WP3. Interstellar dust, PDRs, Disks: Modelisation, Simulation, Observation

Abergel, E. Habart, A. Jones, M.-A. Miville-Deschênes, E. Pantin,
L. Verstraete, N. Ysard
Thomas Bouteraon (PhD Dust micro-physical modeling in disks, 2016-2019)
+ collab with the experiment WP4 **+ collab ext**

- Background
- Key questions where JWST should provide answers
- JWST physical observables (+ complementary)
- JWST working group / program (ERS, GTO, GO)
- Tasks
- Analysis tools: Models, Simulation

WP3

A) Microphysics of PDRs/disks

B) Structure/dynamics of disks

- Background
- Key questions where JWST should provide answers
- JWST physical observables (spectroscopy & imaging) + complementary
- JWST working group / program (ERS, GTO, GO)
- Tasks

Models

- Dust properties evolution: charge, size, composition, optical properties (THEMIS)
- Dust emission/extinction according to the local physical conditions (DustEM)
- Dust radiative transfer

↔

Models, Simulation

- Hydrodynamical simulations: dust size evolution
- Dust radiative transfer
- Disk thermodynamical structure
- Dynamical simulation : accretion disks

- What is expected of the P2IO project in the long term

A) Microphysics of PDRs/disks

Abergel, E. Habart, A. Jones, M.-A. Miville-Deschênes, L. Verstraete, N. Ysard, T. Bouteraon

+ collab with the experiment WP4 (Dartois, Godard, ..)

+ **collab ext**: M. Bocchio, J. Bernard-Salas (Open University), M. Kohler (Queen Mary University)

Our (common) background

- ✓ **Dust content in ISM in relation with the gas properties**
- ✓ **Energetics, Stellar feedback**
- ✓ **(Circumstellar Material: PPDs, AGB, PNe)**
- ✓ **Local (& Extragalactic)**
- ✓ **Expertise on IR spectroscopy and imaging in Space**

→

- Processes (e.g. coagulation, accretion, photo-processing, grain destruction)
- Properties: (charge), Size distribution, aC(:H) equilibrium composition, optical properties)
- Emission and scattering, entire SED
- Polarised emission

Reference dust modeling tools
(Dust radiative transfer code)
(PDR code)

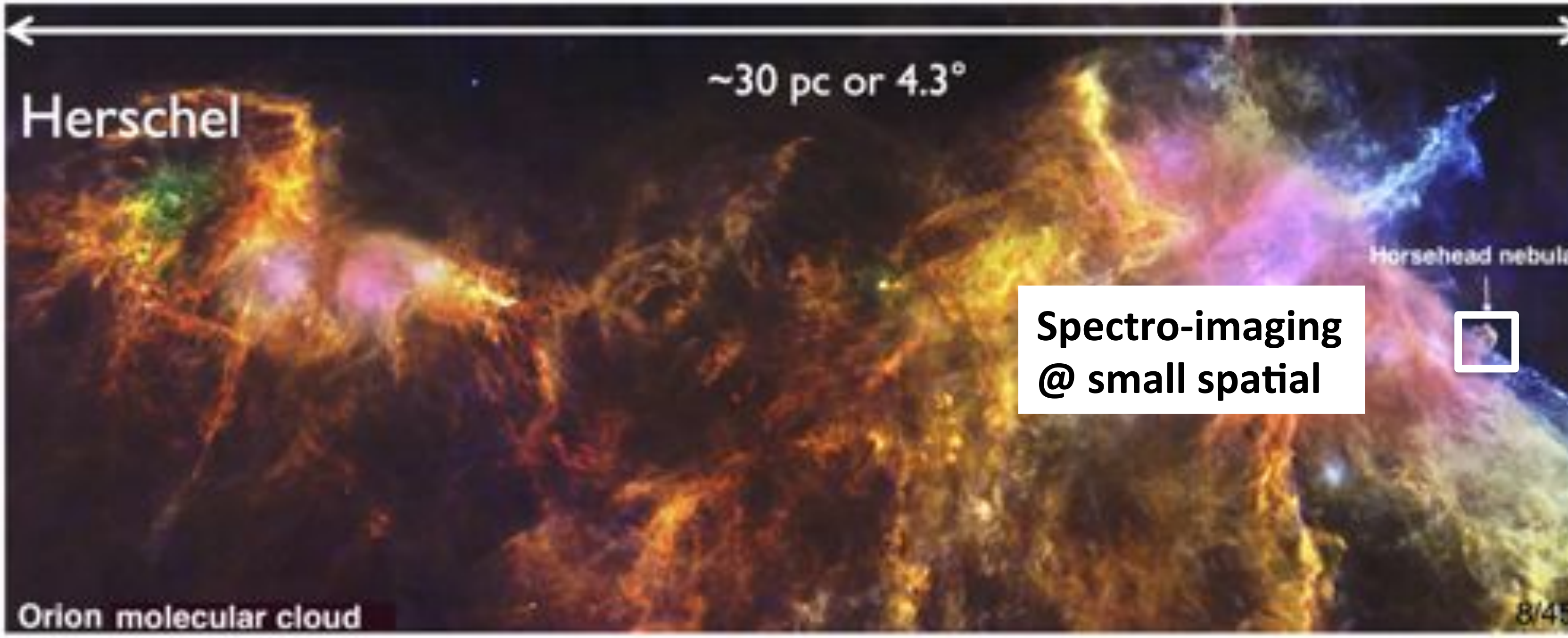
Main topics

1. Evolution from diffuse to dense ISM (see Nathalie talk)

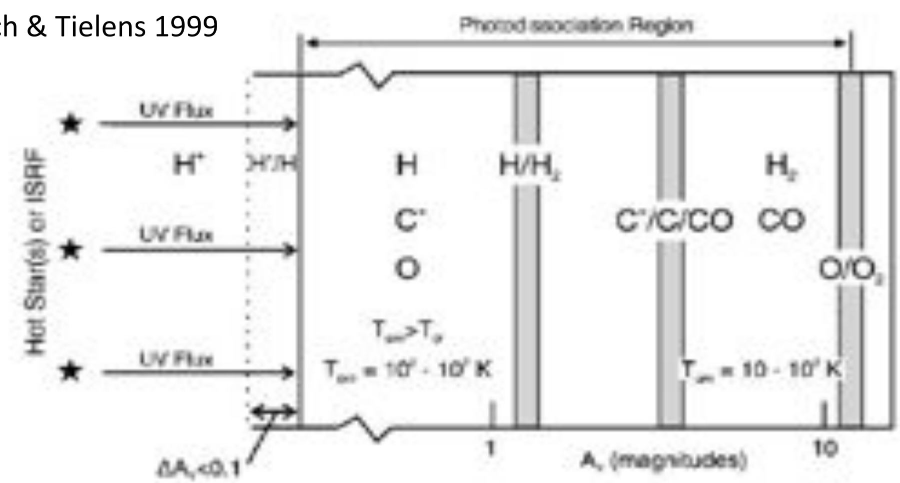
2. Radiation-dominated processes towards molecular cloud interfaces

