

MI²C

Multiscale Investigations of the impact of Mineral Impurities on gas trapping within Clathrate Hydrates

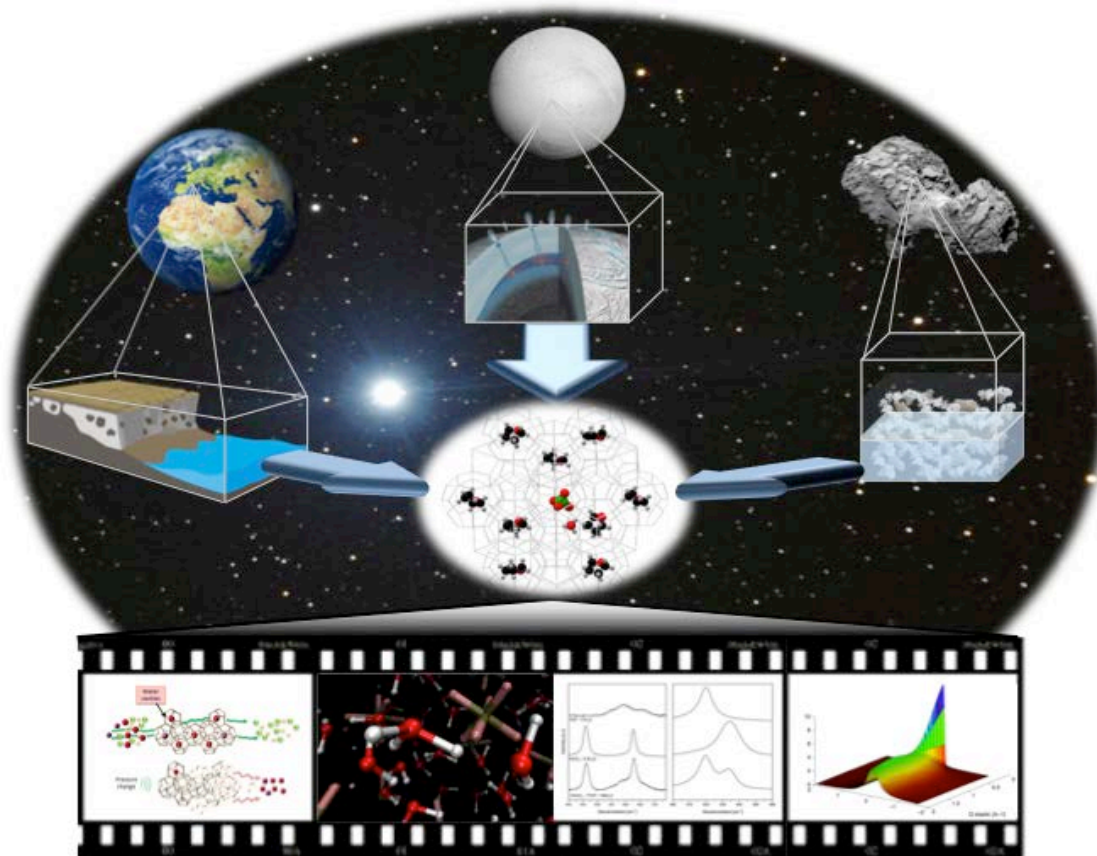
ANR PCR « Défi de tous les savoirs »
2015 – 2020

<http://www.hydrate.eu/MI2C>

Coordinateur: a.desmedt@ism.u-bordeaux1.fr

Groupe Spectroscopie Moléculaire
ISM - UMR5255 CNRS - Univ. Bordeaux I

MI²C?



Central issue: investigation of the physico-chemical properties of clathrate hydrates formed onto/into mineral surfaces, porous sediments or in the presence of salts under geo- or astrophysical thermodynamics conditions.

