

# Evolution of matter from the interstellar medium to exoplanets with the JWST

Etat d'avancement au 15 novembre 2016

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A. Coulais R. Gastaud

# Organisation: 4 work-packages

**WP1 Scientific coordination:** Alain Abergel (IAS)

**WP2 Preparation of JWST observations:** P.-O. Lagage (SAp/AIM)

**WP3 Modeling and simulations :** E. Habart (IAS)

**WP4 Laboratory experiments :** C. Engrand (CNSNM) & A. Aléon-Toppani (IAS)

# WP1 : Scientific coordination

## **Réunion de Kick-off le 19 septembre 2016 (journée complète)**

Présentation des différentes équipes

Questions scientifiques pour lesquelles le JWST devraient apporter des réponses ?

Quelles sont les observables du JWST qui seront utilisées ? Et comment ?

Quelles observations du JWST GTO, ERS, GO, archives?

Programme de travail prévu dans le cadre du projet et au-delà.

## **Suite: Réunions de travail articulées autour de 6 axes :**

Nuages exoplanètes/naines brunes

Disques, spectroscopie JWST

Signatures poussière disques (carbonnées et silicatés)

Modèles/labo

Observations JWST sur les PDRs

Modèles dynamiques, simulations et liens avec les modèles de grains, PDR et disques

## **Mise en place d'un site web interne pour diffusion des documents**

## **En cours: organisation conférence internationale en 2018 ?**

# WP2 : Preparation of the JWST observations

## 1. Prior to launch (2016-2018)

- Task 1:** Simulations of JWST observations,  
Improving the MIRI simulator to extended sources (disk case)
- Tasks 2 & 3:** Keep on acquiring expertise (Optics, Detector, etc)  
Data reduction pipeline: Implementation, use, improvement  
Participation in the data challenges (planned for exoplanets)

## 2. After launch (2019 - ...)

As soon as data are available (great advantage : access to the commissioning data)  
run the data reduction pipeline, assess the uncertainties

**→ to be rapidly in a position to interpret the data**

French Center of Expertise for MIRI located at Paris-Saclay (support from CNES)

**→ 1 PhD (2017-2020, exoplanet atmosphere characterization with the JWST)**

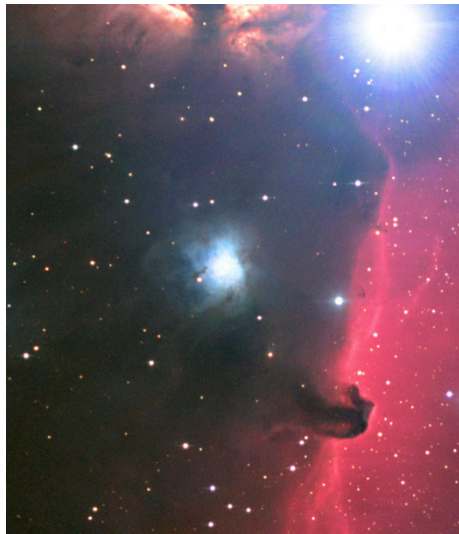
# WP2 : Preparation of the JWST observations

	WP2 : Preparation of JWST observations	Date	People in charge	Deliveries	Progress since mid-2016
1	Improvement of the MIRI observation simulator: - add simulated disk observations with the coronagraph - other improvements necessary for our programs	2016	R. Gastaud, P. Bouchet, A. Coulais, C. Cossou P.-O. Lagage, E. Pantin	Software + upgrade of the user manual	- In progress  - Improvement coronagraphy simulator (implementation of various OPD René)
2	Data reduction pipeline (imager): - Providing data reduction algorithms to the STScI - Implement/test the STScI standard pipeline at Paris-Saclay - High level pipelines not implemented by STScI	2016 2017-2019 2016-2017	P. Bouchet, K. Dassas A. Aberger, A. Coulais, D. Dicken, R. Gastaud, P.-O. Lagage, E. Pantin, PhD	Software, Documentation, Test reports  Software & documentation	- Done for 2016 (Patrice)  - Done for the 2016 version (Alain - Christophe)
3	Exoplanet specifics: 1) MIRI Detector test campaigns at JPL (one per year); Definition, participation, data reduction and interpretation. 2) Specific data pipeline • Member of the STScI WG to specify data pipeline for long observations (mainly exoplanet transit observations) 3) Data challenges: • data reduction, retrieval techniques benchmarking • pipeline improvement following the data challenge results	2016-2018  2016-2017  2017-2018	D. Dicken, P. Bouchet, A. Coulais, R. Gastaud, P.-O. Lagage +collaboration with JPL and MPIA  D. Dicken, P. Bouchet, A. Coulais, R. Gastaud, P.-O. Lagage. M. Ollivier +collab. (STScI and MPIA, SRON...)  P.-O. Lagage P. Bouchet, A. Coulais, R. Gastaud, P. Tremblin, E. Pantin, PhD + STScI, MPIA, SRON, ...	Test report  Technical note  Document with results 1 paper probably in PASP  Software and associated documentation	La campagne de tests de 2016 a eu lieu. Réunion à Tucson (du 14 au 18 novembre) pour discuter des résultats et de la suite (Dan, Patrice)  Participation in the teleconf of the WG

- Organisation de journées JWST à l'IAP (8-10 novembre 2016) pour la préparation de la communauté française à l'exploitation scientifique du JWST (CNES, CEA, CNRS, P2IO) (voir le site <https://jwst-2016-2.sciencesconf.org/>)
- Implication des les réunions consortium MIRI, en particulier pour la définition du temps garanti
- Coordination avec la communauté (participation à divers ateliers nationaux et internationaux) pour la préparation de programmes d'observations JWST

