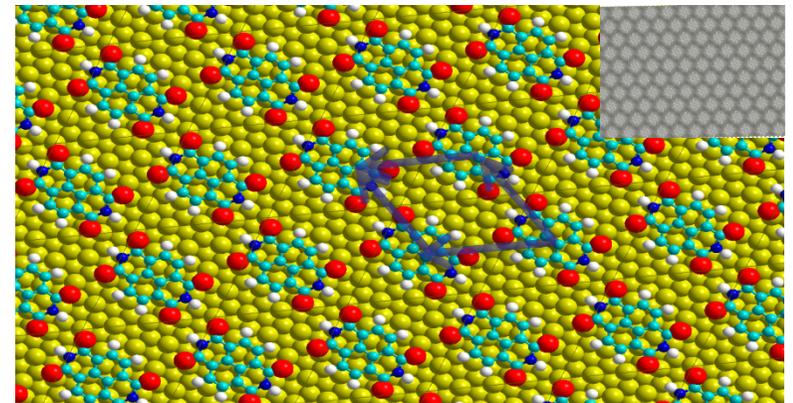
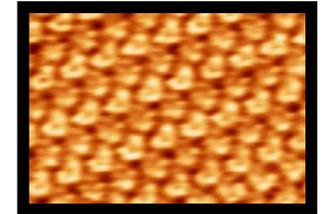
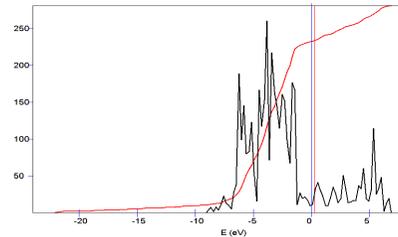
Gas phase: from aggregates to 2D network

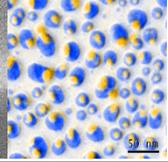
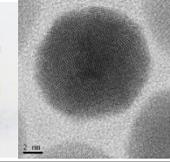
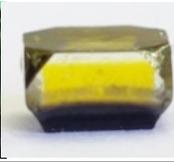
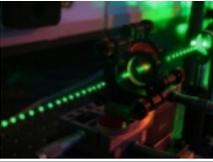
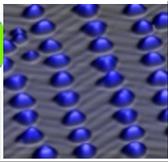
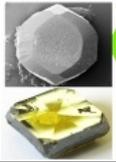
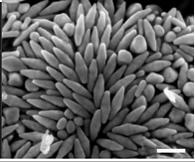
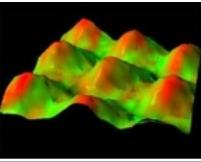
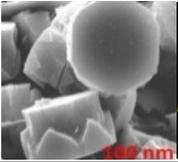
Effect of the surface and characterization: density of states, frequencies, STM image simulation, comparison with experiments



Adsorption on a surface

Surface characterization





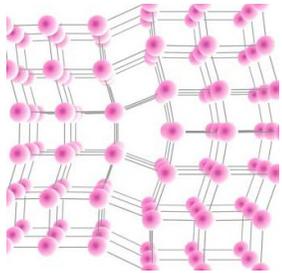
# LABEX SEAM

## Modélisations pour les Matériaux de structure (LSPM +...) Relations Microstructure / Propriétés-Comportement

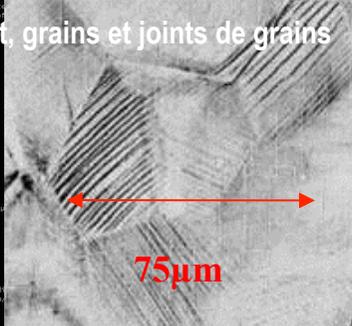
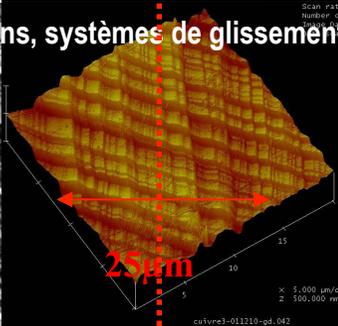
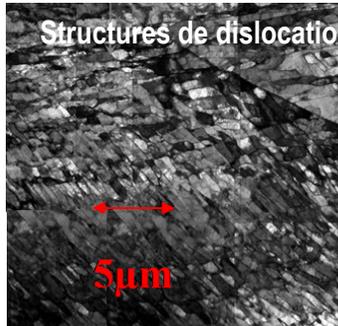
### Thermo-Elasto-Visco-Plasticité : ductilité, écrouissage, dommage, rupture

- Matériaux Métalliques (métaux, alliages, composites)
- Matériaux (poly)cristallins (métalliques; céramiques, composites metal-oxydes)
- Matériaux hétérogènes, architecturés
- Autres si applicatif

### Modélisations Multi-Echelles



structures cristallines



Structures de dislocations, systèmes de glissement, grains et joints de grains



énergie, transports, ...

### Simulations Multi-Echelles

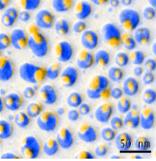
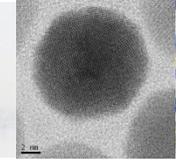
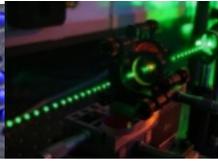
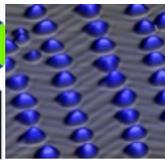
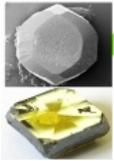
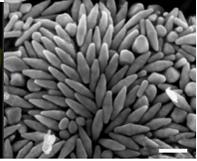
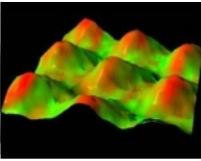
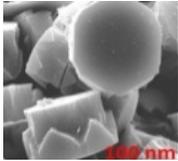
### Couplages d'échelles

### Micro-Macro I

### Micro-Macro II

Amont <<< Deux sous-domaines complémentaires >>> Aval

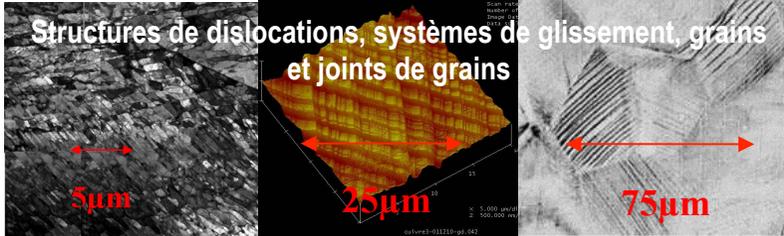
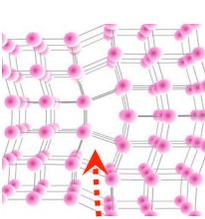




Modélisations Multi-Echelles

LABEX SEAM

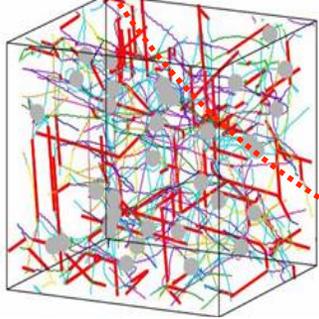
pour les Matériaux de structure



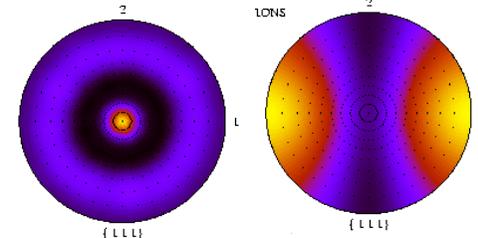
**Micro-Macro I :** De la loi *Microstructurale* de comportement local au comportement effectif par méthodes d'homogénéisation, méthodes statistiques, méthodes de champs

Mécanismes élémentaires + Lois physiques de déformation, d'écroutissage & restauration (dislocations, parois, joints)

Dynamique moléculaire



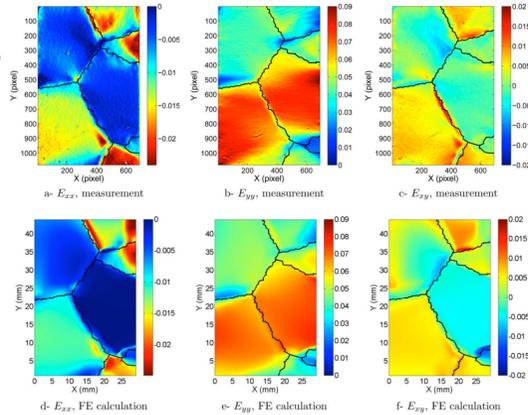
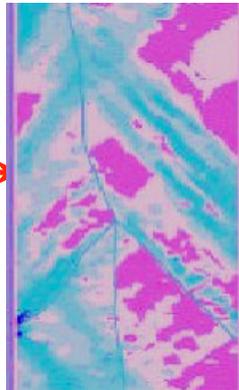
Dynamique des dislocations



Calcul des distributions statistiques d'orientations cristalline (textures)

