

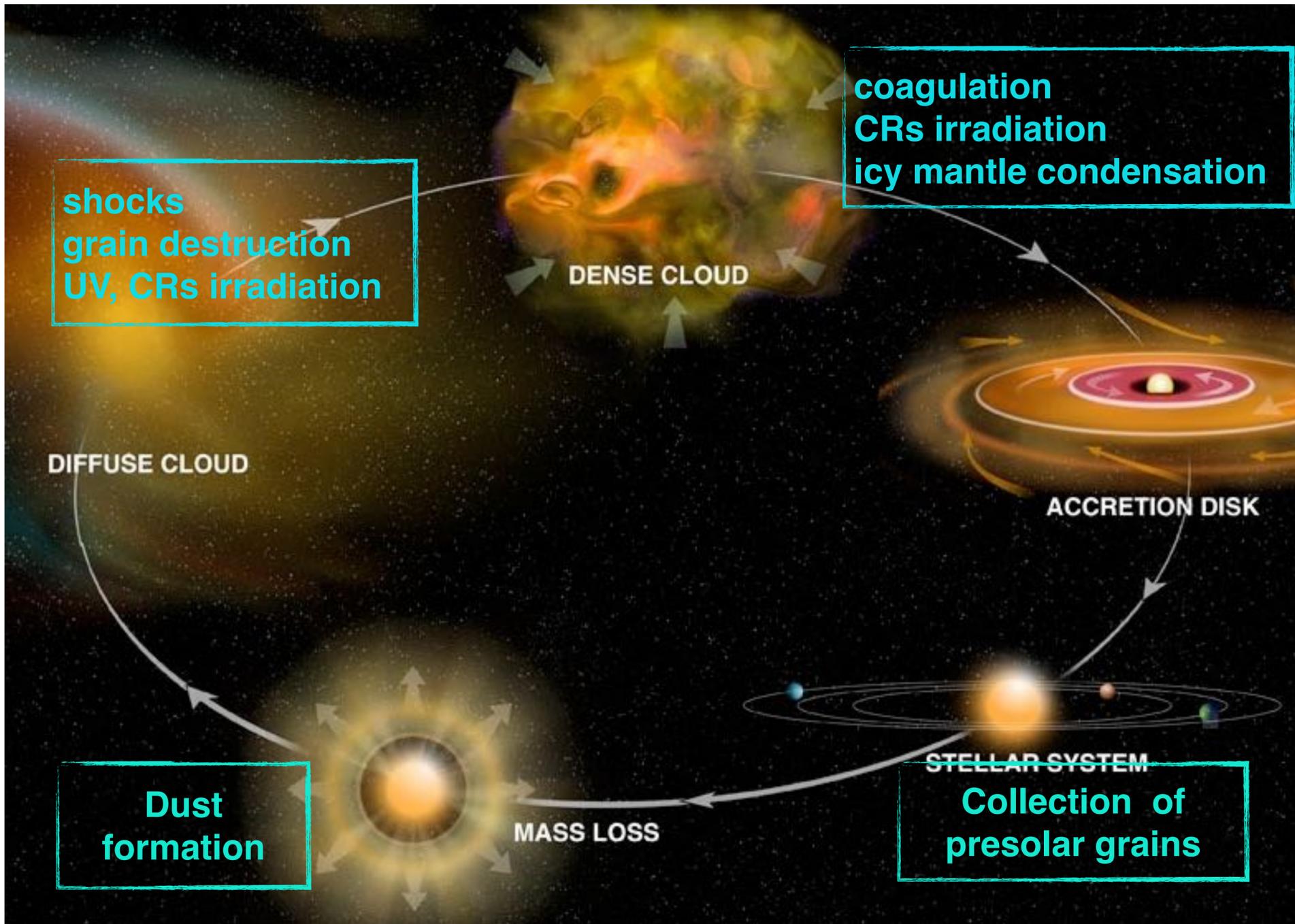
INTERSTELLAR DUST PROPERTIES AND COSMIC DUST MODELS

Karine Demyk, IRAP

Outline

- Observational constraints & dust properties
- Dust evolution
- Modelling dust extinction and emission
- Cosmic dust models

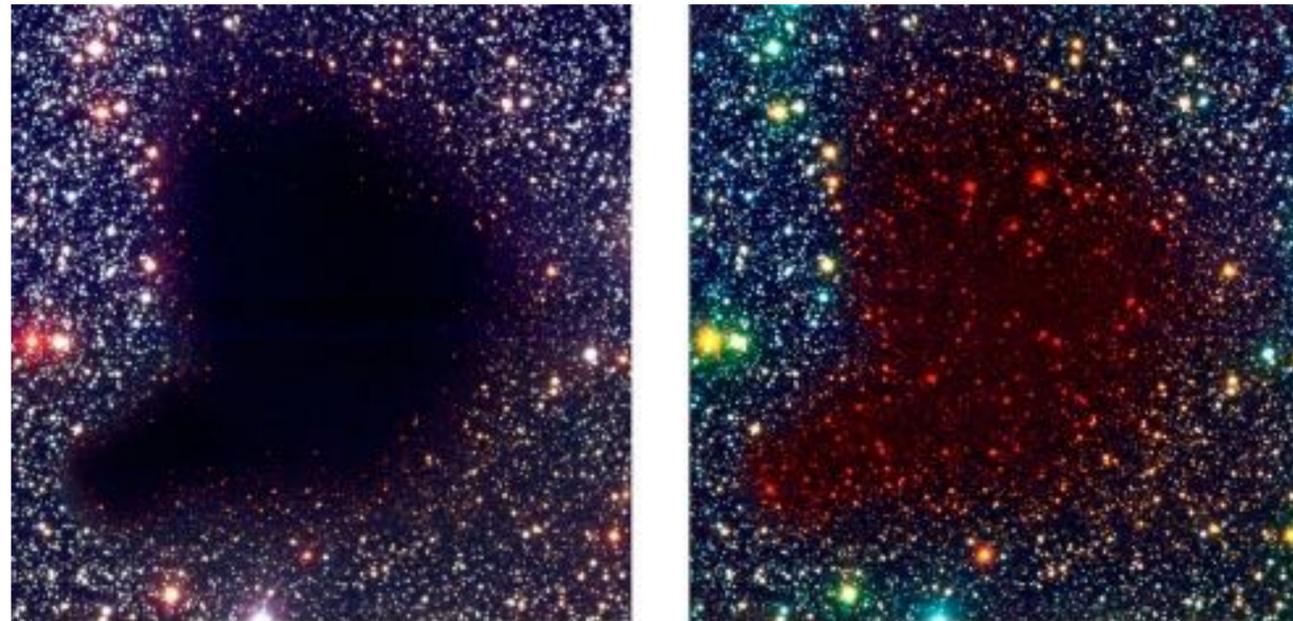
The dust cycle



- The life cycle of the ISM, of stars and dust are intimately related
- Dust is everywhere
- Dust is a probe of the physical and chemical conditions of astronomical environments
- Dust is one of the drivers of ISM evolution and hence of galactic evolution
- Dust is key to promote chemical complexity

Observational constraints & dust properties

Extinction



B, V, I

B, I, K

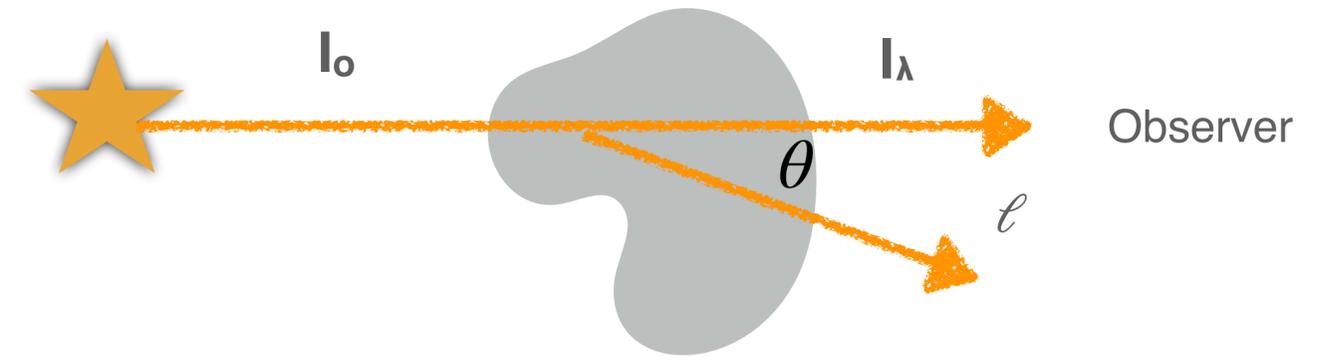
Pre-Collapse Black Cloud B68 (comparison)
(VLT ANTU + FORS 1 - NTT + SOFI)

ESO PR Photo 02c/01 (10 January 2001)

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- 1930: Trumpler proposes that matter attenuates the visible light from stars depending on their distance
- 1934 : Stebbins makes the first measures of extinction in the UBV bands
- 1940-50: Stellar reddening by comparison of stars of the same spectral type



$$I_{\lambda} = I_{\lambda 0} e^{-\tau_{\lambda}}$$

$$\tau(\lambda) = \int k_{ext}(\lambda) dl$$

$$A_{\lambda} = -2.5 \log_{10} \left(\frac{I_{\lambda}}{I_{\lambda 0}} \right) = 1.086 \tau_{\lambda}$$

I_{λ} : Specific intensity
($W \cdot m^{-2} \cdot sr^{-1}$)

k_{ext} : Extinction
coefficient (m^{-1})

The extinction curve

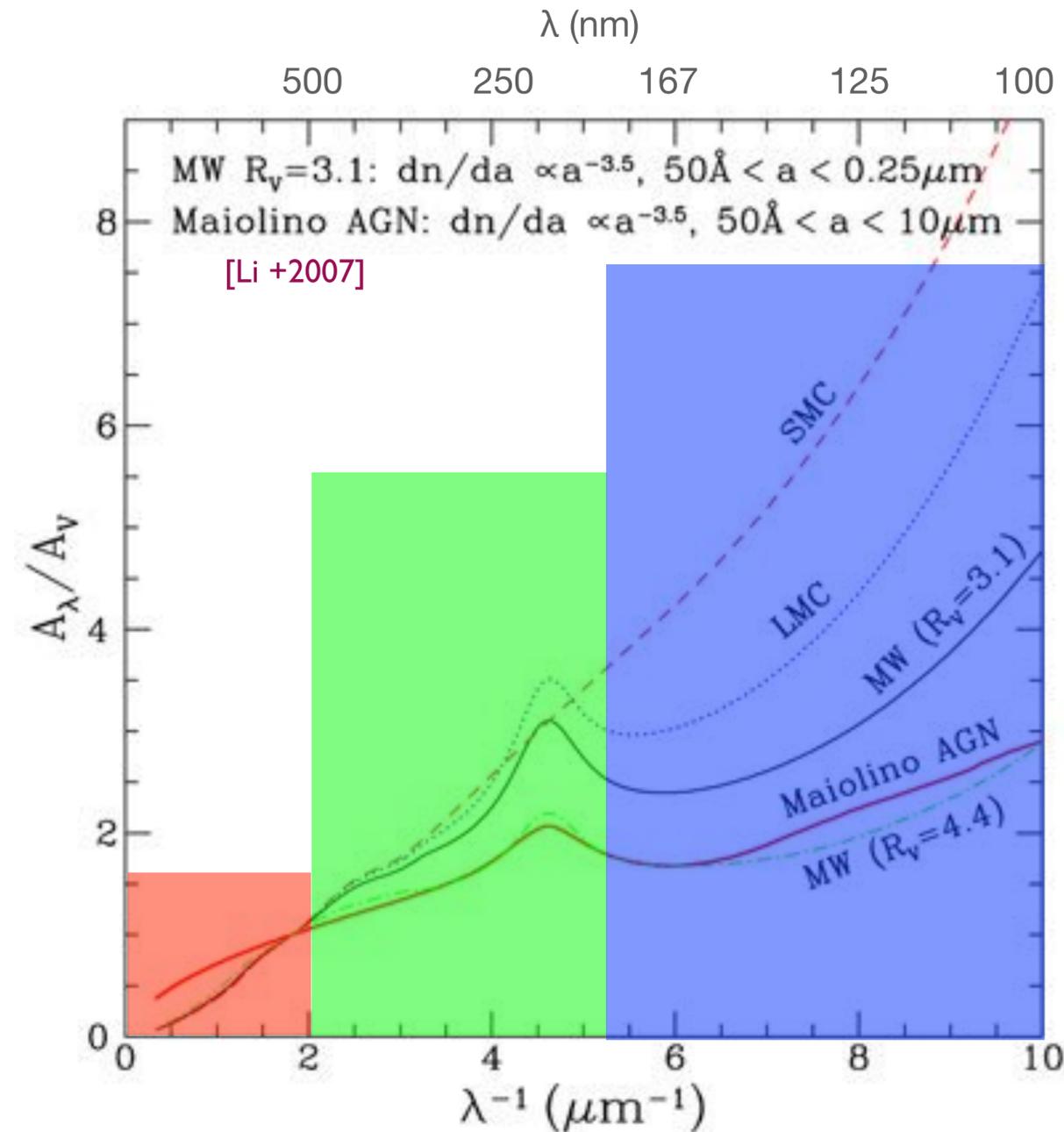
The extinction curve gives information on the size and composition of grains:

- UV rise \Rightarrow grains with radius $a \ll \lambda$ ie. $a < 10$ nm
- 2175 Å bump \Rightarrow carbonaceous grains (electronic transition)
- U, B, V bands \Rightarrow extinction in $\lambda^{-1} \Rightarrow$ grains with radius $a \sim \lambda$ ie. $a \sim 0.1 \mu\text{m}$
- MIR domain : vibrational transitions \Rightarrow silicates, carbonaceous dust, ices

Color excess: $E(B - V) = A_B - A_V$

Total-to-selective visual extinction ratio: $R_V = \frac{A_V}{E(B - V)}$

R_V characterise the extinction curve



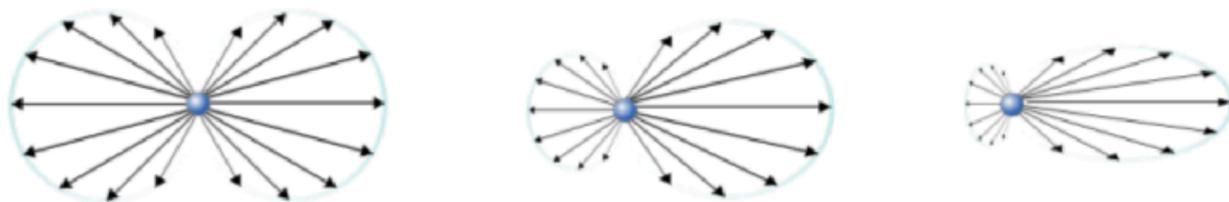
Scattering

- Scattering depends on the size, shape and composition of the grains
 - Grains of radius $a \sim 0.1 \mu\text{m}$ scatter light in the visible
 - Larger grains scatter light at longer wavelengths, in the NIR
-
- Scattering depends on the albedo ω and the phase function g

$$\omega = Q_{sca}/Q_{ext}$$

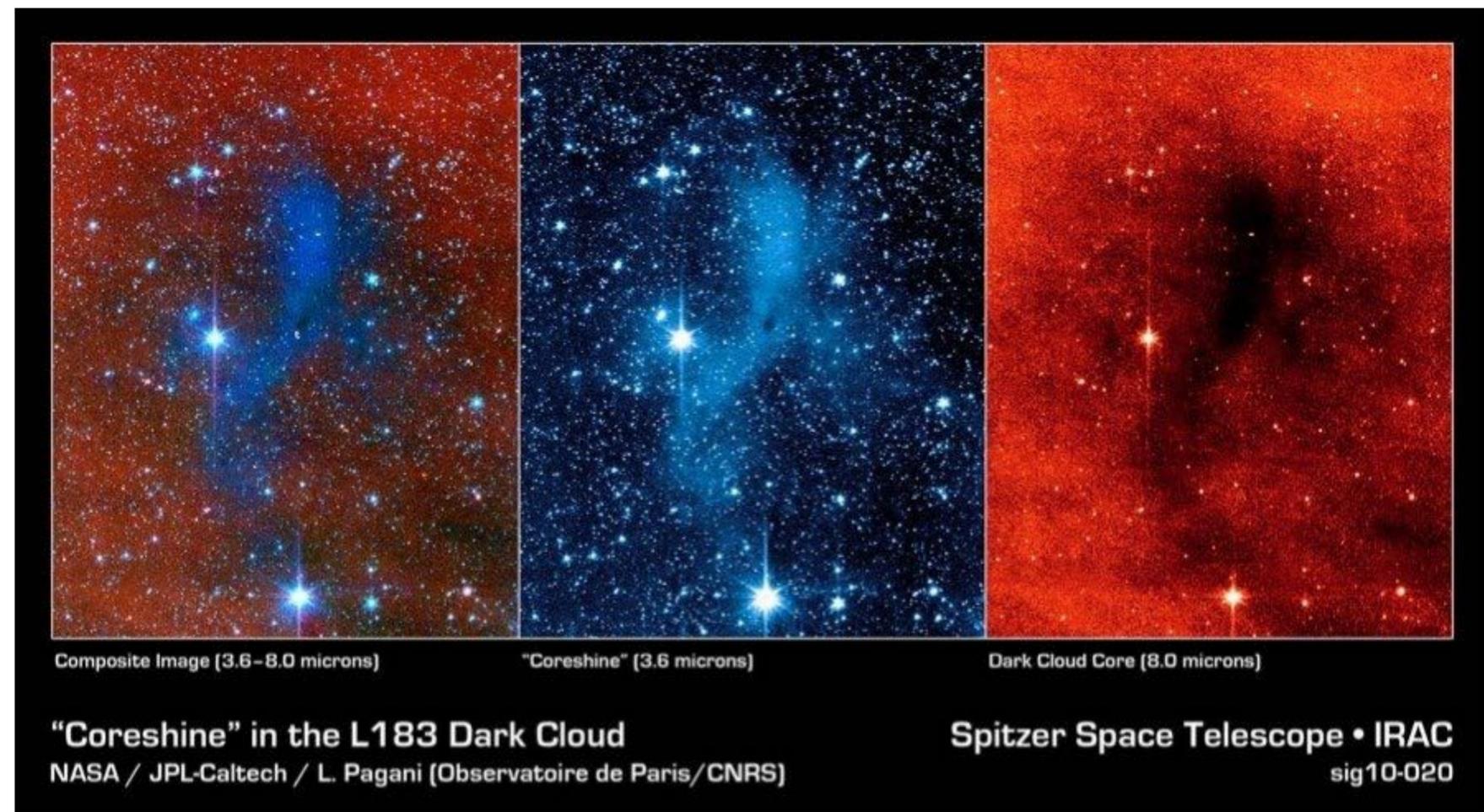
$$g = \langle \cos(\theta) \rangle = \frac{\int_0^\pi I(\theta) \cos(\theta) d\Omega}{\int_0^\pi I(\theta) d\Omega}$$

Rayleigh and Mie scattering phase function



Crédit : Sharayanan CC-BY-SA

Pléiades (Rogelio Bernal Andreo)



Emission

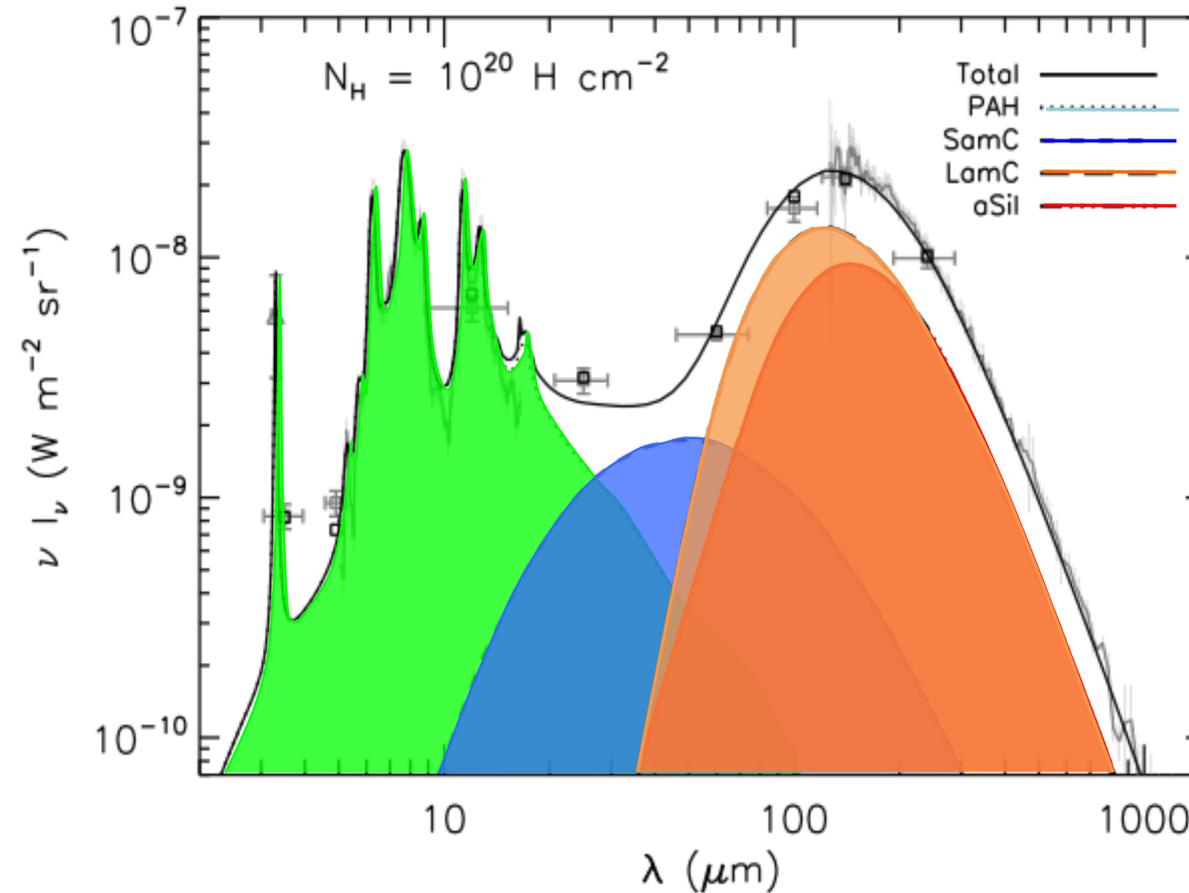
On a given line of sight, dust emission depends on:

- Column density of gas: N_H (cm^{-2})
- Dust abundance: X_d
- Intensity of the ISRF
- Emmissivity of dust: ϵ ($\text{erg}\cdot\text{s}^{-1}\cdot\text{sr}^{-1}\cdot\text{cm}^{-1}\cdot\text{g}^{-1}$)

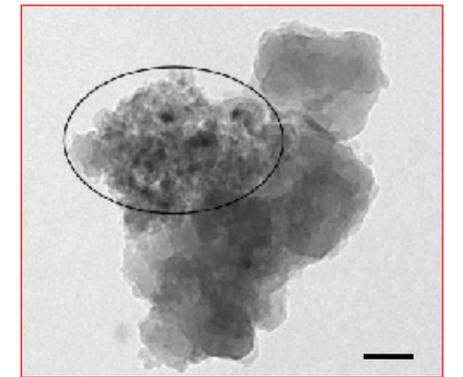
$$I_\nu \propto \int_{LOS} \epsilon \times N_H \times X_d \times ISRF$$

Different emission mechanisms depending on the grain size and nature

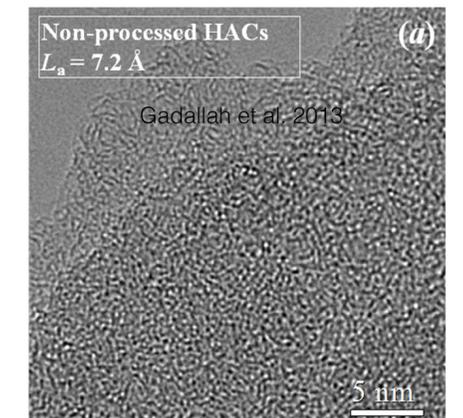
Diffuse ISM emission: [Compiègne+2011]



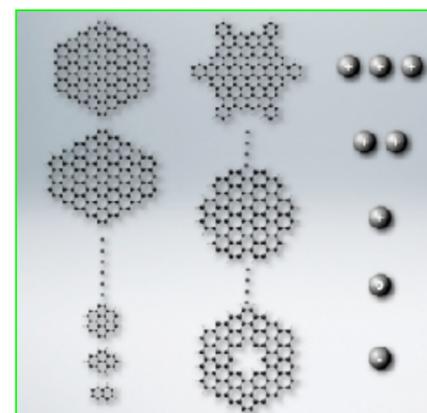
SILICATES
10-300 nm



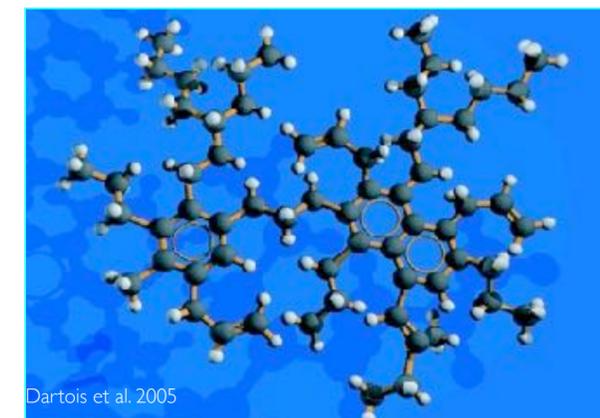
Amorphous carbon



PAHs



VSG 5-10 nm



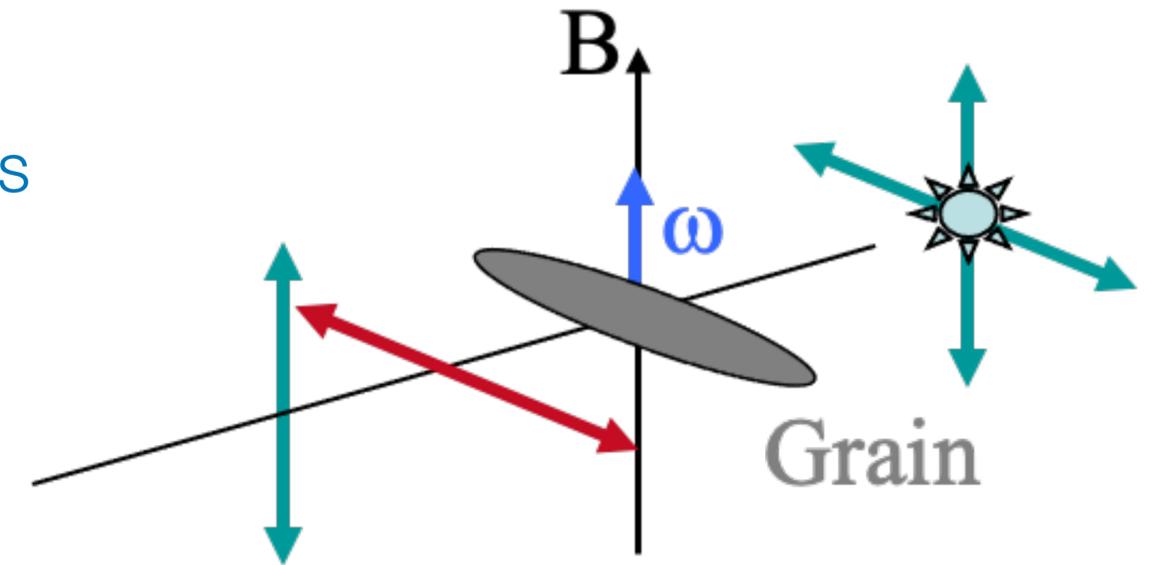
Polarization

- Due to the presence of non-spherical and partially aligned grains

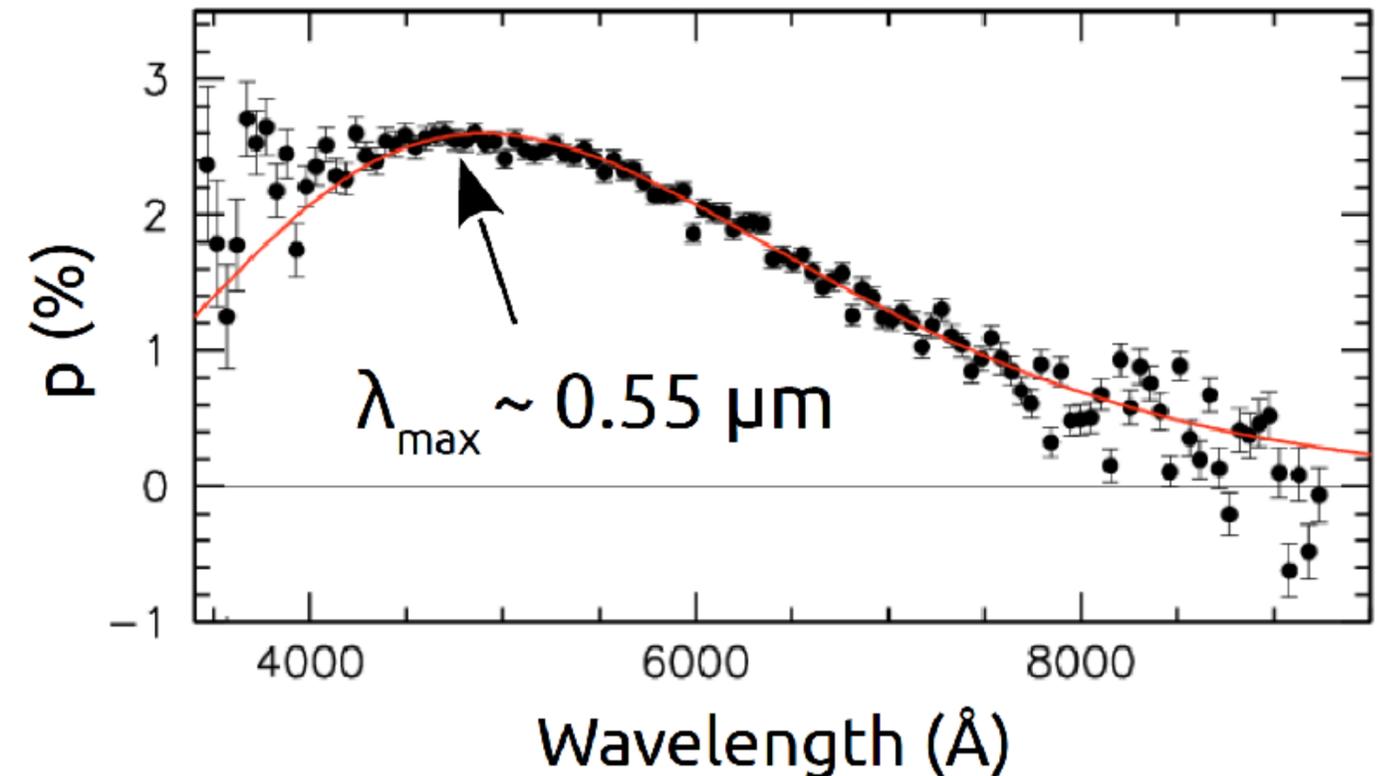
- In absorption starlight is polarised // to B field lines

$$p_{\lambda} = p_{max} e^{-k_p (\ln(\lambda_{max}/\lambda))^2} \quad [\text{Serkowski 1975}]$$

- $\lambda_{max} \sim 0.55 \mu\text{m} \Rightarrow$ grain radius $\sim 0.1 \mu\text{m}$
- The peak position is sensitive to grain size
- $p_{max} \sim$ a few %
- The $10 \mu\text{m}$ feature is polarised