# Dust evolution in photo-dominated regions (PDRs)

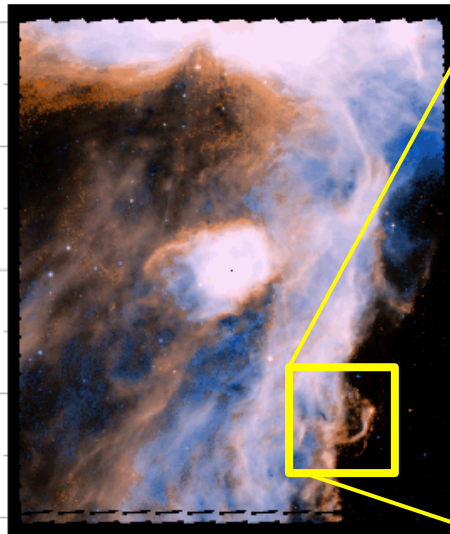
Visible



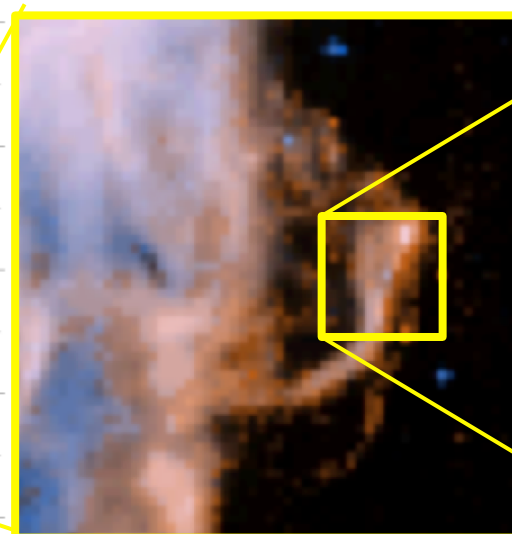
NRAO

IR emission:

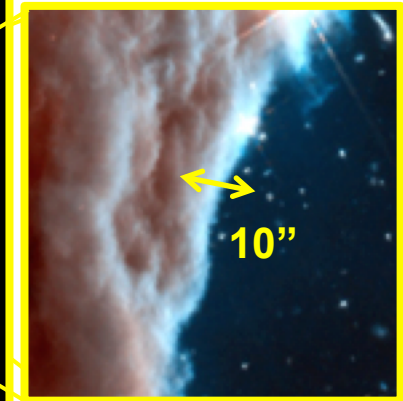
Aromatic 5-8  $\mu\text{m}$   
Continuum at 15  $\mu\text{m}$



ISO (Abergel et al. 2002, telescope diameter: 60 cm)



1-2  $\mu\text{m}$



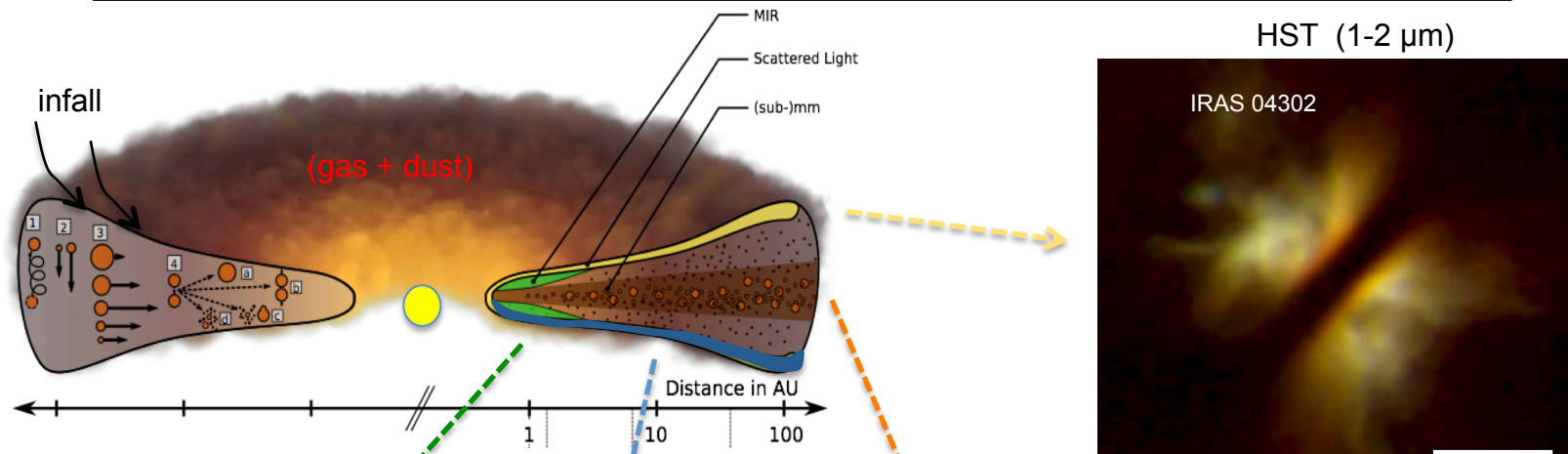
HST

10''

## **JWST : How dust properties change at the interfaces ?**

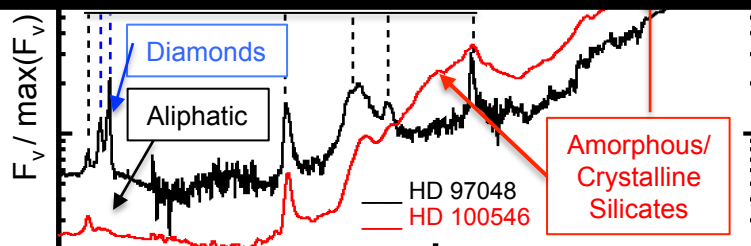
- The JWST has the angular resolution (0.1''-1'') to resolve the interfaces in the IR
- Dust evolution : growing, accretion, fragmentation, charge state, ...