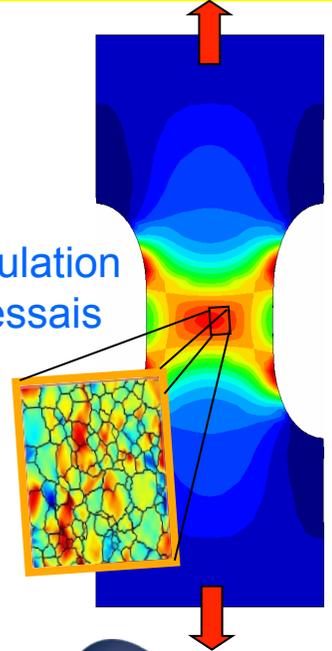
Glissements

Structures de Dislocations



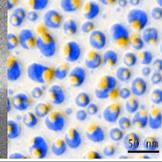
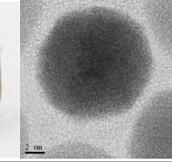
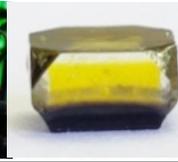
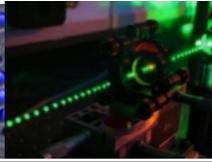
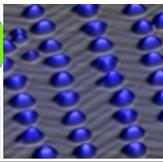
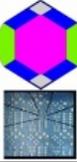
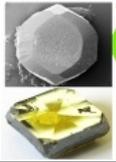
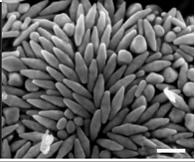
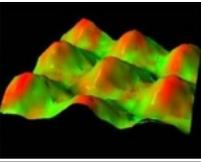
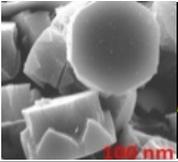
Estimations de champs cinématiques

simulation d'essais



Echelles et couplages d'échelles en développement





## LABEX SEAM

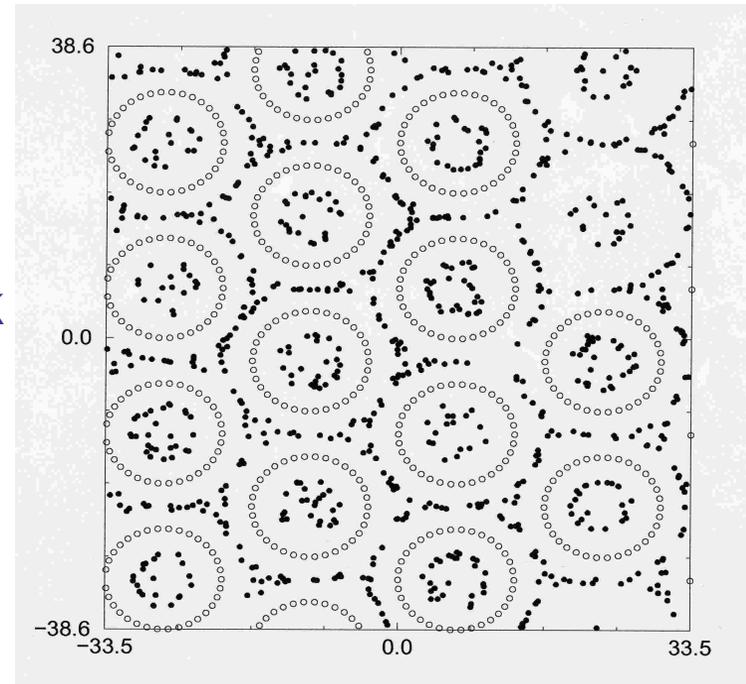
### Hydrogen adsorption on CNT arrays

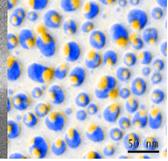
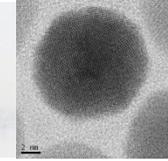
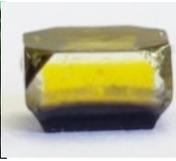
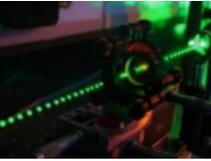
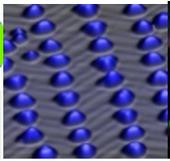
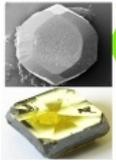
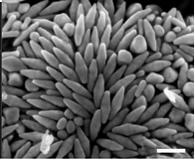
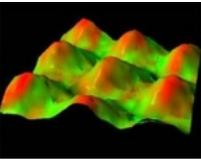
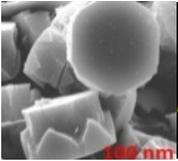
MC Molecular simulation  
ensemble grand canonique

Metropolis Algorithm  
Energy minimization

- 20 MPa
- 293 K et 77 K
- $D = 1$  à  $2$  nm
- $d = 0.3$  à  $1.3$  nm

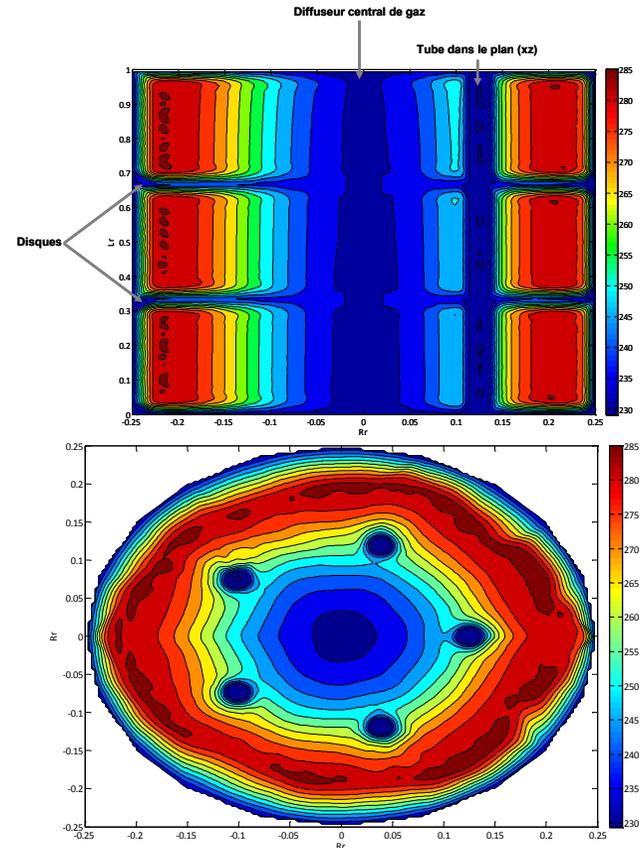
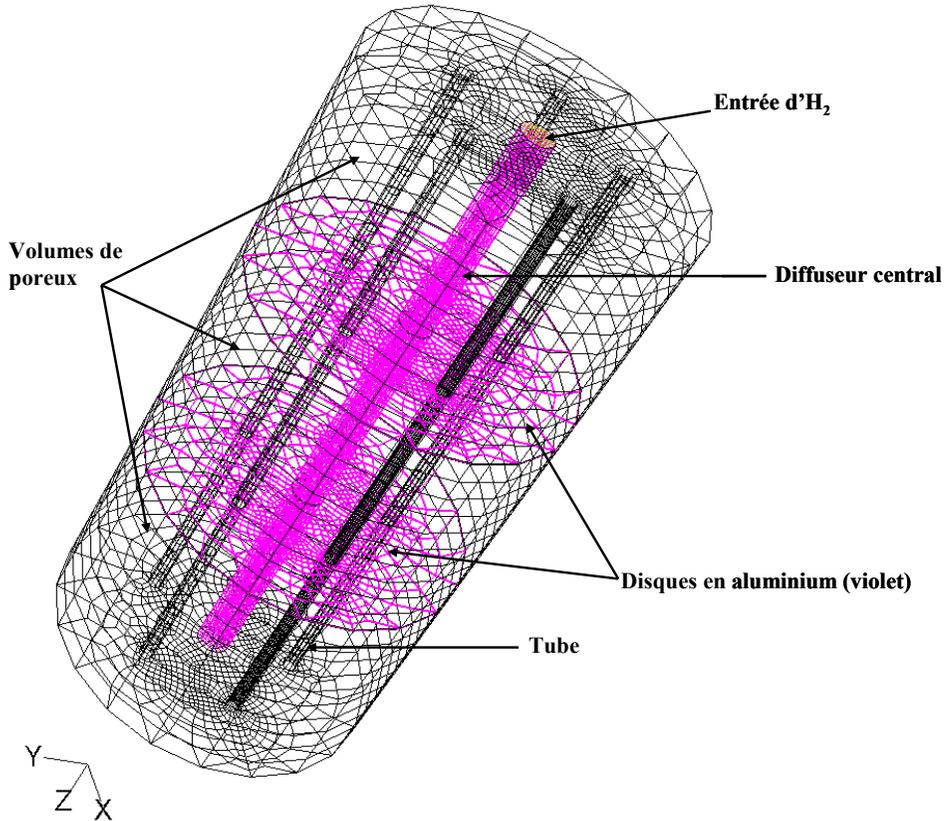
**Physical  
adsorption on NTC  
external walls**