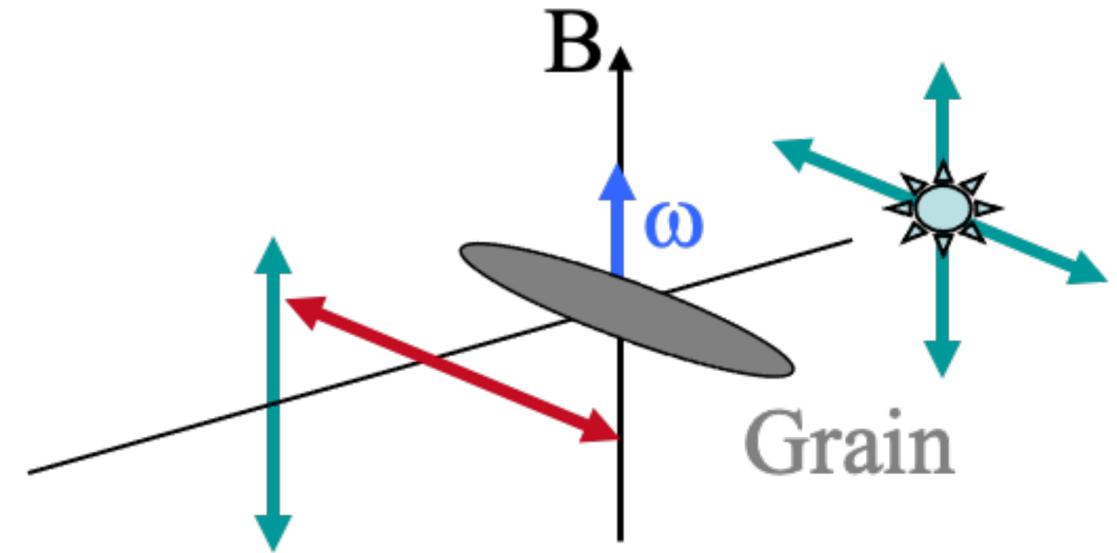


Patat et al. (2010): diffuse ISM

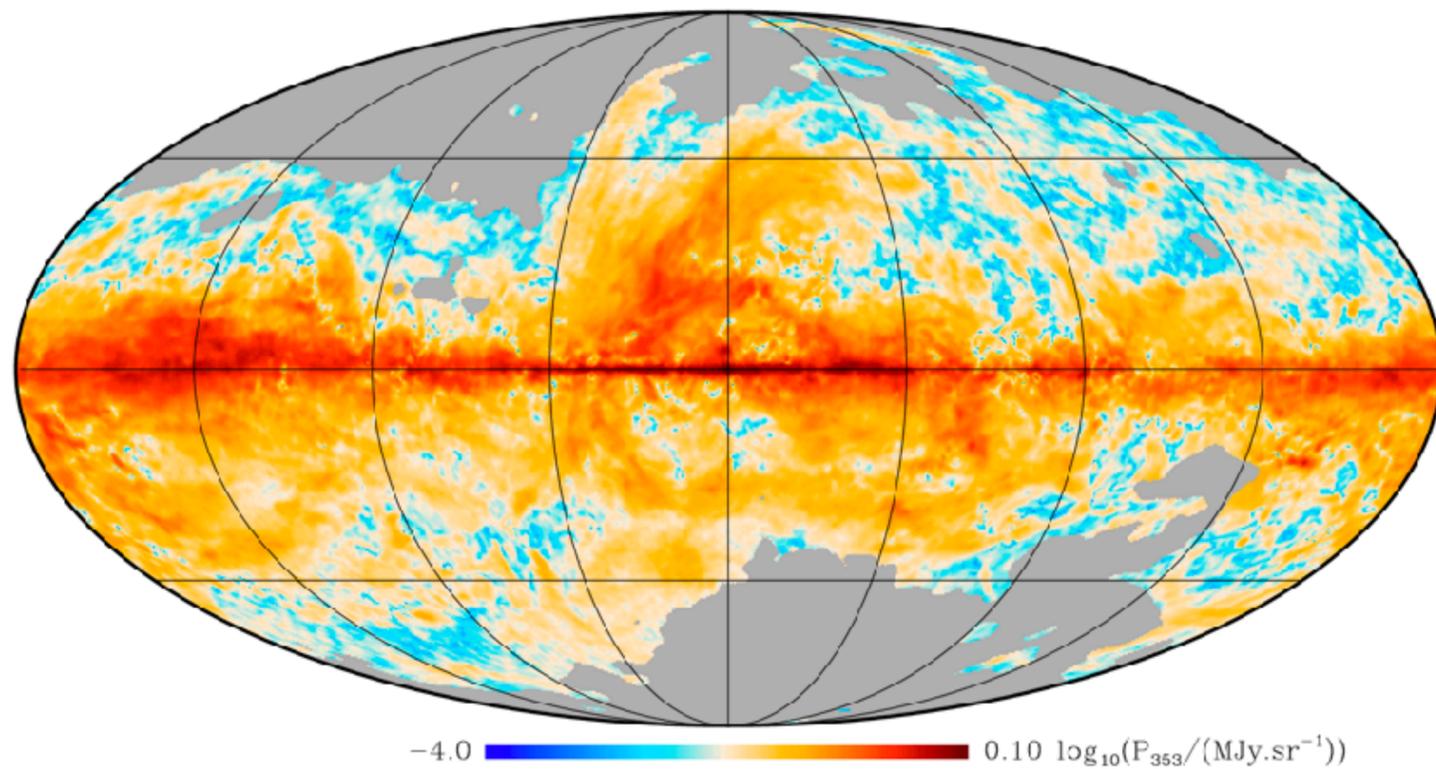


Polarization

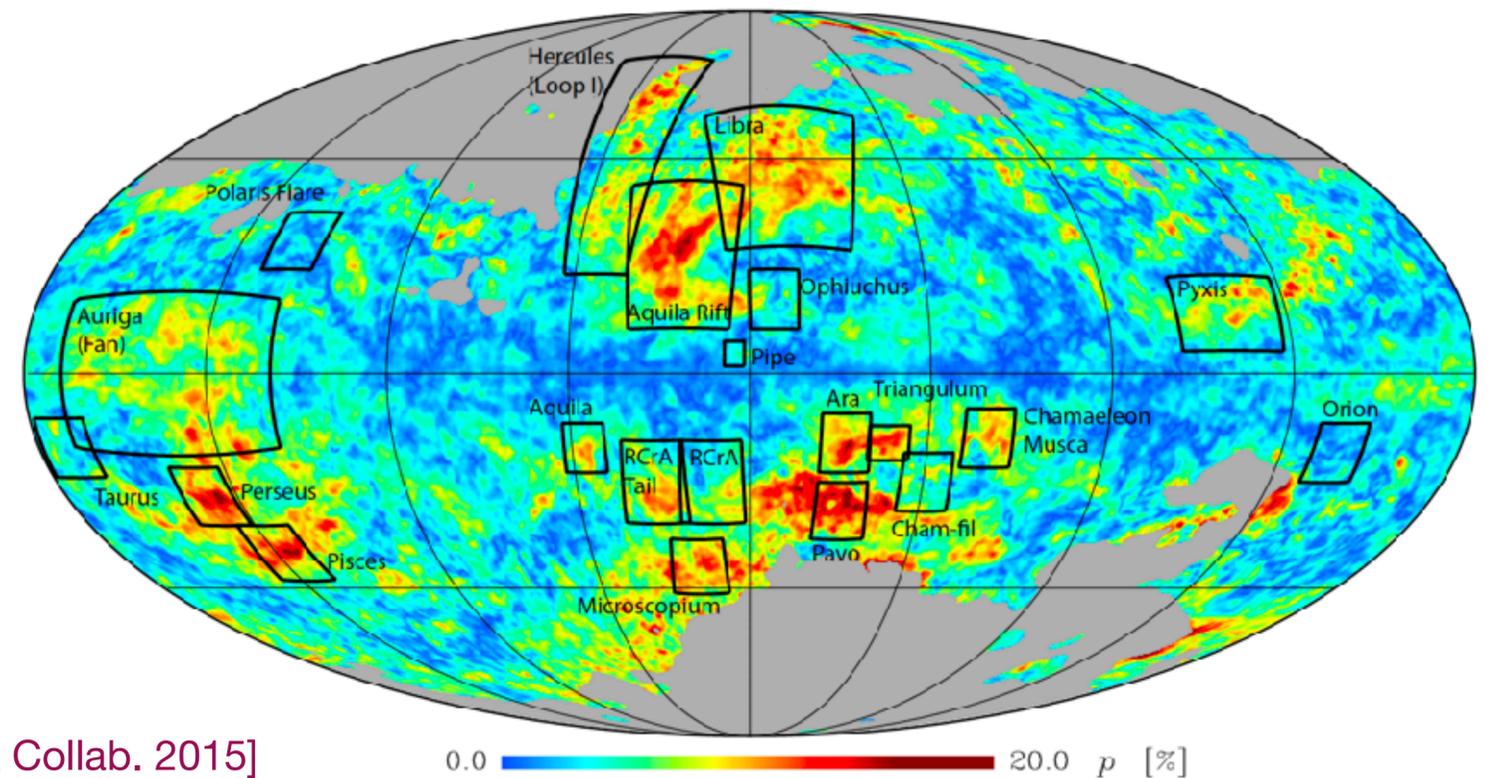
- Due to the presence of non-spherical and partially aligned grains
- Polarized emission is \perp to B field lines
- P/I = polarisation fraction in the FIR/submm
- Observed by ARCHEOPS, WMAP, Planck



Polarised emission (Planck)



Polarisation fraction (Planck)



[Planck Collab. 2015]

Depletion

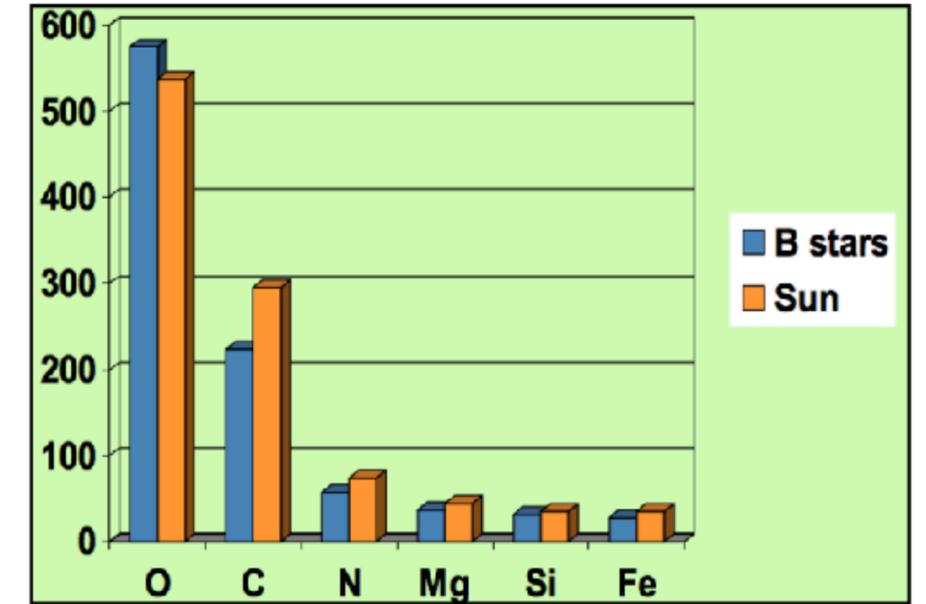
[Jenkins 2009, 2013]

- Electronic absorption lines of atoms or ions
- In the UV spectra of O and B stars
- Copernicus (1972), HST (90's), FUSE (1999)

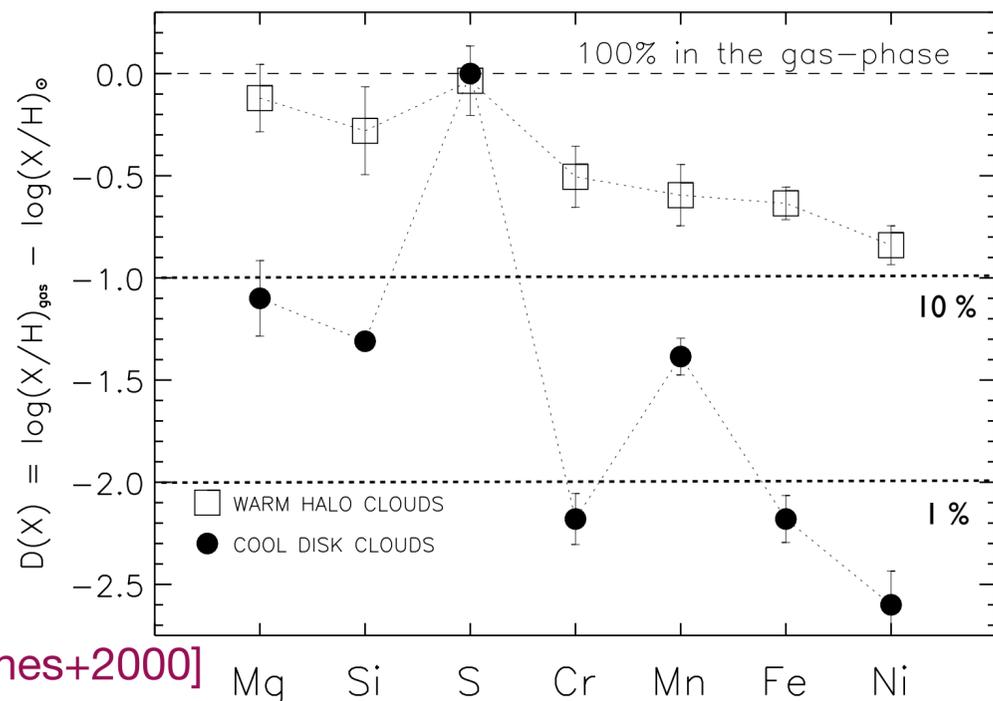
• Depletion factor:
$$\left[\frac{X_{gas}}{H} \right] = \log \left(\frac{N(X)}{N(H)} \right)_{obs} - \log \left(\frac{X}{H} \right)_{ref} \approx \log \left(\frac{X}{H} \right)_0 + A_X \times F_*$$

• Elements in dust:
$$(X_{dust}/H) = (X/H)_{ref} - (1 - 10^{[X_{gas}/H]})$$

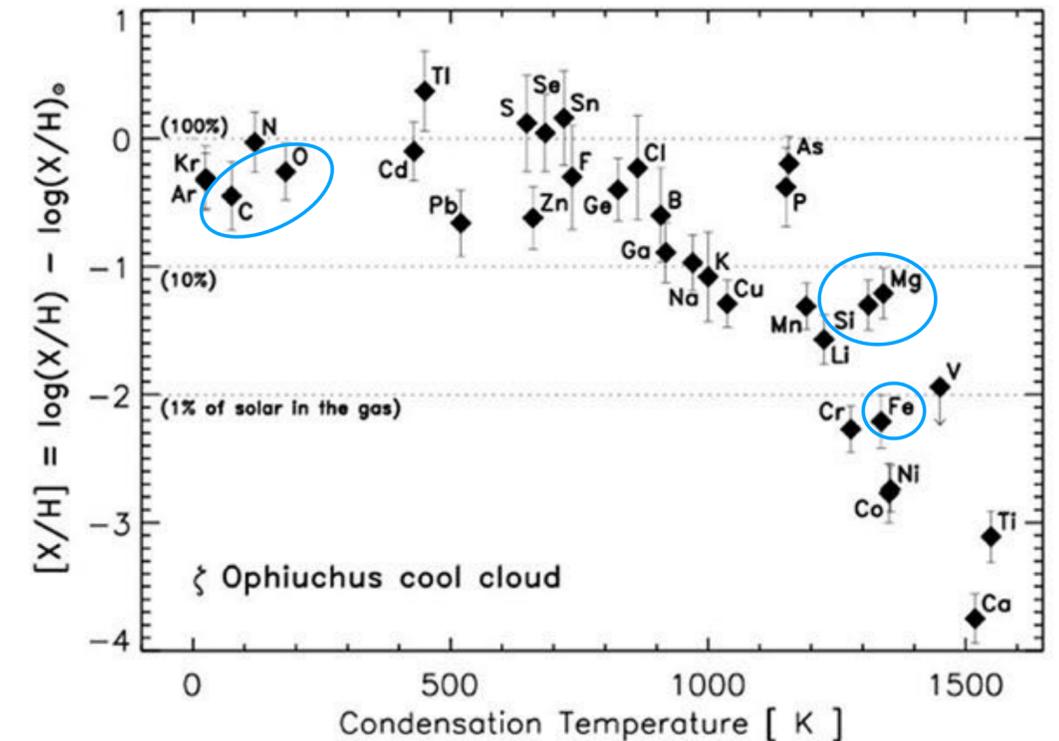
- Low density clouds and high velocity gas have less depletion than dense clouds



Elemental depletions in the ISM



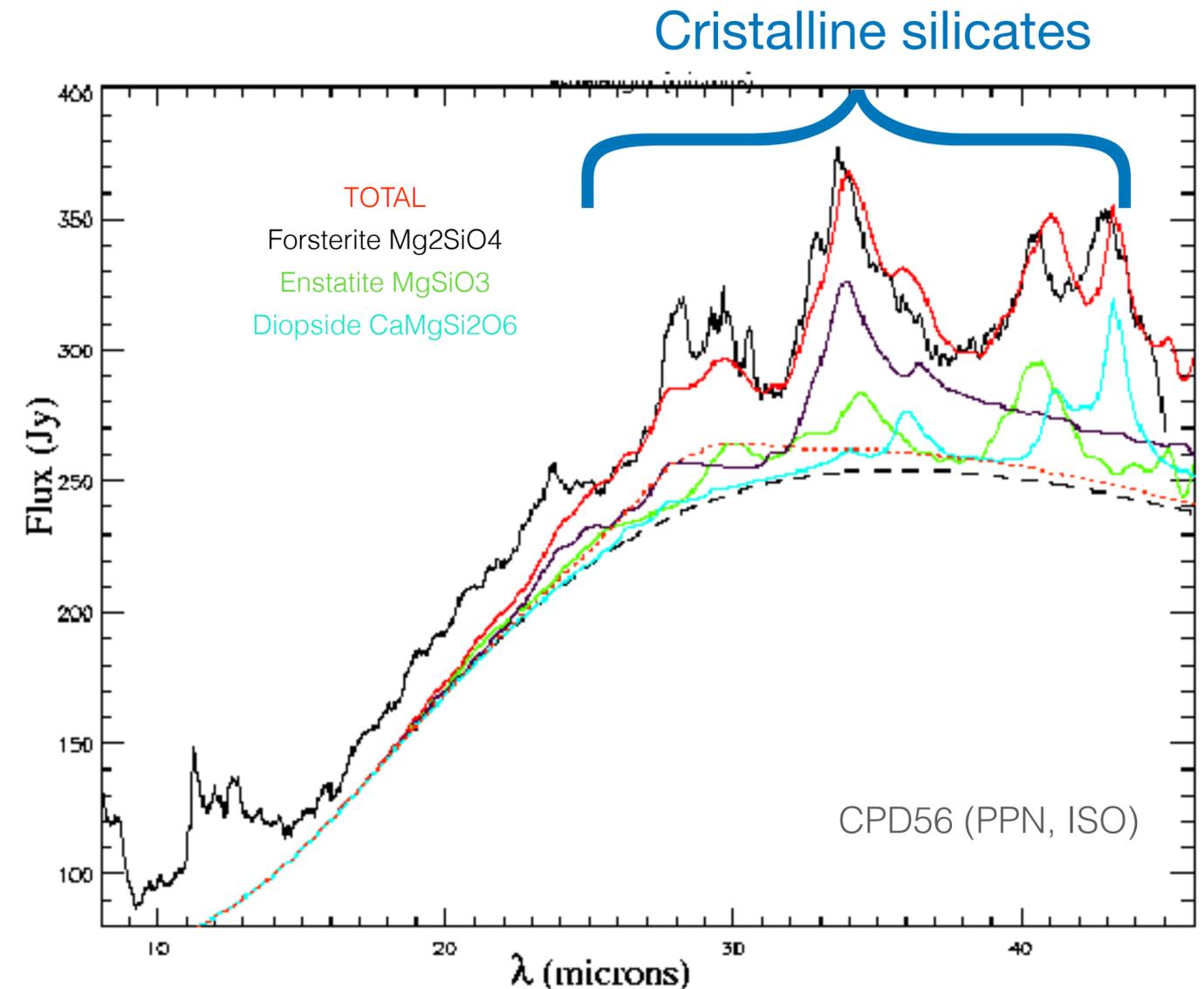
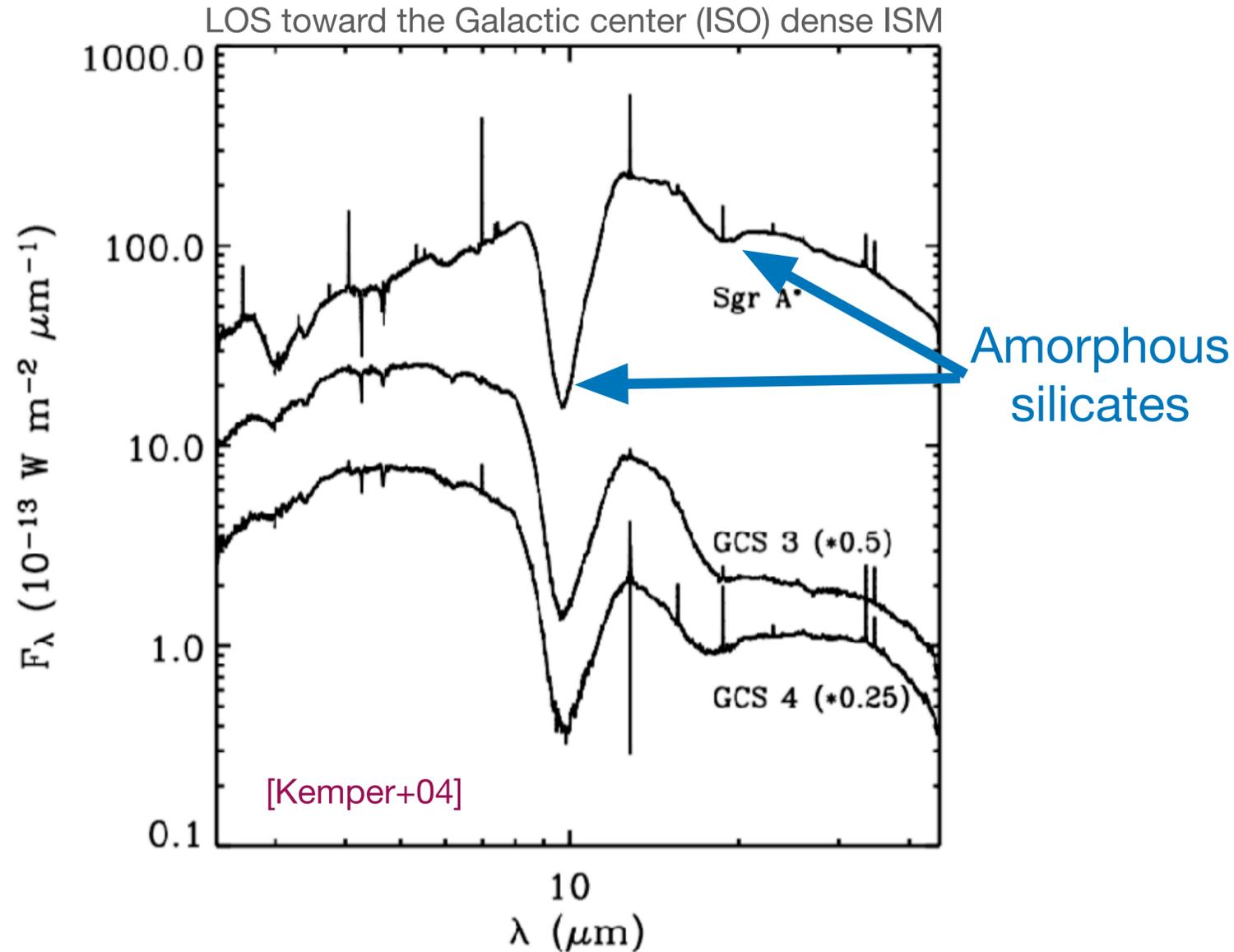
- Depletion varies from one element to the other
- Depletion increases with condensation temperature of the elements



[Jones+2000]

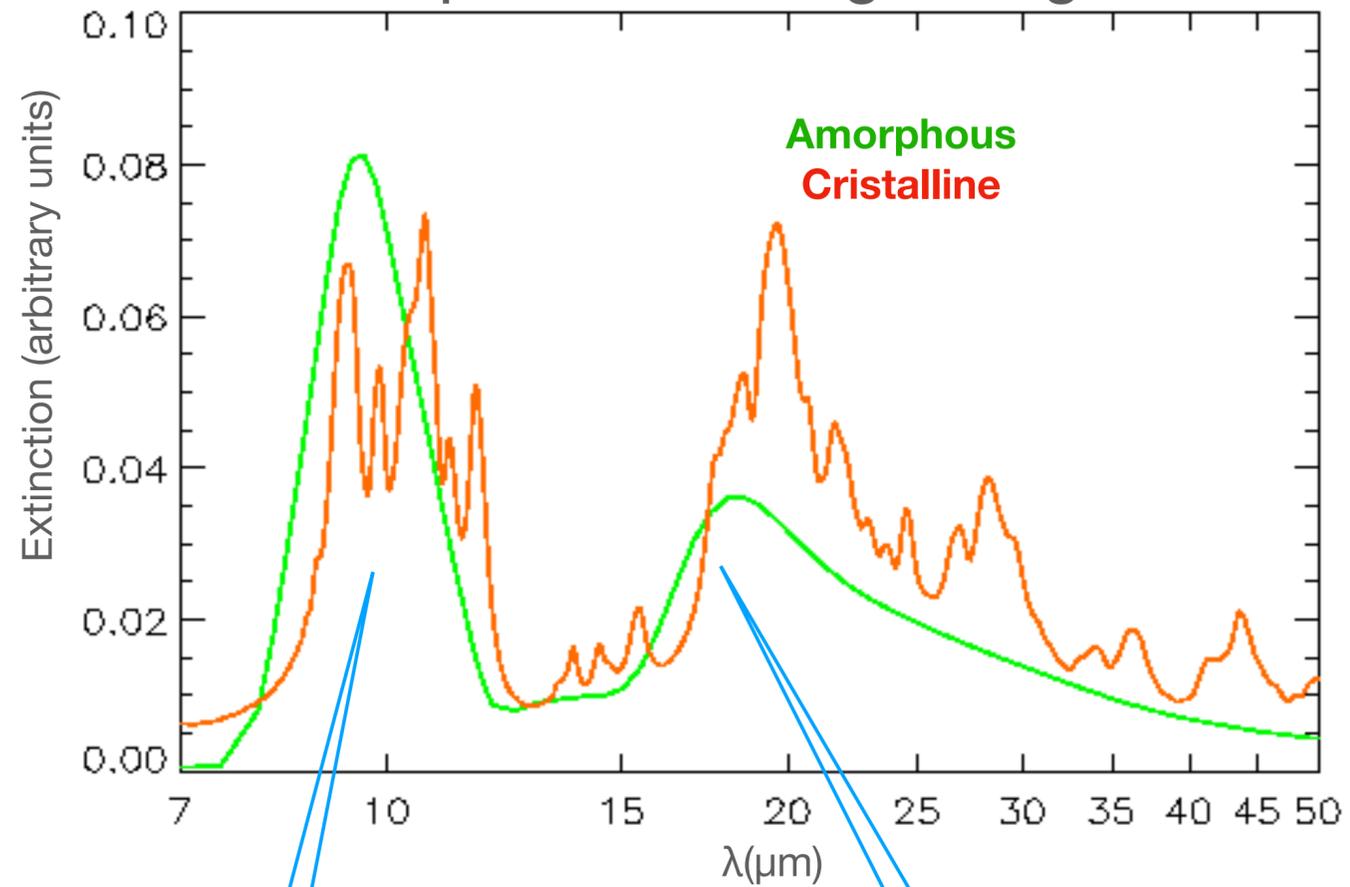
Silicates grains

- Composition and structure constrained by MIR spectroscopic observations
- Silicate grains are submicronic: radius $a \sim 0.1 \mu\text{m}$
- Silicate dust in the ISM is amorphous, at most 1-2 % of crystalline silicates [Kemper+04]
- Mostly Mg-rich silicate such as amorphous enstatite (MgSiO_3) and forsterite (Mg_2SiO_4)