# Dust evolution in protoplanetary disks

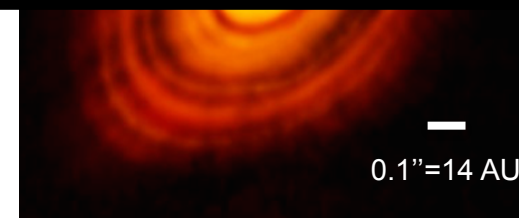


## JWST : How dust properties change at the upper layers of the disks ?

- Spatially & spectrally-resolved dust emission and scattering with a unique sensitivity
- Only JWST can give the warm gas and dust inventory as a function of the local conditions.
- Unique access to large distance from the star (30-500 AU) and T Tauri stars ( $< 2 M_{\odot}$ )
- Dust evolution at the upper layers  $\rightarrow$  Impacts on the growing processes



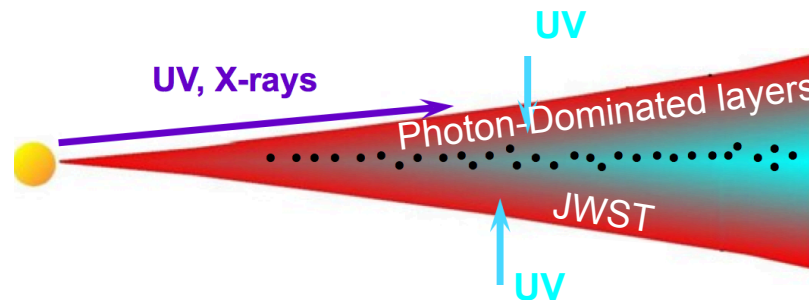
Van Kerckoven et al. 2003  
 Bouwman et al. 2003  
 Habart et al. 2004, 2005



ALMA Partner

## WP3 (Modeling & Simulations) : PDRs & Disks

**Disks: JWST signatures mainly from upper layers → Diagnostics comparable to PDRs**



- Task 1:** Dust properties modeling
- Task 2:** Analysis of pre-JWST data
- Task 3:** Simulation of JWST observations
- Task 4:** Analysis of JWST observations

**Strong interactions with laboratory experiments**

### **Objectives:**

- The modeling is the key to analyse the data:

Realistic dust model in disks based on pre-JWST & JWST data, laboratory experiments

Model calculations: dust (with adaptable properties) & radiative transfer,

→ Survival and interaction of nano-grains with UV photons at the illuminated edges

→ First coagulation of aggregates and settling phases

→ Constrain PDR/disk structures, which is essential for the study of the dynamics & chemistry

→ **2 PhD : 1 for disks (2016-2019) and 1 for PDRs (2017-2020)**

→ **1 postDoc (disks 2017-2019)**



# WP3 (Modeling & Simulations) : PDRs & Disks

	WP3 / ISM, PDRs & Disks	Date	People in charge	Deliveries	Progress since mid-2016
1	<b>Dust properties modeling</b>				
	a) Charge distribution	2016-2017	Verstraete, Bocchio, Jones, Ysard	1 paper for a) & b)	Bocchio, Verstraete, Jones, Ysard, submitted to A&A
	b) Size distribution	2016			
	c) aC(:H) equilibrium composition	2017-2019	Dartois, Godard, Jones, Ysard	1 paper (A&A)	Current analysis on the release of photo-produced H <sub>2</sub> from hydrogenated amorphous carbon (a-C:H) grains and modelled the corresponding diffusion coefficient from temperature-dependent measurements. Martin-Domenech, Dartois, Muñoz-Caro, 2016,
	d) Grain optical properties	2016-2019	<u>Jones</u> , Ysard + collab (Köhler, UK)	2 papers (A&A)	Optical properties computed and incorporated into the THEMIS framework (Jones et al., submitted to A&A). THEMIS web site
	e) DustEM service	2016-2019	<u>Verstraete</u> , Ysard	Updated DustEM tool for the community	Updated data incorporated into DustEM
2	<b>Analysing/ training with pre-JWST data</b> - PDRs - Disks	2016-2019	PDRs PhD, Abergel Disk PhD : Bouteraon, Pantin, Habart, Ysard, Miville-Deschênes Collab. with the lab. experiment team (WP4)	1 paper (A&A) 2 papers (A&A) + Models to be used for task 4	- PDRs : In progress : Modelling of Spitzer + Herschel data using updated dust models (see WP 3.1)  - Disks : Analysis of optic adaptative spectroscopics data (VLT/NAOS-CONICA, L band, angular resolution 0.1") around (pre-)transitional disks. Detection of various carbonaceous dust features (aromatic/aliphatic/diamonds) varying spatially and from source to sources. Modelisation currently in progress.
3	<b>Simulation of JWST observations</b> - PDRs - Disks	2017-2019 2017-2019	ISM PhD, Abergel Disk PhD, Disk postdoc, Habart, Ysard, Pantin	Simulated JWST data	
4	<b>Analysis of JWST observations</b> - PDRs - Disks	2019-2020	ISM PhD, student Abergel Disk postdoc, Pantin, Habart, Ysard Collab. with the lab. experiment team (WP4)	2 papers (A&A) 2 papers (A&A)	