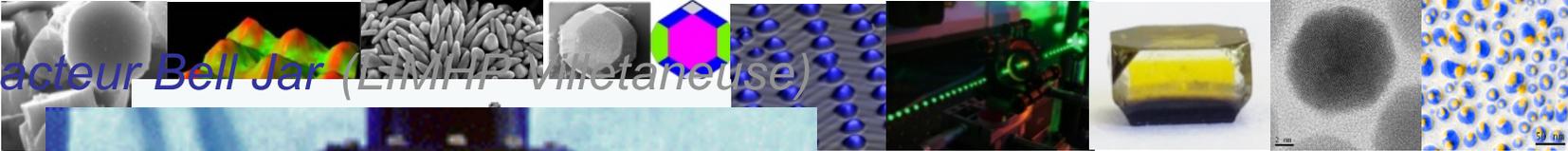
# LABEX SEAM

## *Dynamical Charging process : thermal management and storage performance*

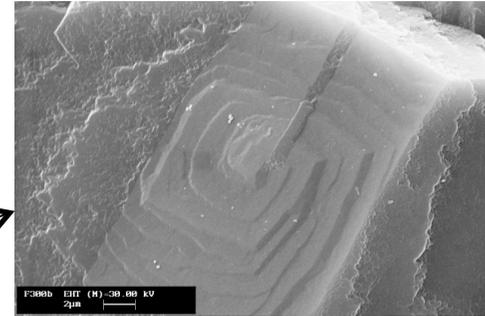
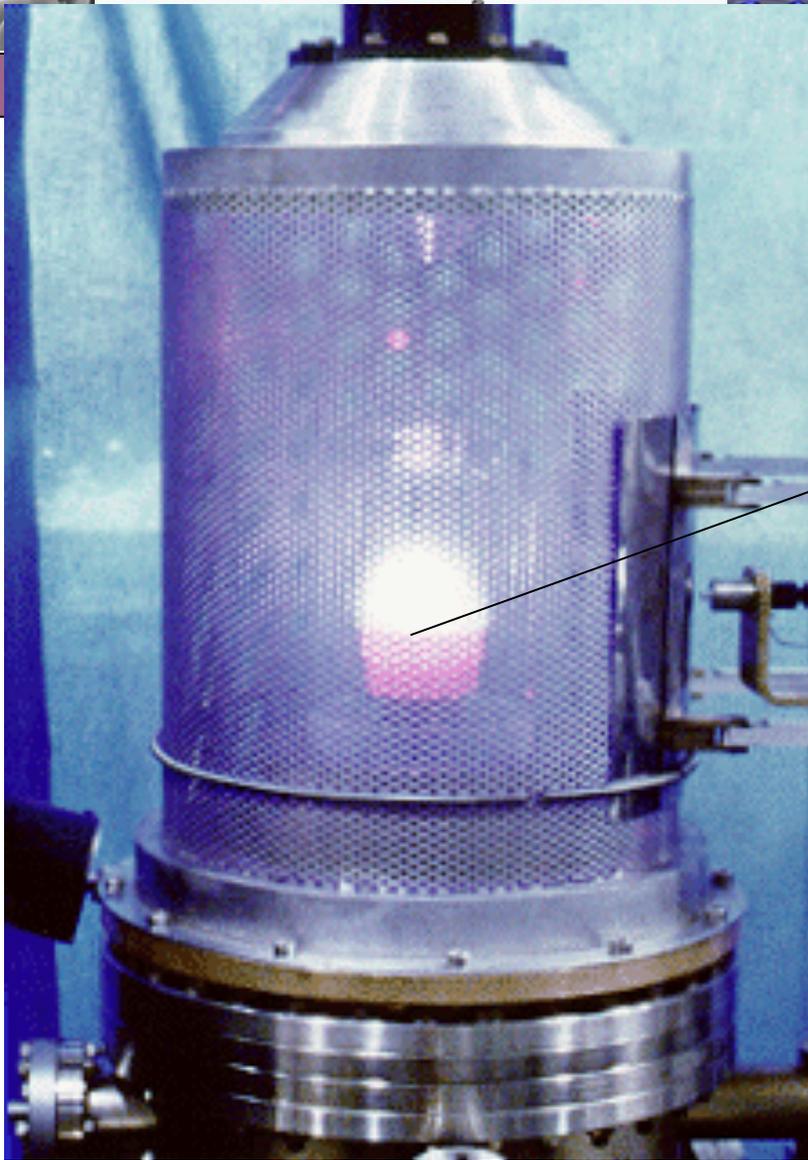




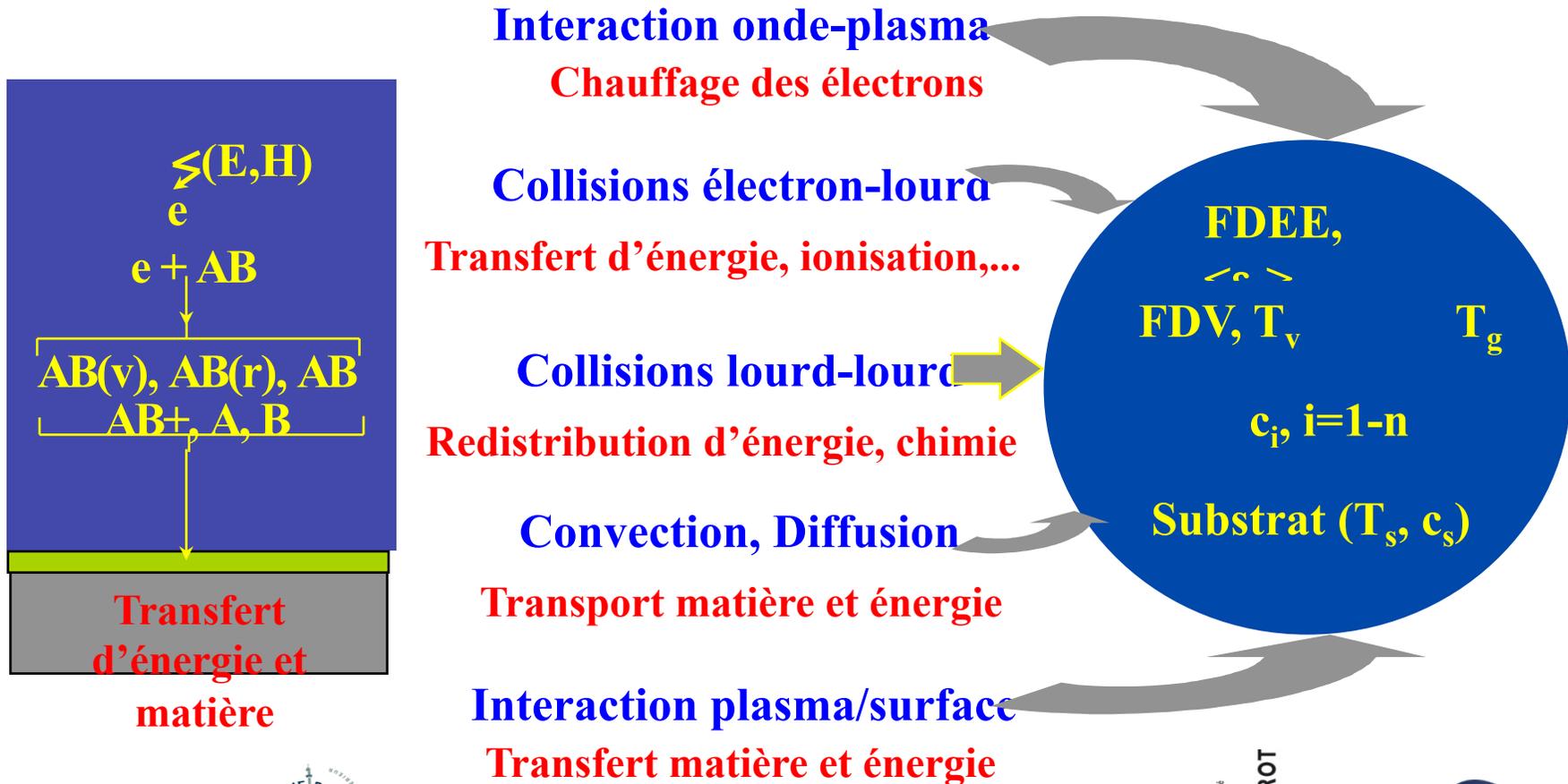
# Réacteur Bell Jar (EMHF-Villetaneuse)

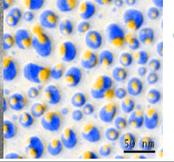
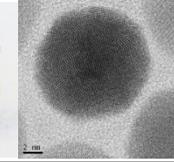
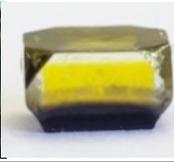
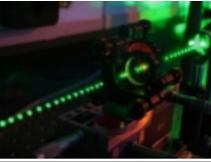
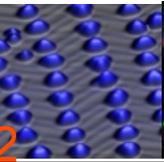
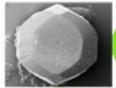
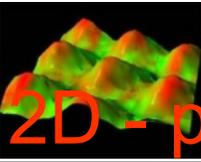
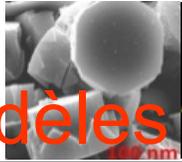


## SEAM



# Modélisation des Procédés d'élaboration des matériaux (exp des procédés plasmas)





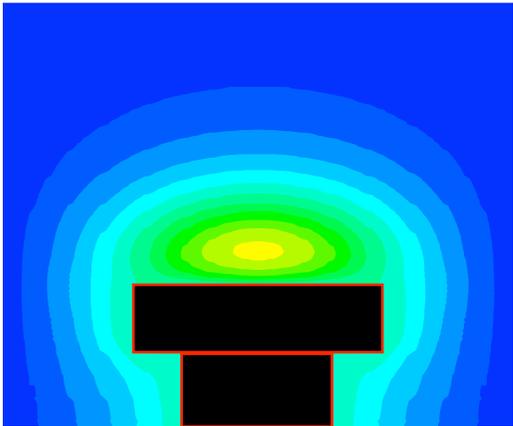
# Modèles 2D - plasma de H<sub>2</sub>

## Résultats - modèle 'auto-cohérent'

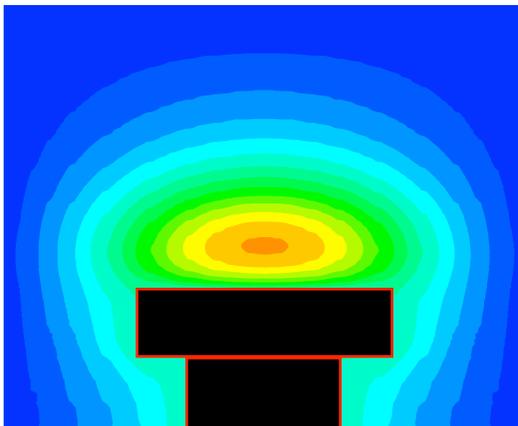
LABEXSEAM

[Puissance optimale à pression donnée : 2500 Pa](#)