3. PDRs diagnostics in the upper layers of proto-planetary disks

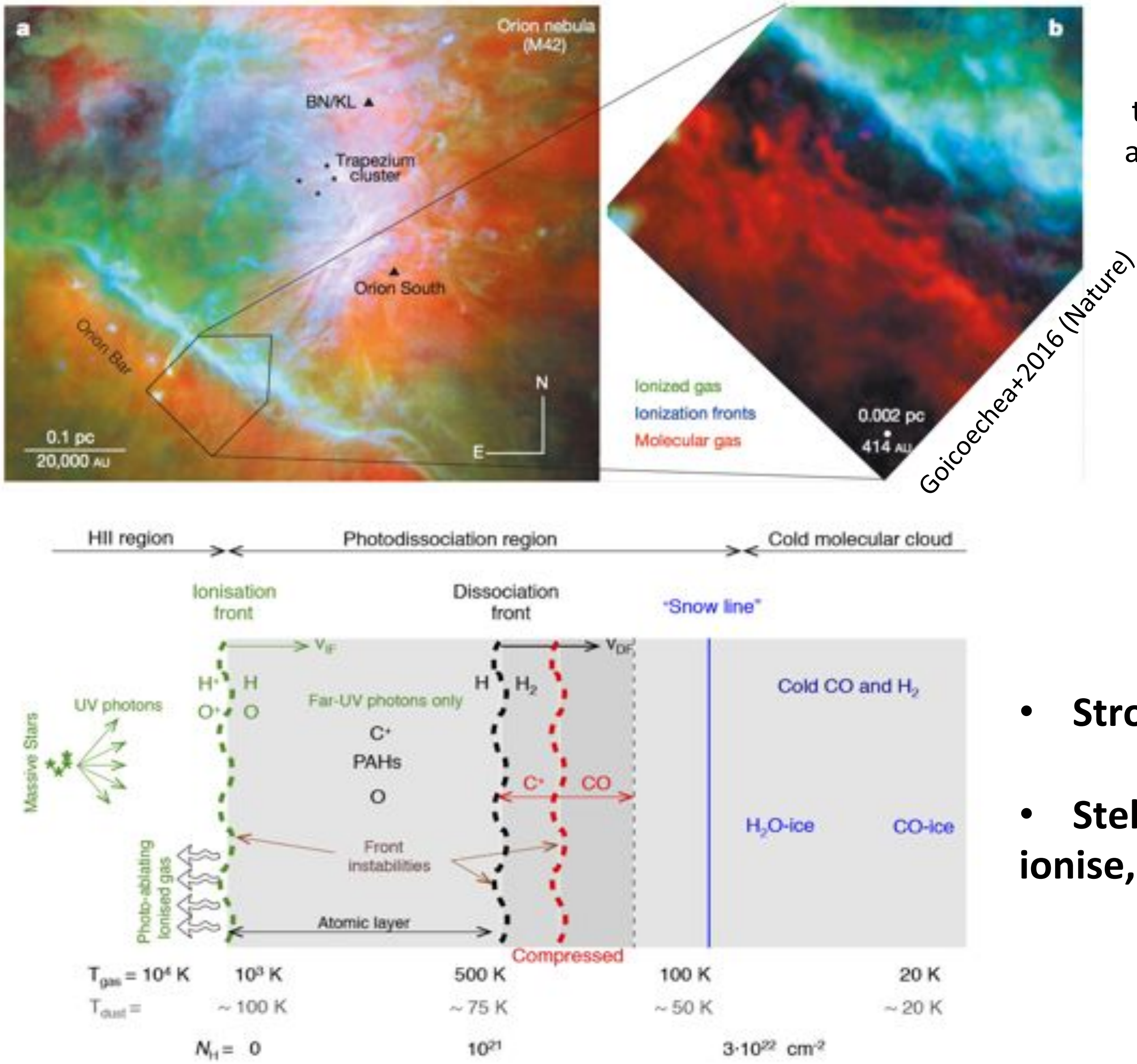
Irradiated molecular cloud interfaces



Hollenbach & Tielens 1999



Extremely structure at small scales

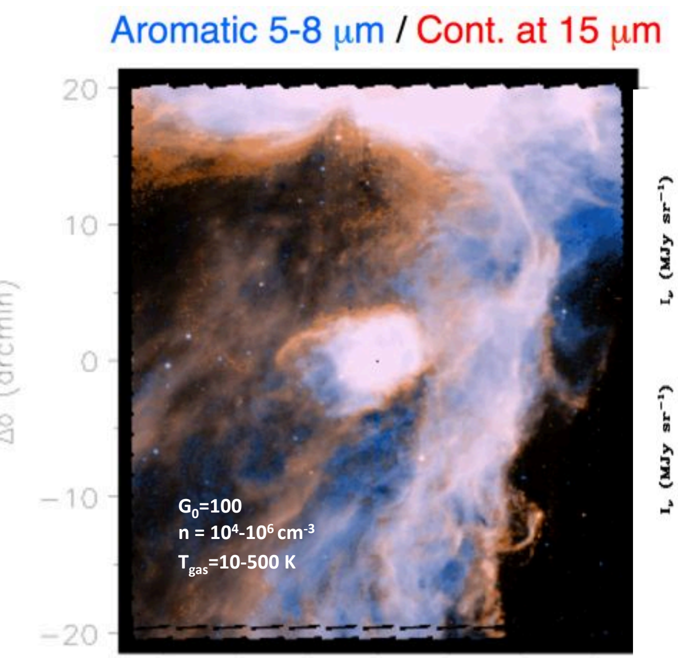


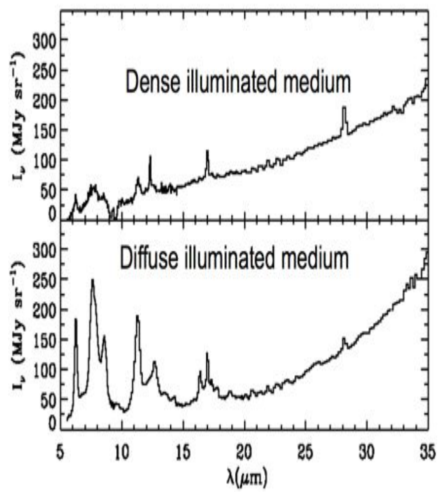
Goicoechea+2016 (Nature)

Multiphase view of
the Orion Bar PDR with ALMA,
a non-equilibrium environment

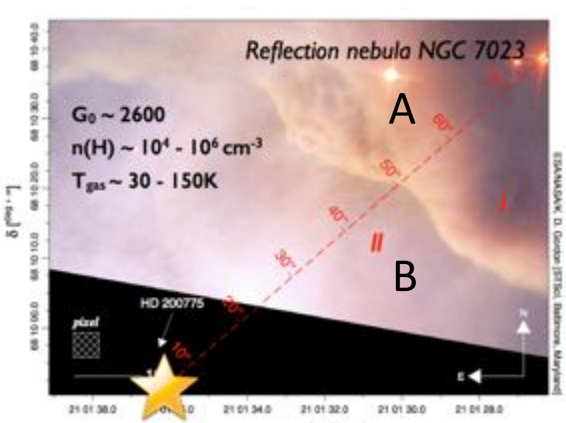
- **Strong dynamical effect**
- **Stellar feedback compress, ionise, heat, photo-evaporate**