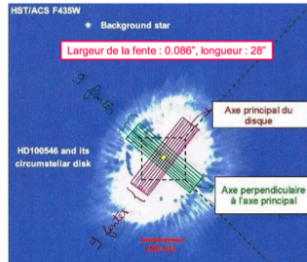
3 papiers soumis à A&A

**Début de la thèse (1/2 financement P2IO) de T. Bouteraon sur les disques (profil nano-matériaux)**

Demande de thèse sur les PDRs faite au CNES

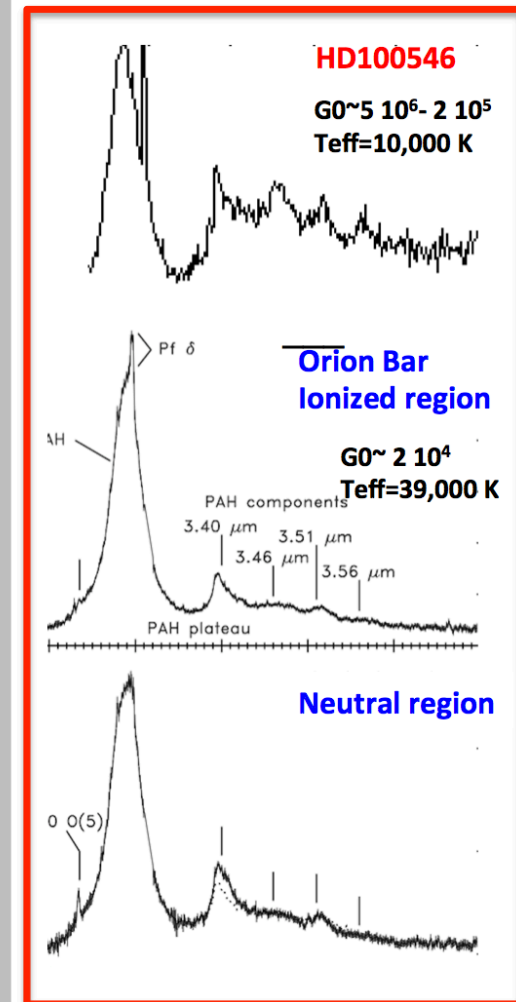
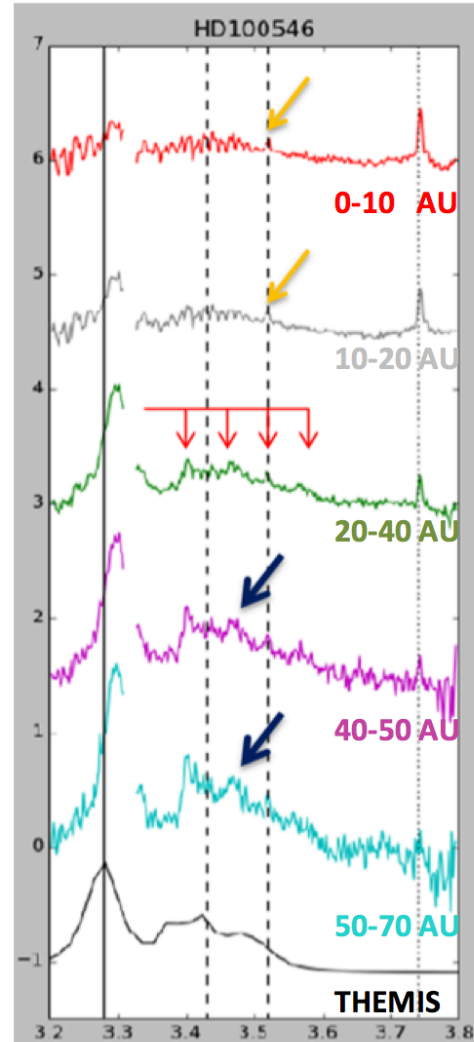
# High resolution spectroscopy of carbonaceous (nano-)particles

In prep.



NAOS/CONICA (VLT)

- 1st results
- Various features;  $\neq$  in each sources
- Present or not in gap
- Similarity and differences with PDRs
- **High aliphatic/aromatic bands ratio!**
- **No significant variation with radius (i.e., UV flux) as observed in PDRs**
- $\Rightarrow$  **constant fresh material resplenish ?**
- Extended IAS dust models to circumstellar environment**
- Follow up with **VLT/MATISSE (1-10 AU)** in 2017-2018



Début de la thèse de T. Bouteron sur les disques

# WP3 (Modeling & Simulations) : Exoplanet atmospheres

→ Test of atmospheric models, circulation models, climate models in new regimes

→ **Link Protoplanetary disks – Atmosphere of giant planets**

Planetary formation starts with the coagulation of icy grains,  
**C/O ratio** = “ f ” (place where the exoplanet forms in the disk)  
(due to different  $T_{condensation}$  for  $H_2O$ ,  $CO_2$  &  $CO$ )

Comparison with the C/O value of the central star

→ discriminate between different formation models

To retrieve the C/O ratio from IR JWST spectra

→ **Need models** (with radiative transfer, opacities...)

- 1D exoplanet atmospheric model of Paris-Saclay (ATMO), one of the best models at the international level

**Task 1:** Benchmarking

**Task 2:** Effect of composition variations

**Task 3:** Include dust clouds (relation with the dust expertise from WPs 3 & 4)

**Task 4:** 3D models to assess the uncertainties when using 1D model

**Task 5:** Analyse first JWST observations

→ **1 two year post doc 2017-2019**

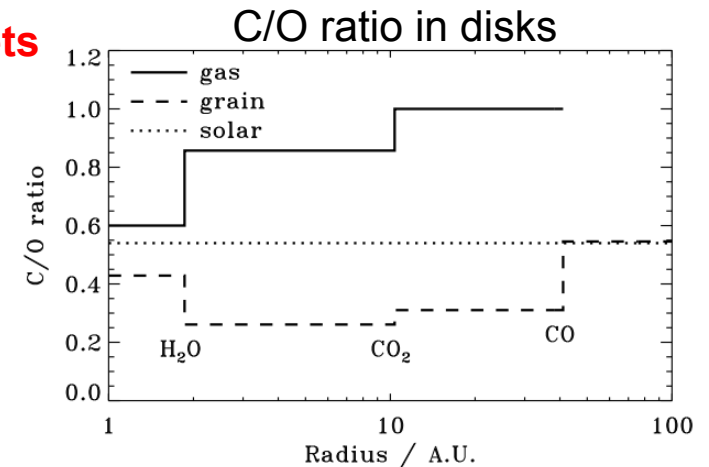


Fig. 1.— The C/O ratio in the gas and in grains, assuming the temperature structure of a ‘typical’ protoplanetary disk around a solar-type star ( $T_0$  is 200 K, and  $q = 0.62$ ). The  $H_2O$ ,  $CO_2$  and  $CO$  snow-lines are marked for reference.