Partners

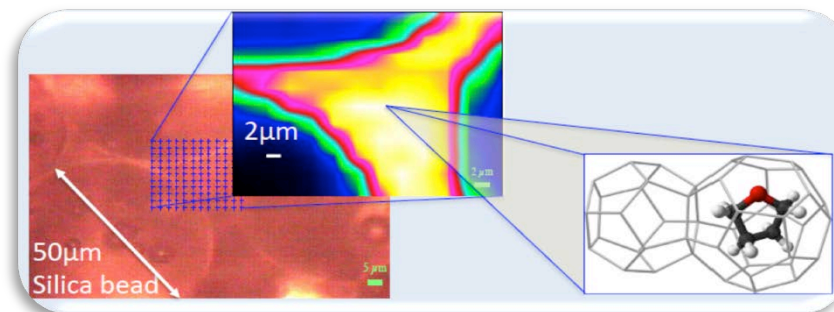
- A. Desmedt, M. Dussauze, C. Petuya, F. Adamietz, D. Talaga, J.L. Bruneel
ISM, Bordeaux
- B. Chazallon, C. Pirim, M. Ziskind, C. Focsa, C. Carpentier
PhLAM, Lille
- J.M. Simon, C. Labbez, M. Salazar
ICB, Dijon
- L. Martin-Gondre, V. Balleneger, S. Picaud
UTINAM, Besançon



➤ Consortium including experimental AND theoretical teams.

Objectives

- The project focuses on the study of:
 - ✓ **mixed clathrate hydrates** in thermodynamics conditions suitable to geological and astrophysical environments,
 - ✓ the **influence of mesoscopic surrogate** properties as present in natural environments.
- Advancing the fundamental understanding of the influence of mineral and sediments impurities:
 - ✓ onto clathrate hydrate **formation/dissociation mechanisms**,
 - ✓ onto the **clathrate hydrate stability**,
 - ✓ **guest-gas selectivity** when exposed to gas mixtures.



Mimicking clathrate hydrates formation into/onto surrogates

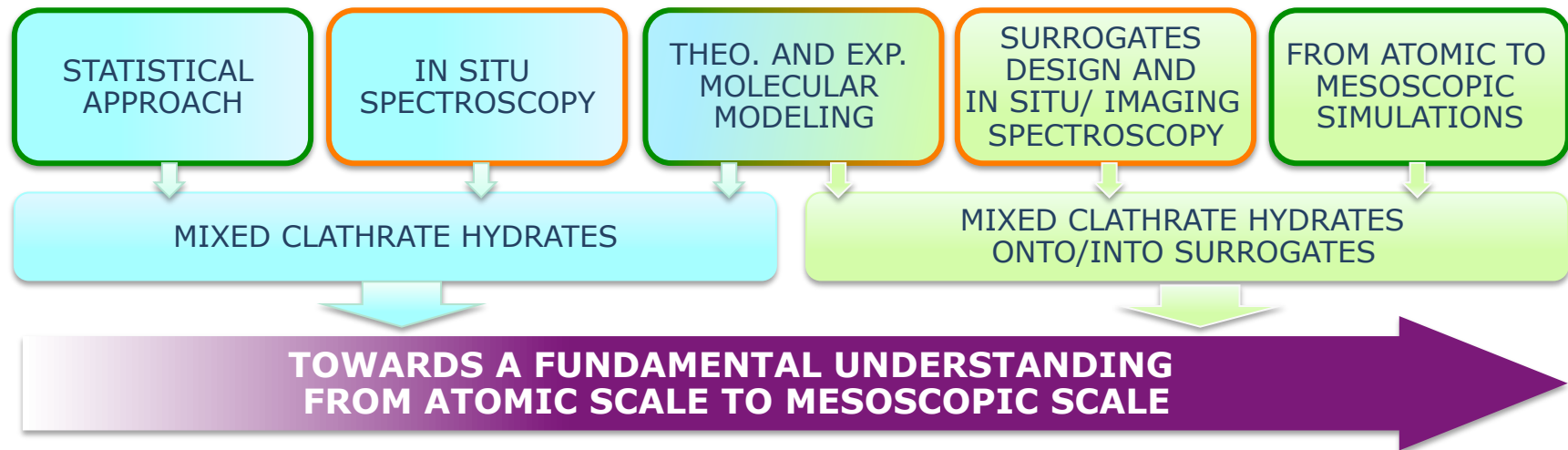


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Clathrate Formation method	Vapour	bulky	Vapour	bulky	Bulky
 H ₂ O Guest 1 Guest 2					
Systems	(a)	(b)	(b)	(c)	(c)
Surrogate	SiO ₂ / SiO ₂ -OH hydrated SiO ₄ ⁻	SiO ₂ / SiO ₂ -OH hydrated SiO ₄ ⁻	SiO ₂ / SiO ₂ -OH hydrated SiO ₄ ⁻	SiO ₂ / SiO ₂ -OH	SiO ₂ / SiO ₂ -OH