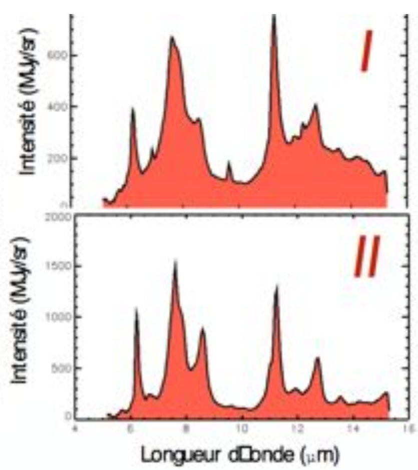
Dust undergoes strong evolution

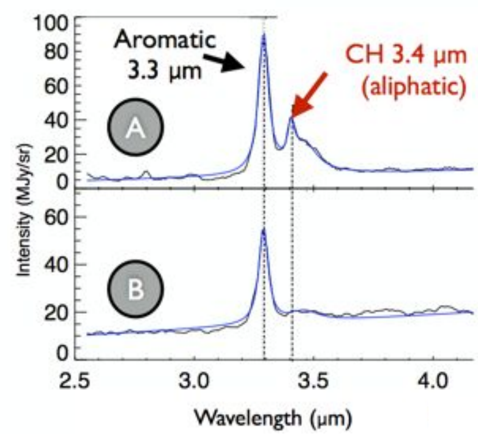


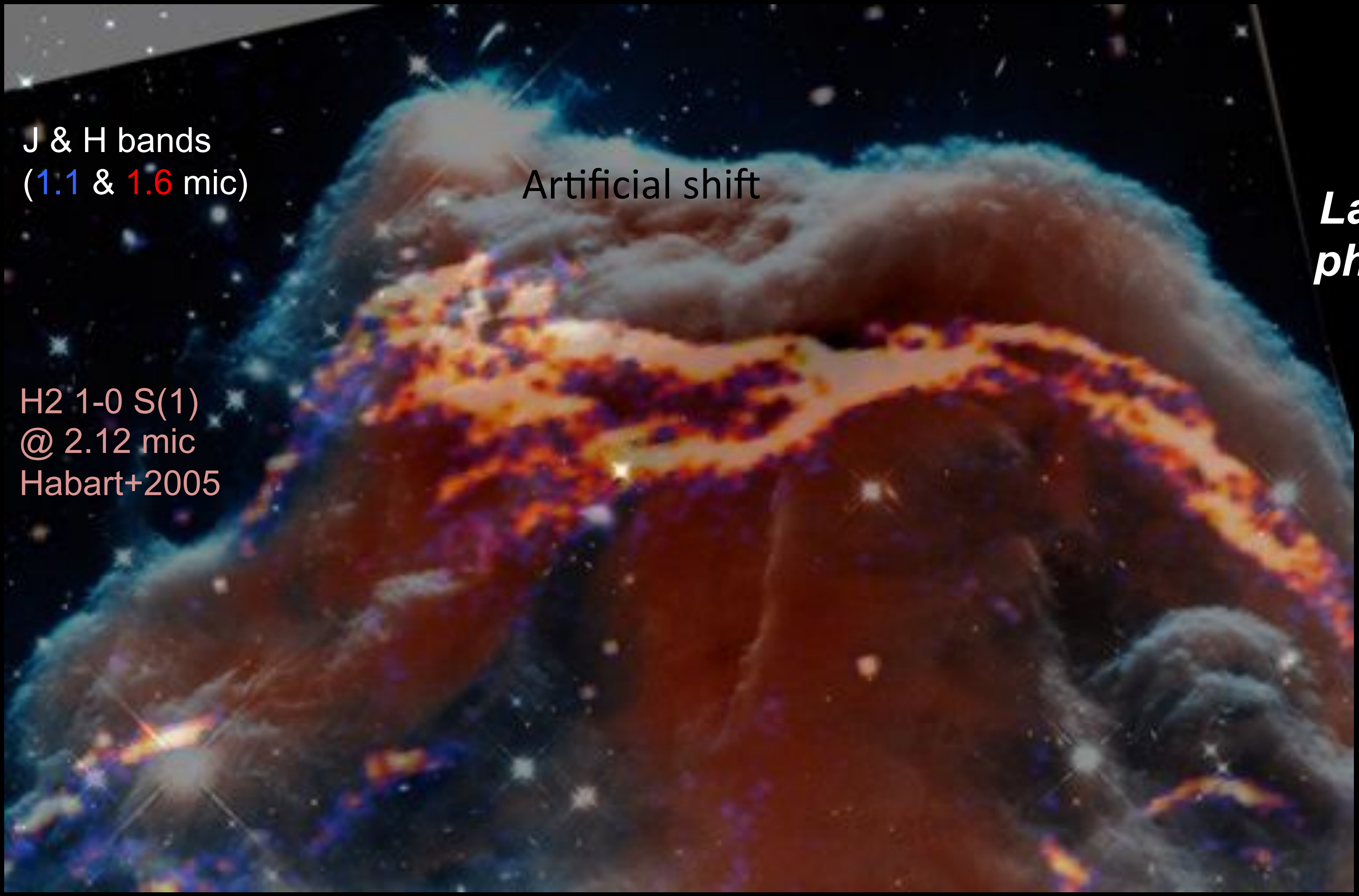


- **Strong colour variations** which due to **evolution of the emitters** (abundance, size distribution, composition...) in response to local conditions (Abergel et al. 2002, Rapacioli et al. 2005, Berné et al. 2007, Compiegne et al. 2008, Arab et al. 2012, Pilleri et al. 2015)
- Dust evolution **: growing, coagulation, fragmentation, charge state, ...**
- Variations not spatially resolved with Spitzer