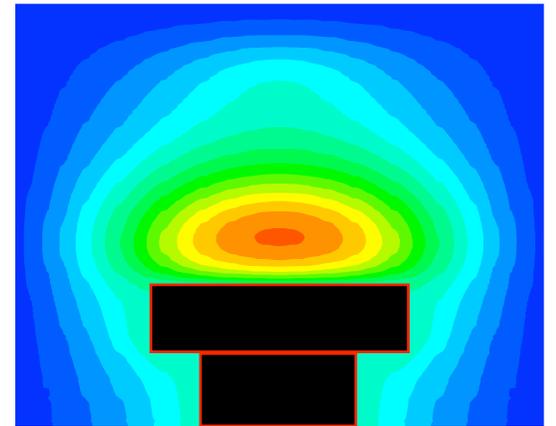
300 W



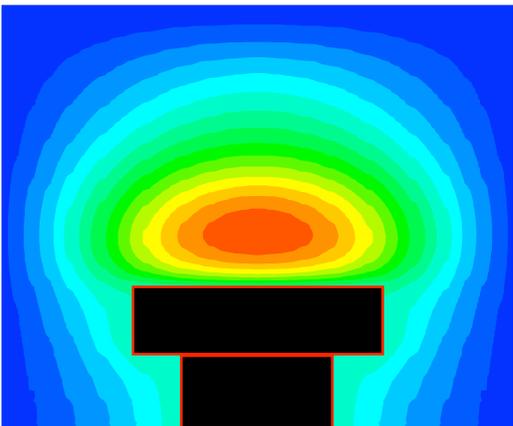
500 W



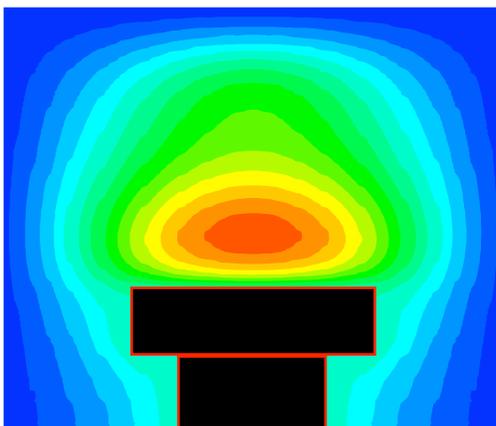
700 W



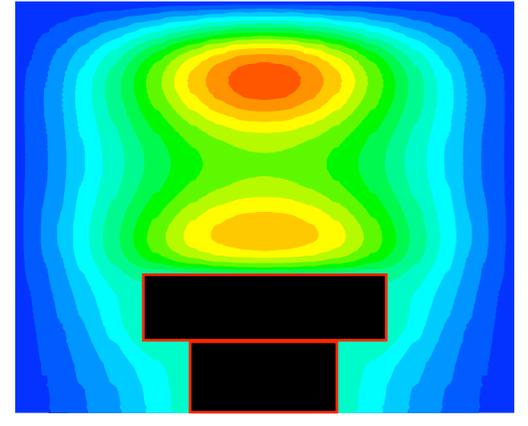
800 W



900 W



1000 W

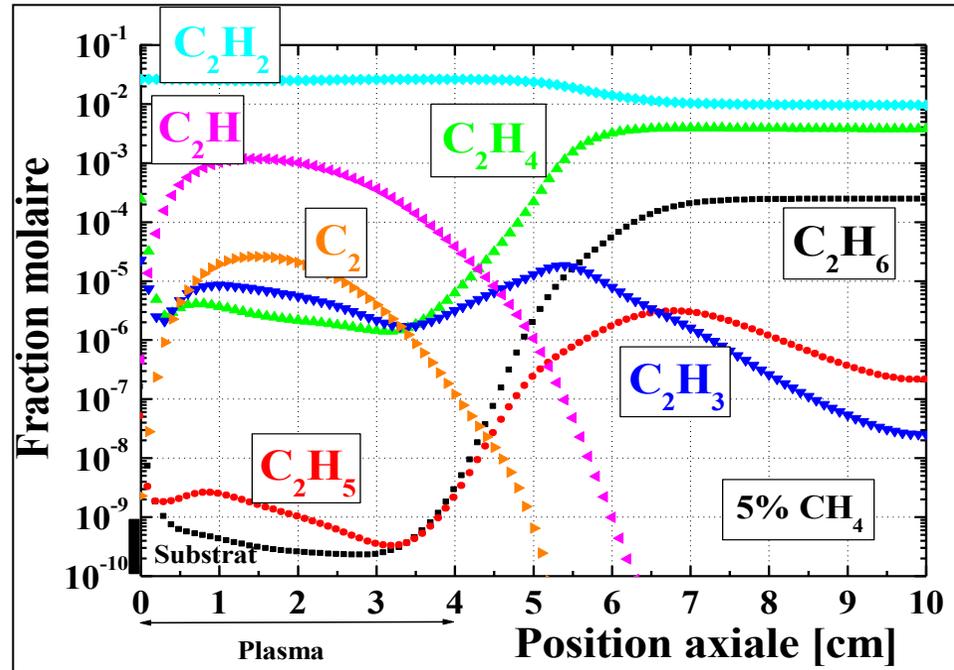
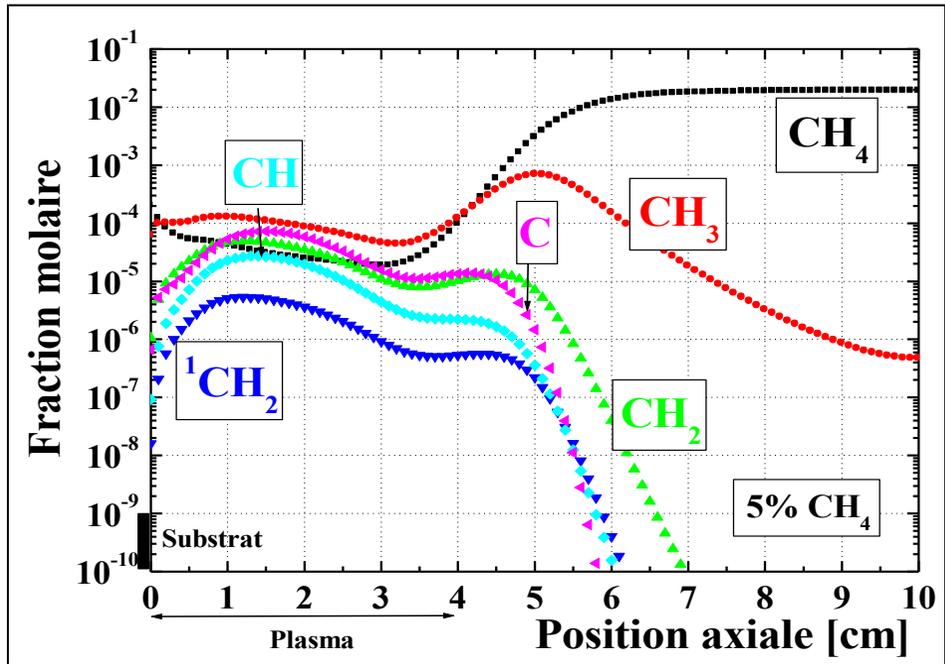


**Profil axial d'espèces carbonées**  
**30 W.cm<sup>-3</sup> (120 mbar / 2 kW)**

$CH_x$

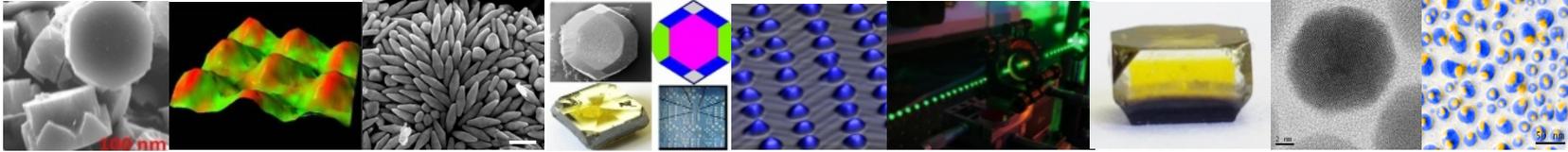
$T_{gmax} = 3200\text{ K}$

$C_2H_y$



- 1/  $C_2H_2$  domine dès l'entrée du réacteur (plasma de  $H_2/C_2H_2$ )
- 2/ Fortes variations en couche limite et au bord de la décharge (raideur spatiale)
- 3/ Forte dissociation de  $CH_4 \Rightarrow$  production de C et  $C_2$  en volume
- 4/ Mesure intégrée  $\Rightarrow$  ce qui se passe hors décharge et non pas dans le plasma





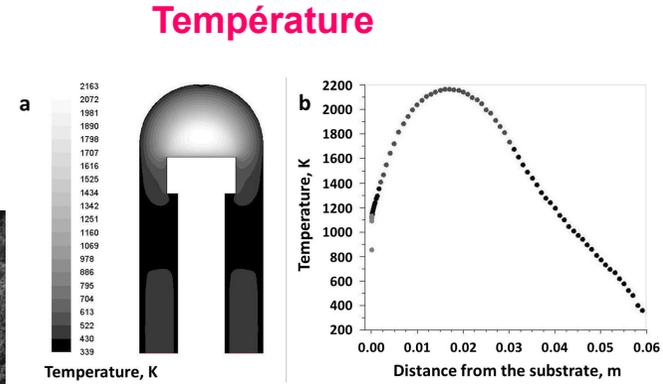
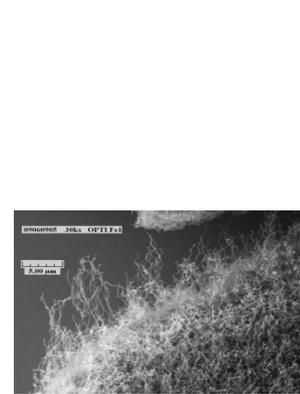
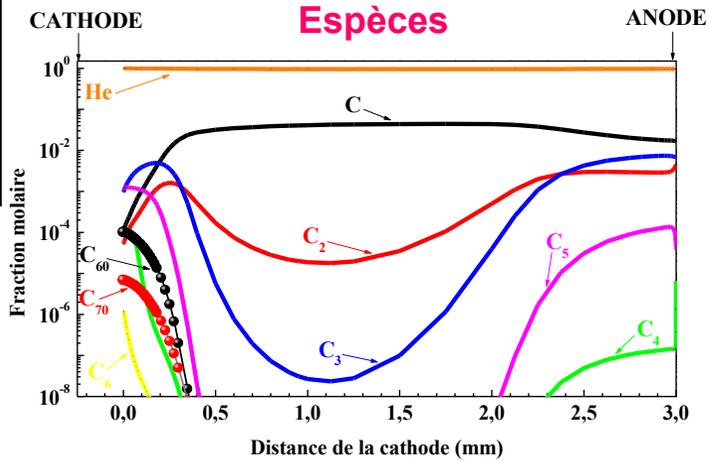
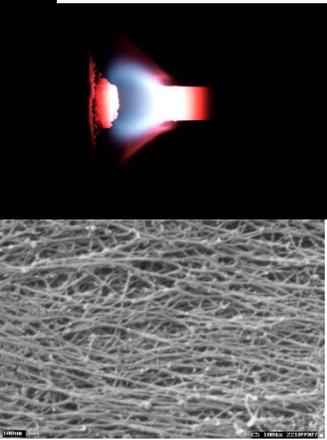
# LABEX SEAM