# WP3 (Modeling & Simulations) : Exoplanet atmospheres

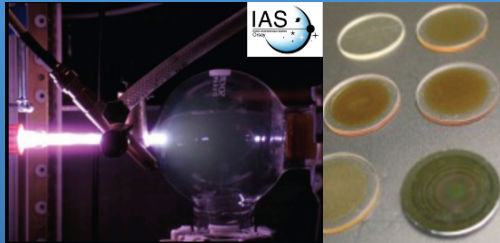
	Description	Date	People in charge	Deliveries	Progress since mid-2016
1	Benchmarking of atmospheric exoplanet models	2016	P. Tremblin . P.-O. Lagage + MIRI consortium exoplanet modeling group	1 paper (ApJ)	Draft paper available
2	Simulate the expected effects of composition variations (e.g., C/O ratio) for different scenarii of planet formation in disks, for direct imaging and for the exoplanets transiting	2016-2017	P. Tremblin, P.-O. Lagage + student at UCL	At least 2 papers (ApJ or A&A)	1 paper accepted in ApJ (Marco Rocchetto et al. sur archive)
3	Implement of clouds in the ATMO model	2017-2018	P. Tremblin, postdoc	1 paper (ApJ or A&A)	
4	Development of 3 D models from the dynamico code: Post-processing of 3D models with ATMO to produce 2D maps of the atmosphere transmission spectra, study of simple clouds prescriptions.	2016-2018	S. Fromang, P. Tremblin + postdoc	1 paper (ApJ or A&A)	Familiarization with the code; proposal to GENSI to get computer time.
5	Analysis of the first JWST exoplanet observations in ERS and in GTO	2019	P.O. Lagage, PhD (of WP2), S. Fromang, M. Ollivier, P. Tremblin and international collaborators	At least 1 paper (Nature or Science)	

1 papier ApJ accepté

Demande de thèse sur les PDRs faite au CNES

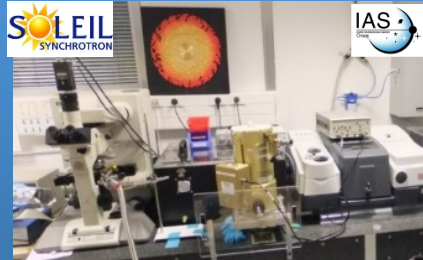
# Laboratory experiments in P2IO laboratories

## ISM Analogues



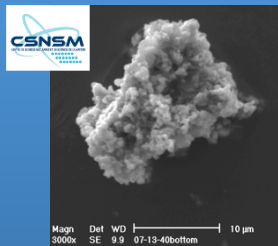
Experimental facilities IAS

## IR microspectroscopy



SOLEIL synchrotron

## Cosmic dust



Concordia collection (CSNSM) + IDP

## Evolution



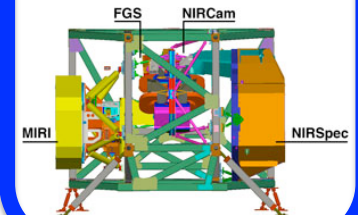
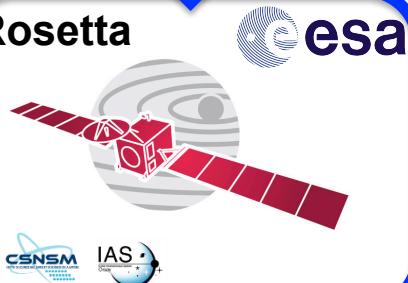
Irradiation facilities CSNSM/IAS-IPNO

## Microanalyses



SIMS, MEB, MET...(CSNSM/IAS + coll.)

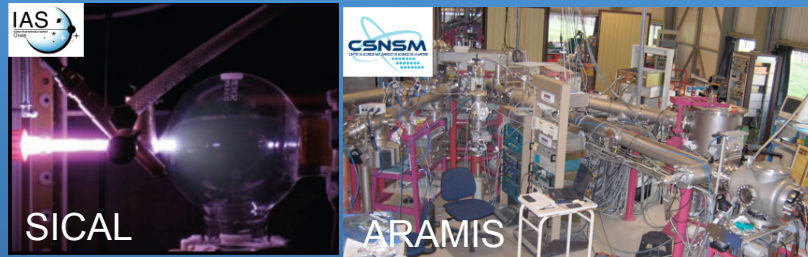
## Rosetta



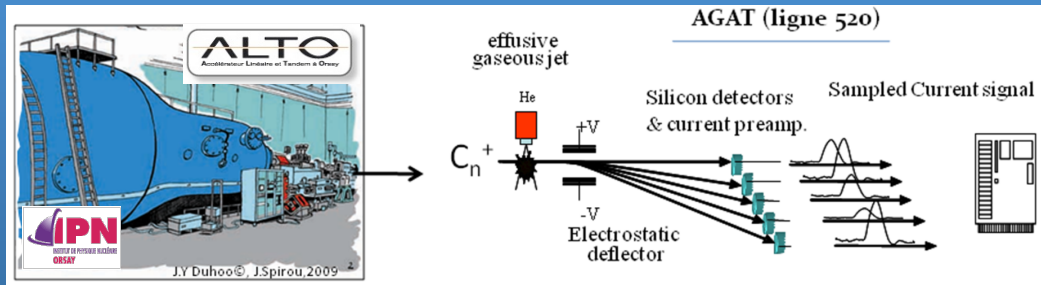
# WP4 Laboratory experiments: Organic Matter