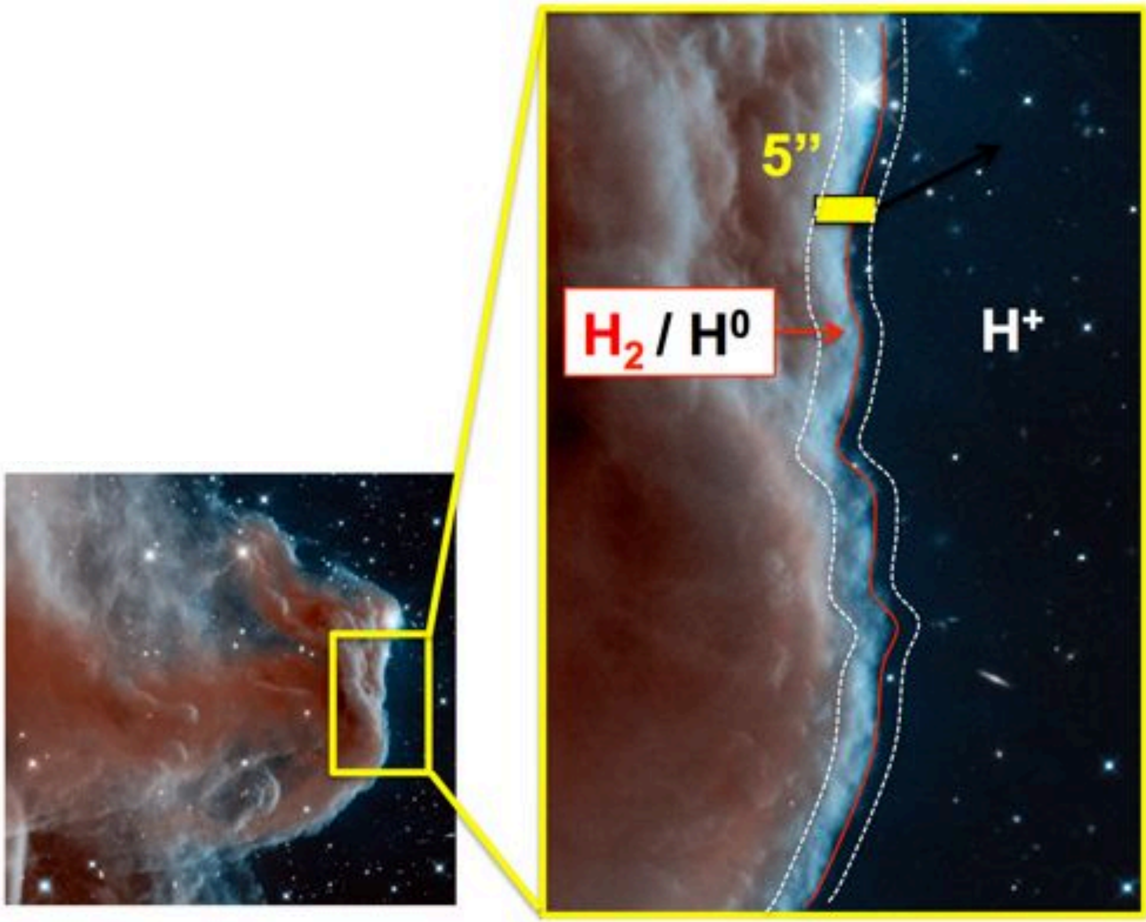


Layers subject to photoevaporation

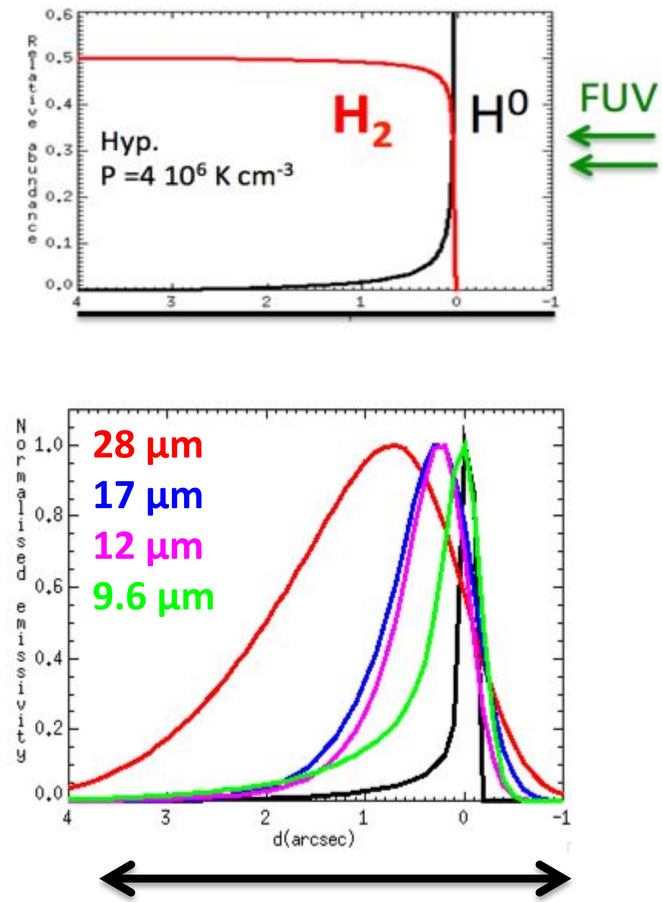
Delineating the H/H_2 transition

H/H2 transition take place on very small scale (<5” or 0.01 pc @ 400 pc)

JWST will spatially resolve the thin interfaces



PDR model predictions



5'' (0.01 pc @ 400 pc)

JWST program

- ❑ **GTO**: ISM program (US/Europe)

- Targets: NGC 7023 North, Horsehead
- Imaging: NIRCAM + MIRI

  Large field (~2' x 2’) in several filters (=>global physical structure of the nebula)
- Spectroscopy: NIRSPEC + MIRI

  1D scan perpendicular to the interface

- ❑ **GO**: PDRs /Diffuse clouds/Boundaries of dark clouds

- ❑ **ERS**: PDRs/proplyds ?

JWST observables

- **Resolved spatial emission of the H_2 rotational and rovibrational lines**, **atomic fine-structure** (O0, C0, N0, Ne+, Ar+, S++...) **and hydrogen lines**
- rotational transition from isotopes (HD 0-0 R(3) to R(5); HDO)
- ro-vibrational lines of CO, rotational and ro-vibrational lines of OH and H2O
- ro-vibrational lines of simple organic molecules (HCN, CO2, …)
- ro-vibrational lines of hydrocarbons
- **Bands of aromatic/aliphatic carbon**, C60
- **Continuum emission**
- **Dust scattering, extinction in the NIR**
- **ice mantle evaporation (released of complex molecules)**

Physical parameters, processes

- **Pressure profile** in the photodissociation front. **Amount of fresh H_2** forming in the cold gas. **H_2 microphysics** (Excitation, Formation processes (physisorption vs chimisorption vs HAC irradiation), Ortho/Para conversion mechanisms

- **Photolysis of hydrogenated HAC** producing molecular fragments (H2, hydrocarbons), aromatisation, destruction of small grains**, impact on the gas chemistry & heating**

- **Dust composition and growth at very high angular resolution**

- Contraints on the penetration of the stellar radiation into molecular clouds strongly depending on the dust properties

Key questions

- How dust properties change in PDRs? What is the influence of the dynamics ?

- What is the evolution of carbonaceous (nano-)particles: a-C:H ?

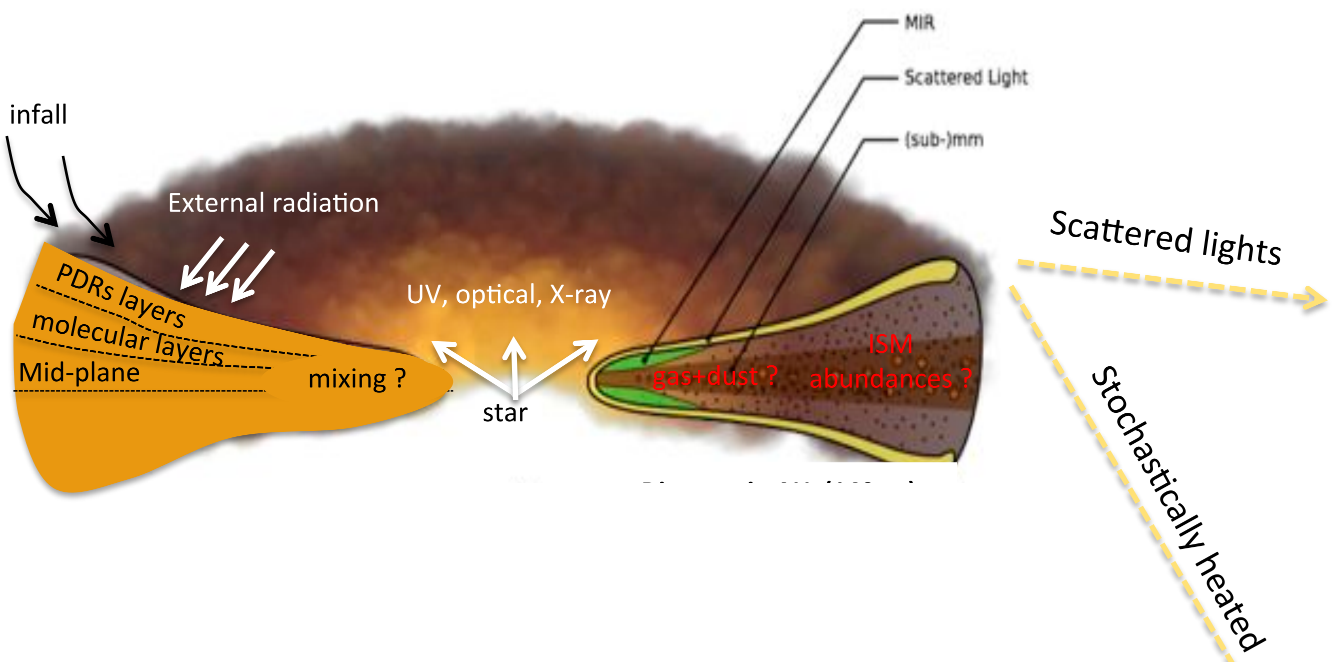
More vulnerable to processing/destruction than their silicate counterparts, this carbon dust component undergoing complex, size-dependent evolution due to photon