- Surrogates:
 - ✓ Various morphologies
 - ✓ Various chemical compositions
- Formation:
 - ✓ vapour co-deposition (10K-230K and 10⁻⁶ mbar-1 bar)
 - ✓ bulky (150K-300K and 1bar-300 bar)

Methodology



- Innovative and challenging approach to address the influence of minerals on clathrates properties by combining state-of-the-art **theoretical** and **experimental** methods.

3 PhD's starting in 2016

- Experimental investigations (**Lille/Bordeaux**):
 - *Vibrational spectroscopy and imaging.*
 - *Elaboration of original silica-based surrogates.*
 - *Investigation of gas selectivity, stability and formation of mixed clathrate hydrates in contact with “geo-like” and “astro-like” surrogates.*
- Theoretical investigations (**Dijon/Besançon**):
 - *Molecular simulation and thermodynamics modelling.*
 - *Elaboration of original simulation codes.*
 - *Study of single- and multiple-guest hydrates in contact with mineral impurities using classical simulation (MC and MD) at an atomic and at a mesoscopic scale.*
- Theoretical/experimental approaches (**Bordeaux/Besançon**):
 - *Ab-initio numerical simulations and neutron/Raman scattering.*
 - *Study of dynamics properties such as vibrational density of state, Brownian dynamics and binding energies of encapsulated gas.*
 - *Investigation of the mechanism involved in gas trapping within clathrate hydrates in contact with silica media.*

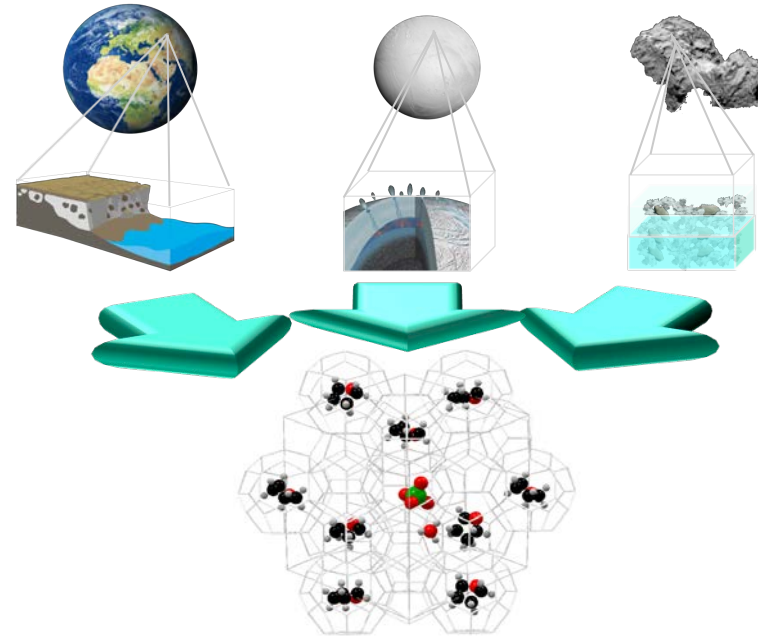
Concluding remarks

ANR MI2C + ANR HYDRE

- Clearly identified national actions for MIGRATE project.

- Challenging objectives for astro- and geo-physics.

- Highly complementary project for investigating hydrates in sediments (probed scales + experiments/modelling)



Molecular

Molecular

Mesoscopic

Macroscopic

Geoscopic

MI2C

HYDRE

- 7 PhD starting in 2016!!

Merci de votre attention