## Origin of organic matter : link ISM – protoplanetary disk?

### Task 1: ISM analogues a-C:H doped in N & O (IAS/CSNSM)

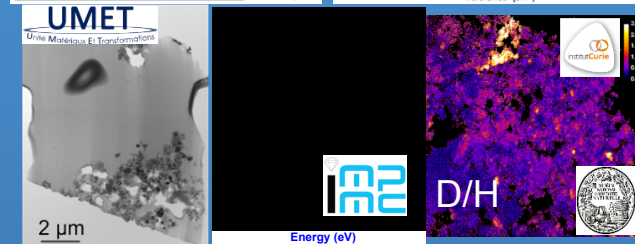
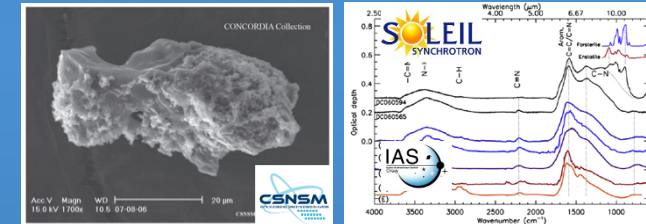


### Task 3: Physico-chemistry in the ISM : irradiation - released species in the gas (IPNO ALTO, CSNSM ARAMIS, CSNSM/IAS Astroline SIDONIE,...)

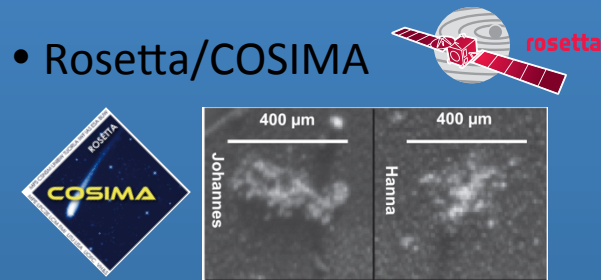


### Task 2: Study cometary matter

#### • CONCORDIA dust collection CSNSM



#### • Rosetta/COSIMA



### Task 4: Synthesis and preparation of interpretation of JWST data

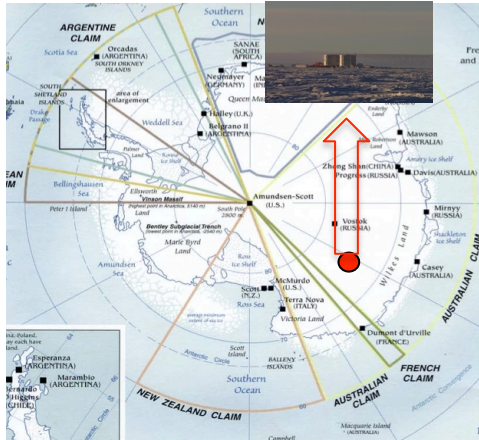


→ 1 two year postdoc already funded by P2IO

# WP4 Laboratory experiments: Organic Matter

	Description	Date	People in charge	Deliveries	Progress since mid-2016
1	Production of doped analogues - N then O-doped a-C:H by plasma (IAS) - N, then O, S-doped by ion implantation (SIDONIE, CSNSM)	2016-2017	Dartois, Godard, Duprat, Charon (PostDoc)	3 papers (A&A, Icarus or ApJ)	- production of CNO standard for NanoSIMS analyses
2	Analysis of cometary organic matter from the CONCORDIA micrometeorite collection (Raman, EDX, SIMS, etc), Comparison with Rosetta/COSIMA data	2016-2018	Engrand, Duprat, Godard, Dartois, Charon (PostDoc)	2 papers (A&A, Icarus or ApJ)	- STXM-XANES analysis of 2 UCAMMs at the SOLEIL-HERMES beam line - TEM analysis of these 2 UCAMMs at UMET in collaboration with H. Leroux - Search for UCAMMs : identification of 1 new candidate
3	Evolution of physico-chemistry in the ISM - Branching ratios & reaction rates (CnNyHz) with AGAT (ALTO/IPNO). - High- (GANIL, GSI, ...) and low- (SIDONIE, ARAMIS) energy ion irradiation	2016-2018 2016-2017	Chabot, Charon (PostDoc) Dartois, Godard, Duprat, Engrand	4 papers (A&A, Icarus or ApJ)  Delivery to the KIDA database	- AGAT Experiment on CnN (Nov. 2016) -
4	Synthesis and preparation of the interpretation of JWST data	2018-2019	Engrand, Dartois, Duprat, Godard, Chabot, Charon (PostDoc) Collab. with the modeling team (WP3)	3 papers (A&A, Icarus or ApJ)	- 1 article accepted by MNRAS as a review article about cometary matter (Engrand et al. 2016)