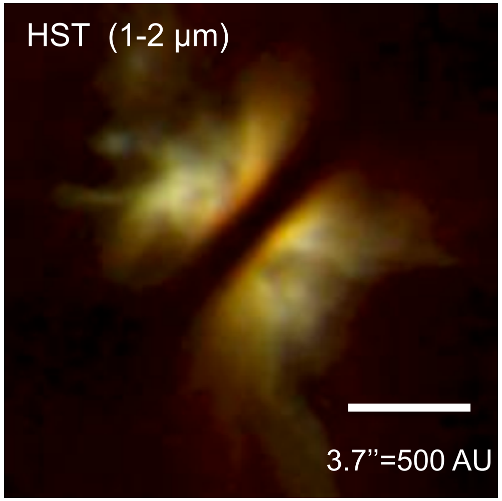
- **How these evolution influence the radiative transfer, temperature and chemistry ?**

Carbonaceous (nano-)particles will be widely observed with the JWST.

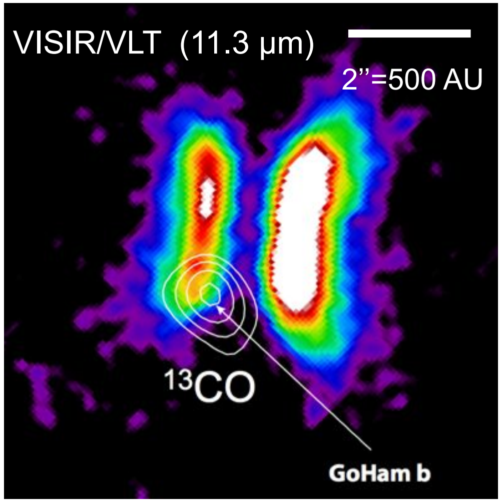
With its resolution and sensitivity, JWST data will show the limits of best current models of dust and gas emission without dust evolution

Upper layers of proto-planetary disks





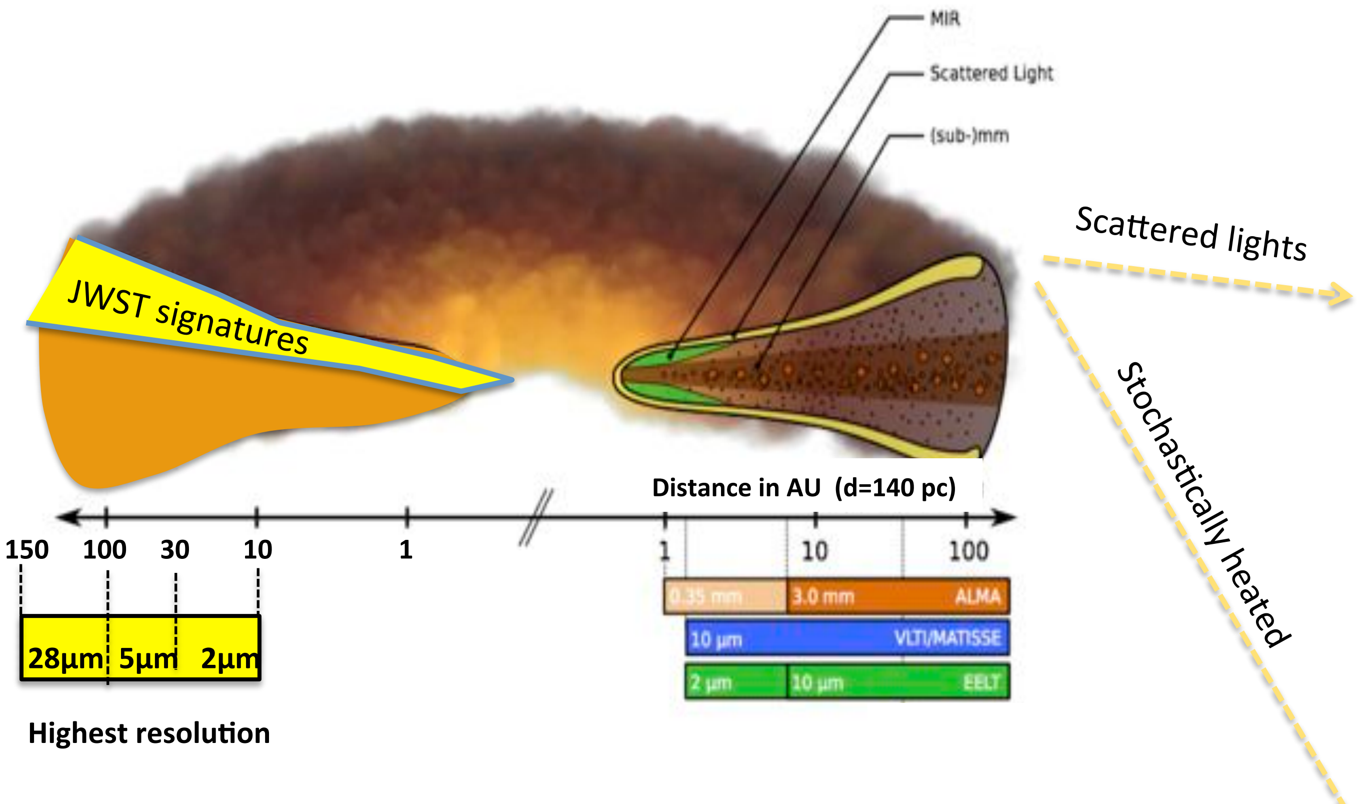
Edge-on disk

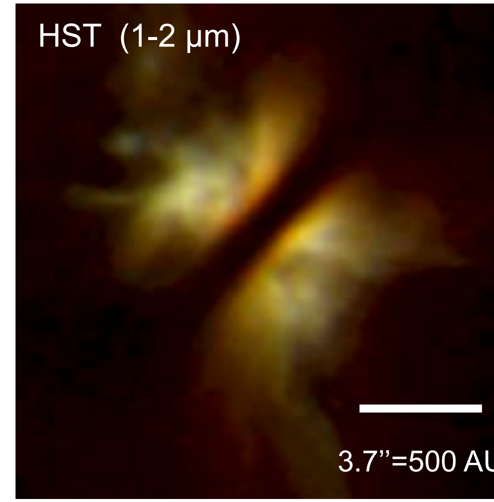


=> Geometry, UV, Av

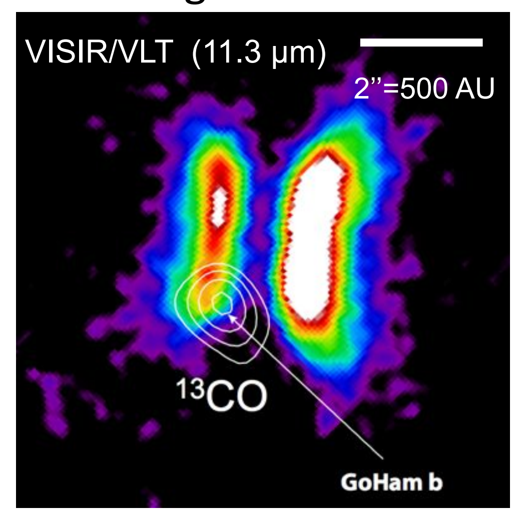
- Active microphysics due to the radiation
- PDR physics and diagnostics are become unavoidable in the interpretation of gas + dust IR signatures (ISO, Spitzer, VLT, ..) in proto-planetary disks