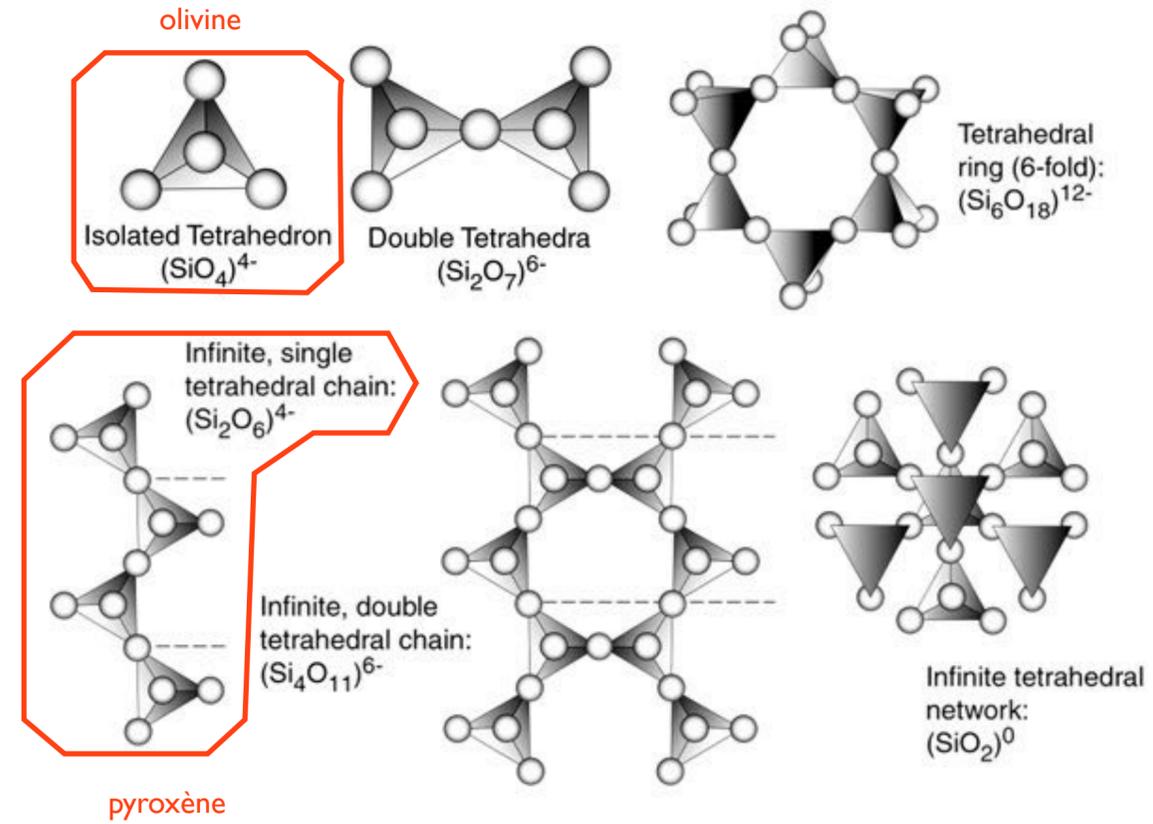
Silicates

MIR spectrum of MgSiO_3 grains



9.7 μm : Si-O stretching mode

18 μm : Si-O bending mode

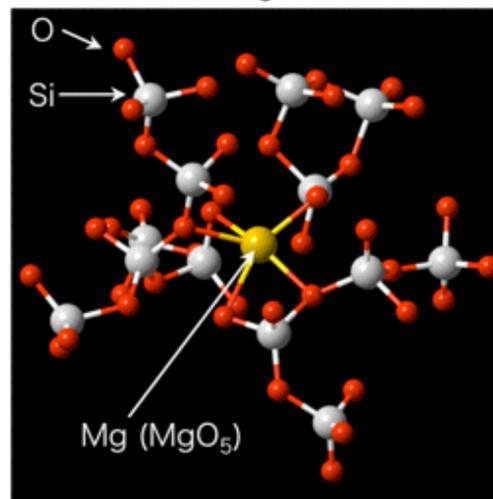


Olivine

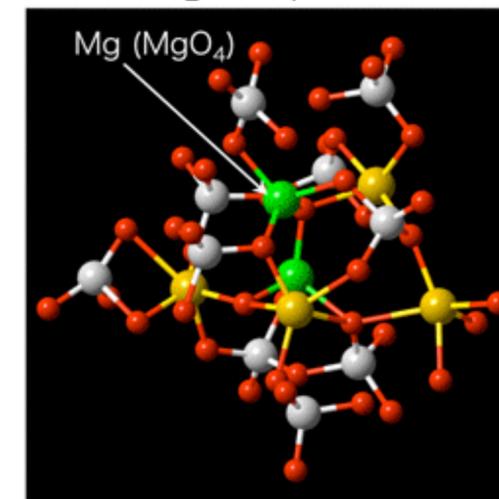


1 cm

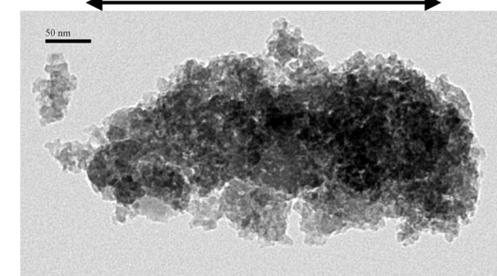
MgSiO_3 glass



Mg_2SiO_4 glass

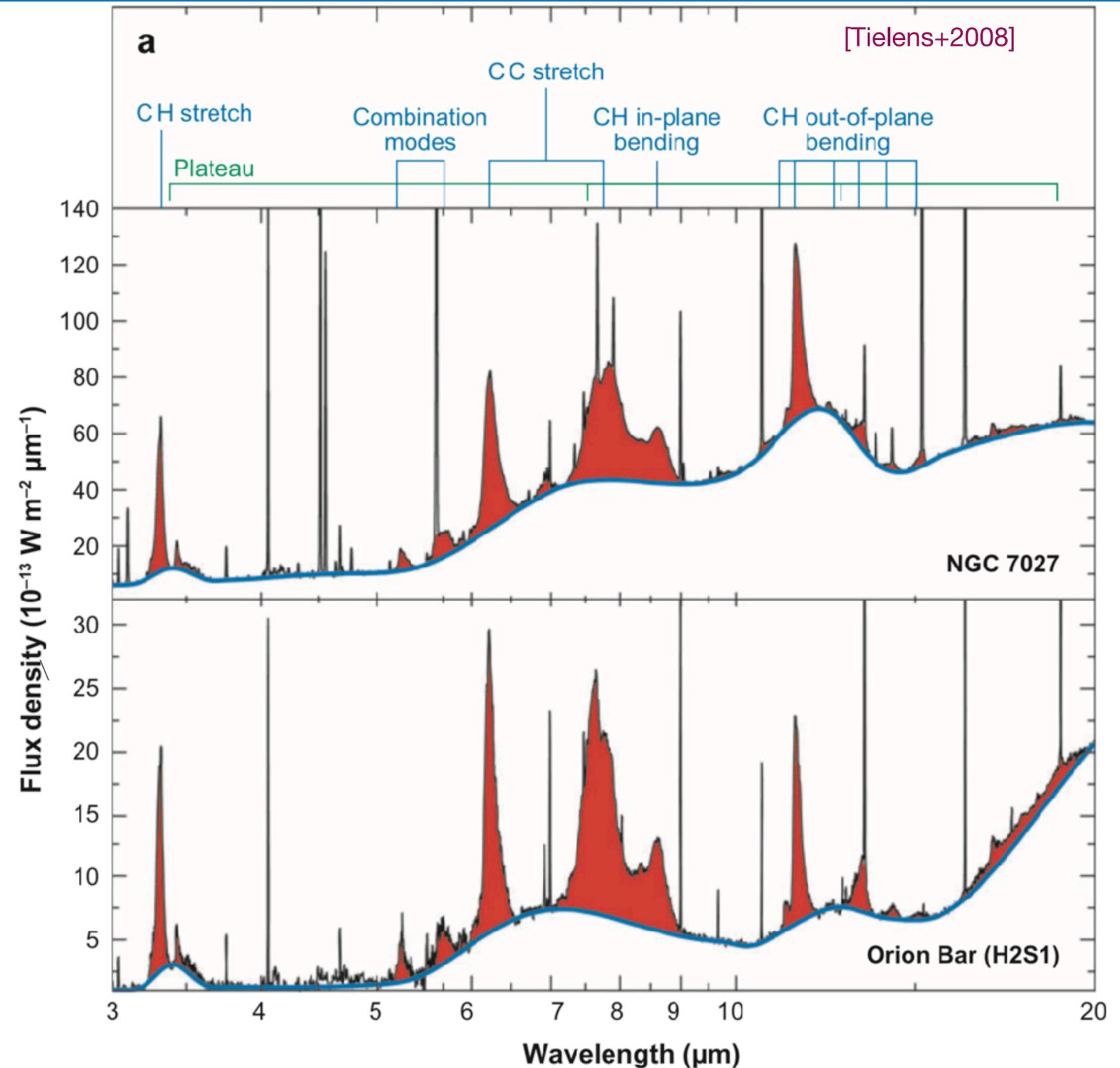


~400 nm



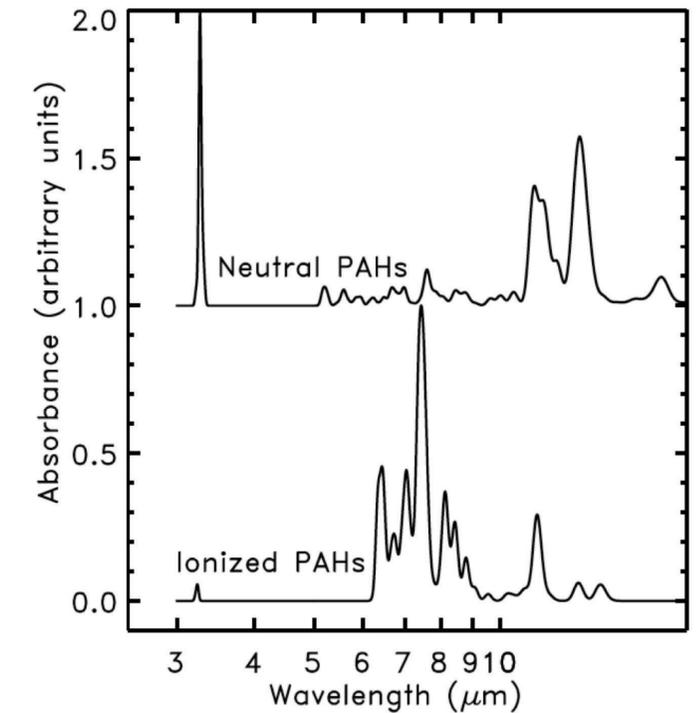
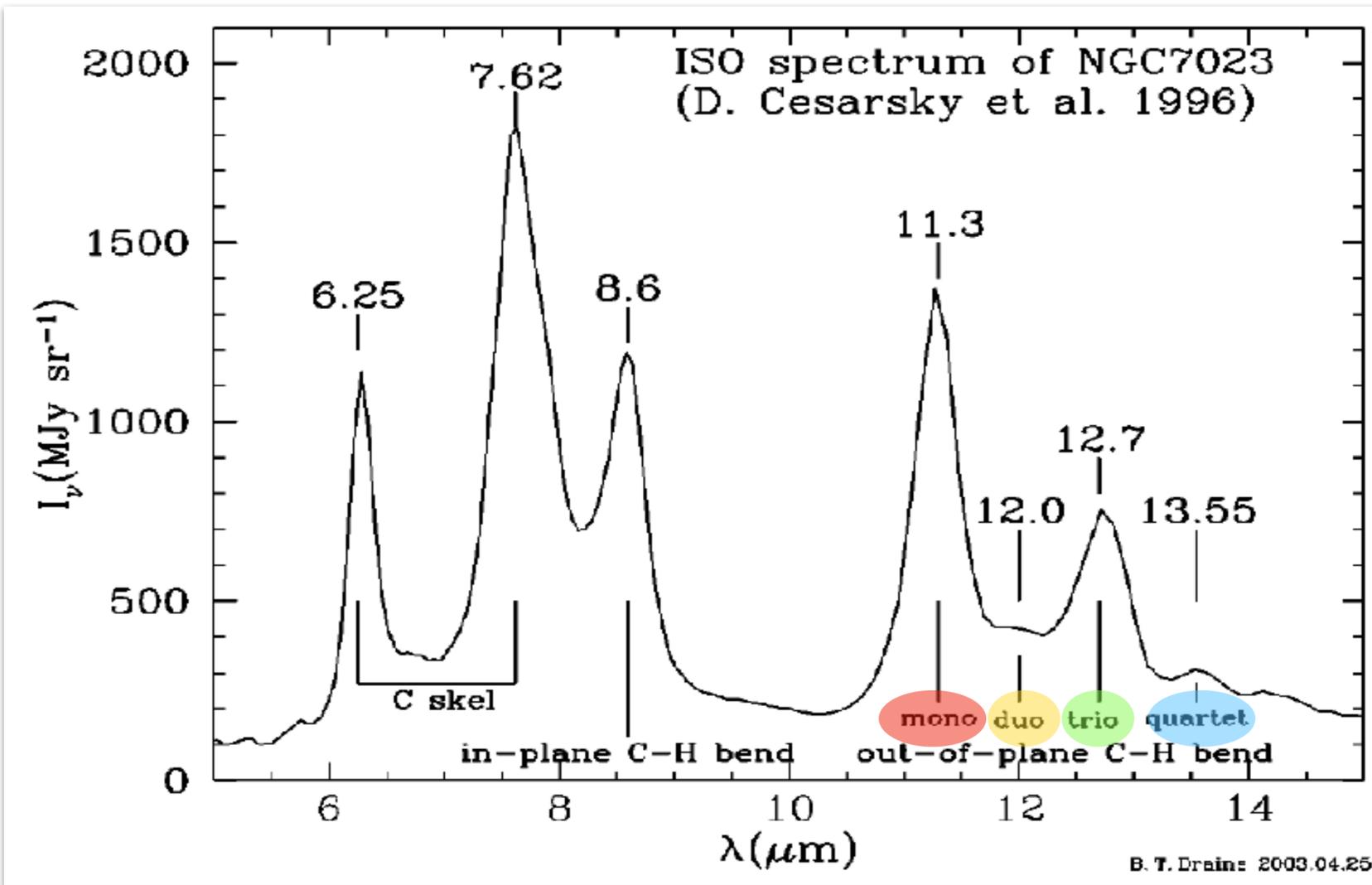
Aromatic carbon-rich dust: the Aromatic Infrared Bands

- Observed in photo-dominated regions, circumstellar shells and disks around evolved and young stars
- ~10-20 % of cosmic carbon
- ~ 5 % of the dust mass
- Band strengths and band ratios vary with the environments

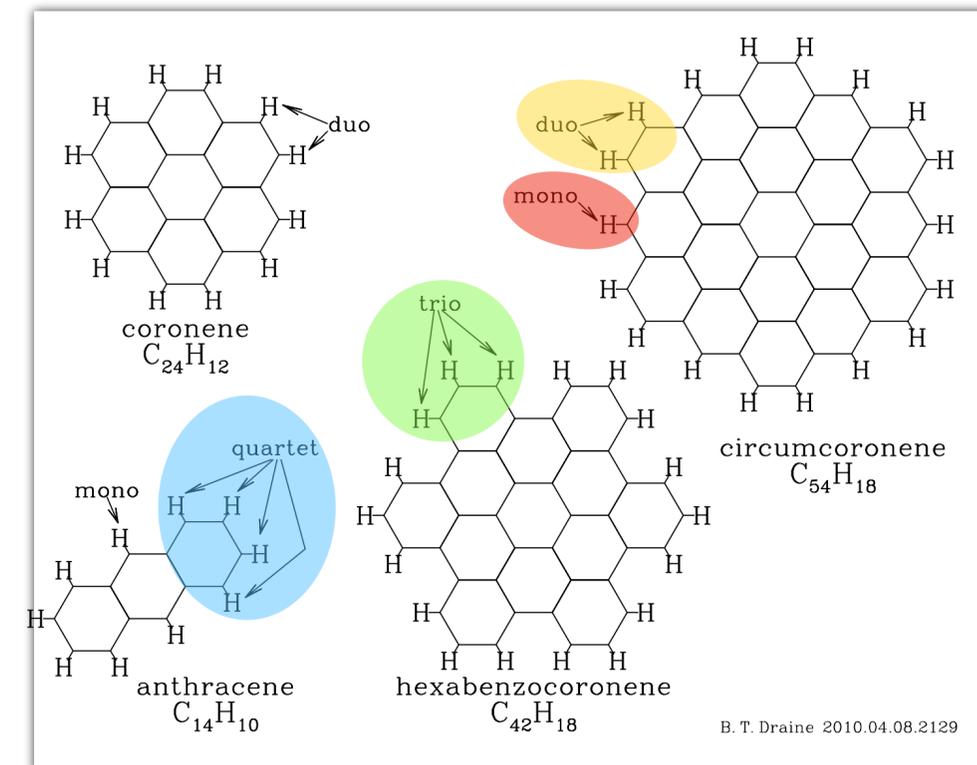


Aromatic carbon-rich dust: PAHs

- Aromatic molecules such as PAHs
 - no single identification
 - distribution of size : ~ several tens of C atoms
 - probably explain some DIBs (ionised PAH)

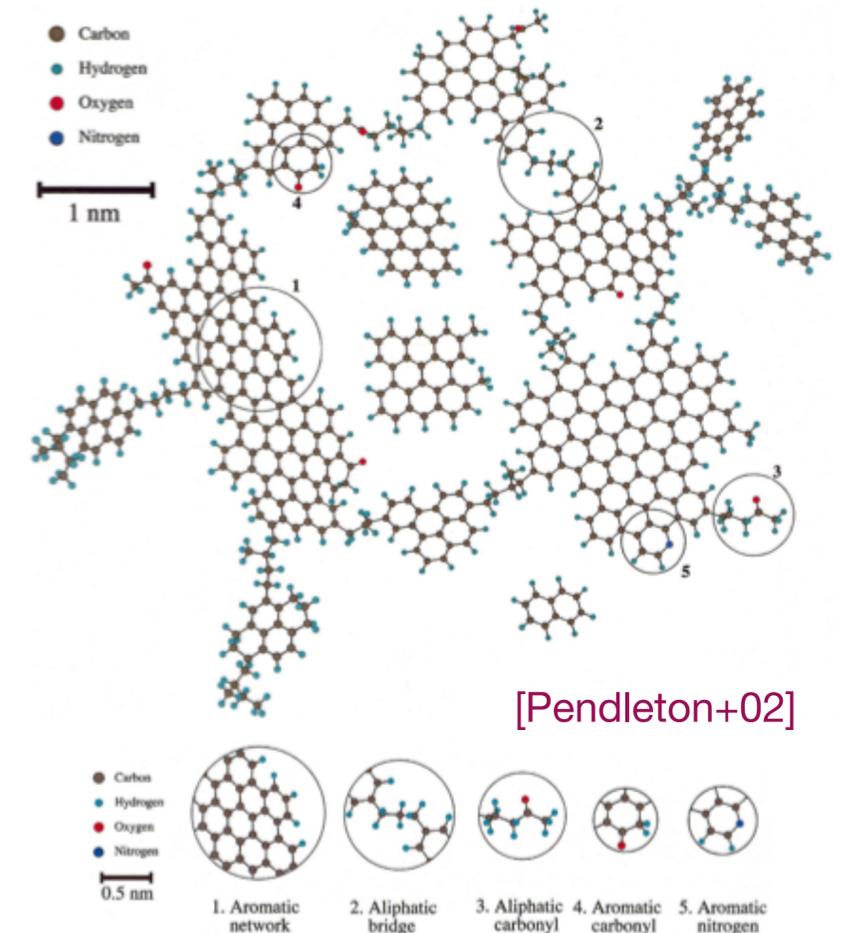
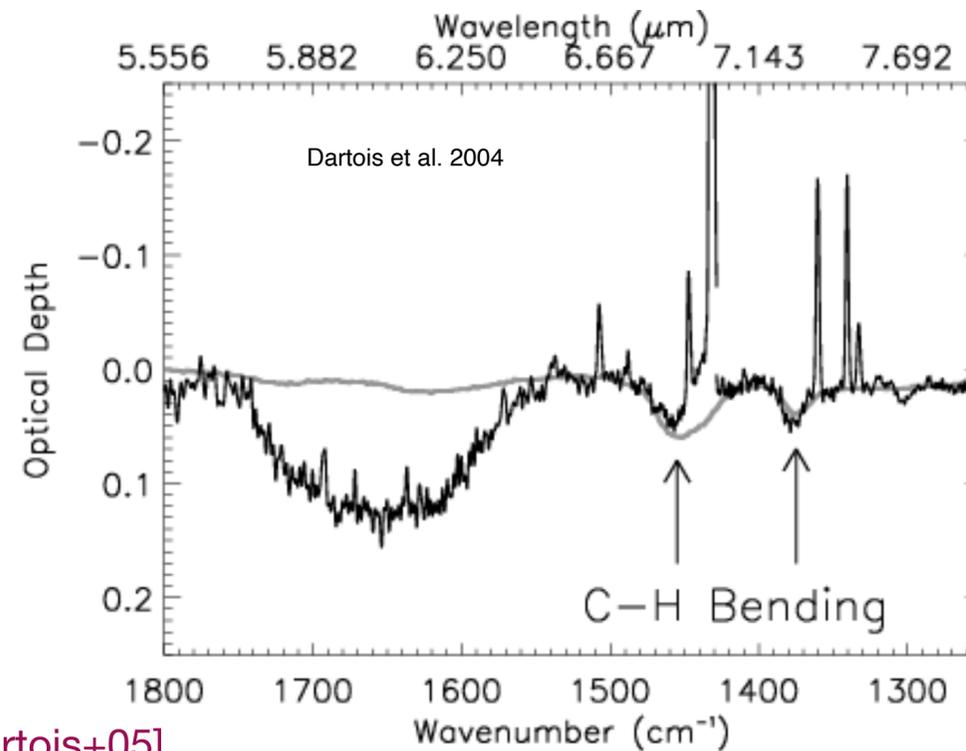
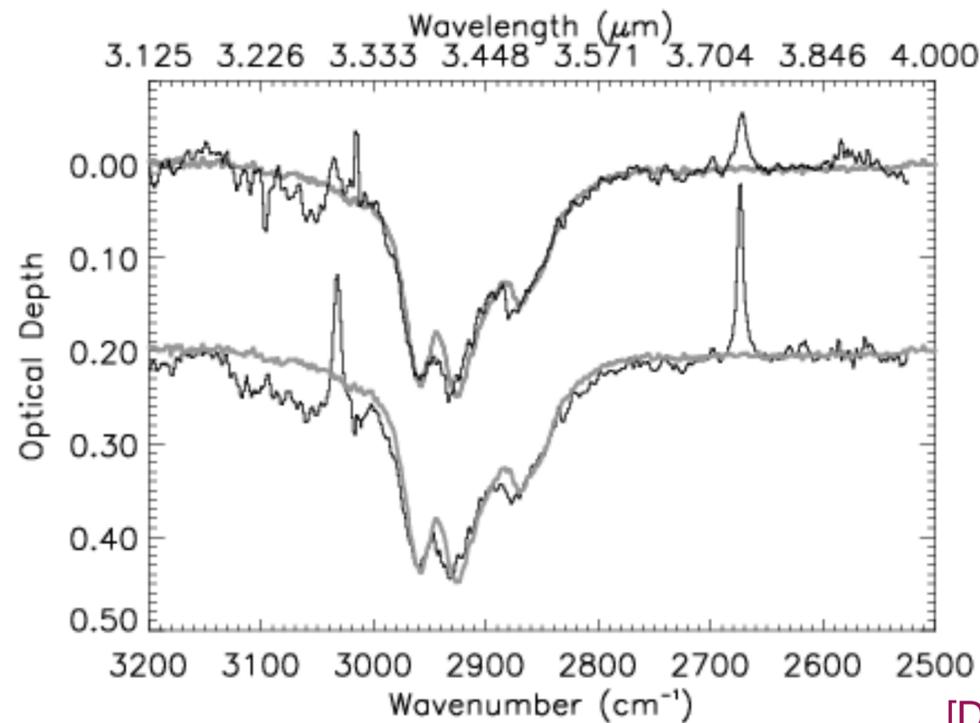


[See review from Tielens 2008]



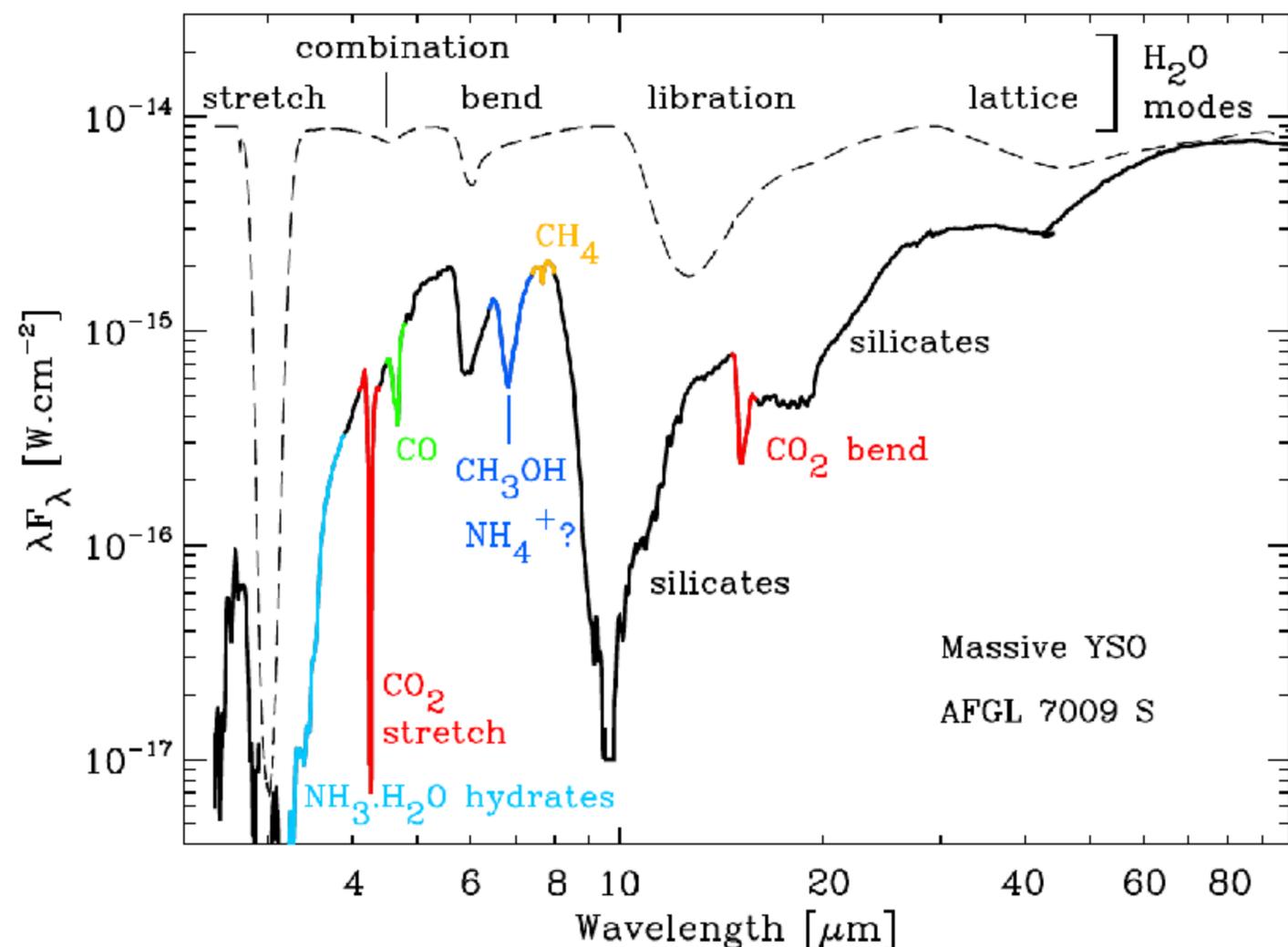
Aliphatic carbon-rich dust: hydrogenated amorphous carbon

- **Hydrogenated amorphous carbon (HAC or a-C:H) :**
 - In absorption in sightlines with sufficient N_H
 - 3.38, 3.42, 6.85 et 7.25 μm features : stretching and bending of C-H bonds in CH_2 and CH_3 groups
 - ratio aliphatic/ aromatic variable:
 - < 15 % aromatic in [Dartois+04](#)
 - ~ 85 % aromatic in [Pendleton+02](#)



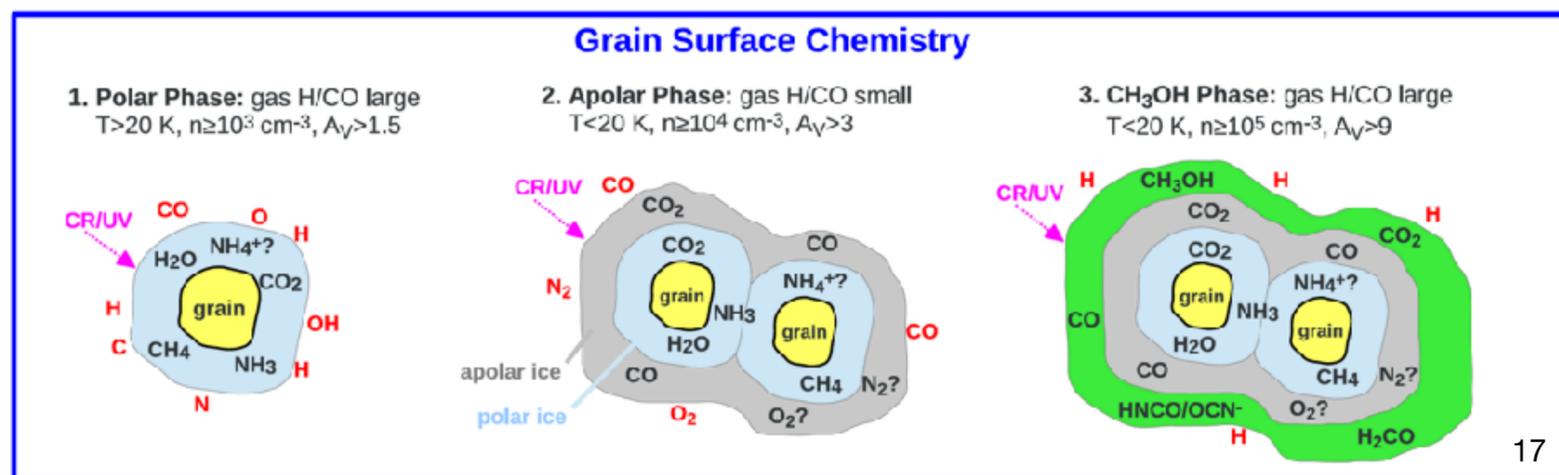
Volatile dust: ices

[Dartois +1998 in Boogert 2015]



- Ices mantles form at $A_v \approx 2-3$
- Dense clouds
- Protostars of all masses
- Circumstellar shells of OH/IR stars and some AGB
- Elemental budget => grain mantle of 5-10 nm
- Main species: H₂O, CO, CO₂, CH₃OH, NH₃, CH₄
- Others likely species: H₂CO, OCN⁻, OCS, HCOOH, CH₃CH₂OH, HCOO⁻, CH₃CHO, NH₄⁺, SO₂, PAH

H ₂ O	100
CO	7-25
CO ₂	15-28
CH ₃ OH	6-9
NH ₃	3-10
CH ₄	1-11



[See review from Boogert+2015]

Dust properties: size distribution

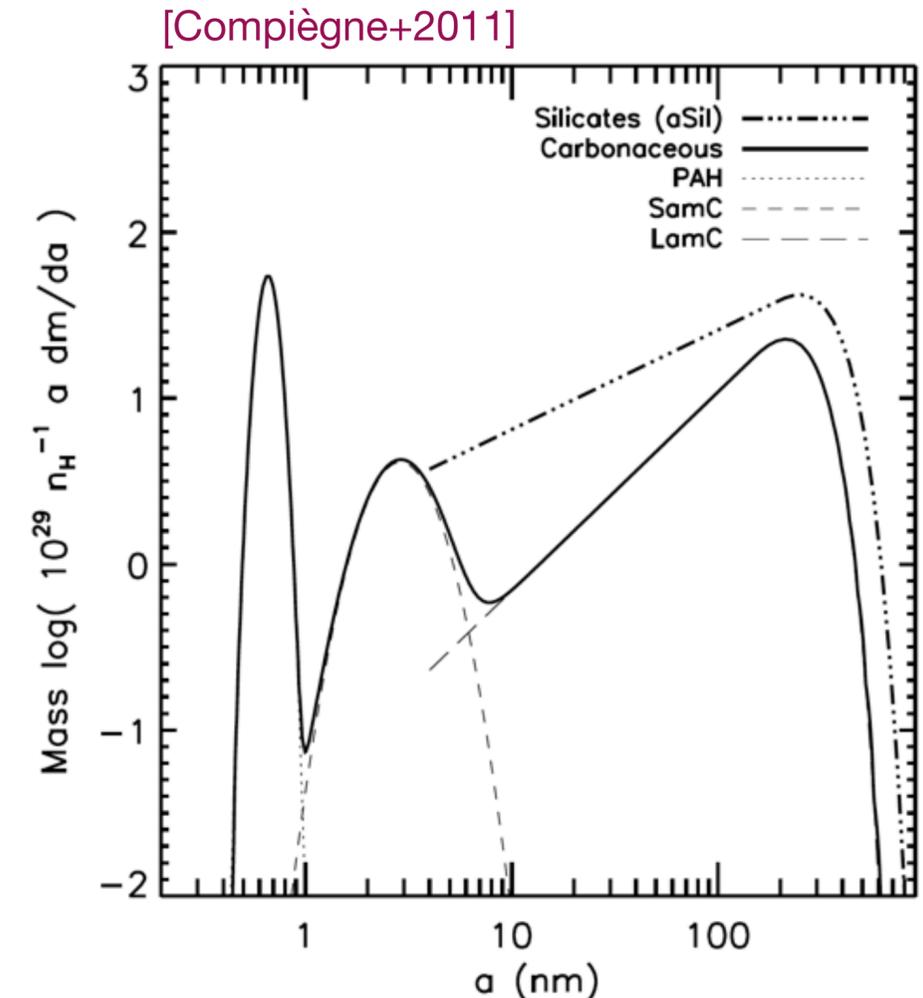
- Constrained by the extinction curve and depletion measurements
- The most used is the MRN size distribution (for spherical grains silicate and graphite grains): [Mathis, Rumpl, Nordsieck, 1977]

$$N(a) \propto a^{-\beta_s} \quad \text{with} \quad a_{\min} = 5 \text{ nm}, a_{\max} \sim 250 \text{ nm} \\ \beta_s \sim 3.3 - 3.6$$

- Many updated versions of the MRN size distribution exist, in particular to include the PAH grain population [see dust models from Compiègne +11, Weingartner & Draine 2001].
- Log-normal grain size distributions are also proposed for large grains [see the THEMIS dust model Jones et al. 2013]