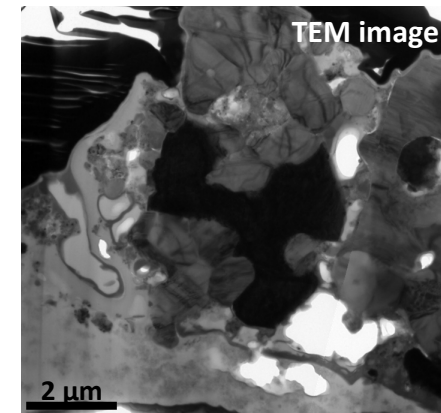
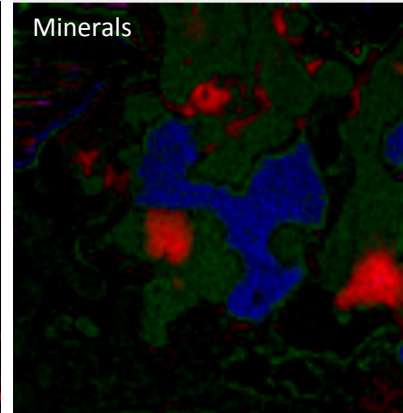
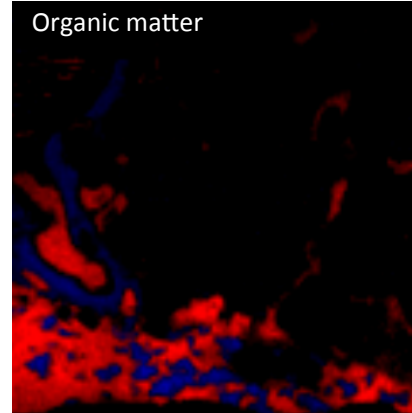
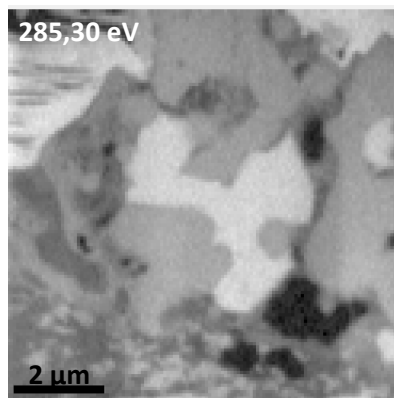
- **Début du postdoc de Emeline Charon (financement P2IO hors projet emblématique) sur la matière organique dans les UCAMMs ...**
- Item2. The budget (CSNSM, IAS) will be used from 2017 (no funding required for 2016)
- Item 3. The P2IO credits only became available in October 2016. The relocation project of AGAT near Andromede and the associated experimental developments, have been delayed by three months for this “administrative” reason.
- Budget execution IPNO (45 k€ equipment + 5 k€ fct):
  - 10 k€ to construct 2 vacuum chambers with optics systems.
  - 7 k€ euros to improve the process of fabrication of the home made silicon detectors (surface barrier on high resistivity epitaxial silicon layers).
  - 5 k€ for the infrastructure (electrical distribution on the experimental area)



CONCORDIA Station,  
January 2016

Collect **dust particles** of cometary origin at the Earth surface: the **Ultracarbonaceous Antarctic Micrometeorites (UCAMMs)**

- ⇒ **UCAMMs** represent a **unique opportunity** to study the association of **low and high temperature phases** in dust coming from the most **remote regions** of the solar system.
- ⇒ The unusually **large concentration** of **organic matter** in UCAMMs is also of uttermost interest for the **input of prebiotic matter** in the early Earth.

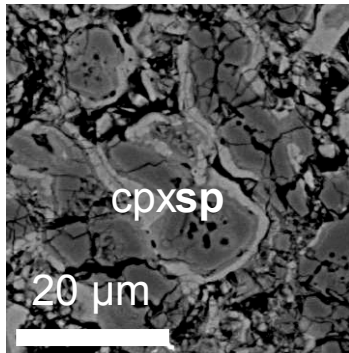


- ⇒ **STXM C-and N-XANES** analyses (Soleil) performed on new UCAMM showed the **presence of small minerals** associated with at least **two organic phases with different nitrogen concentrations**
- ⇒ This sample was analysed by **transmission electron microscopy (TEM)** to precise the **nature of the minerals** present in the UCAMMs (using Tecnaï FEI TEM at UMET in university Lille 1).

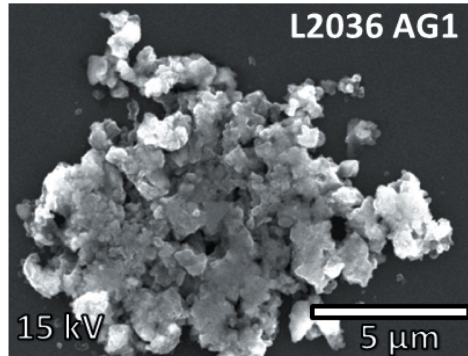


# WP4 Laboratory experiments: Silicate Matter

## IR spectroscopy of primitive extraterrestrial material



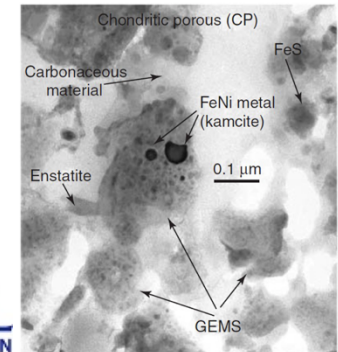
CAI



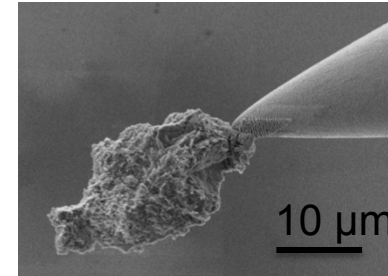
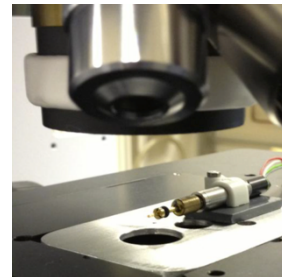
IDP

Merouane et al., 2014

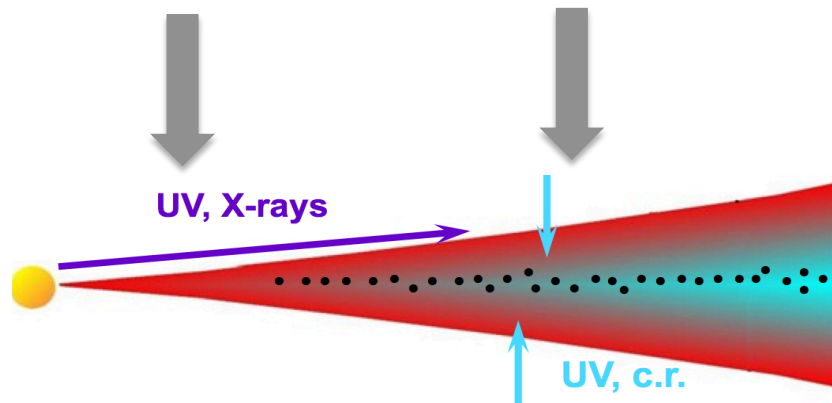
**Task 1 and 2:** IR spectra of bulk and  $\mu\text{m}$  sub-units of meteoritic materials



**Task 3:** 3D IR micro-tomography : porosity of grains



Troadec et Aléon-Toppani, 2015



→ 1 PhD from 2017

**Task 4:** Irradiation experiments in disk conditions  
IAS, CSNSM

**Task 5:** Comparison with pre-JWST & JWST data

- Crystallinity/amorphous and olivine/pyroxene ratios in the disk
- GEMS and CAIs in disks
- Hydrated silicates vs water vapor ?