## Modélisation des écoulements réactifs

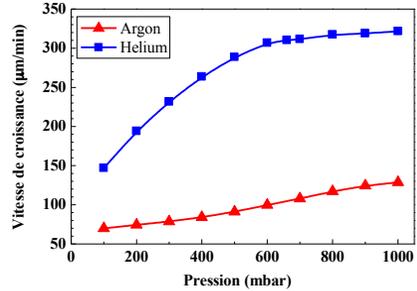
## Simulations thermocinétiques de la croissance de nanotubes

• Simulation de la synthèse de nanotubes par arc

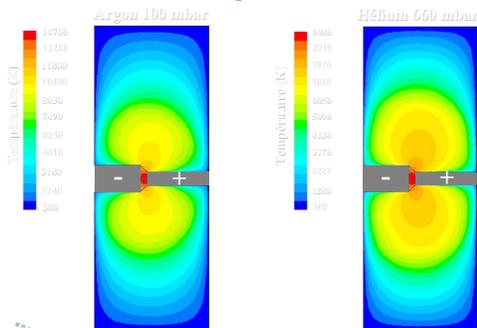
• Simulation de la synthèse de NT Orientés par PECVD



### Vitesse de croissance



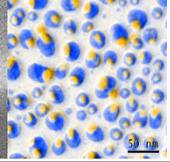
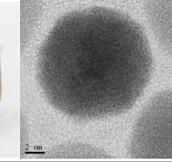
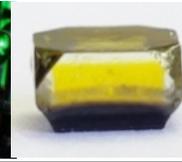
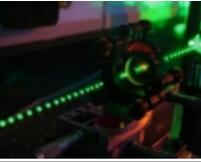
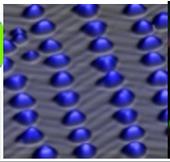
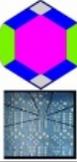
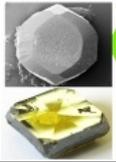
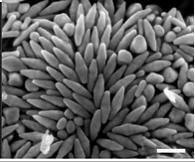
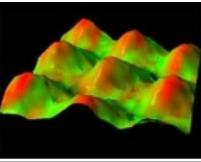
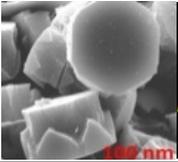
### Température



### écoulement

### Vitesse de croissance





## LABEX SEAM

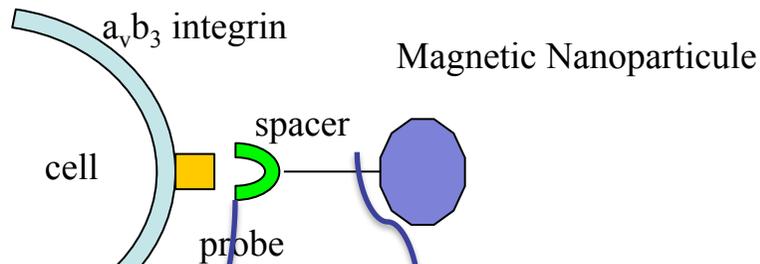
### Conclusion

- Potentiel de synergie sur les approches
  - Chimie théorique
  - Dynamique
  - Simulation électromagnétique
  - Approches statistiques
  - Mécanique des milieux continus→ Potentiel d'adaptation sur plusieurs objets d'études
- Possibilité d'associer des expertises sur différents niveaux de description et approches pour aller sonder des problématiques associant procédé-matériaux(structure)-matériaux(fonctionnalité)-système
- Problématique des « données » en tant qu'input identifiées depuis plus d'une dizaine d'année  
→ **problématique des interprétations des masses de données en output des simulations (3D, particulières)**

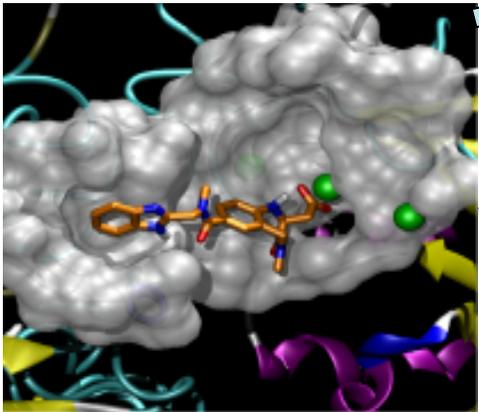


# LABEX SEAM

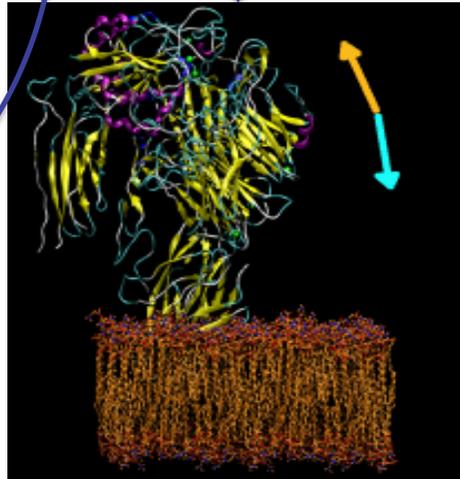
*Molecular modeling for bionanotechnologies can help to:*



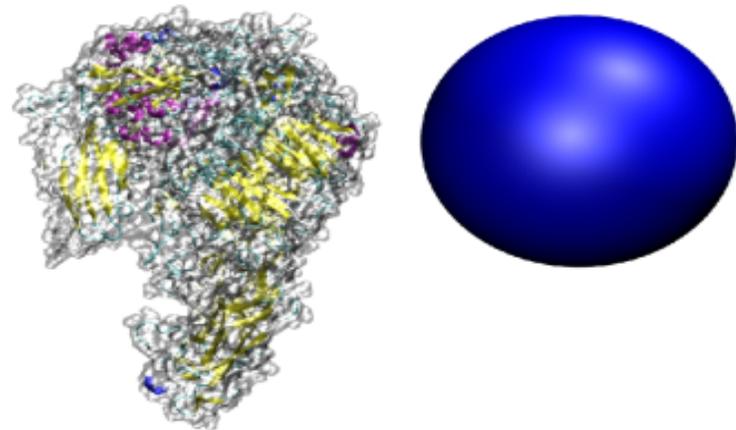
*Toward new selective MRI contrast agents or hyperthermia therapies against cancer*

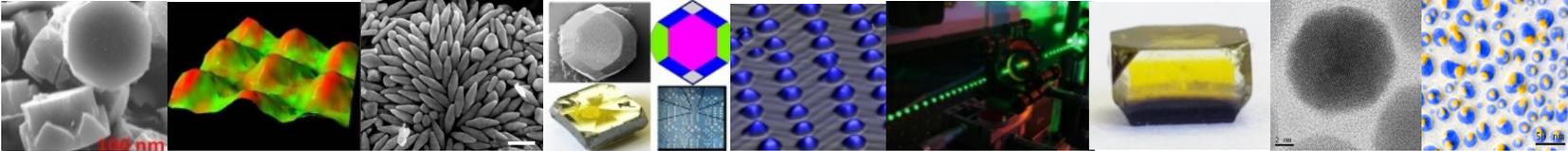


*The design & optimization of the probe (molecular docking calculations)*



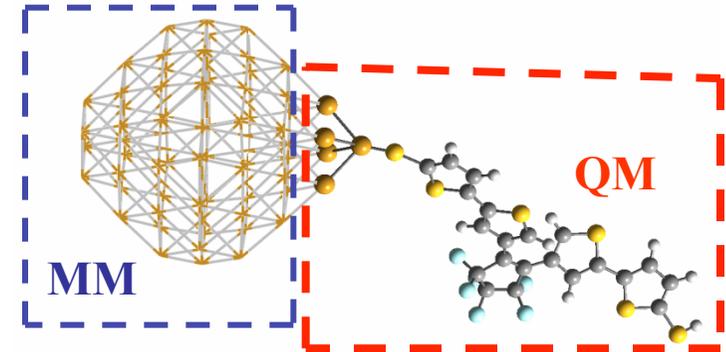
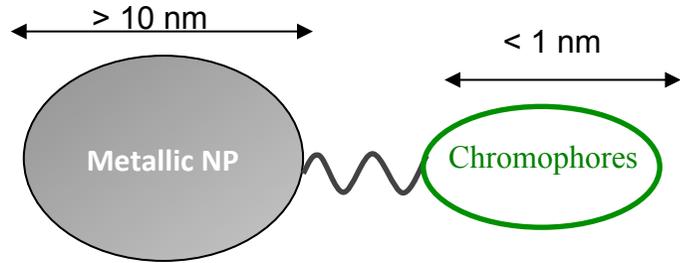
*Orientation and length of the spacer to maintain the structural integrity of the ligand/target recognition (MD & structural analyses)*