⇒ the dust mass is in big grains

⇒ the dust surface is provided by small grains



Observational constraints & dust properties: summary

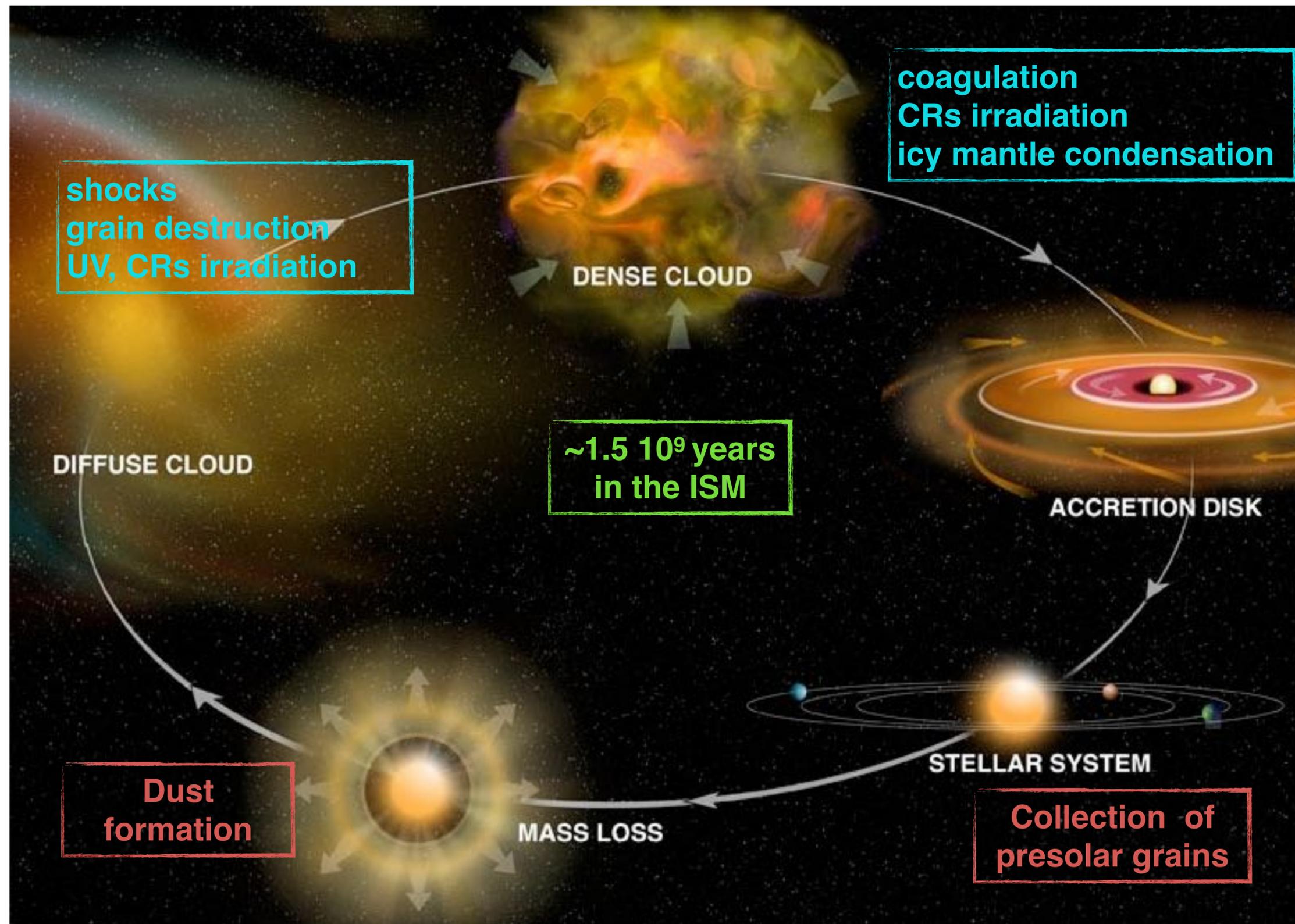
- Observational constraints : depletion, extinction, emission, scattered light, polarisation from X-ray to mm
- Spectroscopic observations provide information on the dust composition and structure
- Additional considerations/constraints should/could guide us:
 - the analysis of presolar grains
 - the dust formation processes
- Several components of dust exist: silicates, carbonaceous grains, ices, PAHs
 - Other minor dust components: oxydes (eg. Al_2O_3 , TiO_2), SiC, TiC?, MgS?, carbonates?
- Distribution of size: from ~ 0.5 nm to up to ~ 0.5 μm in the ISM
- Grains are not spherical and are partially aligned
- Silicates represent $\sim 75\%$ in mass, carbonaceous dust $\sim 25\%$
- Grains evolve in the ISM

Dust evolution

Dust evolution

- **Grain-grain collisions:**
 - At low velocity ($1-2 \text{ km.s}^{-1}$) \rightarrow coagulation
 - At intermediate velocity ($\sim 20 \text{ km.s}^{-1}$) \rightarrow fragmentation
 - At high velocity ($> 20 \text{ km.s}^{-1}$) \rightarrow sputtering & vaporisation
- **Gas-grain reactions:**
 - Grain growth: condensation of molecules on the dust surface
 - Erosion by the hot gas
- **Interaction with photons (UV, X...)**
 - Chemistry on grain surface and within icy mantles
 - Influence the ionisation and stability of PAHs and nano a-C(:H) grains
- **Interaction with cosmic rays (CRs)**
 - Chemistry within icy mantles
 - Changes of the grain structure (amorphization)

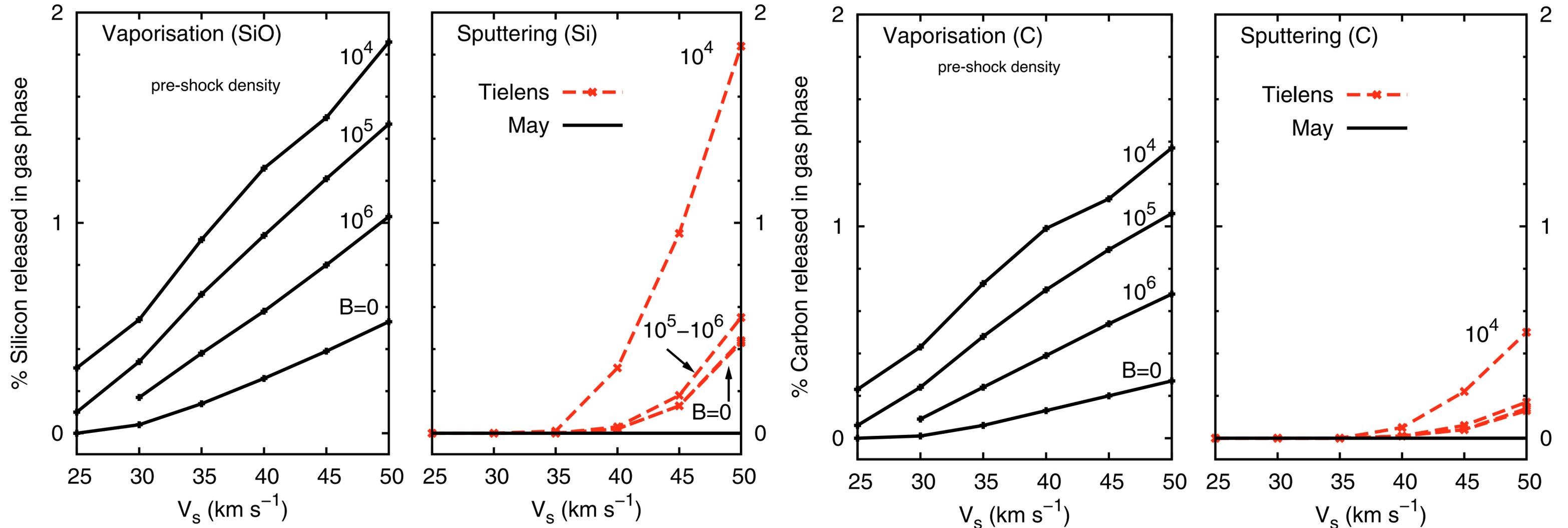
Dust evolution along the ISM life cycle



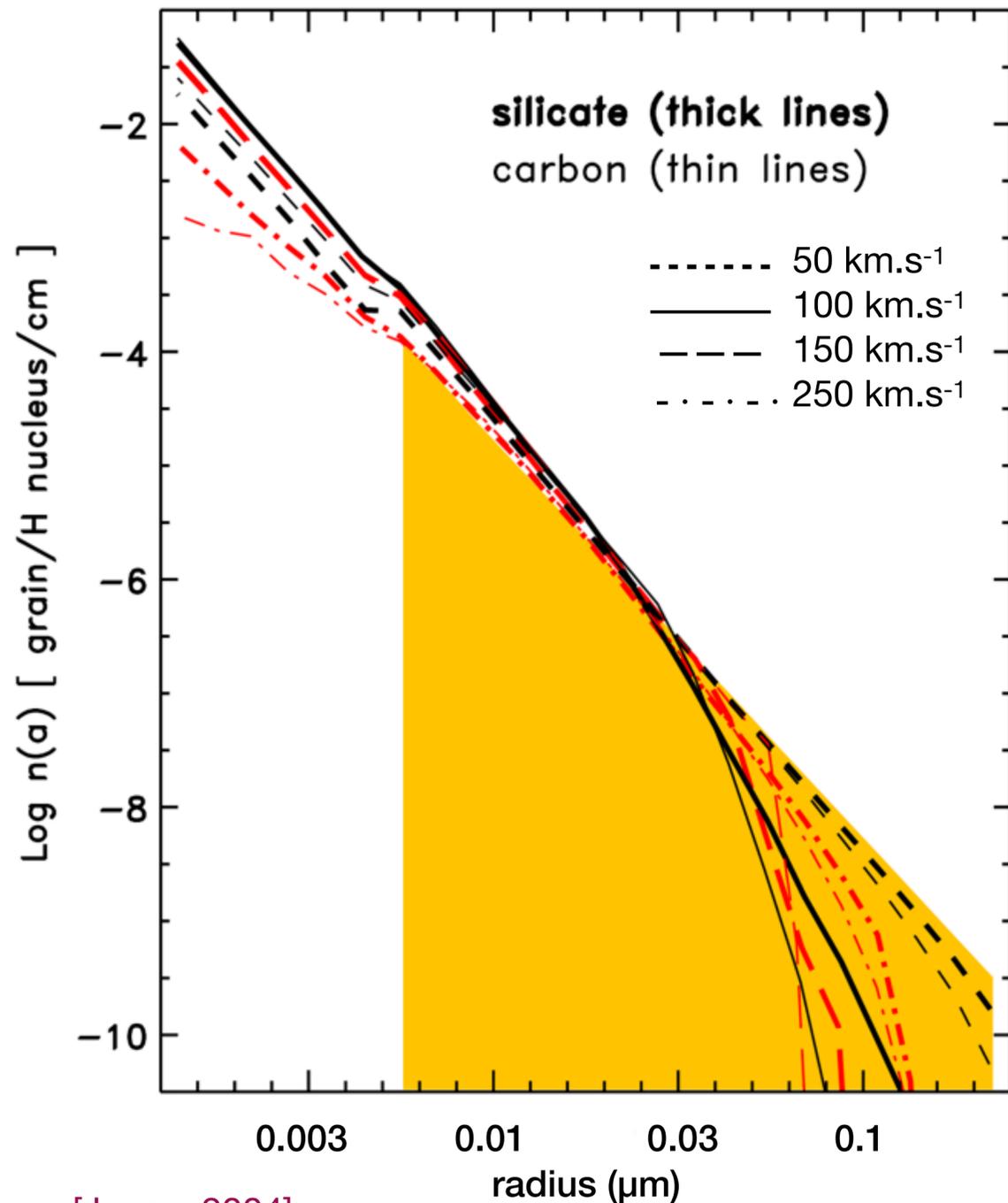
Dust evolution in shocks

- **Gas phase enrichment** with the elements and molecules constituting the grains, both volatile and refractory:
 - vaporisation (complete grain destruction)
 - sputtering (partial destruction)

See Guillet et al. « Shocks in dense clouds I, II, II (2007, 2009, 2011)

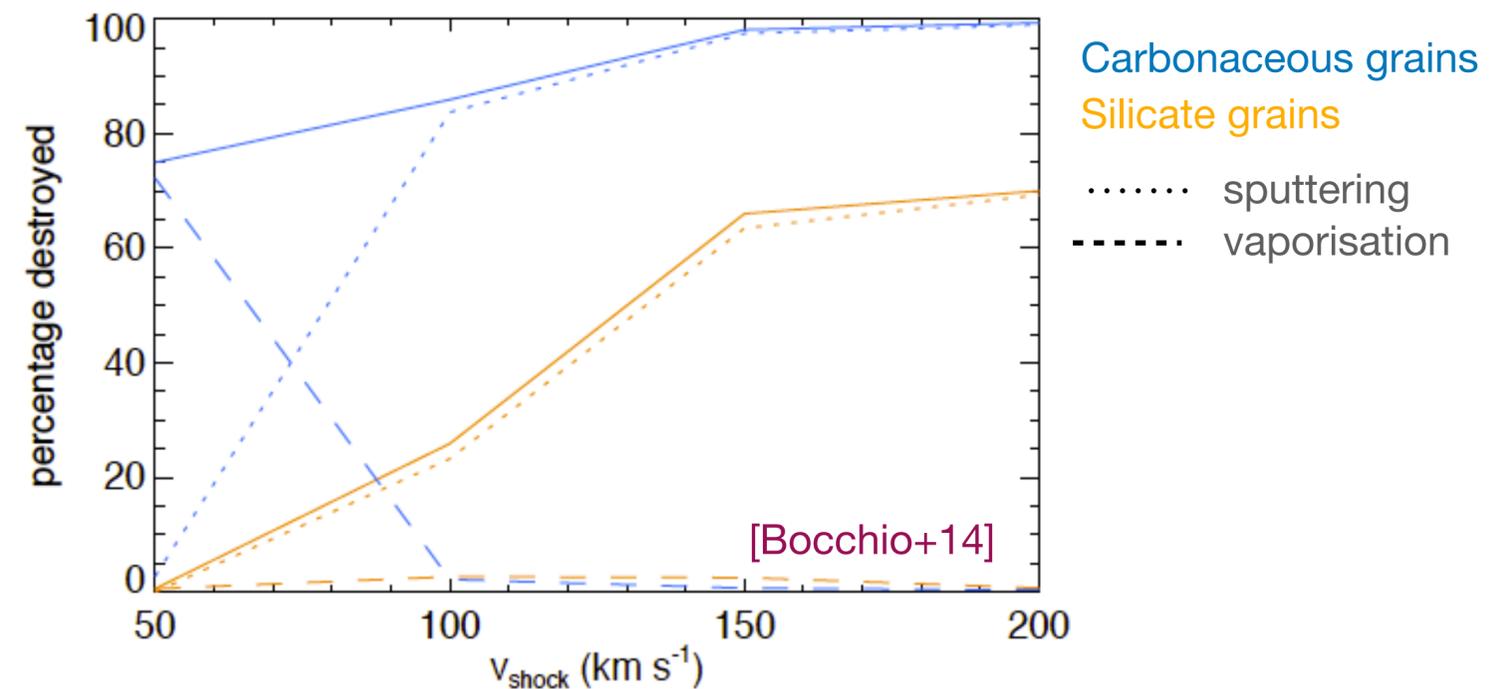


Dust evolution in shocks



[Jones, 2004]

- **Grain size distribution changes:**
- **Fragmentation:**
 - diminution of the number of big grains increase of smalls grains, M_{dust} is constant
 - more important at high density
- **Sputtering:**
 - decrease of grain size and M_{dust}
- **Grain destruction :**

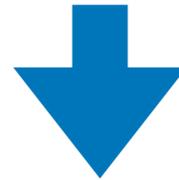


[Bocchio+14]

Dust lifetime

- Grain residence time in the ISM before incorporation in new stars: ~ 1.5 Gyr
- Grain life time against destruction by high velocity (SN) shocks: ~ 0.5 Gyr
- Hydrodynamical models of Giant Molecular Clouds + elemental depletion constraints

[see eg. Jones & Nuth 2011, Bocchio+14, Slavin+15, Zukhoska+2016,2018, Dwek+15,...]



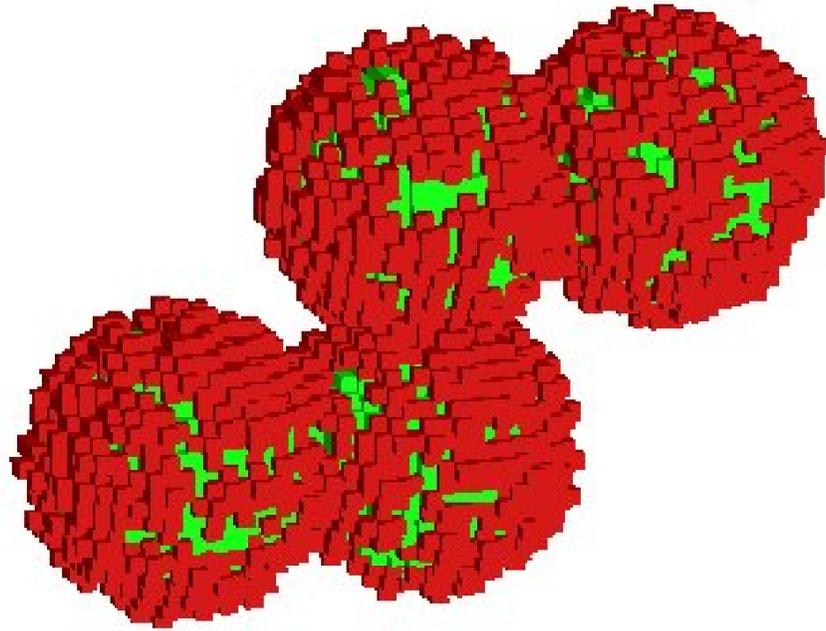
- Most cosmic dust grains are destroyed in the ISM before being incorporated into new stars



- Grains must be formed *in situ* in the ISM
- The proportion of the dust that is formed in the ISM depends on many parameters which are not well constrained
 - Need more observational constraints, more modelling
 - Need experiments on dust growth on the cold surface of grains [Rouillé+2020]

Dust coagulation in dense clouds

- In dense environments: cold clouds, pre-stellar cores, protoplanetary disks



- The time for coagulation is rapid
 \Rightarrow grain have time to coagulate
 before cloud collapse and star
 formation (in $\sim 10^6$ - 10^7 years)

- Coagulation time for a mixture of grains : [Draine+85, Stepnik+03]

$$t_{coa} = \frac{1}{\sigma_{1/2} n_1 v_{1/2}}$$

n_1 : number density of grain 1

$v_{1/2}$: relative velocity between the two grains

$\sigma_{1/2}$: coagulation cross section: $\sigma_{1/2} = \pi \times (a_1 + a_2)^2$

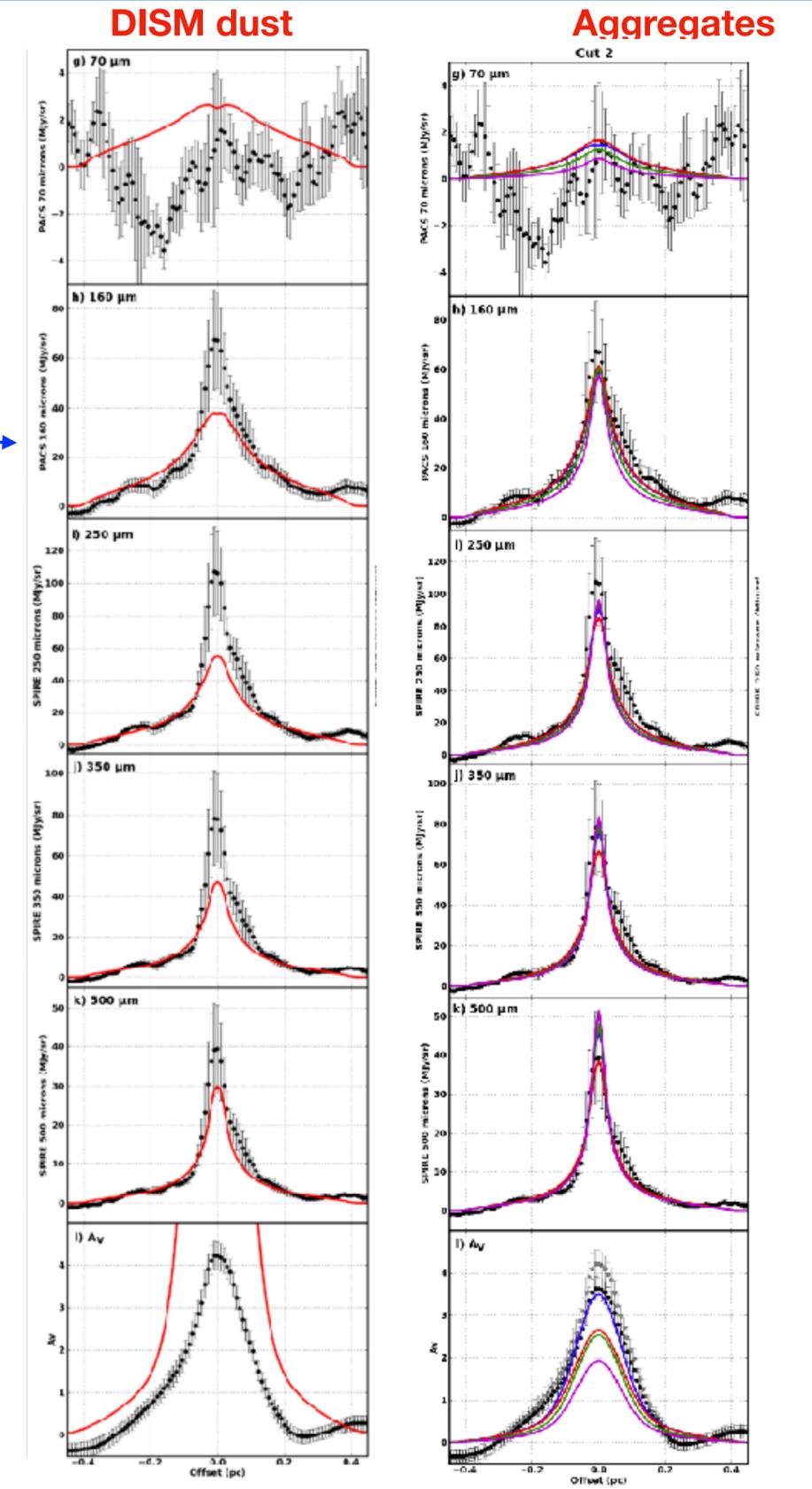
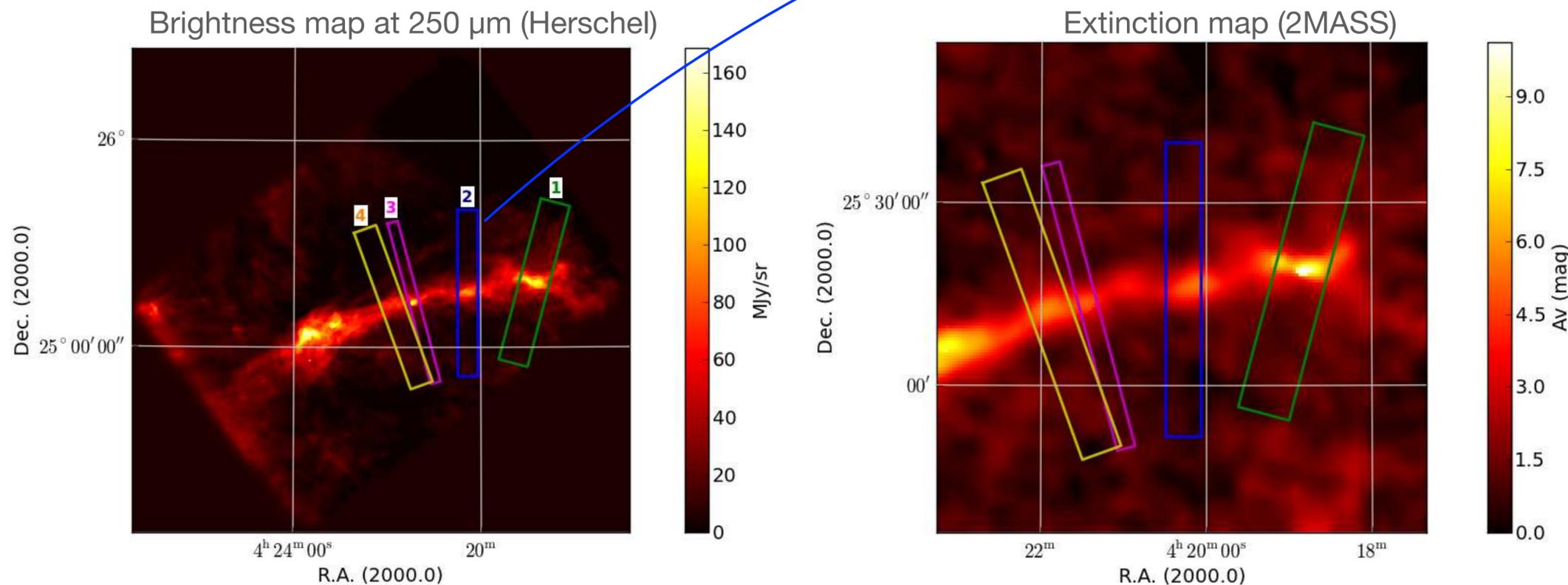
Molecular cloud with $n_H = 4 \times 10^3 \text{ cm}^{-3}$ and a relative velocity of 0.1 km/s

Type of coagulation	Coagulation time-scale [yr]	$n_g \text{ [cm}^{-3}\text{]}$
VSG on VSG	1.4×10^5	1.52×10^{-5}
VSG on BG	1.6×10^3	1.52×10^{-5}
BG (car) on BG	1.1×10^6	6.17×10^{-9}
BG (sil) on BG	4.3×10^5	1.60×10^{-8}

[Köhler+12]

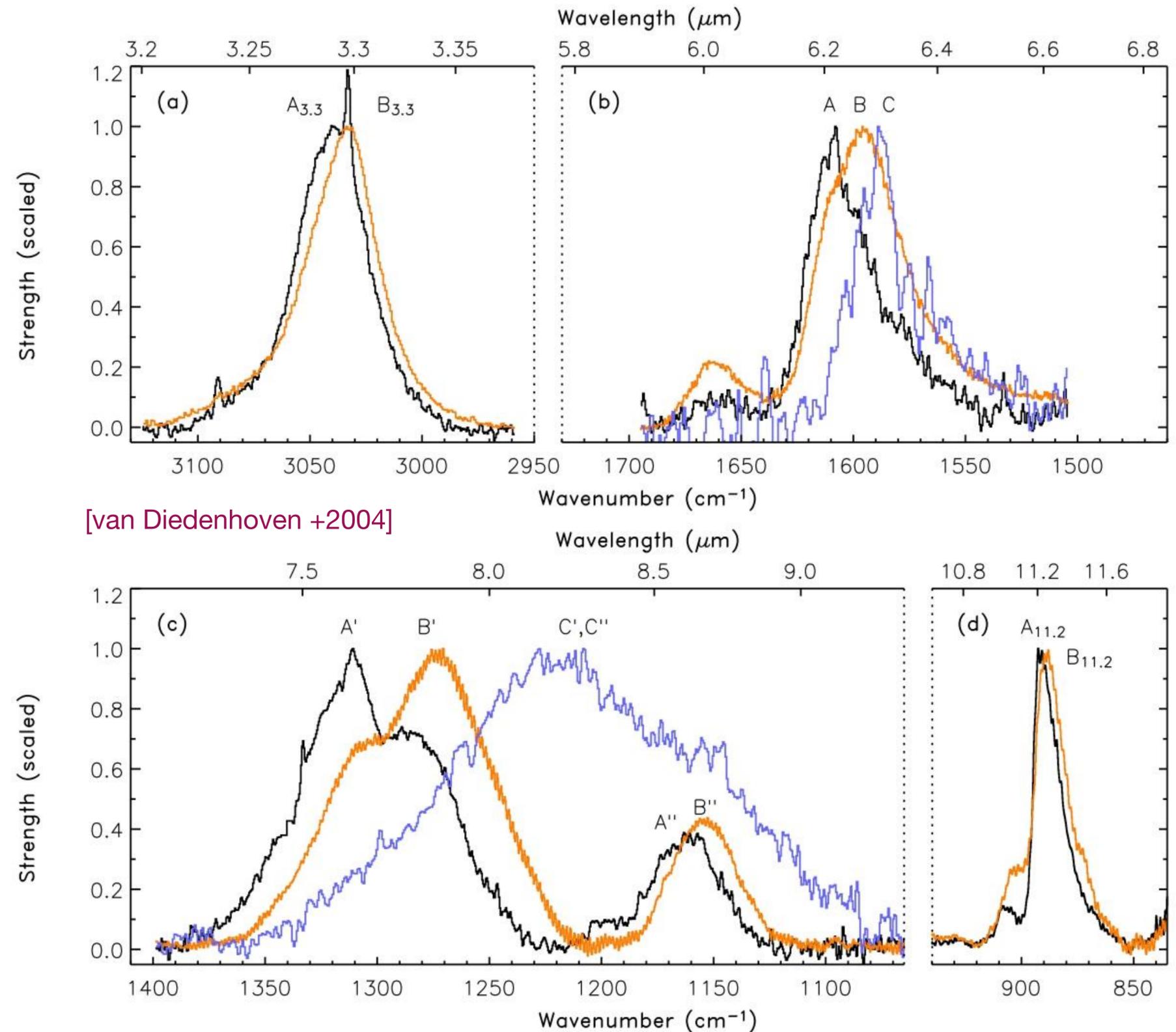
Dust coagulation in dense clouds

- Herschel map of the filament L1506 in the Taurus
- Modelling of the emission along several cuts across the filament
- Aggregates are needed to reproduced simultaneously the extinction and emission data
 - Dust opacity at 250 μm is raised by 1.8-2.2
 - Grain size increases by a factor 5



Evolution of carbon dust: the AIB

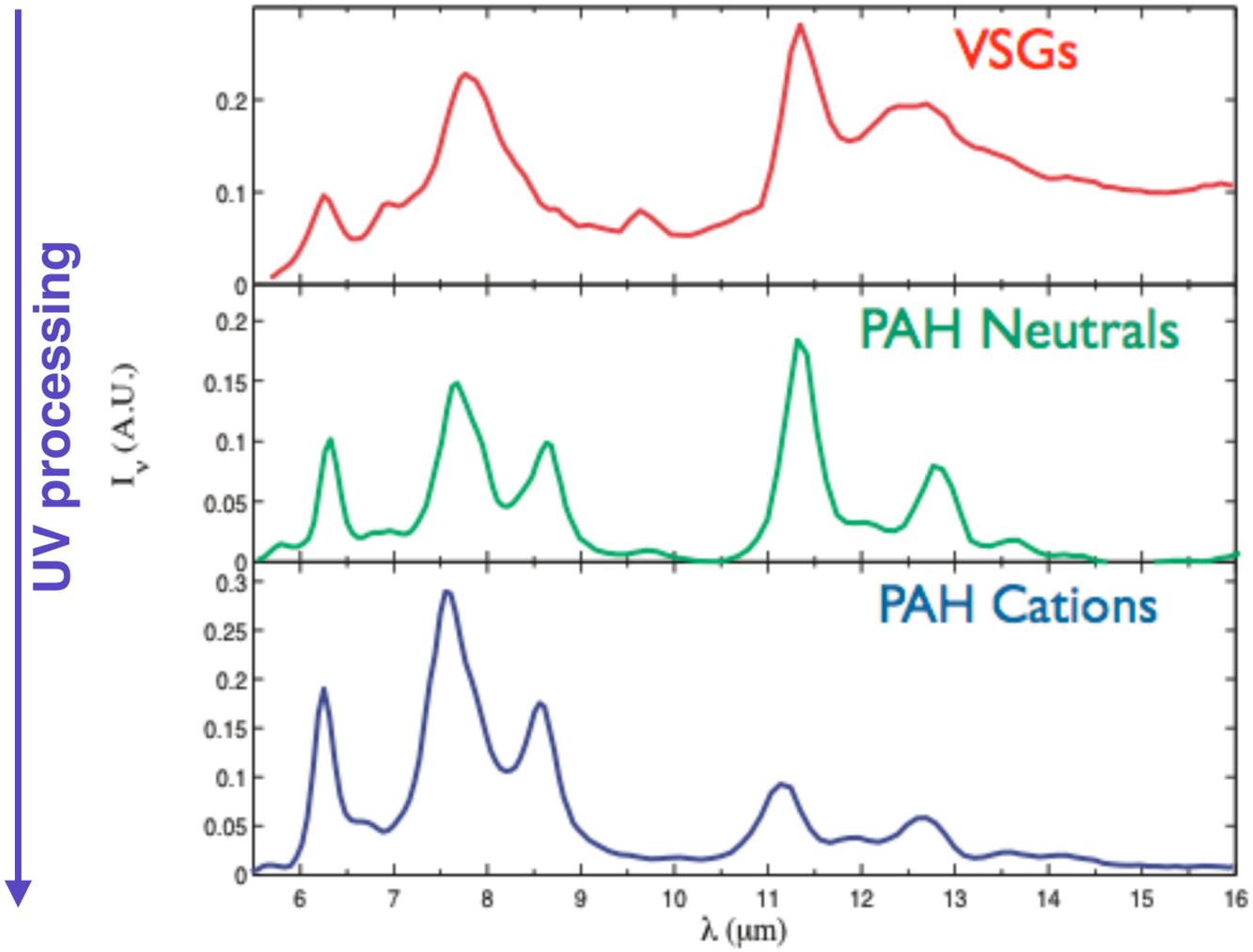
- A (the most common) : HII regions, Herbig AeBe stars, reflexion nebula, post-AGB stars, PPNs, extragalactic sources
- B: Some isolated Herbig AeBe stars, AGB stars, and PPNs
- C: Some post AGB stars and young PPNs
- The AIBs are sensitive to the radiation field → change of the ionisation state & size of the carriers
 - ⇒ band ratios are diagnostics of the physical conditions of environments and of its chemical evolution, see [Galliano+18]