JWST signatures mainly from upper layers





Edge-on disk

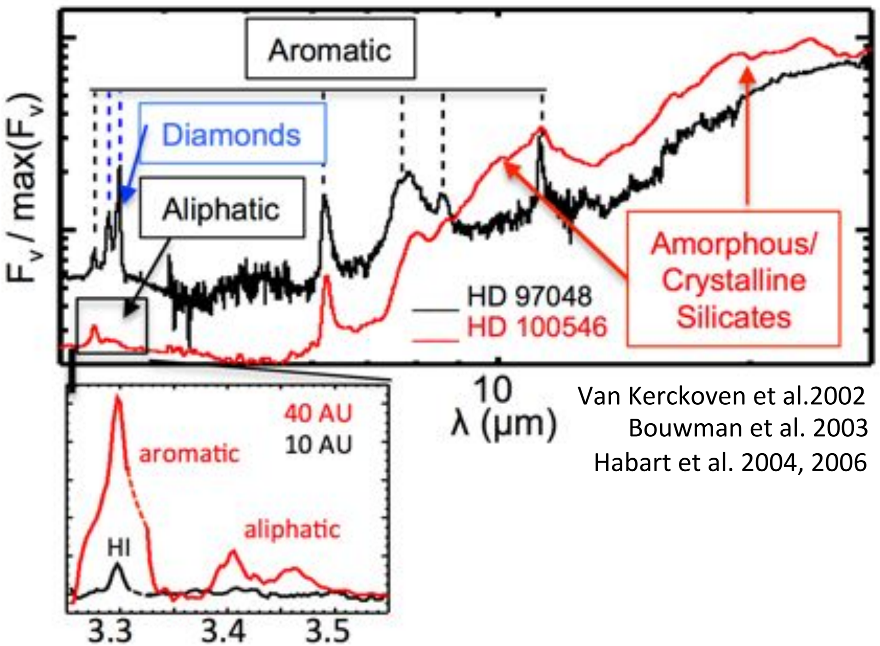


=> Geometry, UV, Av

- Warm thermal emission from the inner disks <10 AU
  ⚠ not spatially resolved
- Spatially- and spectrally-resolved dust scattered light and bands of nano-grains coupled to the gas in the « outer » disk >10 AU
- Access to T Tauri and large distance from the star (30-500 AU)

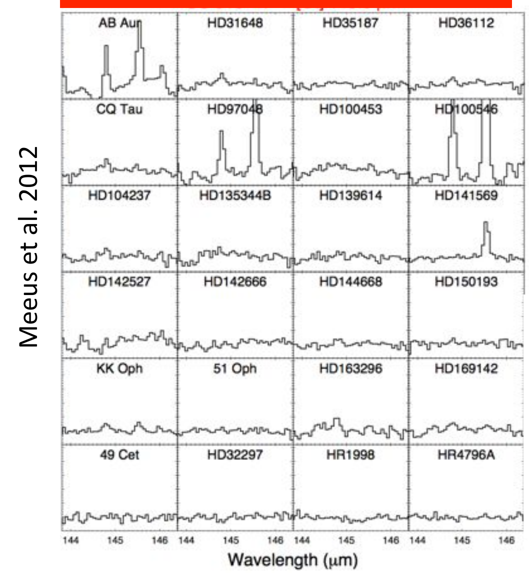
⇒ warm gas and dust inventory as a function of the local conditions

Nano-grains and warm gas signatures in emblematic disk

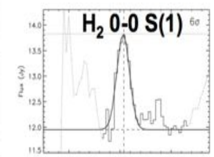


Van Kerckoven et al.2002
Bouwman et al. 2003
Habart et al. 2004, 2006

CO J=18-17 [OI] 145.5 µm

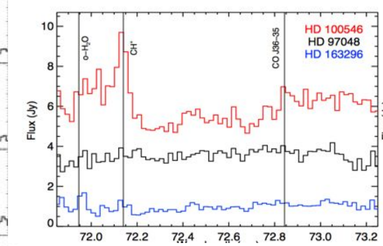


H2 0-0 S(1) 17 µm



- 1st detection!
- T<570 K

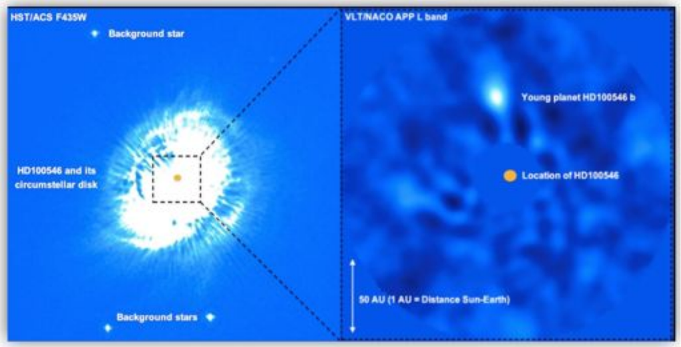
(Martin-Zaidi et al., 2009)

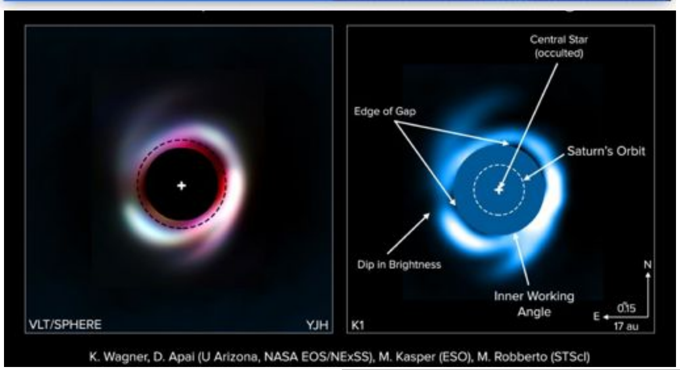


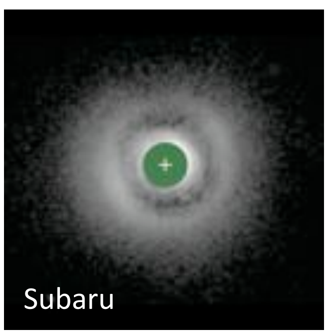
- 70% HAeBe with aromatic features (55% with aliphatic)
- Fresh PAHs (class C)
- PAH-survival in 10% in T Taurii. Turbulent vertical motions ?
  (Acke et al. 2010), Siebenmorgen & Heymann 2012)

- UV heating dominant excitation process
- UV rich chemistry: - gas-phase
  (e.g., CH+, Thi et al. 2011)
  - gas-grain
  (e.g., CCH, Kastner et al. 2015)

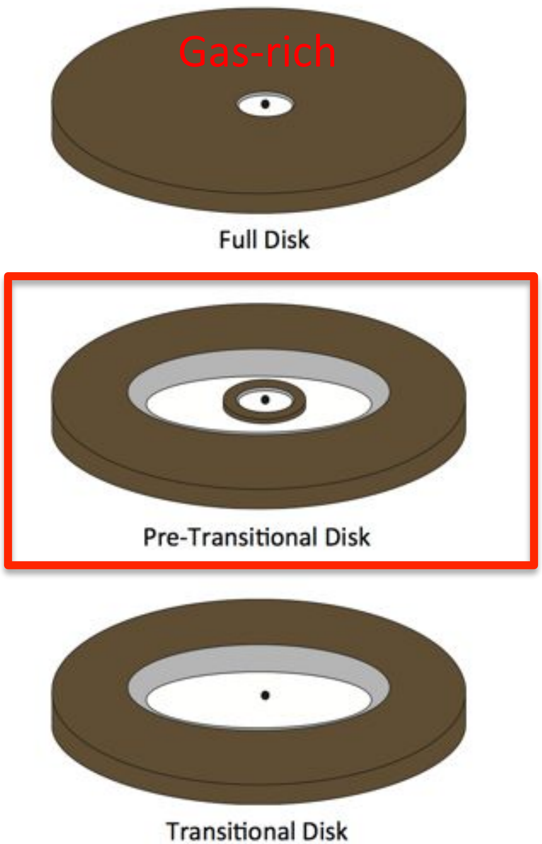
Complex distribution of gas and dust (previously unexpected..)