# LABEX SEAM

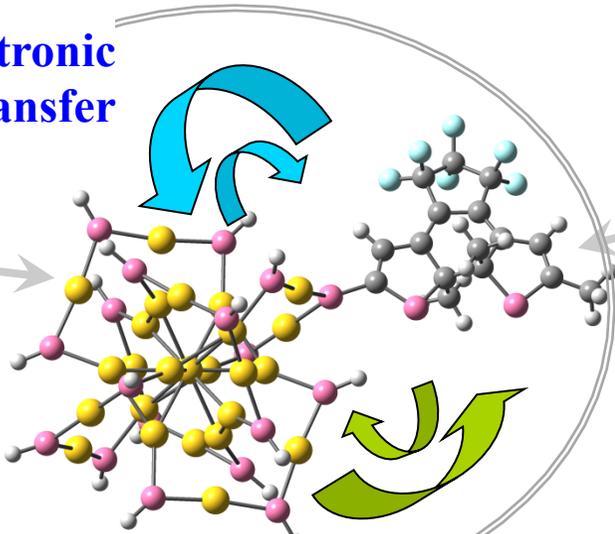
## Towards the "in silico" design of nano-hybrid switches



Study of the electronic transfer

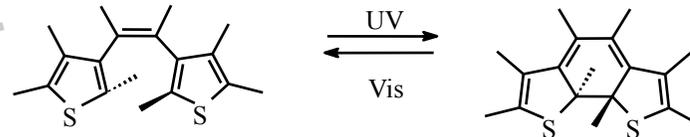
NP :  $\text{Au}_{25}(\text{SH})_{18}$

Plasmonic properties

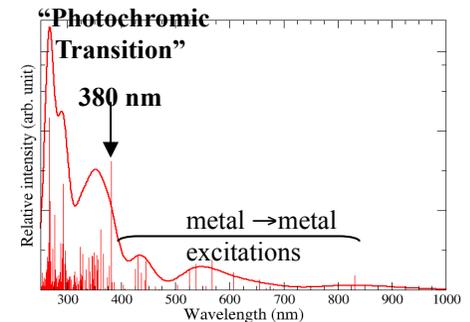


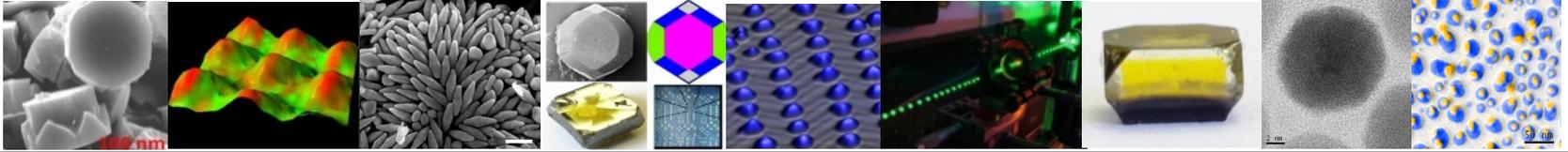
Study of the energy transfer

Photochromic molecule



Simulation of the optical properties of molecules grafted on NP

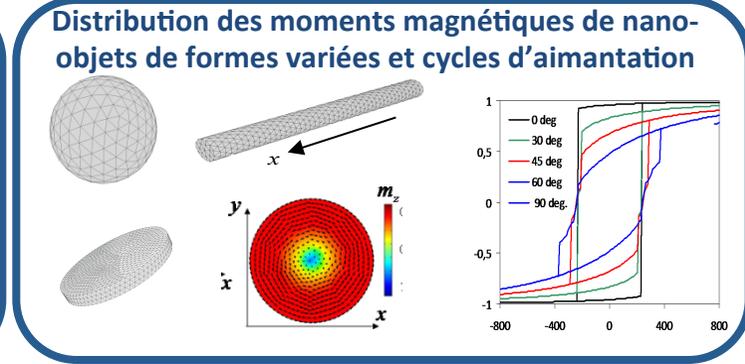
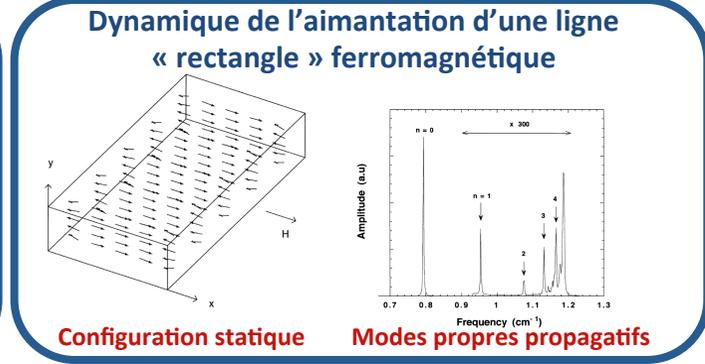
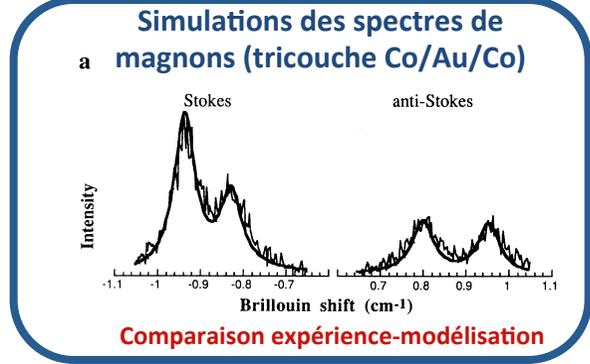




**Groupe FINANO (LSPM) LABEX SEAM**

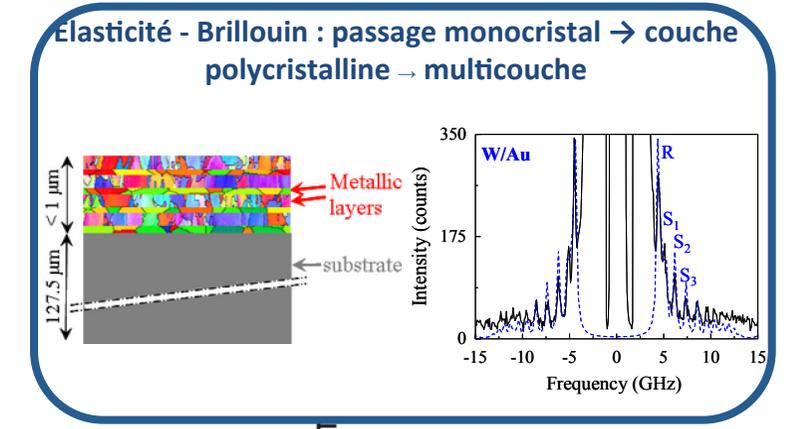
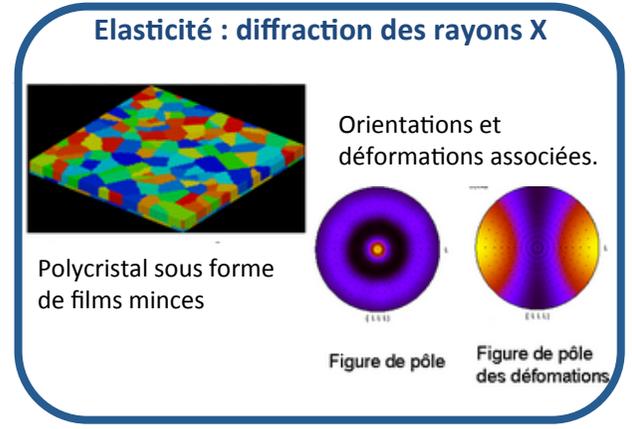
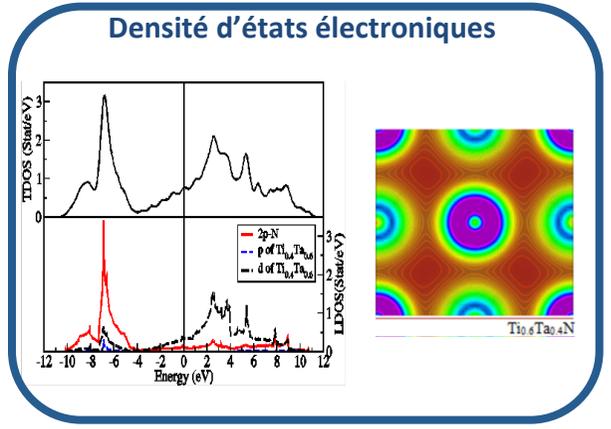
**Théorie du micromagnétisme (codes « maisons » et/ou libres)**

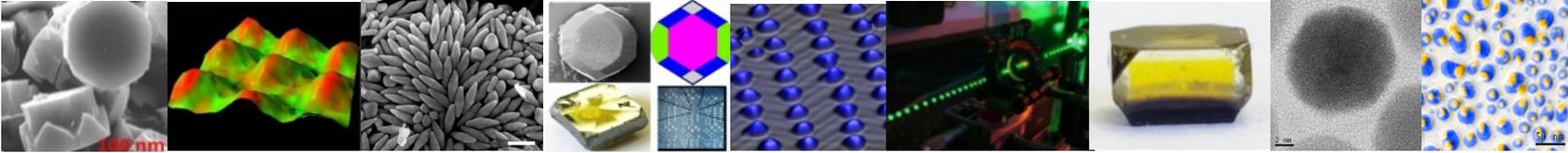
Application à l'étude des propriétés statiques et dynamiques de l'aimantation dans les couches et multicouches ferromagnétiques ainsi que dans des nano-objets ferromagnétiques



**Elasticité: de la théorie de la fonctionnelle de la densité (ABINIT) à l'homogénéisation:**

**Propriétés calculées:** énergie de formation du cristal, paramètre de maille, densité électronique, constantes et modules élastiques, permittivité, phonons