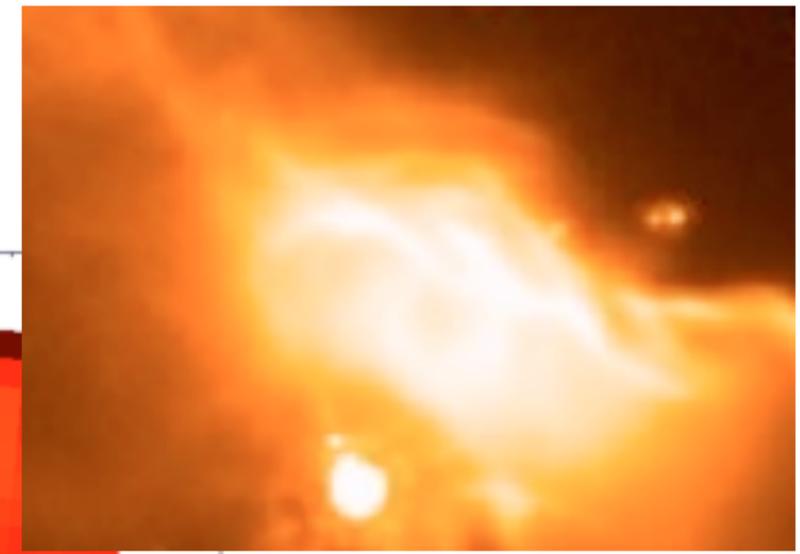
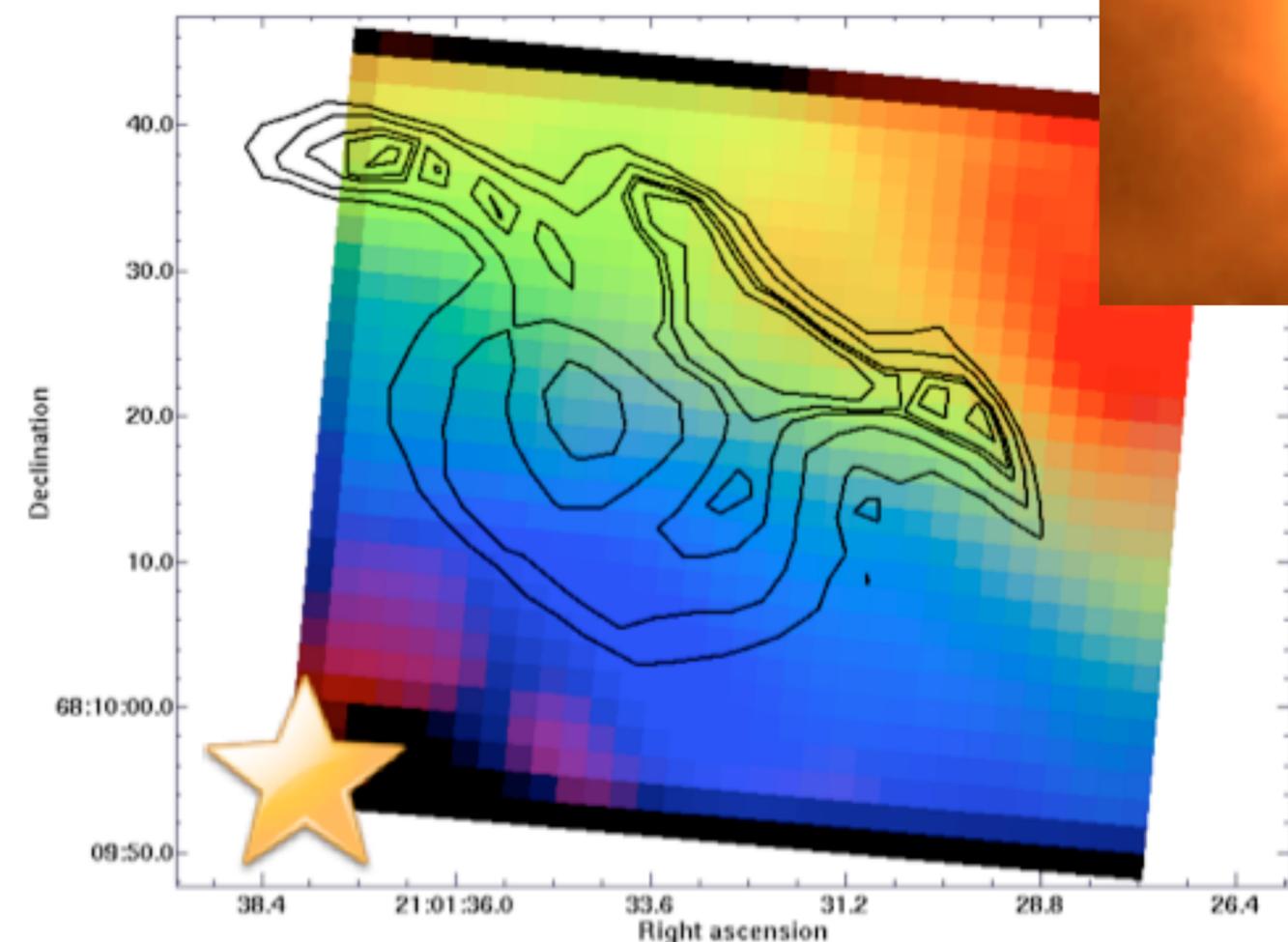
[van Dienenhoven +2004]

Evolution of PAHs

Extracted spectra [Berné +2007, 2010]



Spatial distribution



NGC 7023 reflexion nebulae (Spitzer)

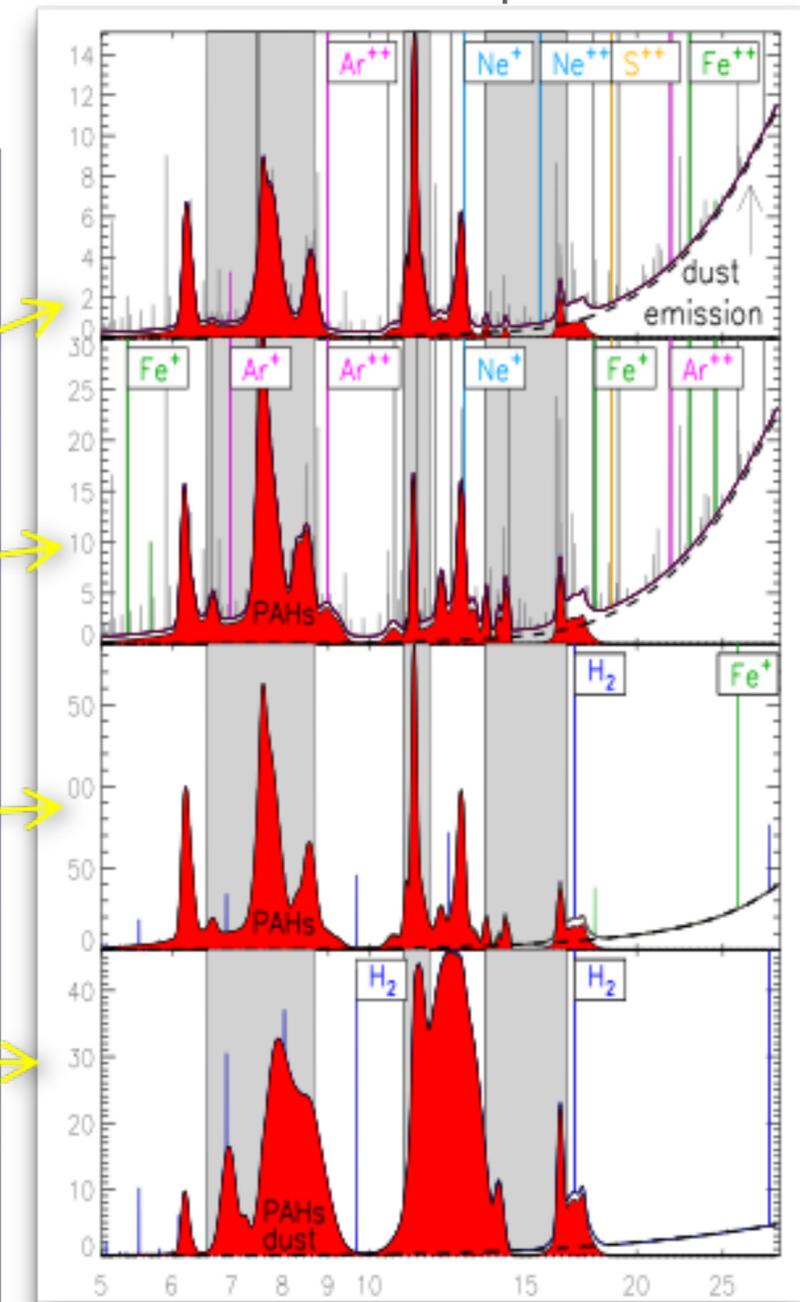
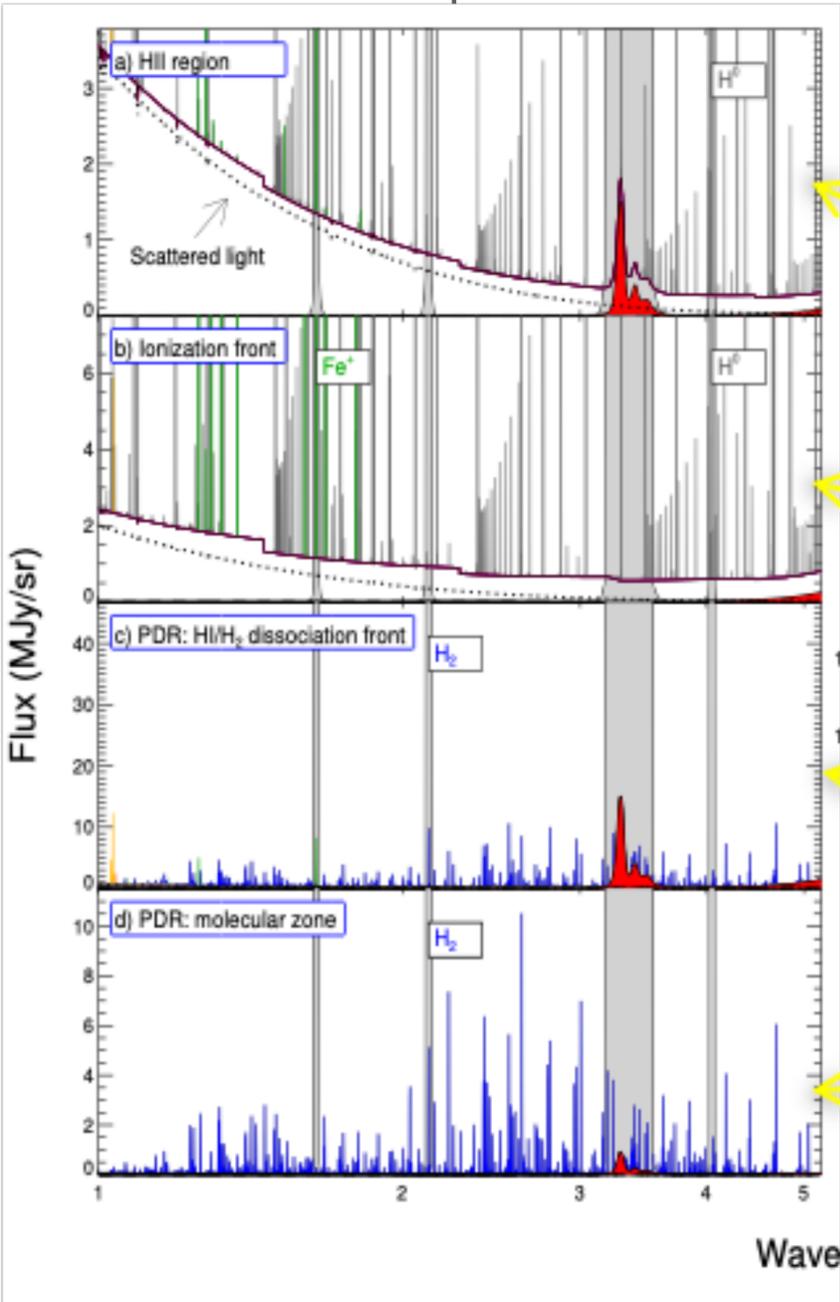
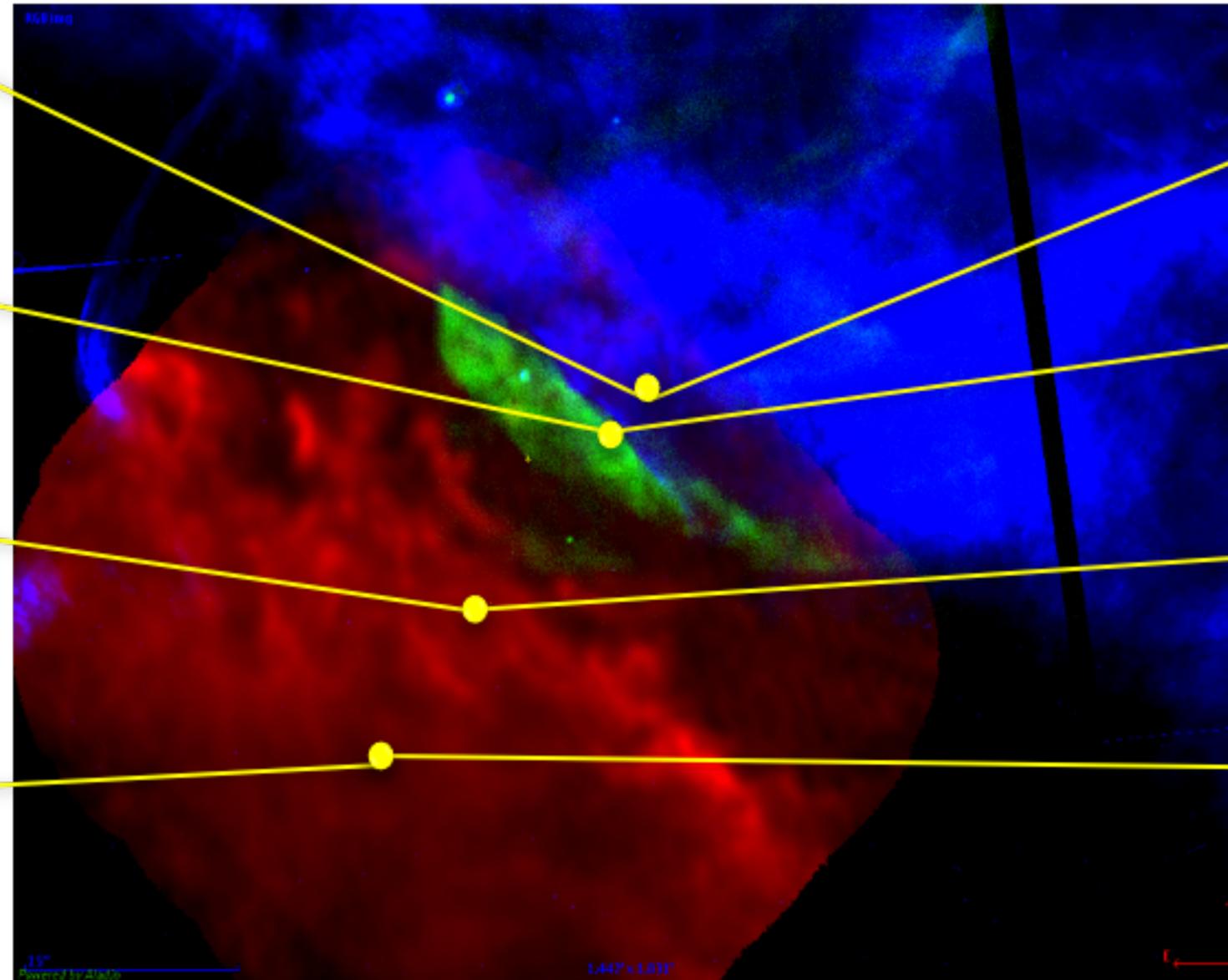
- High radiation field: photo-destruction of VSGs & production of PAHs, ionisation of PAHs
- Possible release of small hydrocarbons from PAHs destruction [Pety +2005]

Evolution of the AIBs

Predicted spectra

Predicted spectra

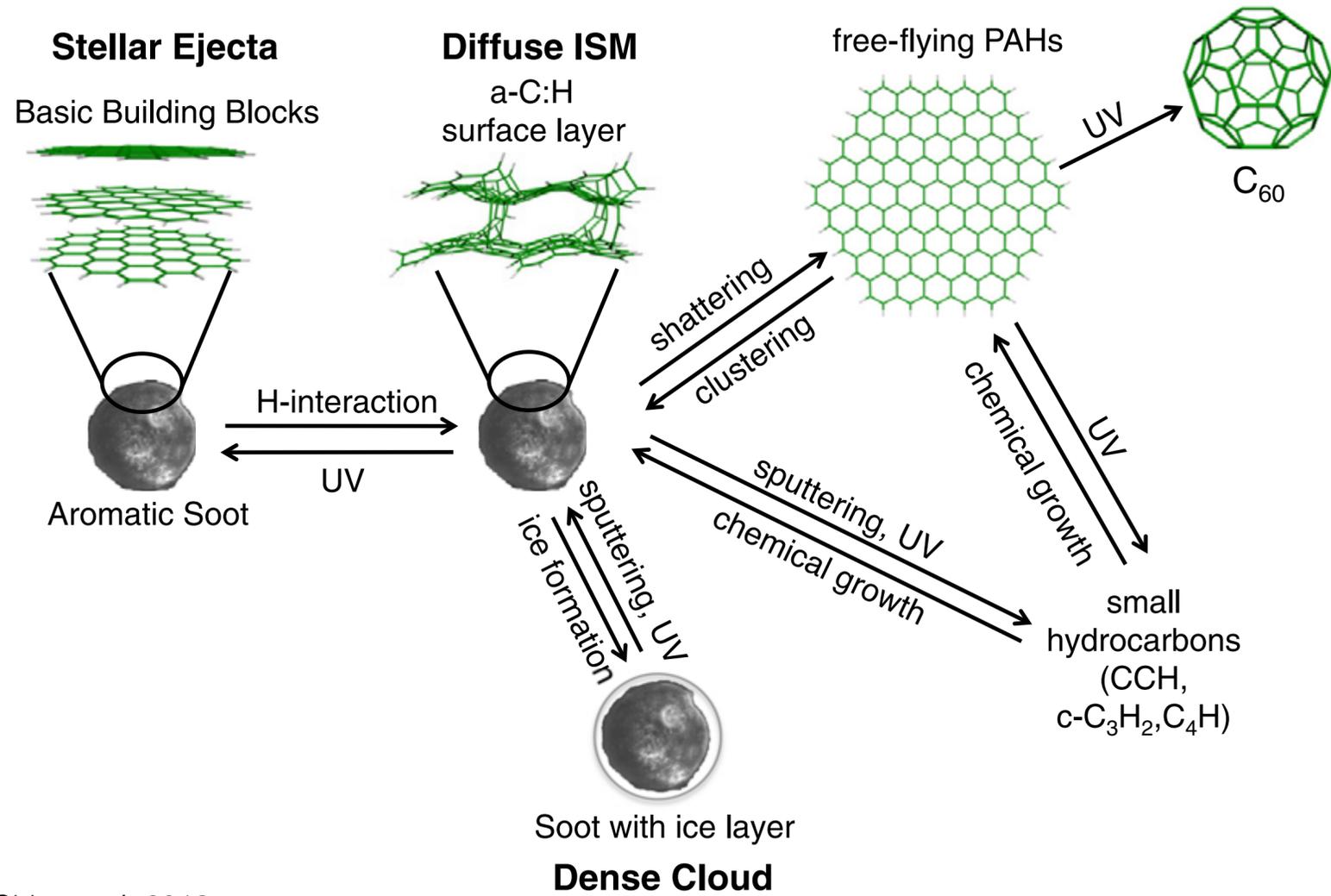
Orion Bar
Barre of Orion (HST, VLT/VISIR, ALMA)



Adapted from the JWST ERS project « Radiative feedback from massive stars as traced by multi band imaging and spectroscopic mosaics » PI O. Berné, E. Habart, E. Peters

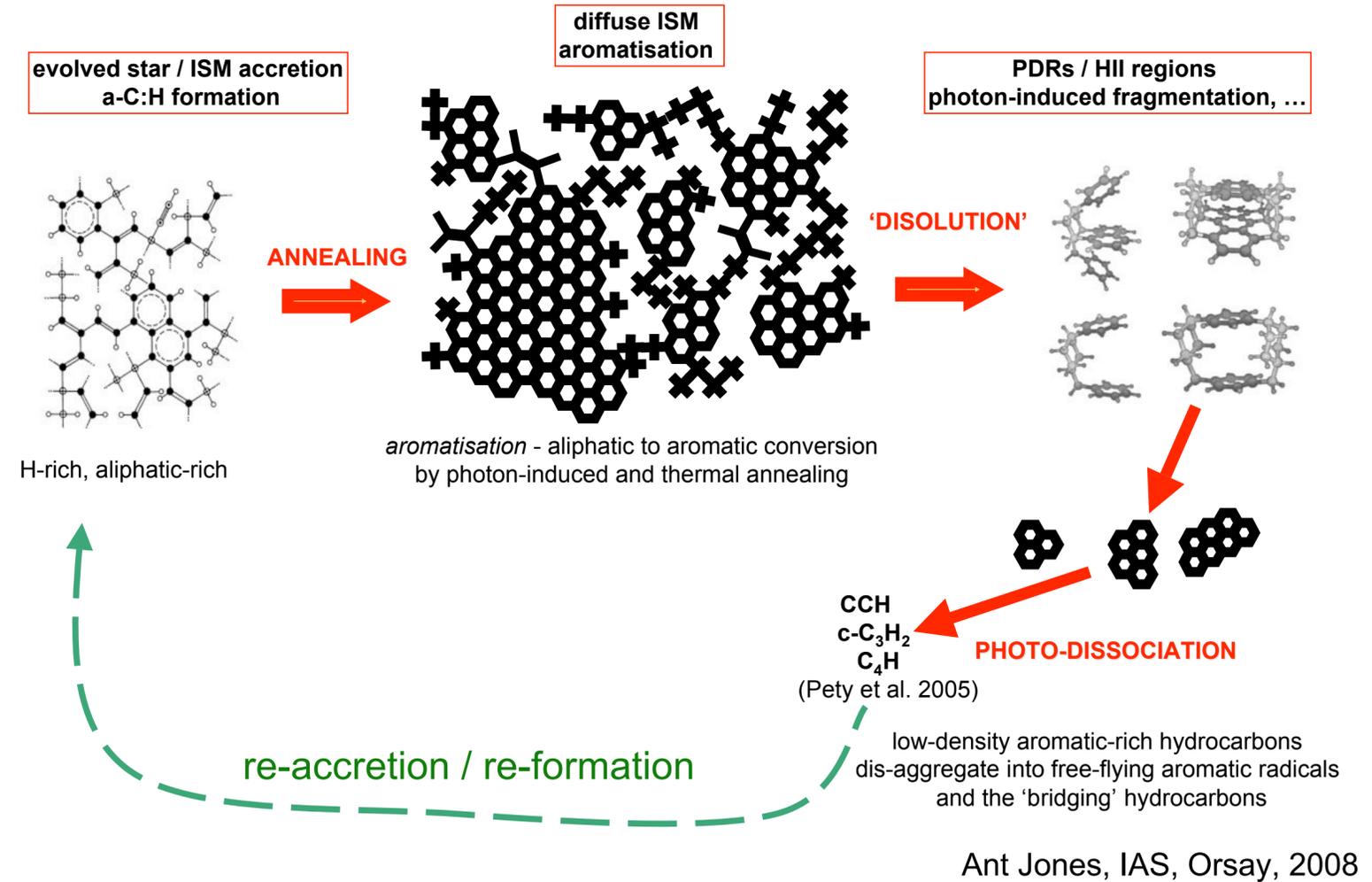
Evolution of hydrocarbon dust

The Lifecycle of Hydrocarbon Dust in the Interstellar Medium



Chiar et al. 2013

Hydrocarbon evolution through the ISM



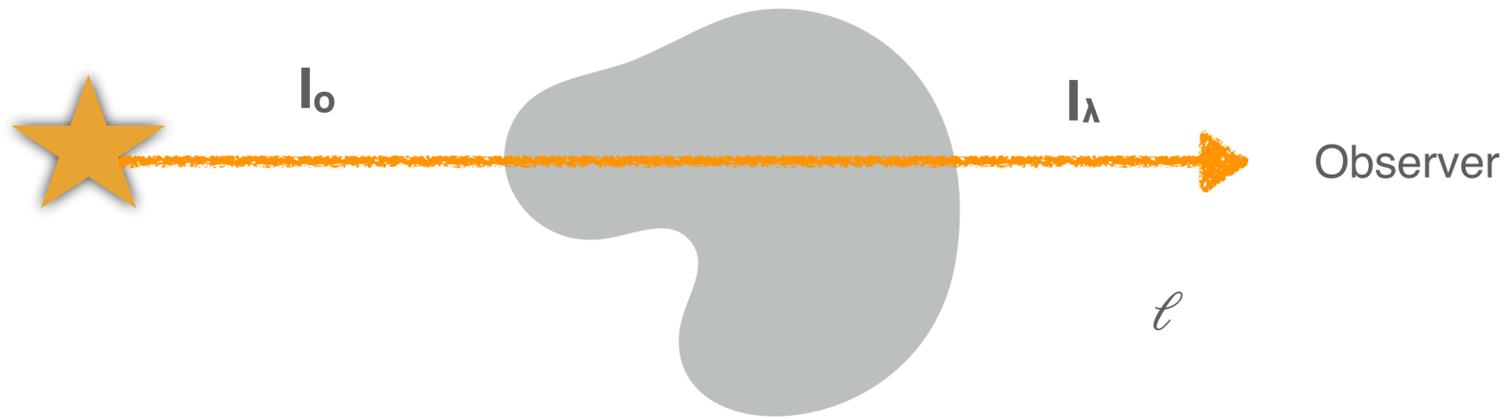
See also Goto+2003, Carpentier+2012

Dust evolution: summary

- Dust properties change along the life cycle of the ISM
- Grains are destroyed in shocks
 - the size distribution changes
 - the ISM is enriched in molecules and heavy elements
 - this suggests that dust grains must be formed also *in situ* the ISM
- In dense clouds, protostars and protoplanetary disks grains coagulate
 - the size distribution changes
 - a complex chemistry occurs on grain surfaces and in ice mantles
- This complexity is partly inherited by the new stellar systems
- Carbonaceous dust composition, structure and ionisation state changes with the interaction with UV photons as well as with the interaction with gas

Modelling dust extinction and emission

Modelling the extinction



$$I(\lambda) = I_0(\lambda) \times e^{-\tau(\lambda)}$$

$$\tau(\lambda) = \int k_{ext}(\lambda) dl$$

Extinction coefficient (cm⁻¹)

$$k_{ext} = C_{ext} \times n = (C_{abs} + C_{sca}) \times n$$

Extinction cross section (cm²)

$$Q_{ext} = \frac{C_{ext}}{\sigma_{gr}} = \frac{(C_{abs} + C_{sca})}{\sigma_{gr}}$$

Extinction efficiency

$$K_{ext} = \frac{C_{ext}}{V_{gr} \rho_{gr}}$$

Opacity or mass extinction coefficient (cm². g⁻¹)

n : number density of dust (cm⁻³)
 N : column density of dust (cm⁻²)
 σ_{gr} : geometrical cross section of the grains (cm²)

$$\tau(\lambda) = l k_{ext} = N C_{ext} = \sigma_{gr} N Q_{ext}$$

$k_{ext}, C_{ext}, Q_{ext}, K_{ext}$ contains the information on the dust properties

Modelling the extinction

- To calculate the absorption, scattering, emission and polarisation cross sections of the grains for each grain population, one needs to understand the interaction of small particles with the electromagnetic radiation
- This interaction is specified by the dielectric function ϵ or optical constants m of the grain material:

$$\epsilon = \epsilon_1 + i\epsilon_2$$

$$m = \underbrace{n}_{\text{refraction index}} + i \underbrace{k}_{\text{extinction coefficient}} = \sqrt{\epsilon}$$

- Need to solve Maxwell's equations with appropriate boundary at the grain surface
- Solution first formulated by Mie in 1908 for spherical grains [See books from Bohren & Huffman (1988) or Van de Hulst (1958)]

Grains smaller than the wavelength

- Electric dipole limit (**Rayleigh limit**) : when the particle size a is $\ll \lambda$, it experiences an EM field nearly uniform. Then :

$$C_{abs} = \frac{4\pi\omega}{c} \text{Im}(\alpha) \quad C_{sca} = \frac{8\pi\omega^4}{3c^4} |\alpha|^2$$

where α is the electric polarisability of the grains, the electric dipole moment $P = \alpha E$

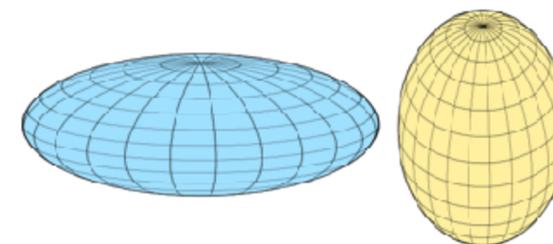
- The polarisability has a simple analytical expression for spheres, spheroids and ellipsoids:

$$\alpha_j = \frac{V}{4\pi} \left[\frac{\epsilon - 1}{(\epsilon - 1)L_j} + 1 \right] \quad \text{where } L_j \text{ is the shape factor, } L_1 + L_2 + L_3 = 1$$