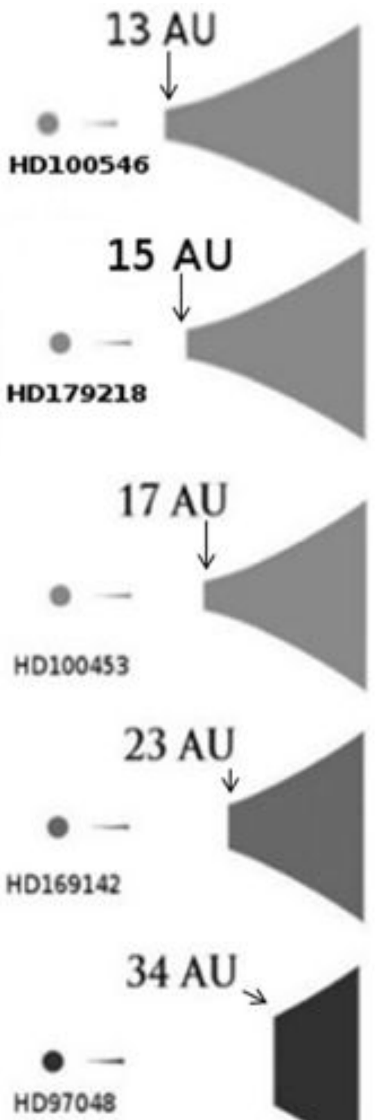




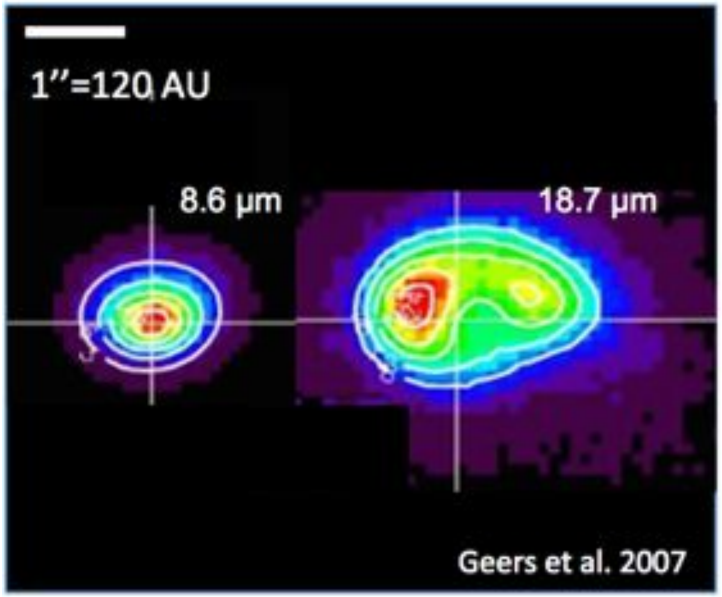
- **inner gaps**
- **Annular gaps**
- **rings**
- **Spirals**
- **dust traps**
- **proto-planets…**

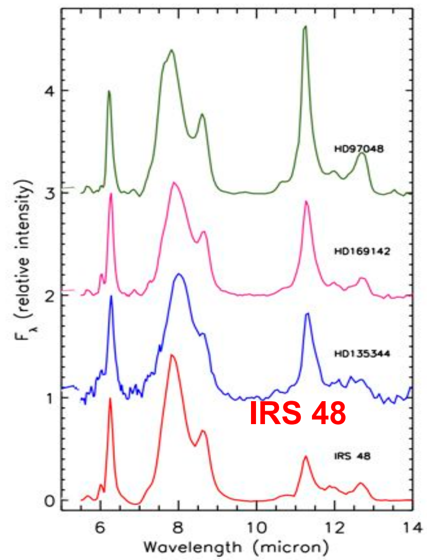


(all Groupe I
=> (pre-)transitional)

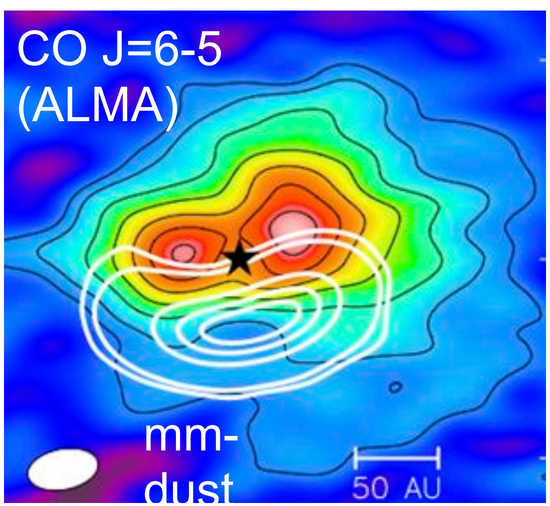


Inner gaps not empty: gas, nano-grains (escape settling)