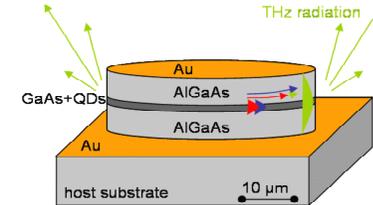




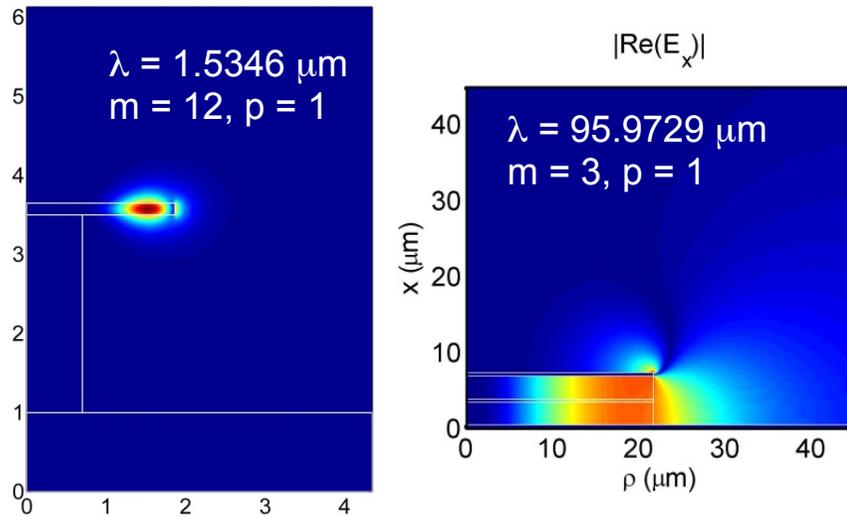
# LABEX SEAM

## Equipe DON

Simulations électromagnétiques  
d'optique non linéaire en  $\mu$ -cavité



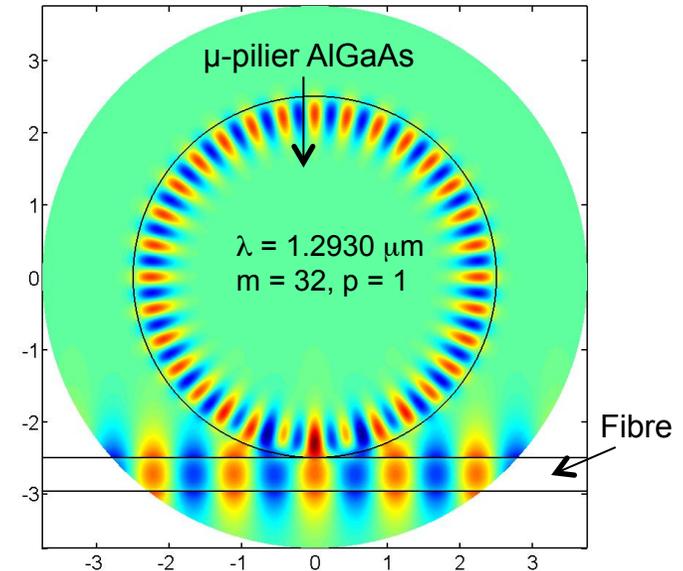
### Domaine des fréquences (FDFD)



Calcul vectoriel des modes de cavité:

- Fréquences de résonance
- Facteurs de qualité

### Domaine du temps (FDTD)



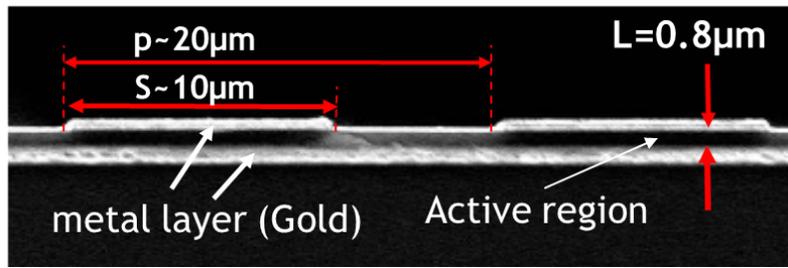
Propagation (2D et 3D) de la lumière dans  
des structures dispersives et non linéaires



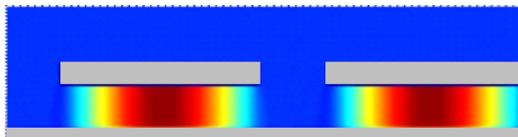
# LABEX SEAM

Equipe QUAD: Simulations des propriétés optiques et électroniques de dispositifs infrarouges

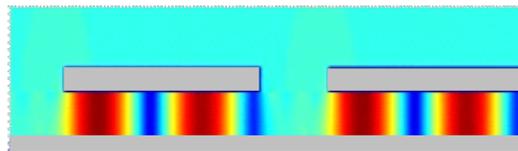
## Modes de cavités plasmoniques



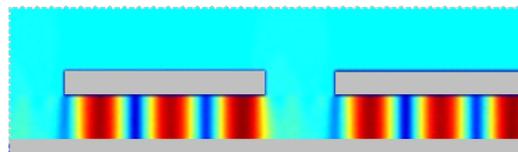
3.5 THz



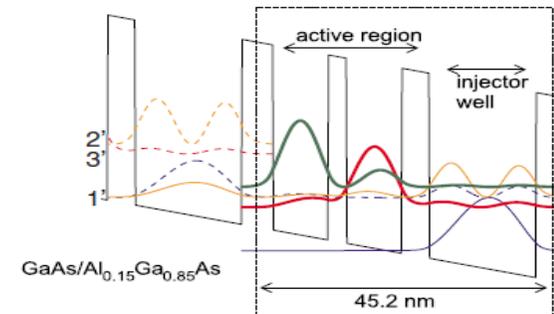
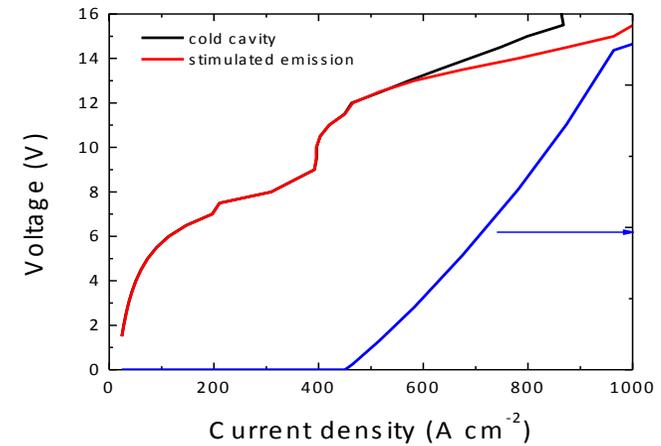
6.5 THz



7.8 THz

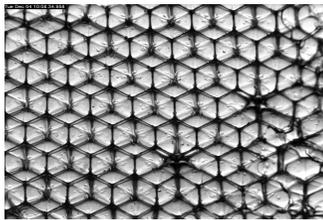


## Caractéristiques électriques et optiques de lasers à cascade quantique



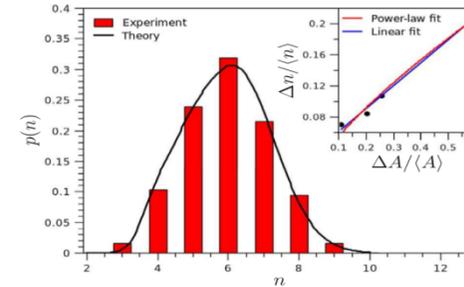
# Mousses au laboratoire MSC

**Mousses gélifiées** Alain PONTON



**Physique statistique des mousses**

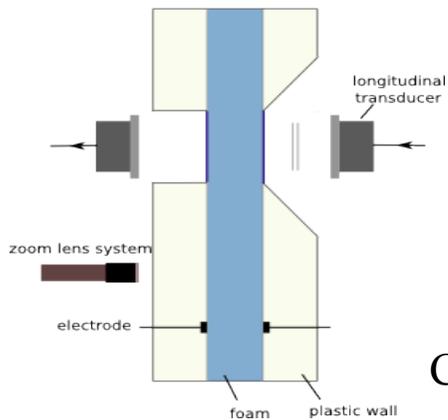
Marc DURAND



**Vibrations et acoustique des mousses**

Valentin LEROY  
transmission configuration

Florence ELIAS  
Caroline DEREK

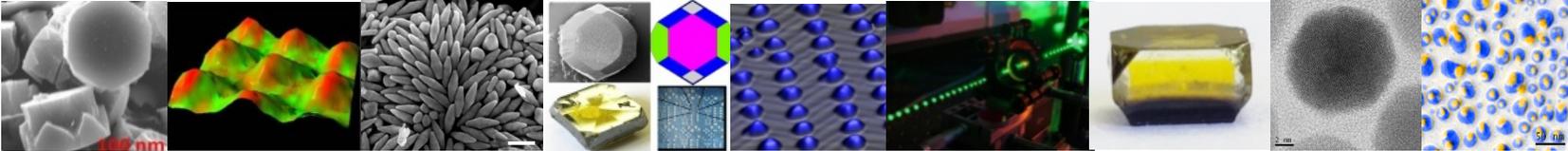


Cyprien GAY

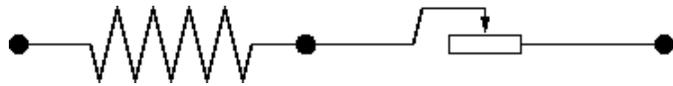
**Rhéologie des mousses**

Cyprien GAY





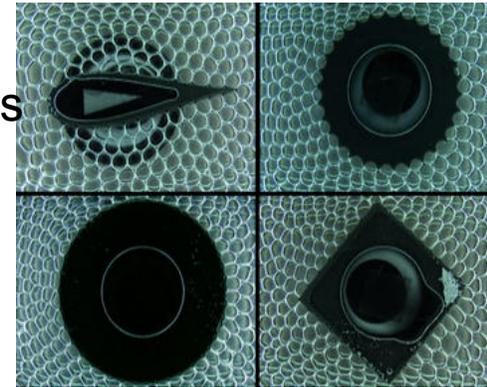
# Rhéologie des mousses



modèles rhéologiques à un tenseur

Marmottant, Raufaste, Graner (2008)  
Bénito et al. (2008)

mousses :  
grandes  
déformations

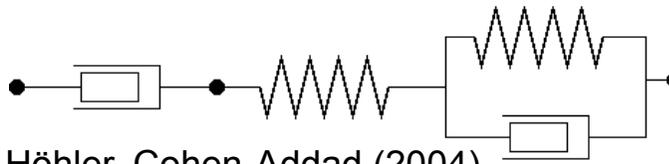


tilt + plasticity = overshoot  
Raufaste et al PRE (2010)