- **For a spherical grain ($L_i = 1/3$) small compared to the wavelength :**

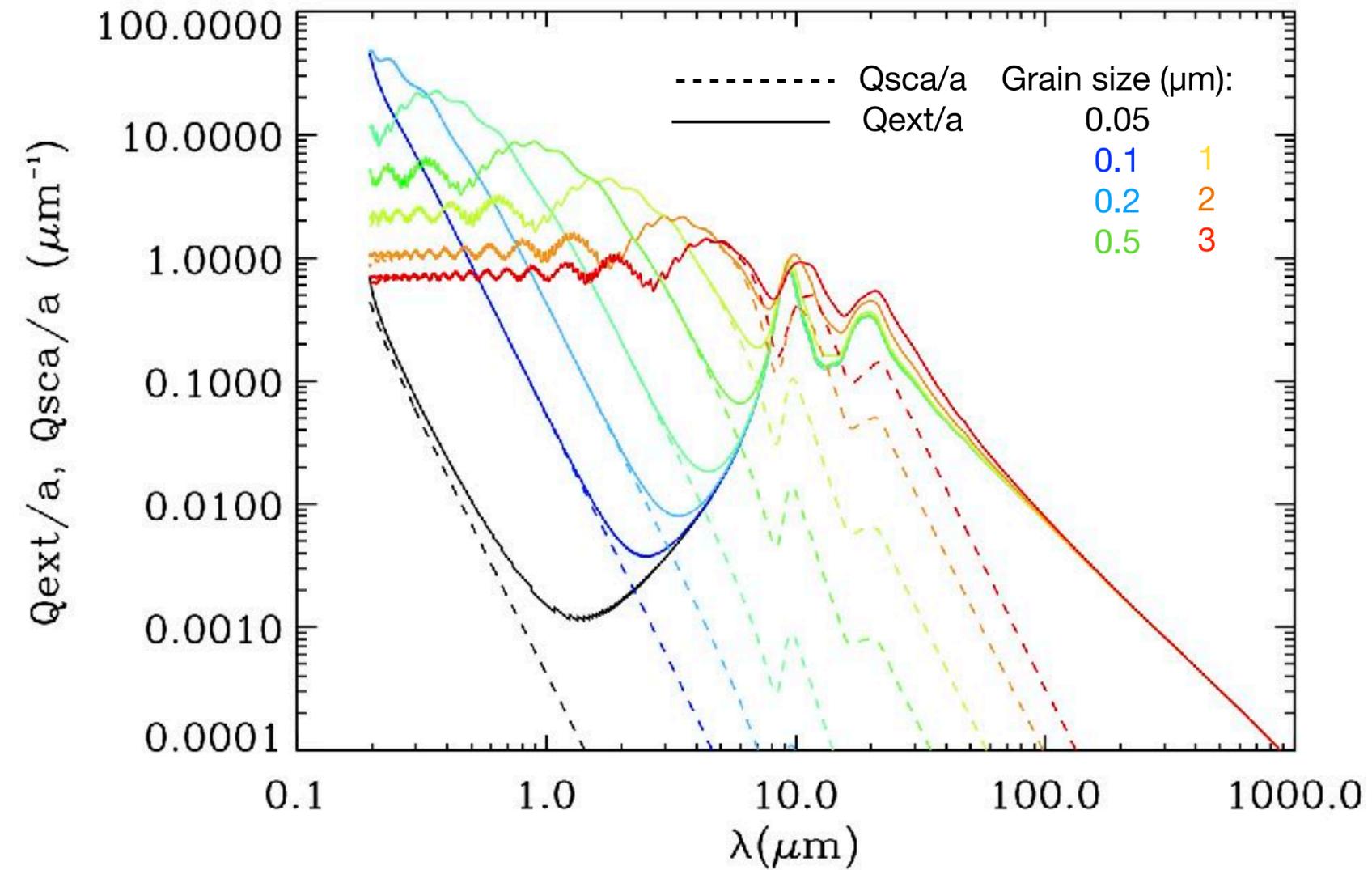
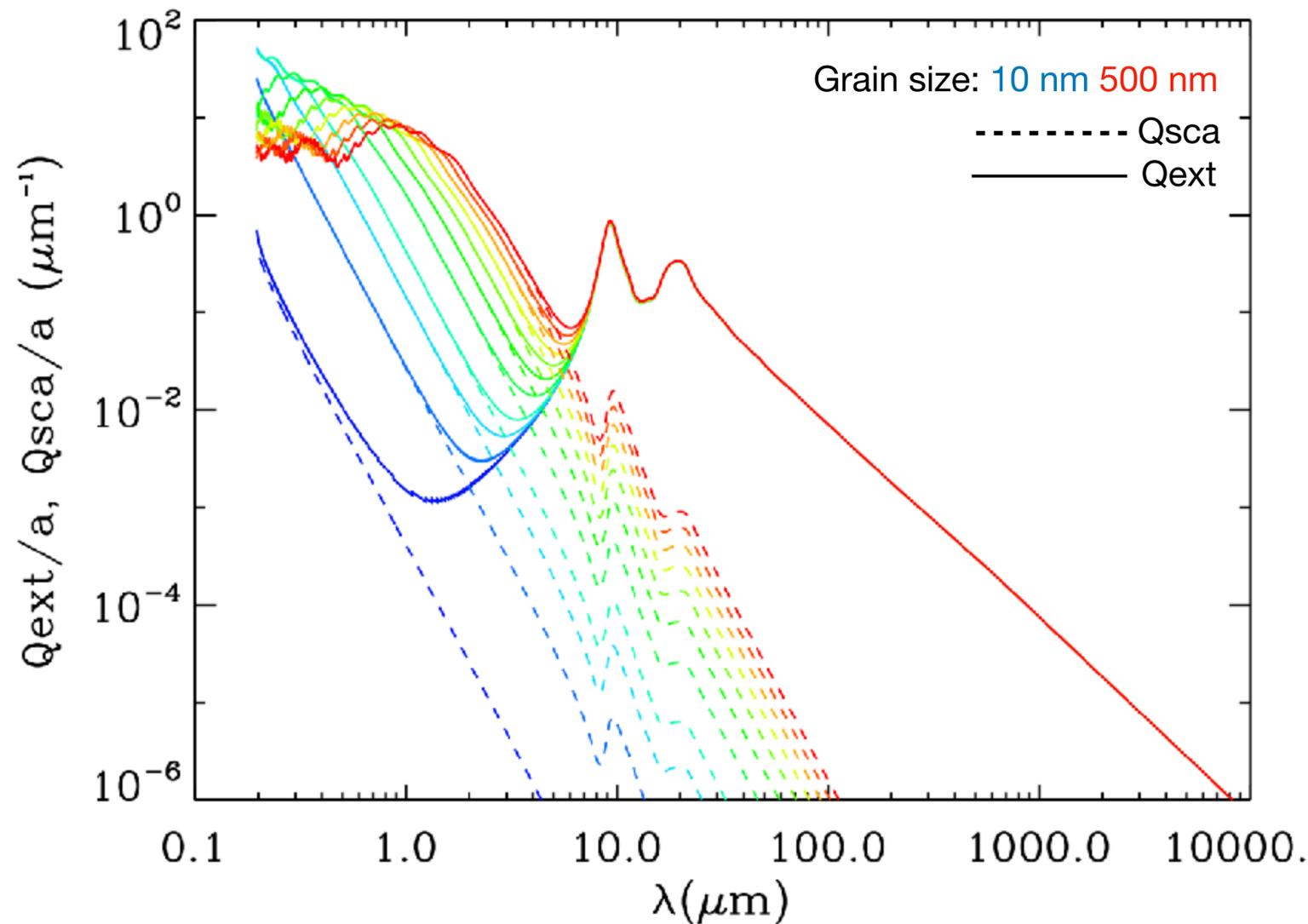
$$C_{abs} = \frac{18\pi V}{\lambda} \frac{\epsilon_2}{(\epsilon_1 + 2)^2 + \epsilon_2^2} \quad C_{sca} = \frac{24\pi^3 V^2}{\lambda^4} \left| \frac{\epsilon - 1}{\epsilon + 2} \right|^2$$

- **Reasonably simple expression also exists for spheroids**



Extinction as a function of size: spherical grains

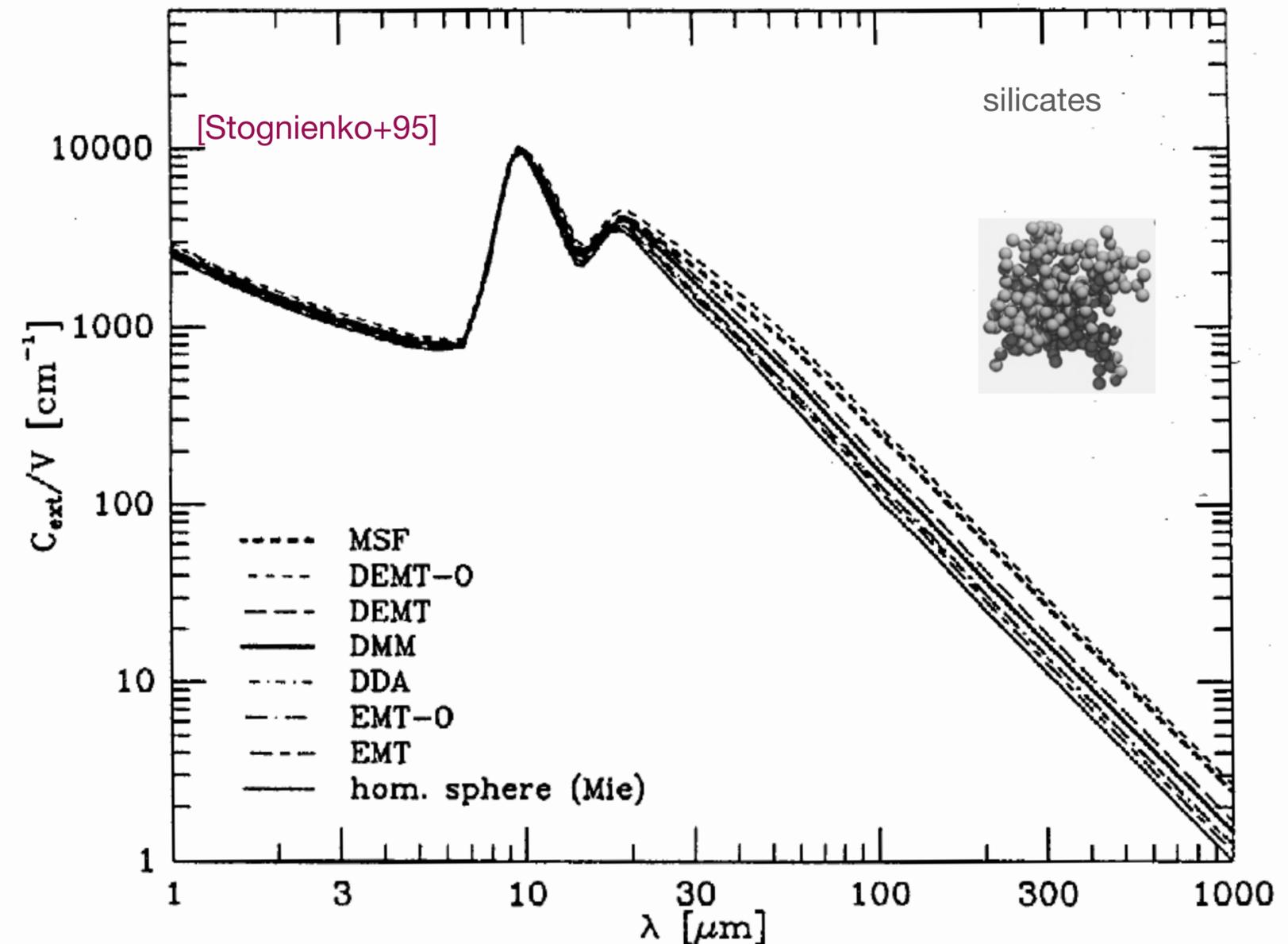
- When the **particle size $a \approx \lambda$** , we have to use different methods to calculate C_{abs} and C_{sca}
- If the particles are **spherical** we can use **Mie Theory** (many public codes exist)



- for $a \ll \lambda$, the absorption and scattering properties do *not* depend on the dust size
- for $a \approx \lambda$ the absorption and scattering properties depend on the grain size

Extinction cross section of aggregates

- If the particles are not spherical or if grains are aggregated, calculation are more complicated. Different methods are used such as **DDA** [Draine & Flatau 2010], **T-Matrix** [Mischenko+1996]. Some codes are public.
- Complex dust grains in term of composition and structure can be treated with **effective medium theories (EMTs)**:
 - core-mantle grains
 - composite grains with inclusions
 - aggregates of grains of different compositions (approached method)
 - [see eg. Min+2008]
- *Each theory has its own limitations*



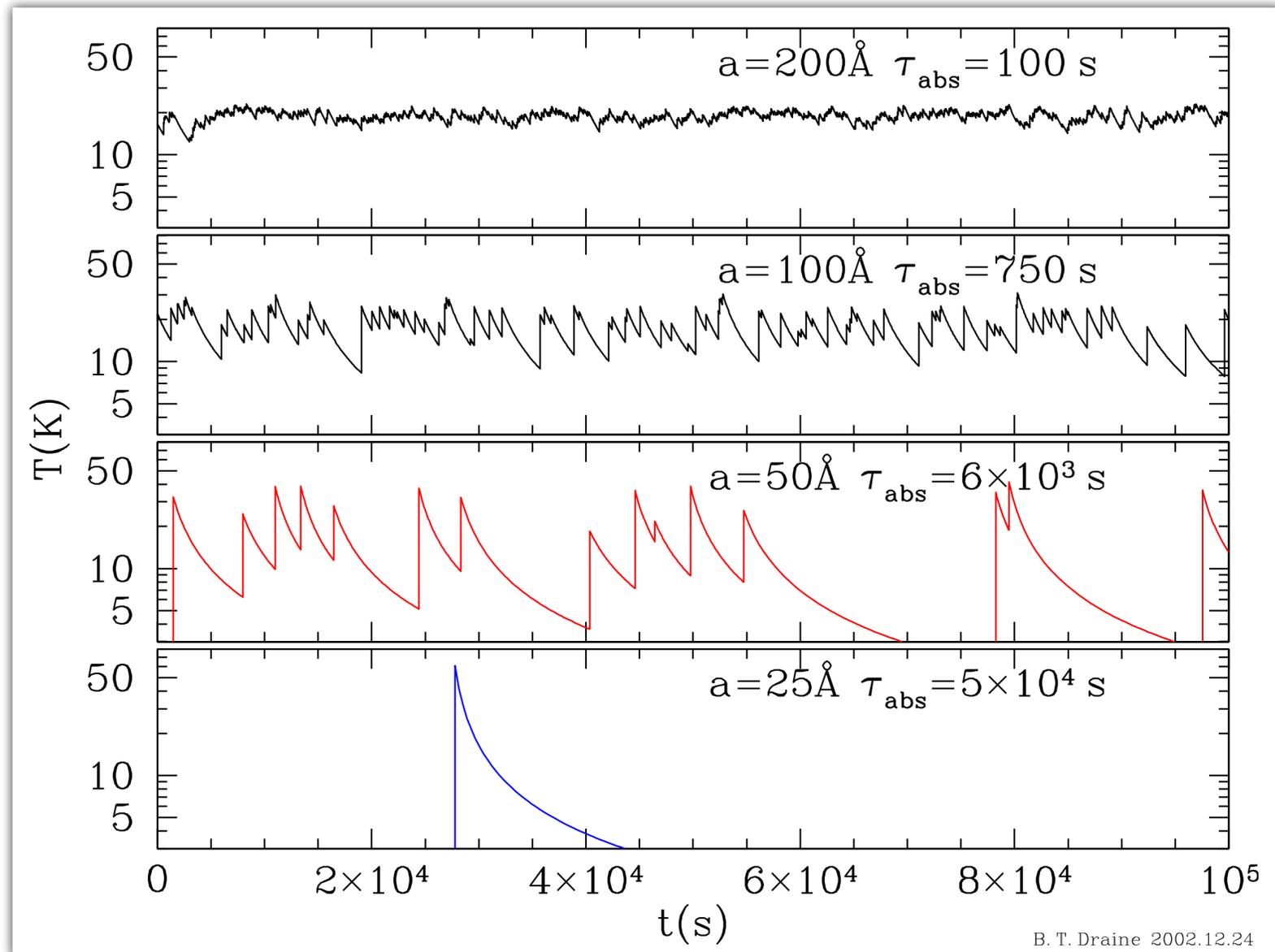
Dust properties: heating & cooling

- **Grains are heated by:**
 - absorption of a photon from the radiation field
 - collision with atoms, electrons, cosmic rays, grains
 - energy delivered by chemical reactions at grains surface
- Radiative heating is the most important in the ISM because of the large energy density of starlight ($\sim 0.5 \text{ eV/cm}^3$) and the high opacity of grains to starlight

- **Grains cool down via:**
 - emission of a photon
 - collision with cold atoms and molecules
 - ejection of electrons, atoms or molecules from the surface
- Radiative cooling is dominant

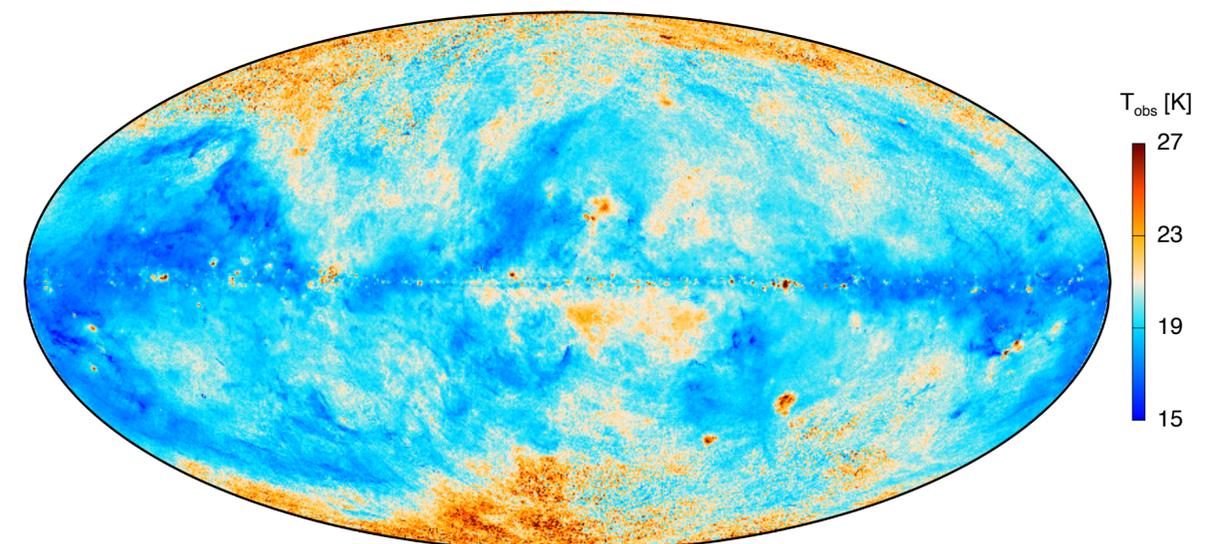
Dust temperature

- Stochastic heating induced by the absorption of photons of the ISRF



- Small grains absorb fewer photons than large particles
- Small grains reach higher temperature than large grains
- Small grains exhibit higher temperature fluctuations than larger ones
- Big grains have a constant temperature
- Big grains in the ISM are cold : 10-100K

All sky Planck observations [Planck Collaboration 2013]



Modelling grains emission: the big grains

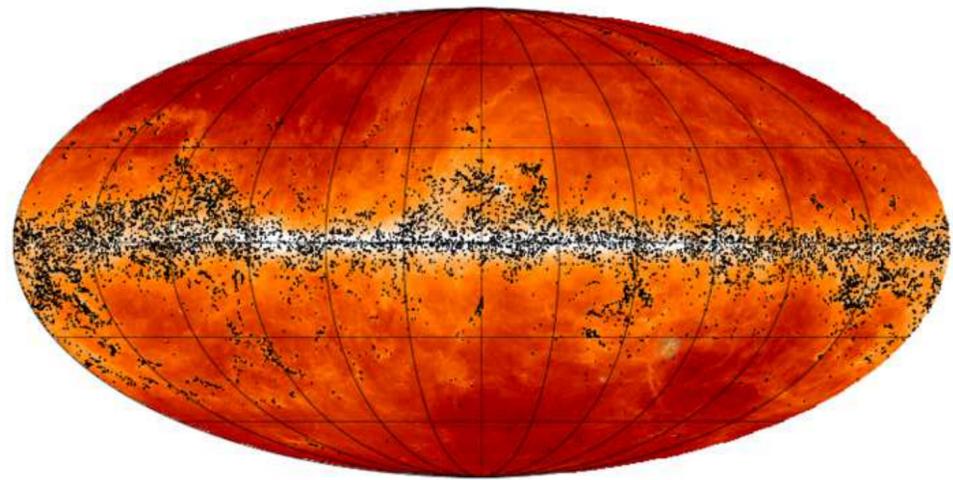
- Kirchoff law \Rightarrow at thermal equilibrium, emitted power = absorbed power $\iff \epsilon \propto K_{\text{abs}}$
- Assuming:
 - the medium is optically thin
 - grains in thermal equilibrium
 - no temperature gradient on the line of sight
- the emission may be modelled with the Modified Black Body model:

$$I_{\nu} \propto B_{\nu}(T) \times \kappa_{\nu} \quad \text{with :} \quad B_{\nu}(T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{(h\nu/kT)} - 1}$$

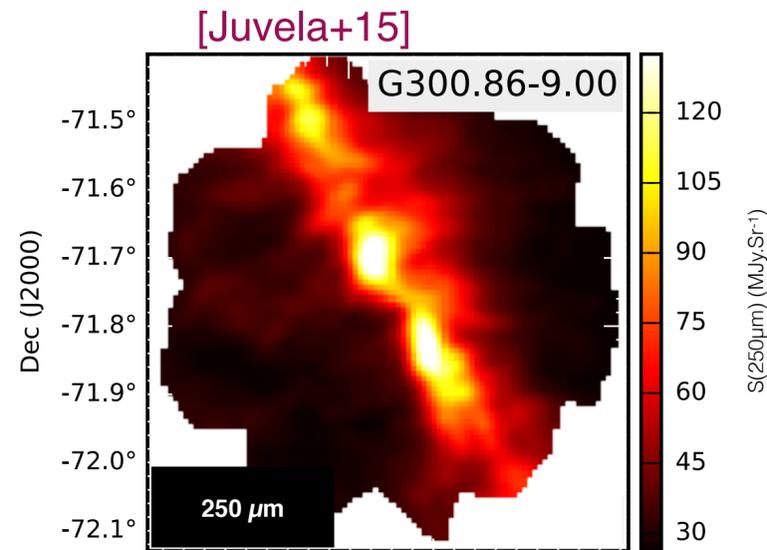
- ISM big grains have $T \approx 100 \text{ K} \Rightarrow$ emit in the FIR/mm domain
- In the FIR/mm, semi-classical physical models assume an asymptotic behaviours : $\kappa_{\lambda} = \kappa_{\lambda_0} \left(\frac{\lambda}{\lambda_0} \right)^{-\beta}$
with:
 - $\beta = 2$ from Lorentz model
 - $\beta = 1-2$ for phonons model

Variation of grain emissivity in the ISM

- Planck: 13188 Galactic Cold Cores:
- Herschel-PACS/SPIRE: 136 cores mapped [Juvela+12]



[Planck 2015 XXVIII]



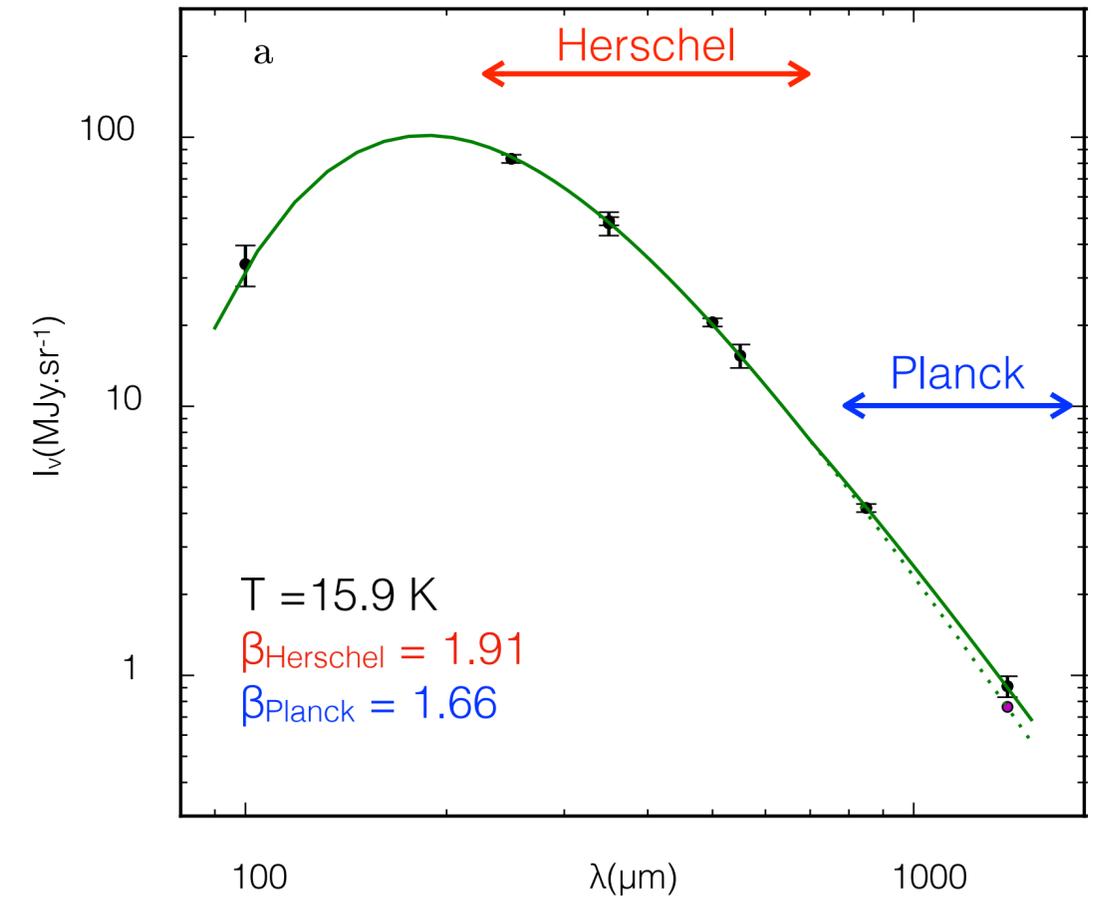
[Juvela+15]

G300.86-9.00

Dec (J2000)

250 μm

$S(250\mu\text{m})$ (MJy.Sr $^{-1}$)



a

Herschel

Planck

$T = 15.9 \text{ K}$

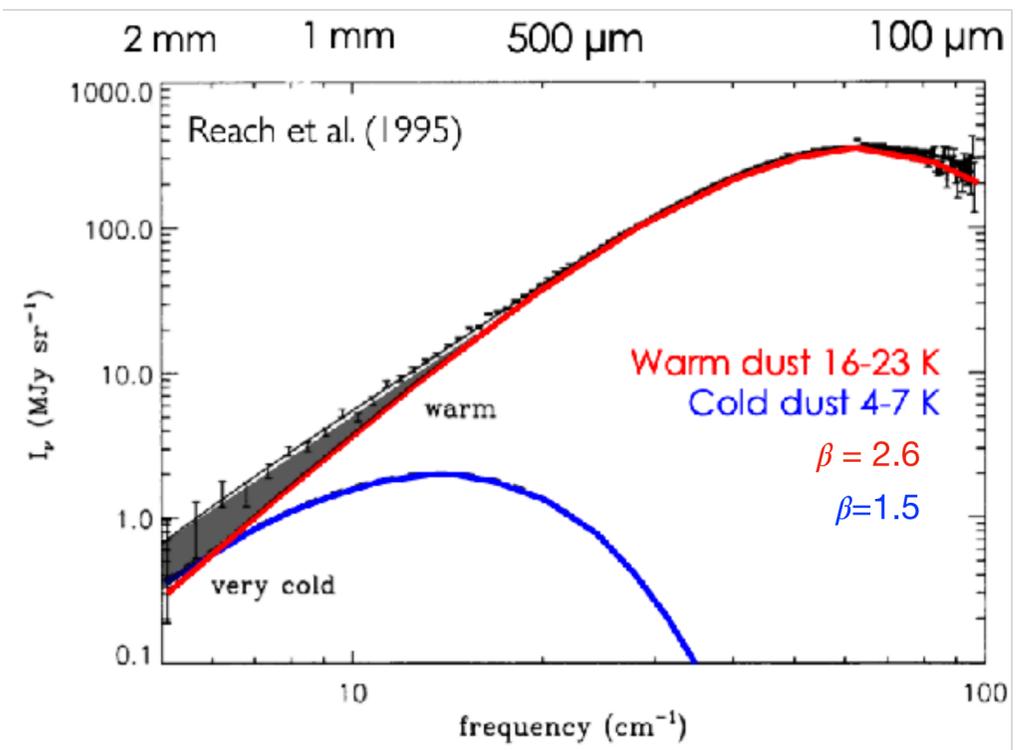
$\beta_{\text{Herschel}} = 1.91$

$\beta_{\text{Planck}} = 1.66$

100

$\lambda(\mu\text{m})$

1000



2 mm

1 mm

500 μm

100 μm

Reach et al. (1995)

Warm dust 16-23 K

Cold dust 4-7 K

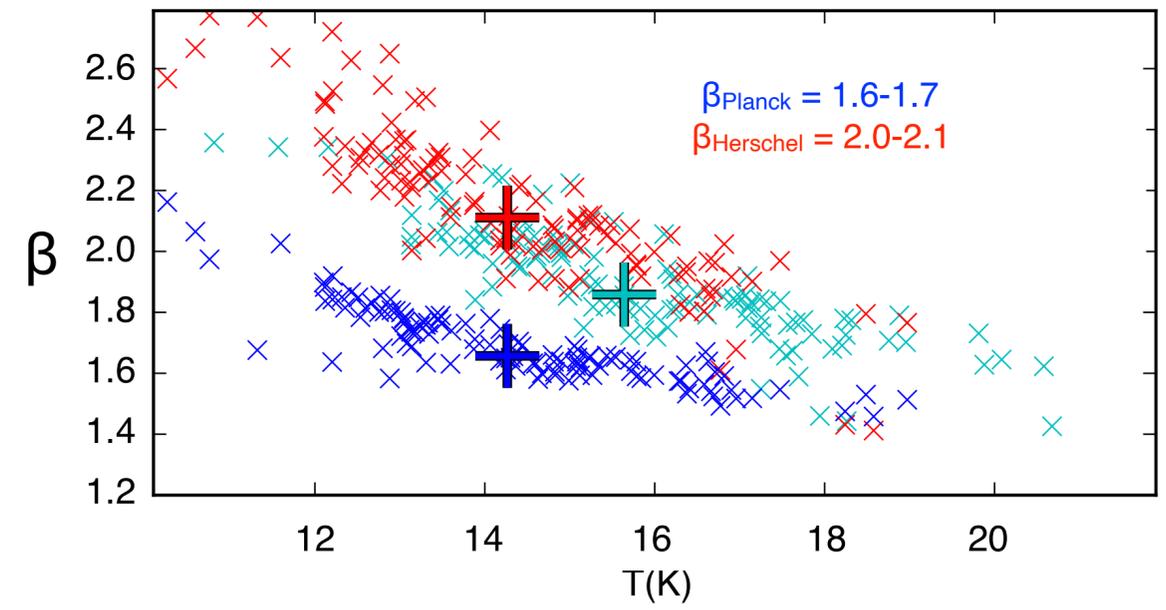
$\beta = 2.6$

$\beta = 1.5$

frequency (cm $^{-1}$)

➔ $\beta \neq 2$ and may be > 2

➔ β varies with λ :
flattening at large λ



$\beta_{\text{Planck}} = 1.6-1.7$

$\beta_{\text{Herschel}} = 2.0-2.1$

β

12

14

16

18

20

T(K)

Modelling big grains emission: cloud mass

- In optically thin medium:

$$I_\lambda = \tau B_\lambda(T) = \frac{M_{dust} \kappa_\lambda B_\lambda(T)}{d^{-2} \Omega^{-1}} \quad \rightarrow \quad M_{dust} = \frac{I_\lambda d^2 \Omega}{B_\lambda(T) \kappa_\lambda}$$

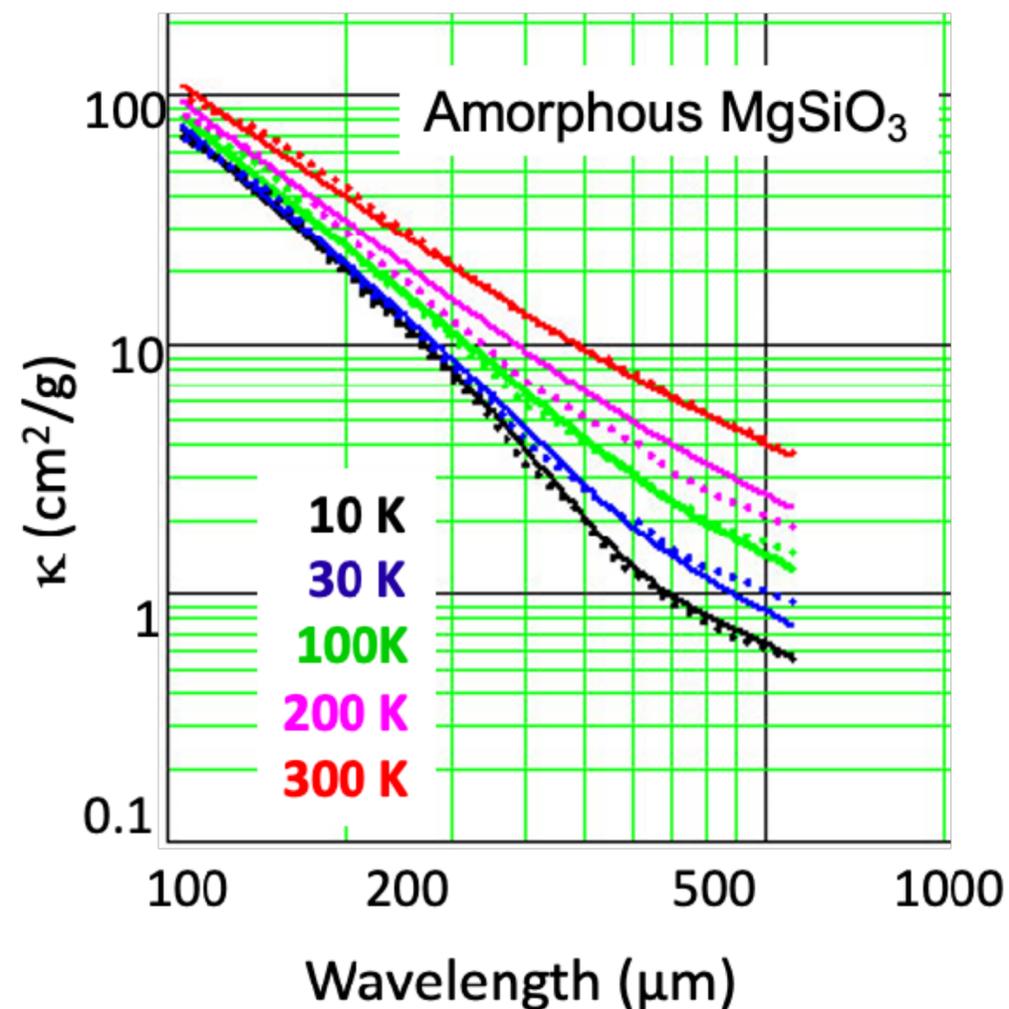
- The determination of the mass depends on the dust temperature and on the dust opacity