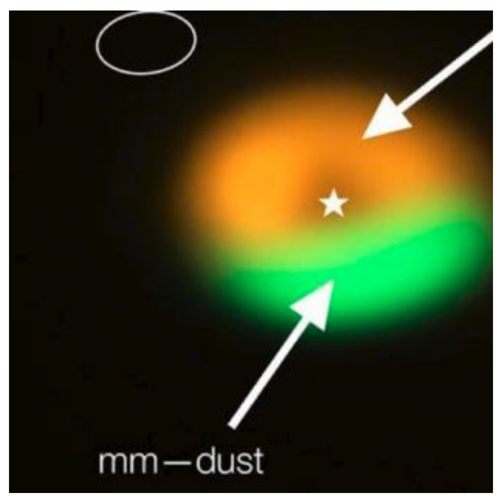




Maaskant+2014



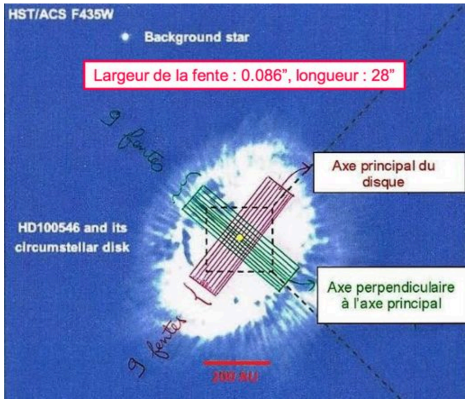
Bruderer+2014



Van der Marel et al.2013

High resolution spectroscopy of carbonaceous (nano-)particles

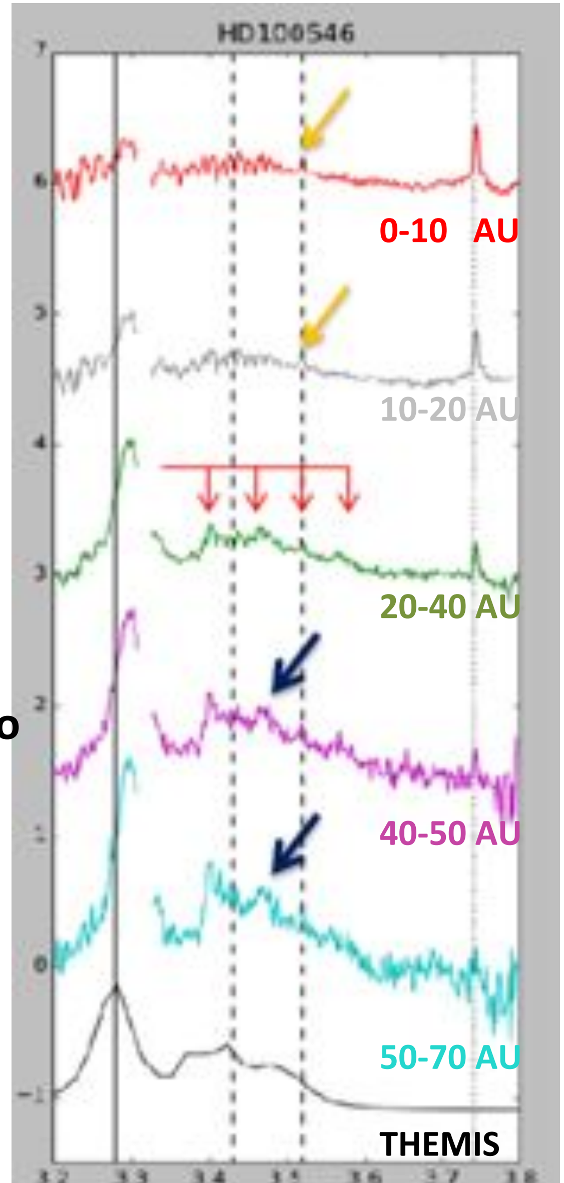
In prep.

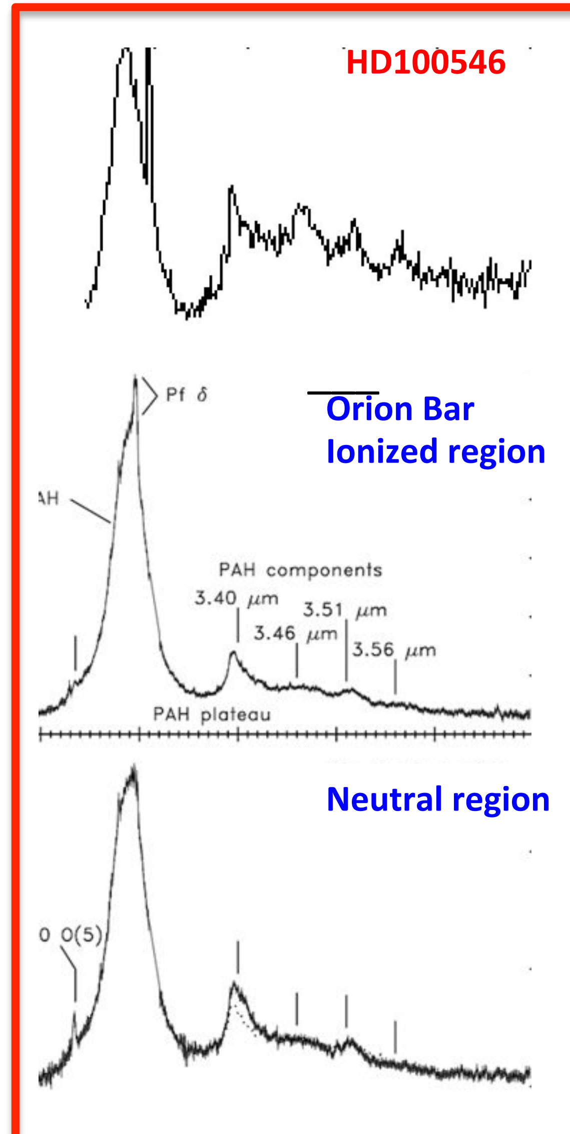


- 1st results
- Various features (≠ in sources)
- Similarity with PDRs
- **High aliphatic/aromatic bands ratio**
- No variation with radius (UV flux)
- **Fresh material resplenish ?**

⇒ **Extended IAS dust models to circumstelar environment**

=> **VLT/MATISSE** (1-10 AU) 2017-2018





Key questions

- **How (nano-)particles evolve in disks ? Difference with PDRs ?**

- **How these evolution influence the radiative transfer, temperature and chemistry ?** Key for physico-chemical models and photoevaporation

- **How are they robust tracers of the physical conditions (UV flux, ionization, extinction) ? Tracers of the disk structure?** The mid-IR surface brightness appears brighter in the planet forming region of disks with PAH emission than in those without PAHs

- **What carbonaceous (nano-)particles become ? What are the links with the primitive solar system materials (meteorites, interplanetary dust) ?**

Tasks

WP3 / ISM, PDRs & Disks	Date	People in charge	Deliveries
Dust properties modeling			
a) Charge distribution	2016-2017	Verstraete	1 paper for a) & b)
b) Size distribution	2016	Bocchio, Jones	
c) aC(:H) equilibrium composition	2017-2019	Dartois, Godard, Jones, Ysard	1 paper (A&A)
d) Grain optical properties	2016-2019	Jones, Ysard + collab (Köhler, UK)	2 papers (A&A)
e) DustEM service	2016-2019	Verstraete, Ysard	Updated DustEM tool for community
Analysing/ training with pre-JWST data - PDRs - Disks	2016-2019	PDRs PhD, Abergel, Wagle Disk postdoc, 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 t
Simulation of JWST observations - PDRs - Disks	 2017-2019 2017-2019	 ISM PhD, Abergel Disk PhD, Disk postdoc, Habart, Ysard, Pantin	 Simulated JWST data
Analysis of JWST observations - 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)

PhD

- **PhD Thomas Bouteraon (2016-2019)**

  Dust micro-physical modeling in disks; preparation of the analysis of JWST data

  – 2016-2017 : Analysis of the carbonaceous nano-particle spectra in the near- and mid-IR (VLT, Spitzer) around Herbig Ae/Be stars using the dust models available at IAS.

    Determination of the composition (aromatic/aliphatic rich) and the size distribution (a_{min}) as a function of UV field strenght and spectral distribution

  – 2017-2018 : **Dust model + radiative transfer code**. Prediction of the **spatial distribution** of the various emission features to be observed with the JWST for different **disk density structures**, inclinations

  – 2018-2019: Comparison with ground-based spatially resolved data (VISIR/VLT) and JWST data simulations in collaboration with SAp. Participation to the preparation of open time observing proposals.

- **PhD : Dust emission in PDRs with the JWST (2017-2020)**

  – 2017-2018 : Modeling of the dust emission in nearby PDRs using Spitzer, Herschel and ground-based data (dust model + radiative transfert code). Evolution of the composition, the relative abundances, the size of the dust particles.

  – 2018-2019 : Simulation of JWST data. Preparation of the analysis of first JWST data.

  – 2019-2020 : Analysis of first JWST data. Modeling of the dust emission in nearby PDRs observed with the JWST (emission of small carbonaceous dust, scattered emission of large grains). Participation to the preparation of open time observing proposals.