Maxwell = un tenseur



mais les mousses sont plus riches



Höhler, Cohen-Addad (2004)

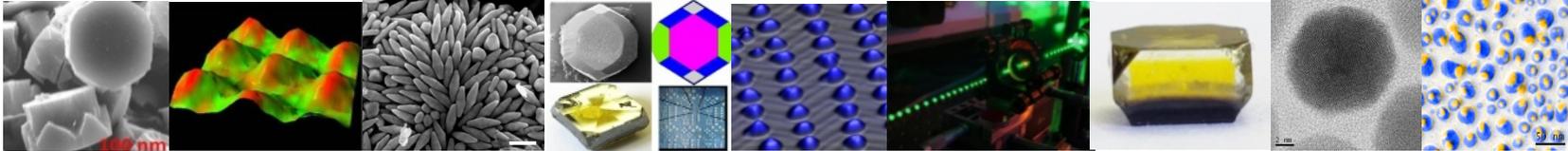
Cyprien GAY, Isabelle CANTAT (2011/2012)



modèle  
rhéologique  
à deux tenseurs







Modélisations Multi-Echelles

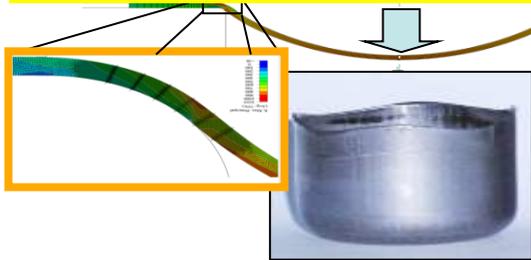
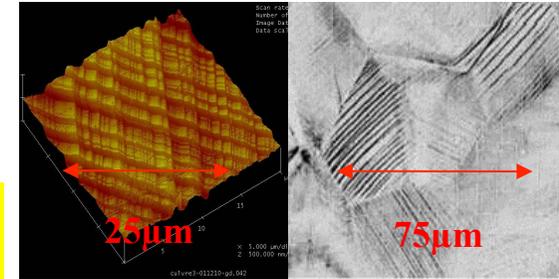
LABEX SEAM

pour les Matériaux de structure

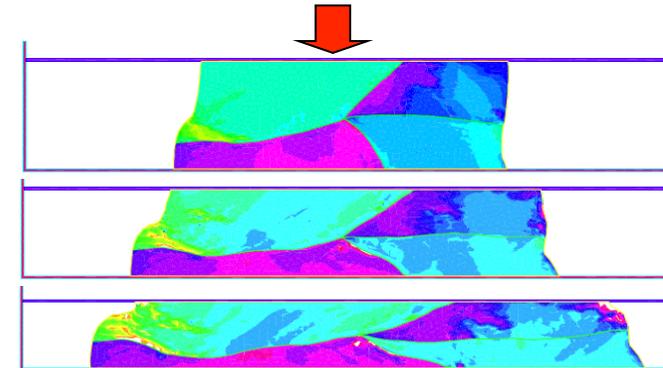
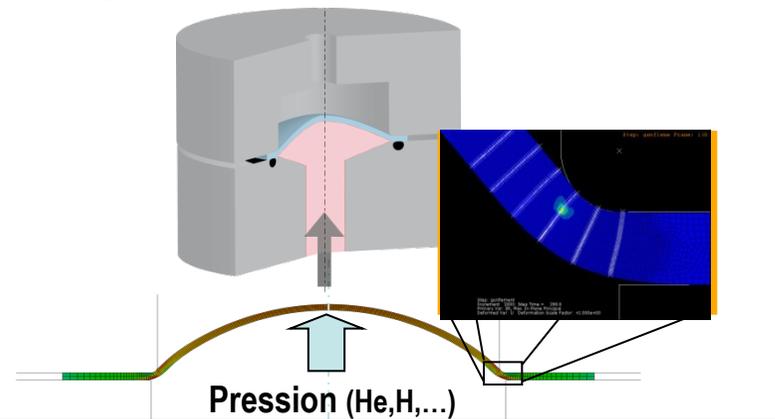
### Micro-Macro II:

De la loi de comportement local Homogénéisé ou phénoménologique, Au comportement global par *Calculs de structure*

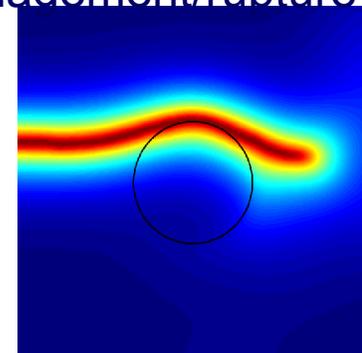
Grandes Déformations Statiques (formage), Dynamiques (impact), Prise en compte des hétérogénéités de phases (grains, sous-grains, inclusions,)



### Chargements/enviromnements complexes



Endommagement/rupture

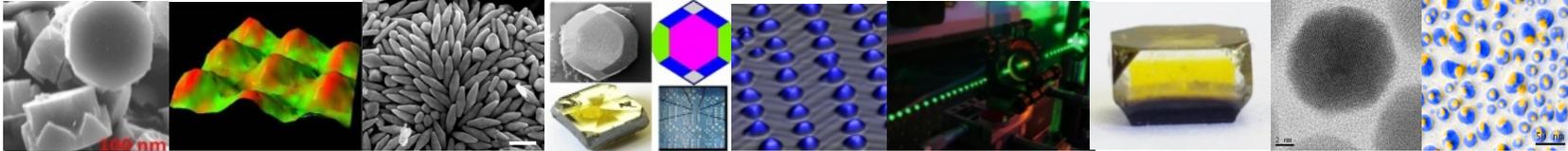


Autres couplages mécanique/chimie/physique en développements

PEEQ (Avg: 75%)  
+6.000e-01  
+5.500e-01  
+5.000e-01  
+4.500e-01  
+4.000e-01  
+3.500e-01  
+3.000e-01  
+2.500e-01  
+2.000e-01  
+1.500e-01  
+1.000e-01  
+5.000e-02  
0.000e+00

laminage





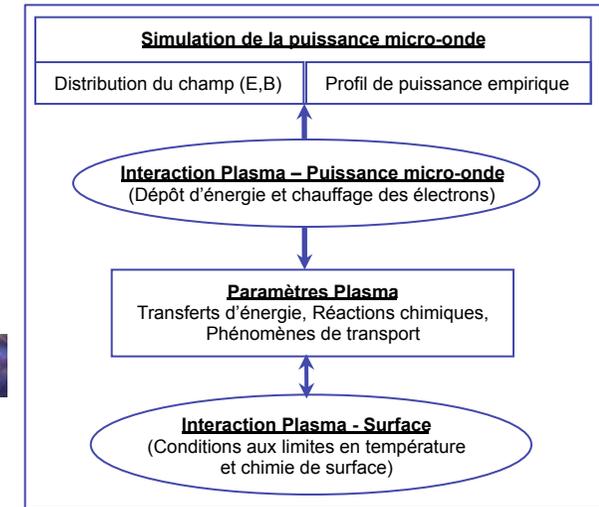
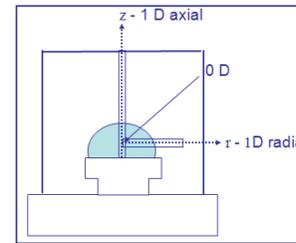
# LABEX SEAM

## Modélisation des écoulements réactifs

### Simulations thermocinétiques de la phase gaz pour la croissance de diamant

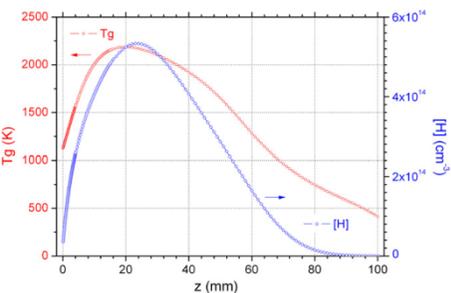
#### Outils de simulations

Géométrie	Chimie considérée	Spécificité	Réacteurs
0D	H <sub>2</sub> , H <sub>2</sub> /CH <sub>4</sub> , H <sub>2</sub> /CH <sub>4</sub> /Ar, Suies		Bell Jar Métallique
1D	H <sub>2</sub> , H <sub>2</sub> /CH <sub>4</sub> , H <sub>2</sub> /CH <sub>4</sub> /Ar, H <sub>2</sub> /CH <sub>4</sub> /B <sub>2</sub> H <sub>6</sub>	Axial – Radial	
2D	H <sub>2</sub>	Auto cohérent	

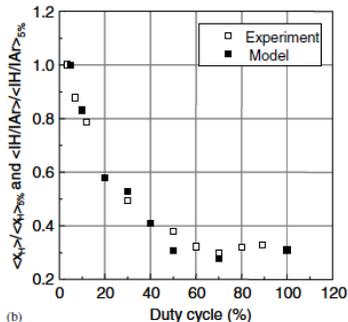


#### Exemples de résultats obtenus

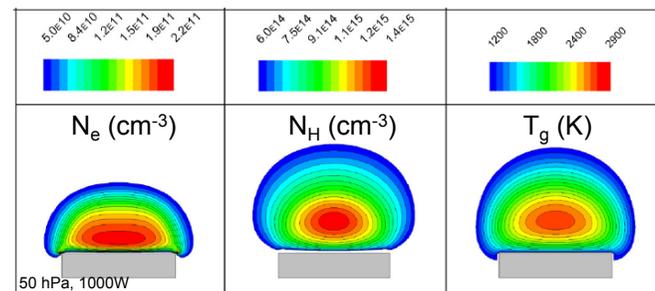
Profil 1D des températures, densités d'espèces et taux de production



Evolution temporelle (T, n<sub>i</sub>) pour plasma pulsé



Cartographie 2D des densités et températures



(T, n<sub>i</sub>) plasma à la surface du diamant