- Assuming: $\kappa_\lambda = \kappa_{\lambda_0} \left(\frac{\lambda}{\lambda_0} \right)^{-\beta}$ \rightarrow $M_{dust} = \frac{I_\lambda d^2 \Omega}{B_\lambda(T) \kappa_{\lambda_0}} \left(\frac{\lambda}{\lambda_0} \right)^\beta$

- If β varies with the temperature and wavelength
 - and if the emissivity (κ_0) varies in the ISM
- \rightarrow The mass determination is wrong

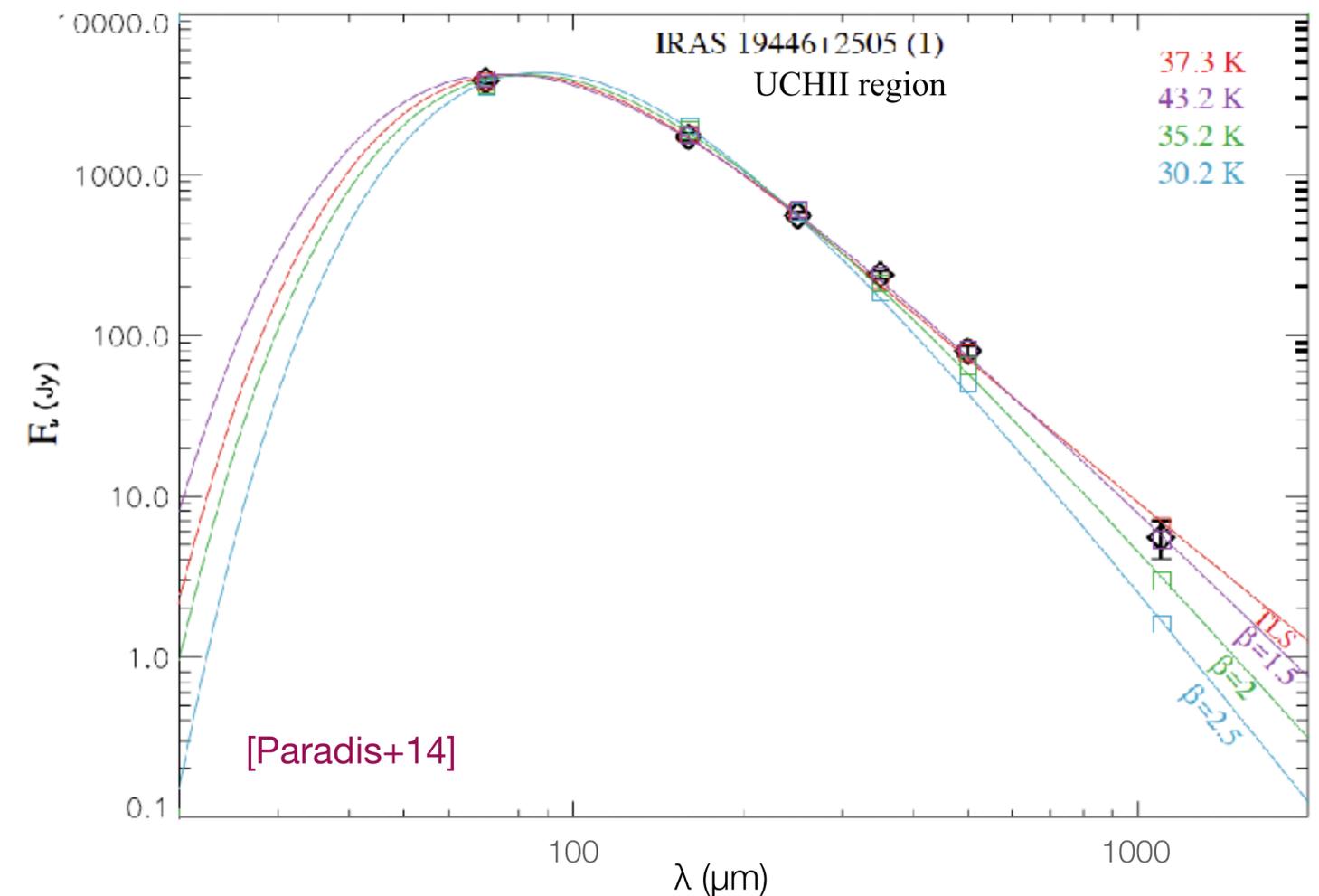
Modelling grains emission: the TLS model

- Proposed by solid state physicists to describe the low temperature behaviour of disorder material
- Adapted for astrophysical studies by [Meny et al. 2007](#)
- Sum of two different models: DCD and TLS:
 - temperature dependent absorption mechanisms
 - β values greater than 2 and β variation with λ



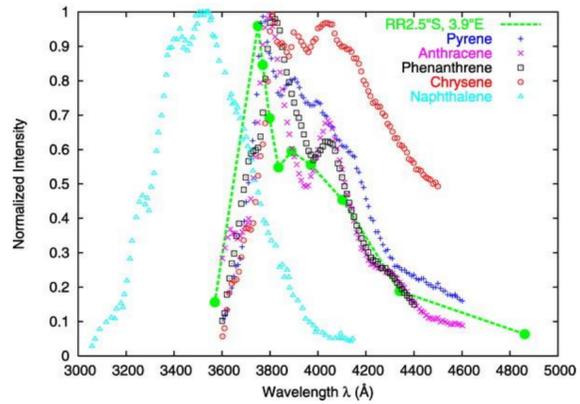
- The TLS model is able to reproduce the SED of warm and cold regions
[Paradis+12,14]

$$\kappa_{dust} = \kappa_{IR} + \kappa_{DCD} + \kappa_{TLS}$$

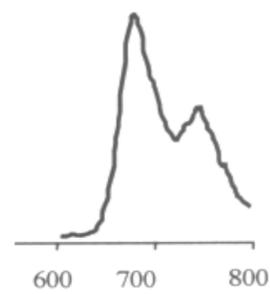


Modelling the AIBs:

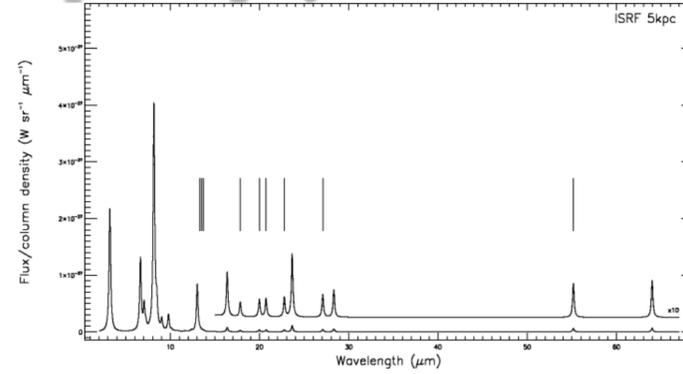
A unified vision of PAH photophysics



Fluorescence



Phosphorescence

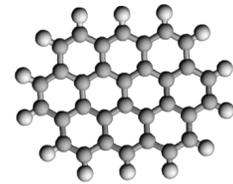


Vibrational emission

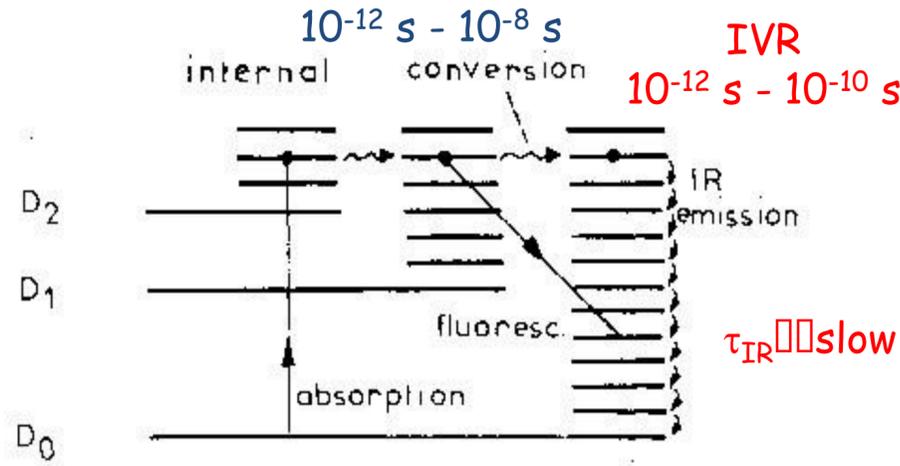


UV radiation field

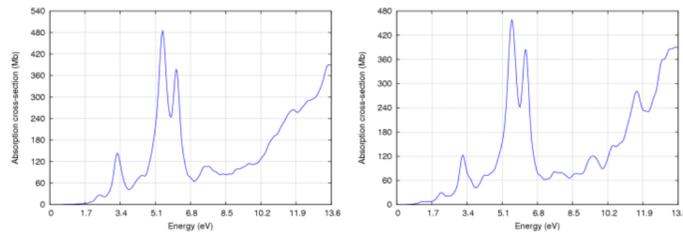
emission



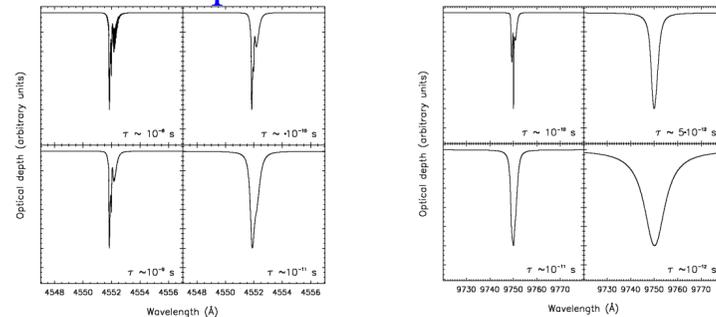
absorption



Discrete absorption features in the visible



Broad absorption in the UV



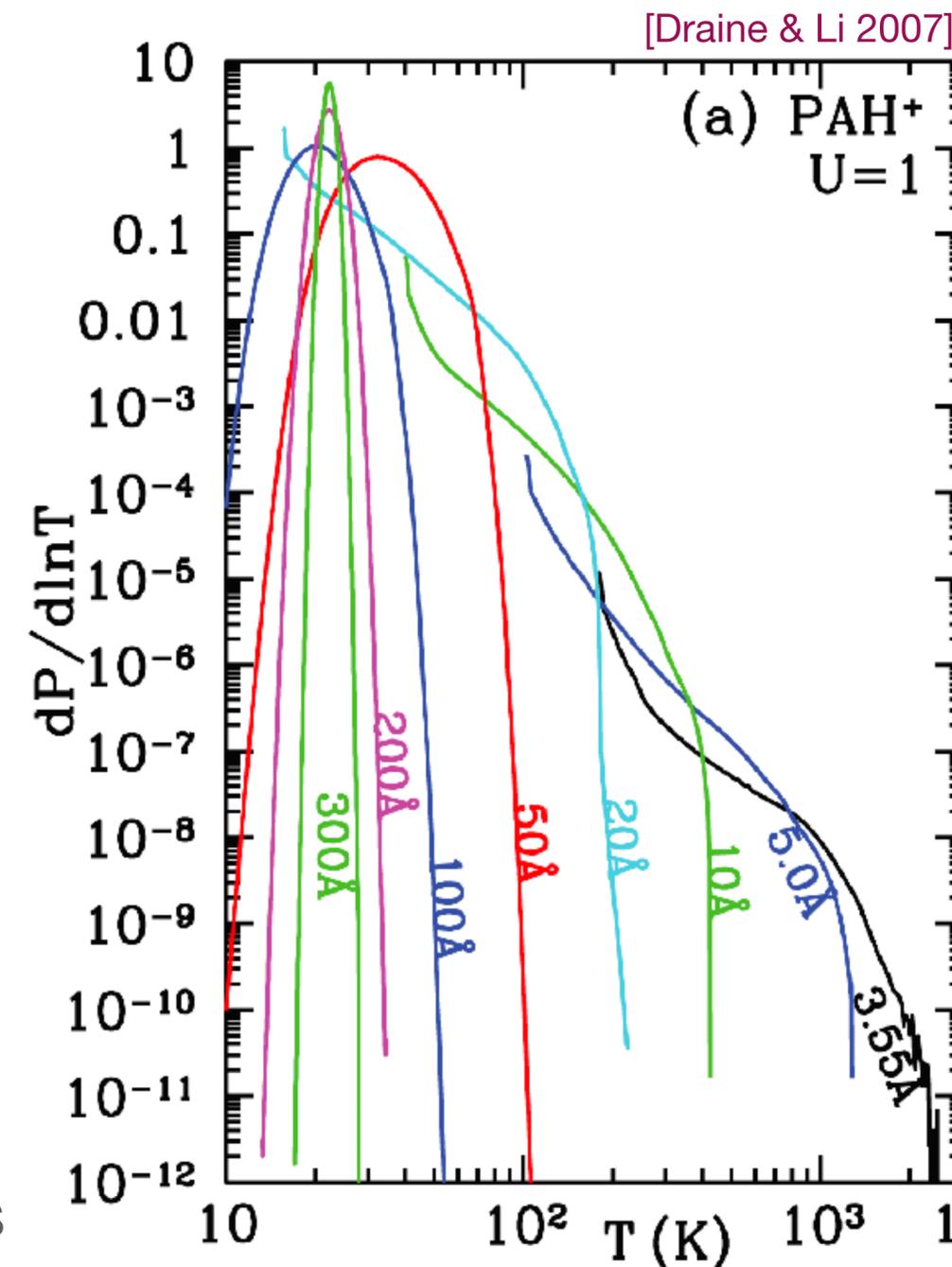
- Modelling of AIB emission requires to simulate the spectrum of a family of PAH in a given radiation field knowing :

- the excitation conditions (physical conditions, UV)
- molecular complexity
- photo-absorption cross-sections
- vibrational modes
- IR band positions and widths as a function of T

- Detailed physical model very time consuming [see eg. Joblin+02, Mulas+06]

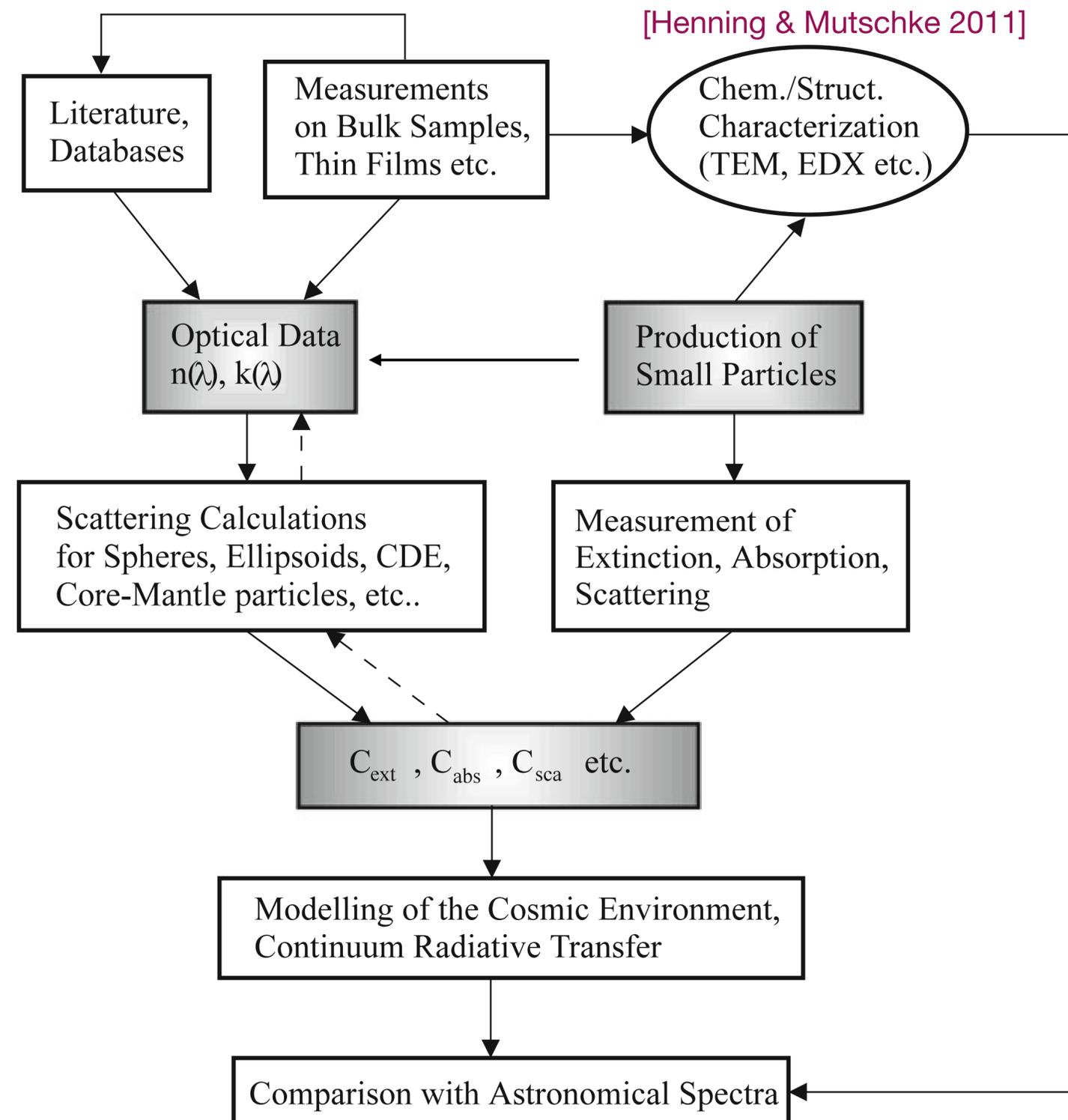
Modelling the AIBs:

- Other approaches: [eg. Désert+90, Draine & Li 2001]
 - C_{abs} taken from laboratory measurements (but very few data [eg. Joblin+95]) and/or quantum chemical theoretical calculations [eg. Bauschlicher 2009]
 - C_{abs} calculated from the Drude model (classical Lorentz oscillators model modified for conducting material to take into account free electrons)
 - C_{abs} calculated from optical constants simulated with the new optEC model developed from solid state physical models for amorphous hydrocarbon materials [Jones 2012a,b,c]
- Need to calculate the temperature probability distribution of the different species -> need to know the heat capacity of the species
- Empirical approach:
 - from a combination of templates spectra derived from observations [eg PAHTAT toolbox, Pilleri+2010]



Modelling dust extinction and emission: summary

- Modelling dust extinction and emission relies on the description of the interaction of matter with light
- It is necessary to know the physical characteristics of the dust :
 - dielectric constants
 - size distribution, shape distribution
 - heat capacity for emission modelling
 - photo absorption cross-section
- These data comes from laboratory astrophysics studies of dust analogues



Cosmic dust models

From observations to cosmic dust models

- Cosmic dust models are built to interpret observations of various astrophysical environments
- **Many** dust models exist, they differ because they consider different:
 - sets of observations used to constrain the dust populations
 - reference abundances
 - grain components: nature, number, size distribution...
- For each dust components :
 - They provide the optical constants
 - They calculates the extinction cross sections for a given grain shape and size distribution
- These cross sections may be used in astronomical modelling

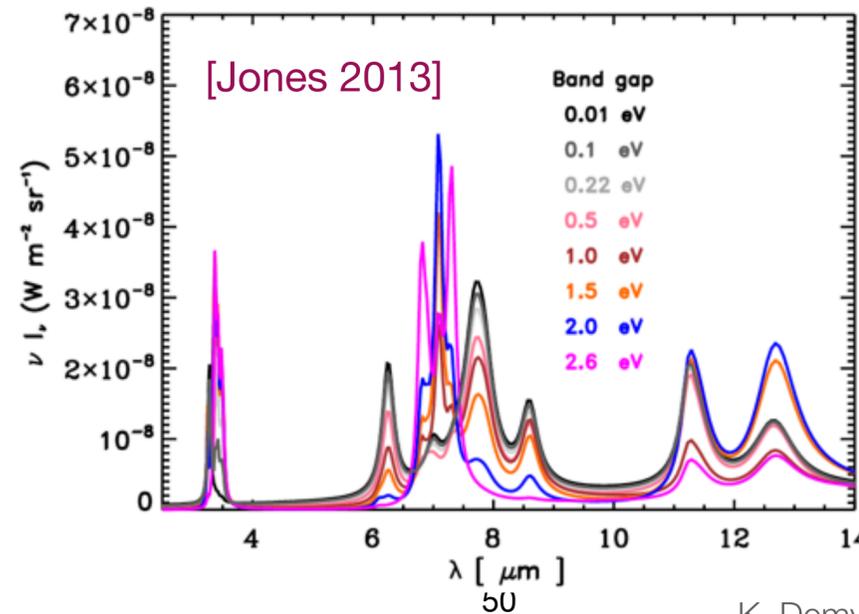
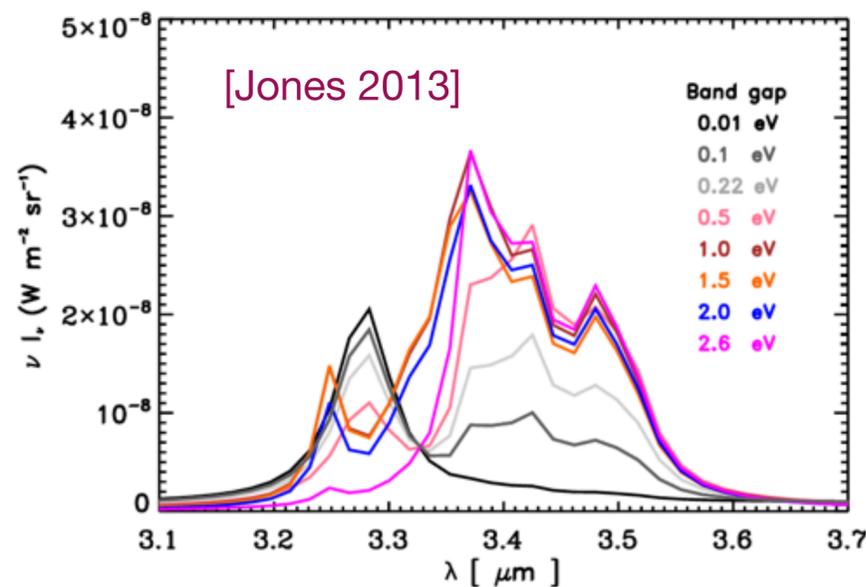
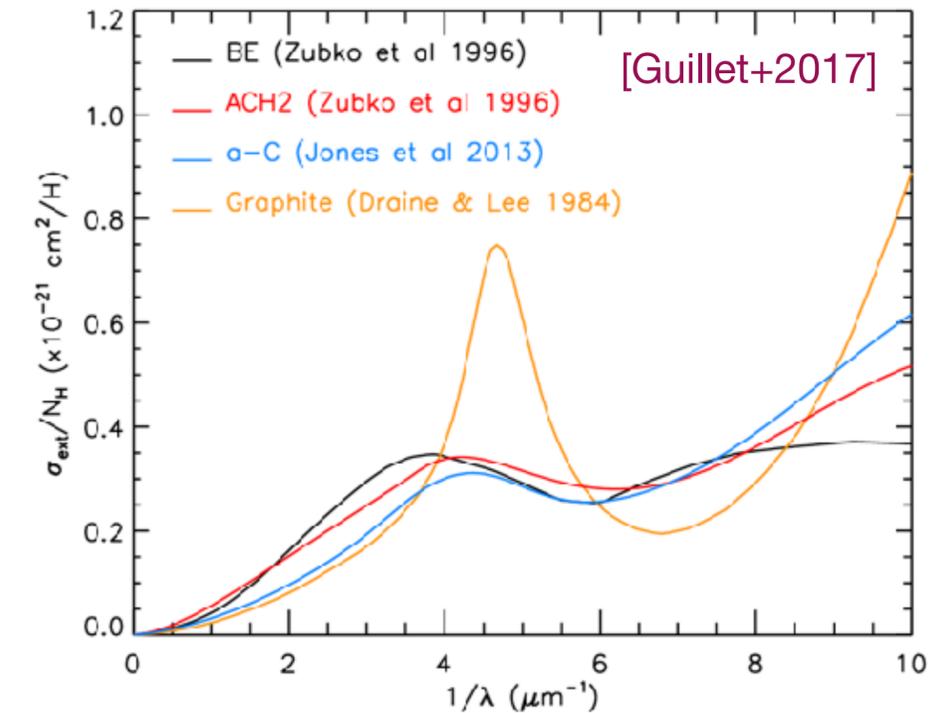
Optical constants used in cosmic dust models:

- Optical constants are derived by inversion of :
 - laboratory measurements of spectra of dust analogues
 - theoretical calculations from physical description of dust analogues
 - observational constraints
 - extrapolations

• Amorphous carbon

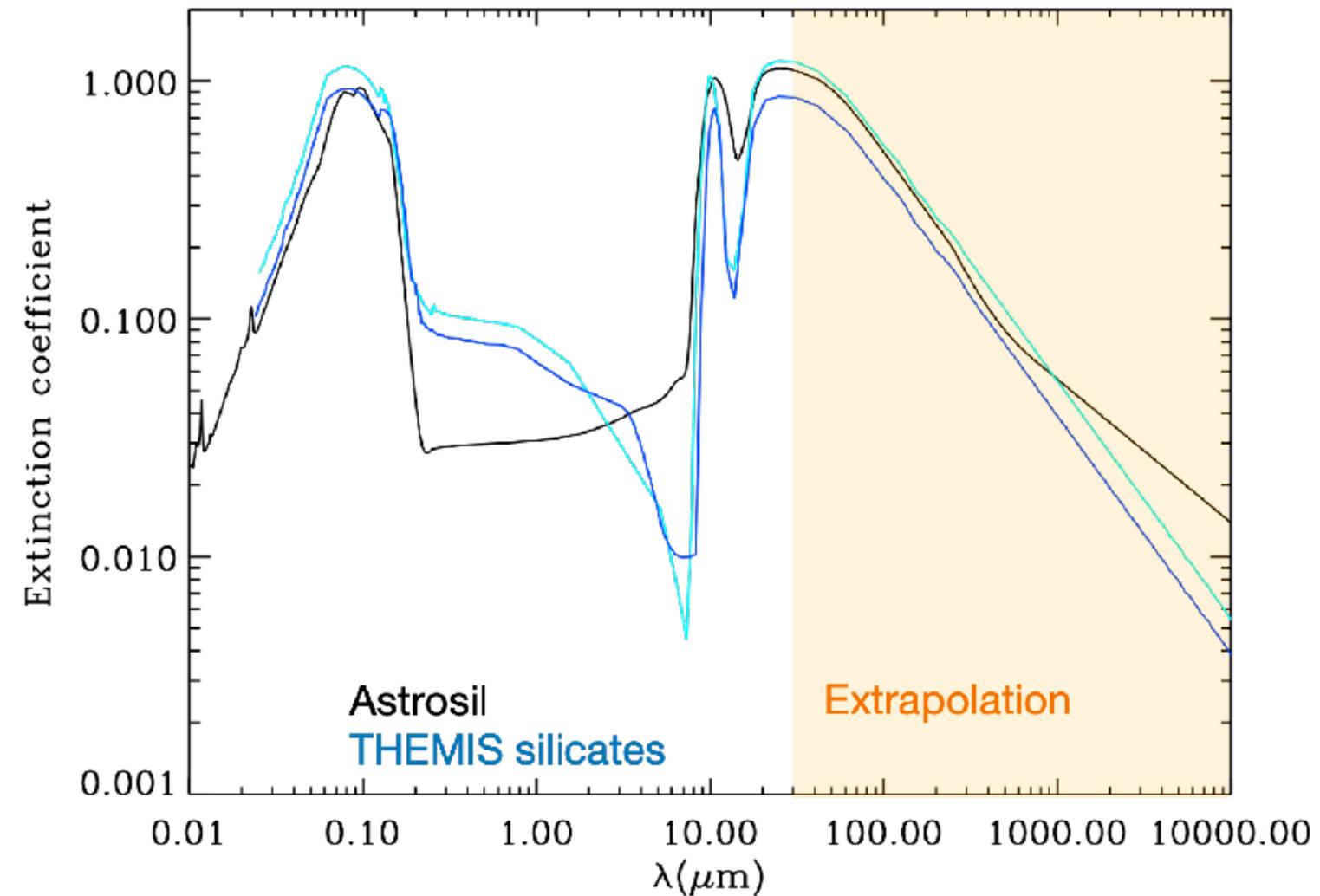
- Lab data from [Zubko et al. 1996](#) in the MIR-FIR domain for more or less hydrogenated material (BE & ACH)
- a-C(:H) : theoretical calculations (eRCN and DG models) [\[Jones 2012\]](#)

- **PAHs** : lab data & theoretical calculations for neutral and ionised PAHs



Optical constants used in cosmic dust models:

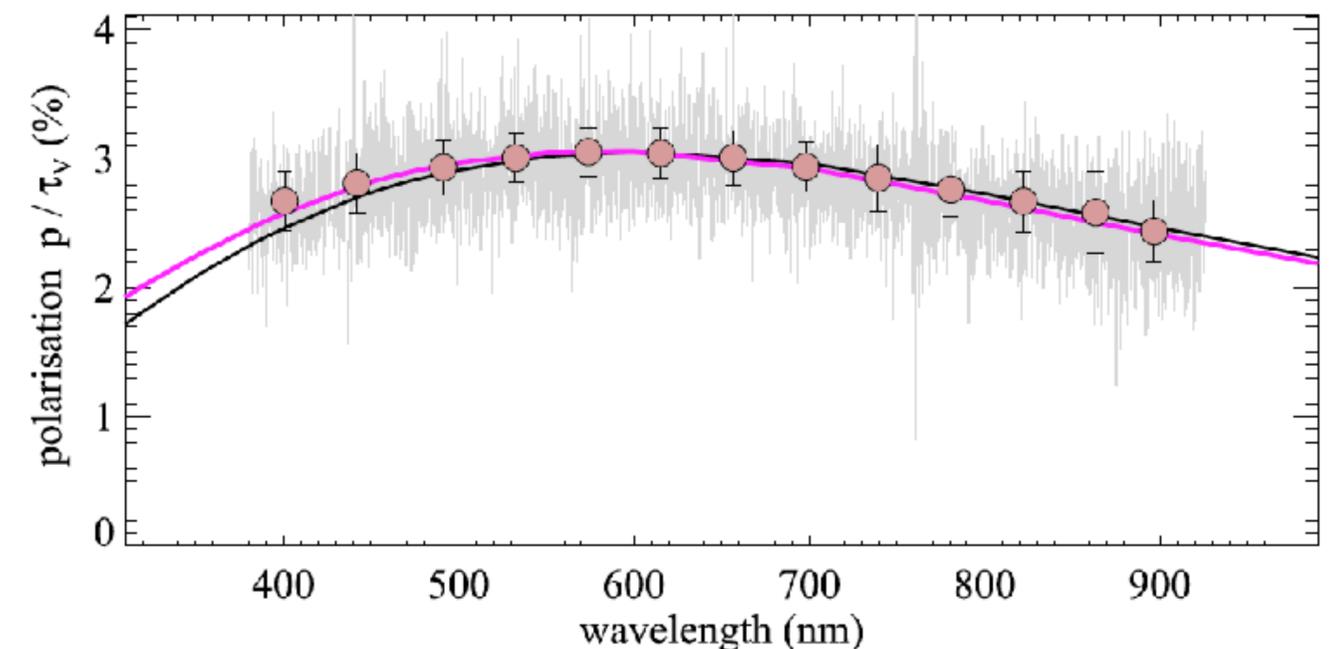
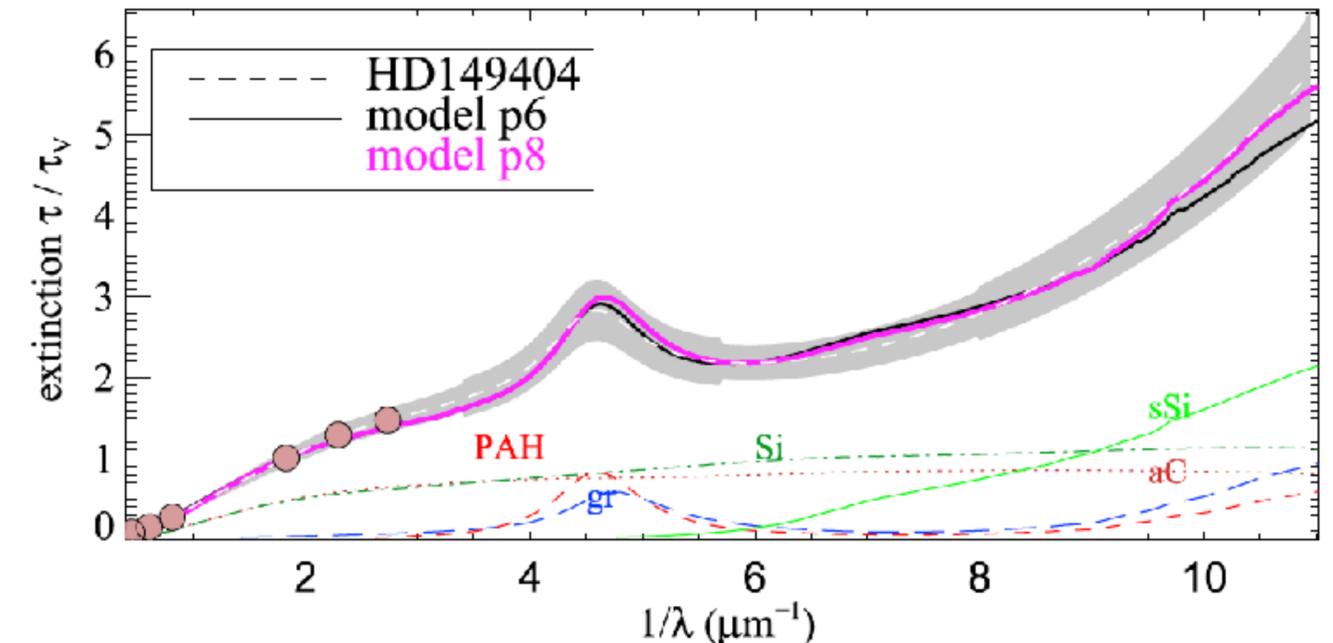
- *astrosilicates* :
 - MIR : optical constants constructed from the astronomical observations
 - NIR - UV: experimental data on crystalline silicates
 - FIR: extrapolation
- **Lab data for MgSiO₃ and MgSiO₄**
 - MIR from Scott & Duley (1996) and Day (1981)
- See the DOCCD and STOPCODA databases on the SHAADE portal [Schmitt+2018] for more optical constants on silicates :
 - <https://www.sshade.eu/db/doccd>
 - <https://www.sshade.eu/db/stopcoda>