# WP4 Laboratory experiments: Silicate Matter

	Description	Date	People in charge	Deliveries	Progress since mid-2016
1	Sample preparation	Sep 2016-mid 2017	Aléon-Toppani, Djouadi, PhD	Samples ready for analyses	Test (using the FIB) to split a 30 microns grain in 3 slices of different thickness
2	IR spectroscopy - bulk IDPs, meteorite matrix, CAIs - extraterrestrial objects at micron scales	Jan 2017-mid 2018	Aléon-Toppani, PhD, Brunetto, Djouadi	Database of IR signatures (0.4-60 $\mu$ m) of extraterrestrial materials 2 papers (A&A, GCA or Icarus)	Installation of our new spectroscope equipped with a FPA detector. First tests on crushed meteorite sample and on CAI FIB slice.
3	Measurements of the porosity of IDPs, and meteorite matrix	June-Dec 2018	Brunetto, Aléon-Toppani	Database of dust porosity 1 Paper (A&A, GCA or Icarus)	
4	Evolution of the primitive extraterrestrial dust under irradiation	mid 2018-mid 2019	Djouadi, Brunetto	1 paper (A&A, GCA or Icarus)	
5	Comparison between laboratory and Spitzer/JWST data	mid 2017- 2020	PhD, Aléon-Toppani, Djouadi, Brunetto Collab. with the WP3 team	4 papers (A&A or Icarus) : GEMS, Olivine/Pyroxene, Irradiation/Evolution, CAIs	

- Tests performed in order to improve the sample preparation of micron grains both for classic IR spectroscopy and for IR tomography. To be able to perform IR tomography on 30-microns grains, the grains need to be welded on the tip of a very thin needle..
- IR spectroscopy : in collaboration with SMIS-SOLEIL, we have acquired a new FTIR imaging microscope equipped with a 128x128 pixels matrix detector, which provides simultaneously a large number of spectra on surfaces ranging several centimeters to a few microns. The system also allows to conduct analyzes in 3D. The microscope has been installed during summer 2016.
- P2IO funding will be used in 2017
- Demande de thèse (oct. 2017) faite au CNES

## PhD and post-doc

- 3 two year post-doc:
  - 1 cometary matter (financement P2IO hors projet emb.): début sept. 2016
  - 1 disks 2017-2019 (P2IO)
  - 1 exoplanets 2017-2019 (P2IO)
- 4 PhD (seulement 2 ½ PhD financés par P2IO)
  - 1 Disks oct. 2016 (½ P2IO et ½ allocation Paris-Sud)
  - 3 autres (exoplanets, PDRs, silicate matter) à partir de 2017  
(3 demandes de financement CNES faites à la rentrée)

# Budget

	Laboratory	Actions/equipments	Total cost	Requested to P210	Budget total	Gestion	2016	2017	2018	2019	2020
3 thèses thèse mais missions  1 post-doc		Actions collectives			10	IAS	10,00				
	Missions total	Missions à réparer			19,8						
	IAS	Missions			9,9	IAS		3,30	3,30	3,30	
	SAP	Missions			6,6	SAP		2,20	2,20	2,20	
	CSNSM	Missions			3,3	CSNSM		1,10	1,10	1,10	
	IPN	Missions			0	IPN		0,00	0,00	0,00	
<b>Total WP1</b>	<b>All</b>	<b>Scientific animation</b>	<b>60</b>	<b>60</b>	<b>29,8</b>		<b>10,00</b>	<b>6,60</b>	<b>6,60</b>	<b>6,60</b>	
<b>Manpower</b>											
WP2	SAP/IRFU	PhD 2017-2020	100	50	0	SAP					
WP3	IAS	PhD 2016-2019	100	50	50	IAS	4,17	16,67	16,67	12,50	
WP3	IAS	PhD 2017-2020	100	50	0	IAS	0,00	0,00	0,00	0,00	
WP3	SAP/IRFU	2 postdoc 2016-2018	200	200	200	SAP		50,00	100,00	50,00	
WP4	IAS	PhD 2017-2020	100	50	0	IAS		0,00	0,00	0,00	0,00
WP4	CSNSM/IAS	1 postdoc	100	0	0	CSNSM					
<b>Total Manpower</b>			<b>700</b>	<b>400</b>	<b>250</b>		<b>4,17</b>	<b>66,67</b>	<b>116,67</b>	<b>62,50</b>	<b>0,00</b>
<b>Equipments</b>											
WP2	SAP/IRFU	Meso-machine	504	63	63	SAP		63,00			
WP4	CSNSM	EDX for scanning electron microscopy	72	50	50	CSNSM		50,00			
WP4	IAS	Optical microscope	40	40	40	IAS	40				
WP4	IAS	Low temperature cryohead interfaced	50	50	50	IAS	50				
WP4	IPNO	Single Side strip silicon Detector (SSD)+ mounting.	50	50	50	IPNO	50				
<b>Total Equipment</b>			<b>716</b>	<b>253</b>	<b>253</b>		<b>140,00</b>	<b>113,00</b>	<b>0,00</b>	<b>0,00</b>	
WP4		Participation to the analysis costs at IAS & CSNSM	30	30	15			5,00	5,00	5,00	
		IAS						2,50	2,50	2,50	
		CSNSM						2,50	2,50	2,50	
<b>Total</b>			<b>1506</b>	<b>743</b>	<b>547,8</b>		<b>154,17</b>	<b>191,27</b>	<b>128,27</b>	<b>74,10</b>	<b>0,00</b>