Cosmic dust models for the DISM

Model from Siebenmorgen et al. 2017:

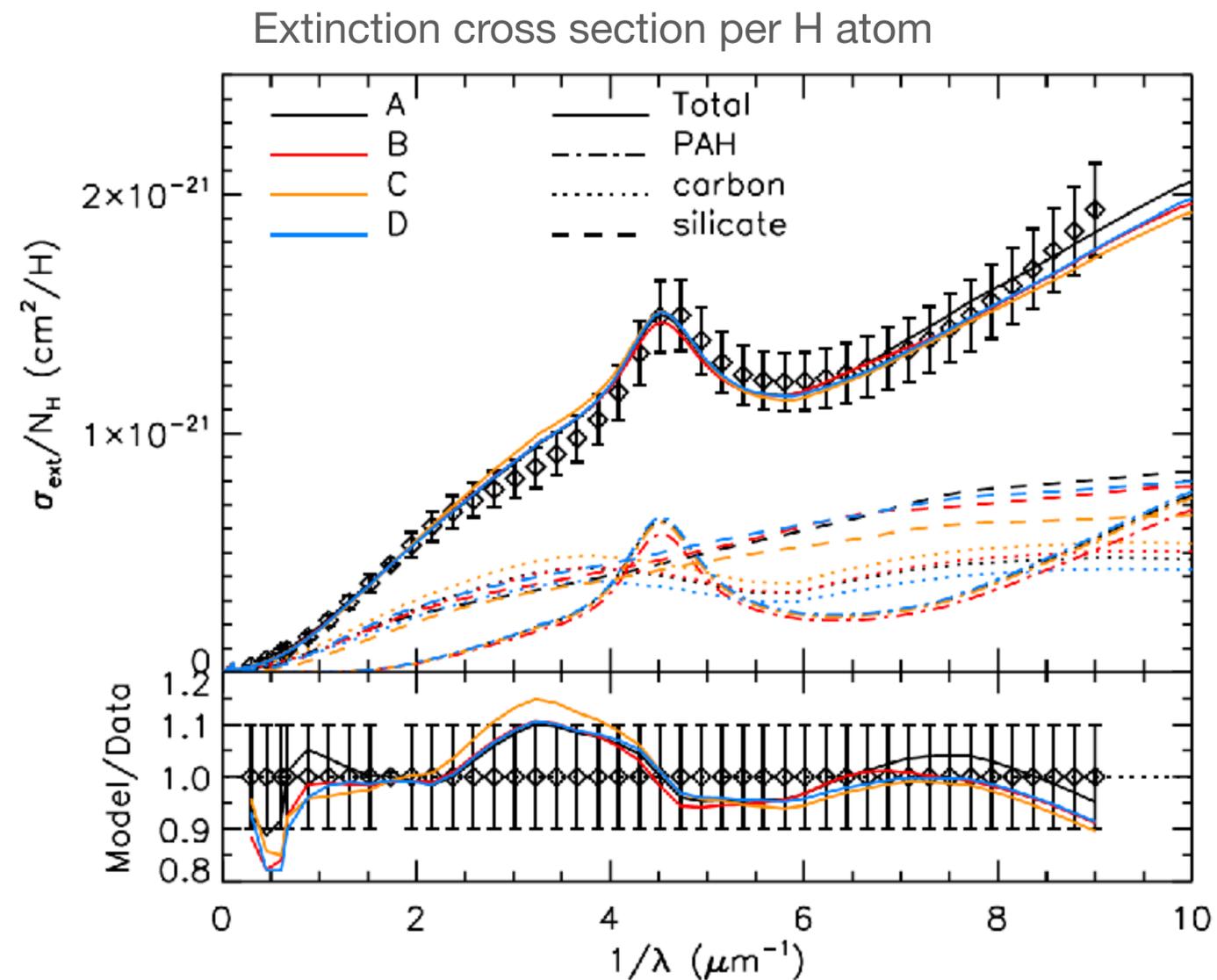
- DISM environments towards the Sco OB1 association
- Constraints on extinction and spectra-polarimetry (not on emission)
- Big spheroidal grains of
 - *astrosilicates*
 - amorphous carbon (Zubko+96 and Jones+12)
 - up to 350 nm, power law
- VSG (spherical) with Drude profile for the UV bump
 - 0.5 - 6 nm
 - graphite and silicates
- PAHs with 60 and 150 atoms



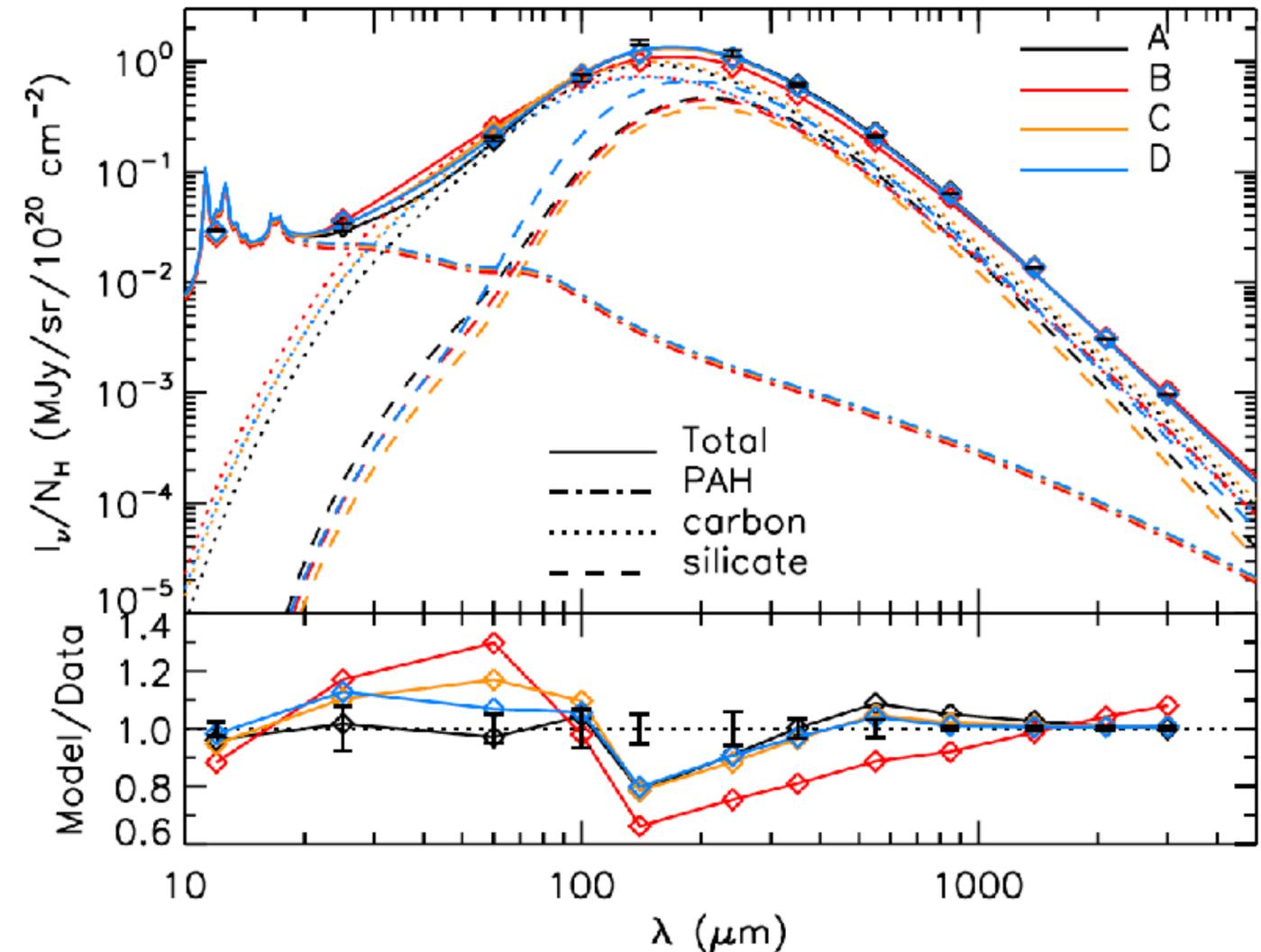
Cosmic dust models for the DISM :

Model from Guillet et al. 2018 (1/2):

- Constraint on translucent lines of sight ($0.5 < A_v < 2.5$)
- Adaptation of Compiègne et al. 2011 model :
- Consider *astrosilicates* prolate grains with porosity (20%), amorphous carbon inclusions, different size distribution



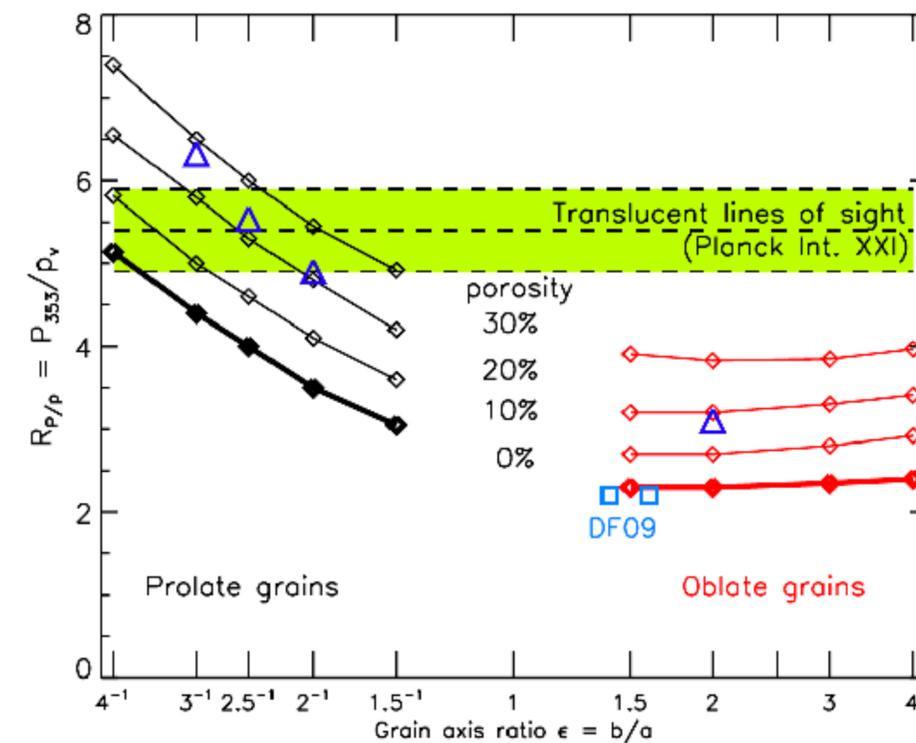
Dust emission SED



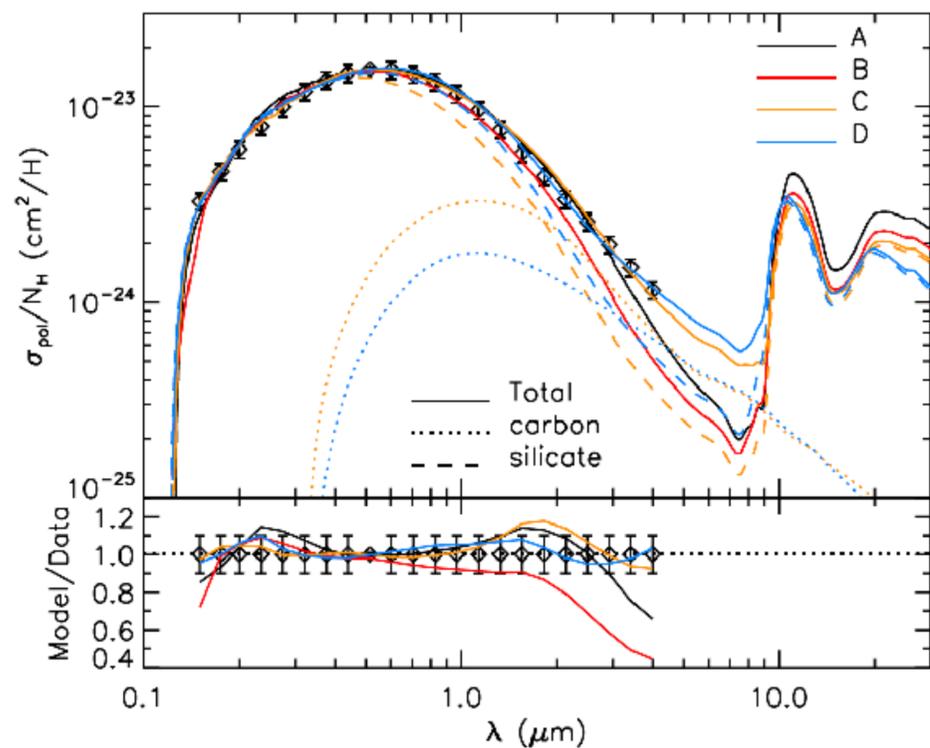
Cosmic dust models for the DISM

Model from Guillet et al. 2018 (2/2):

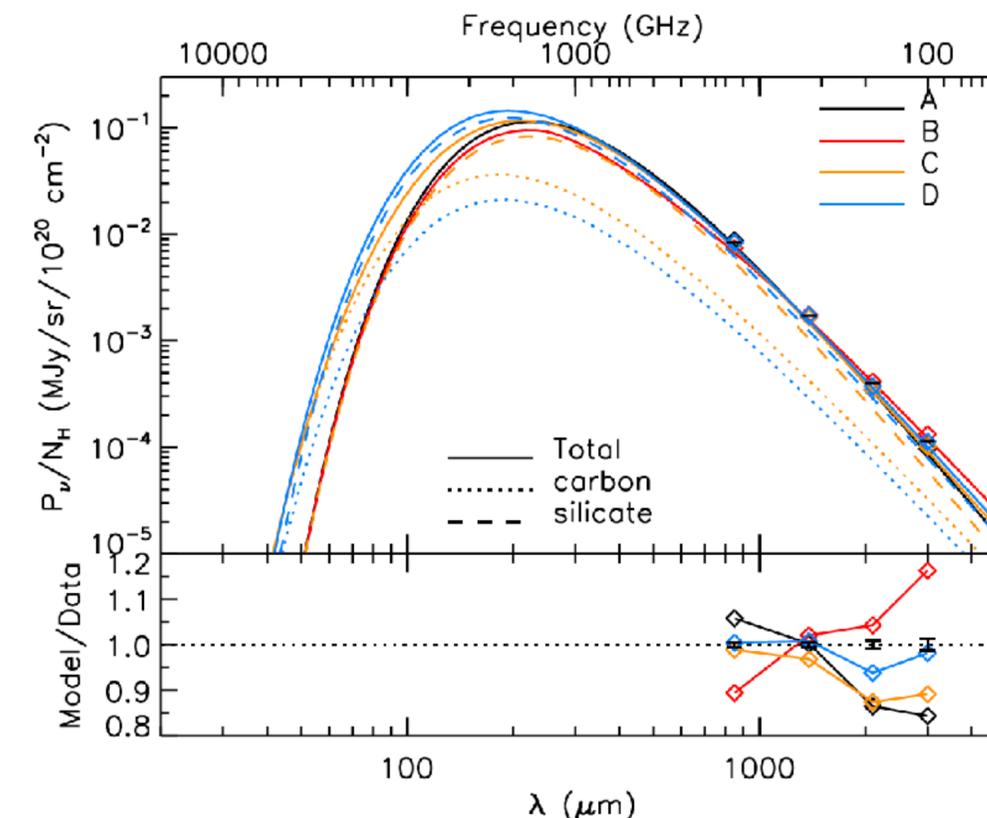
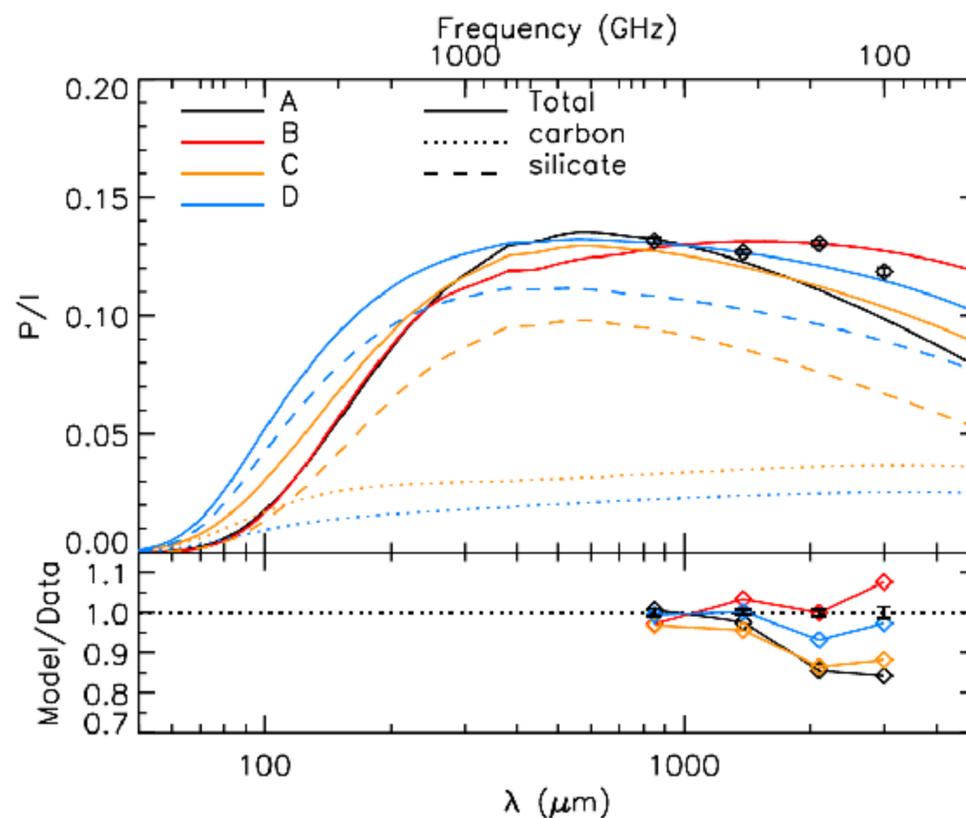
- Prolate grains are more emissive than oblate grains \Rightarrow better fit of the emission to extinction polarisation data from Planck data
- The addition of a-C in the silicate grains is equivalent to porosity



Polarisation cross section per H atom



Polarisation fraction in emission



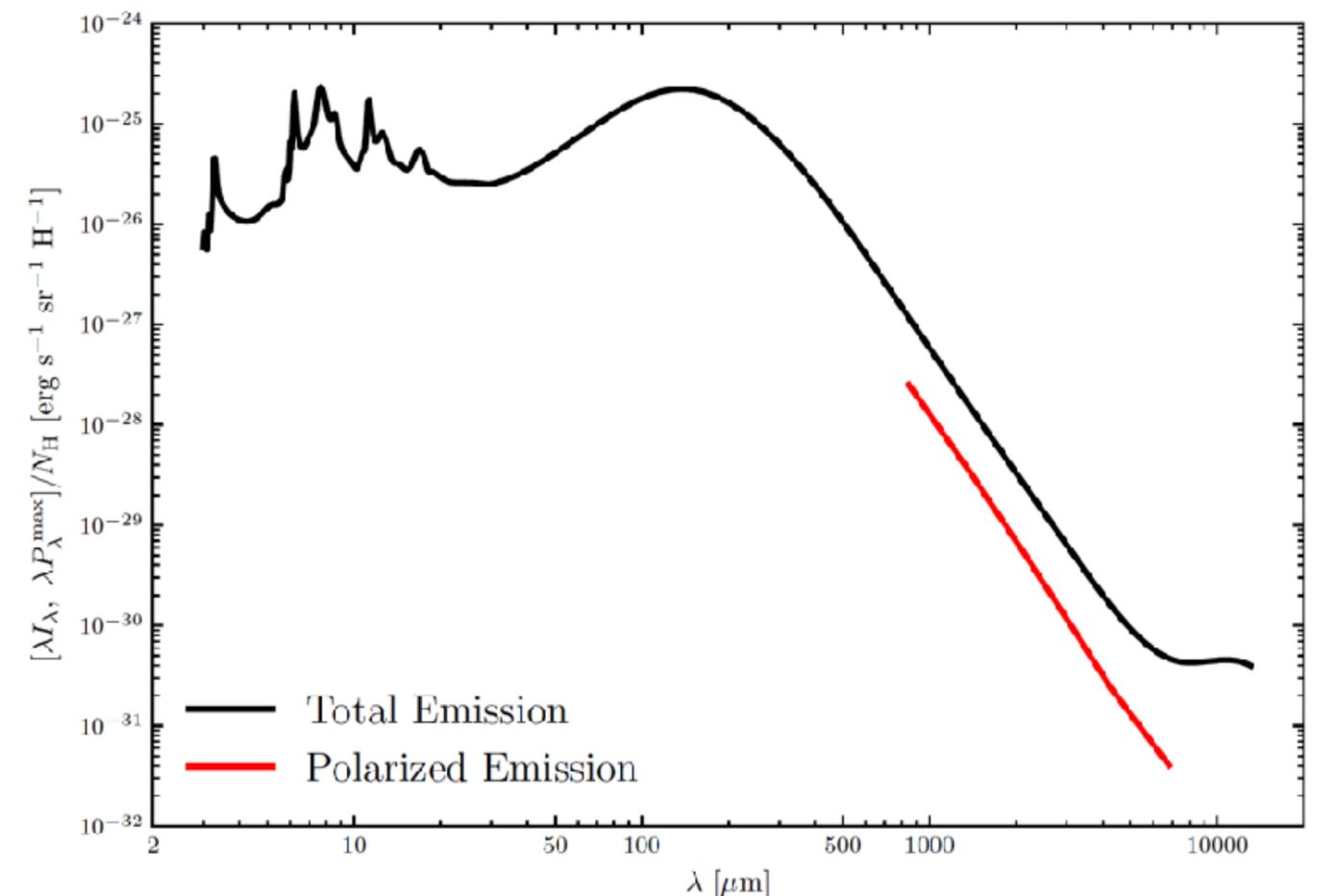
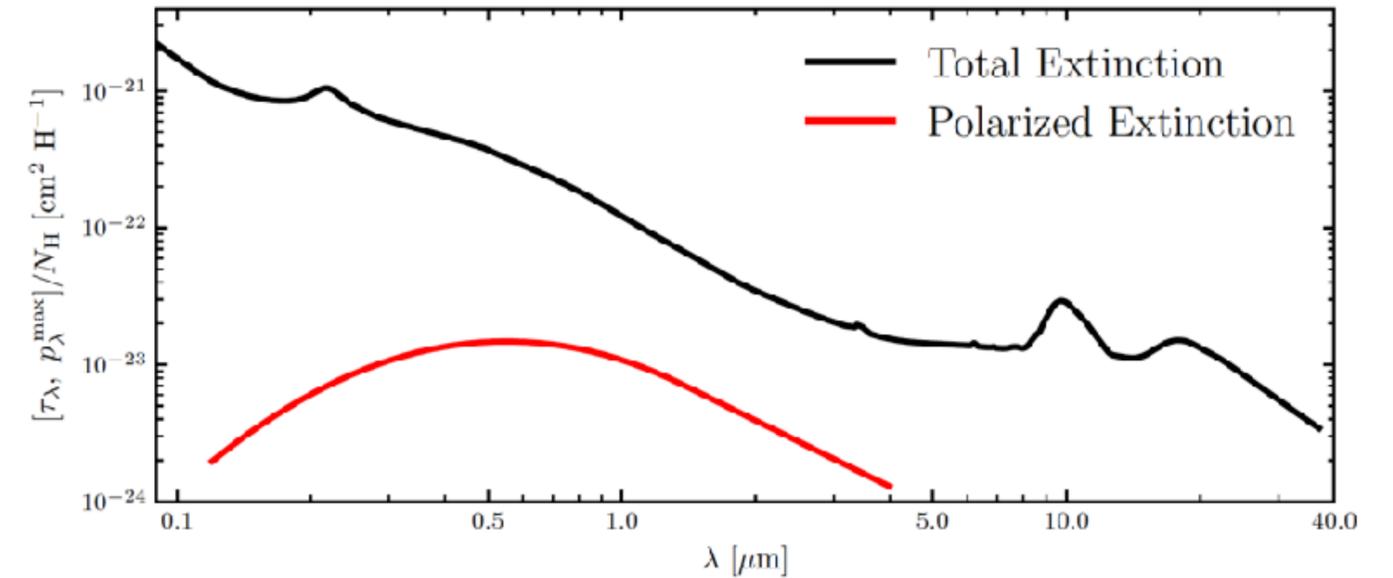
Cosmic dust models for the DISM

Model from Draine & Hensley (2021) (1/2):

- Observational constraints and adopted cosmic abundances: [Hensley & Draine 2020](#)
- Many sets of extinction and emission observations through different DISM sightlines from X-rays to mm
- Polarisation is calculated in the submm but not used to constrain the model

Table 5. Adopted Values of Select Quantities for the Diffuse ISM

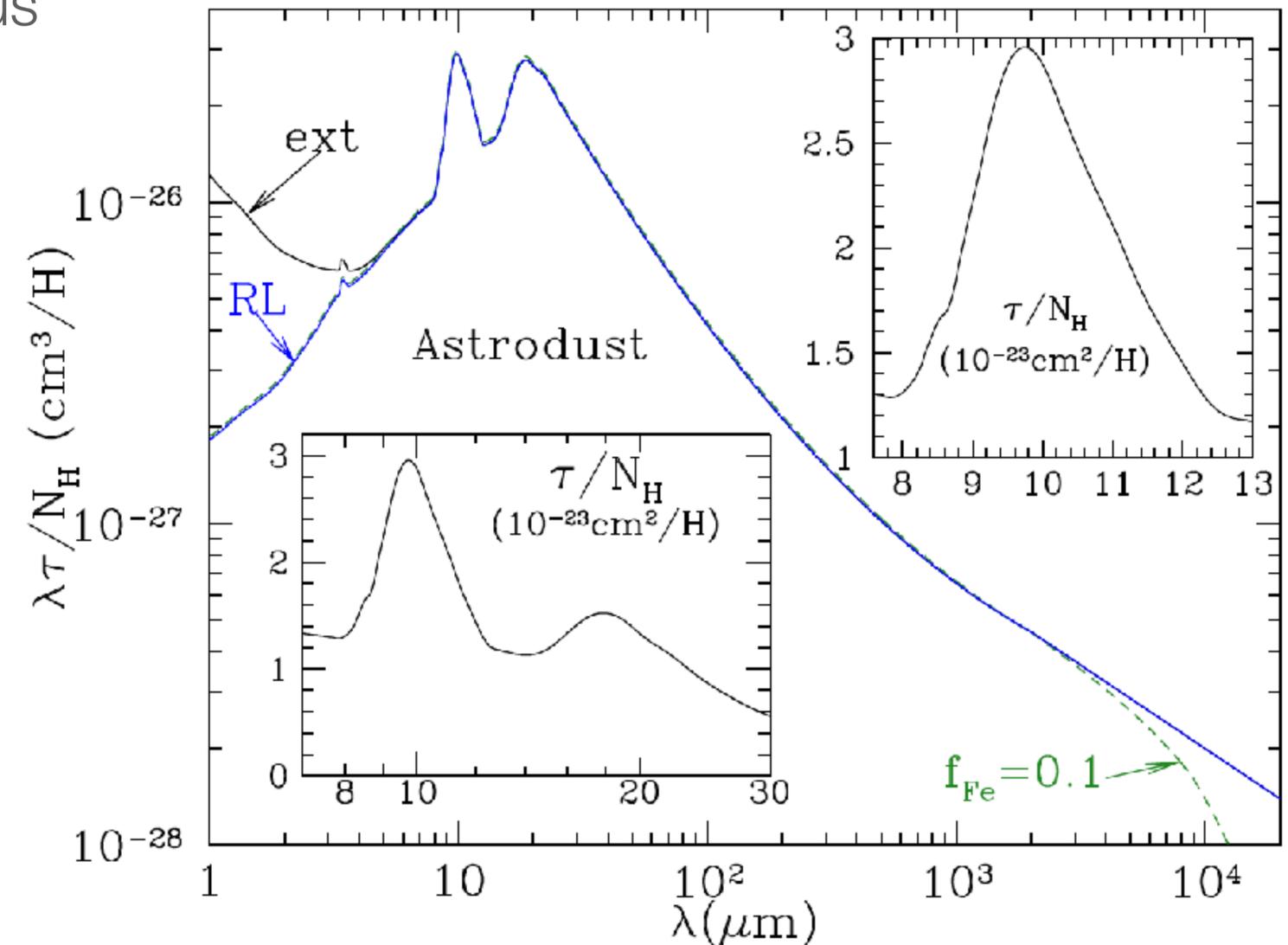
Reference Quantities		
Quantity	Value	Reference
$A(5500 \text{ \AA})/E(4400 \text{ \AA} - 5500 \text{ \AA})$	3.02	Fitzpatrick et al. (2019)
A_H/A_{K_s}	1.55	Indebetouw et al. (2005)
$N_H/E(B - V)$	$8.8 \times 10^{21} \text{ cm}^{-2} \text{ mag}^{-1}$	Lenz et al. (2017)
$[p_V/E(B - V)]_{\text{max}}$	0.13 mag^{-1}	Planck Collaboration XII (2018)
$p_{353}/(p_V/\tau_V)$	4.31	Planck Collaboration XII (2018)
Derived Quantities		
Quantity	Value	Reference
R_V	3.1	Fitzpatrick et al. (2019)
Λ_V/N_H	$3.5 \times 10^{-22} \text{ mag cm}^2$	
p_{353}^{max}	19.6%	
P_{353}/p_V	4.8 MJy sr^{-1}	



Cosmic dust models for the DISM

Model from Draine & Hensley (2021) (1/2):

- Two dust components:
 - **astrodust**: porous mixture of silicates & carbonaceous matter on grain surface
 - **PAHs**
- Optical constants build from:
 - observations in the X-ray - VIS domain
 - 300 oscillators in the IR (Lorentz model)
- Constrained from the silicates and aliphatic bands in extinction and polarisation

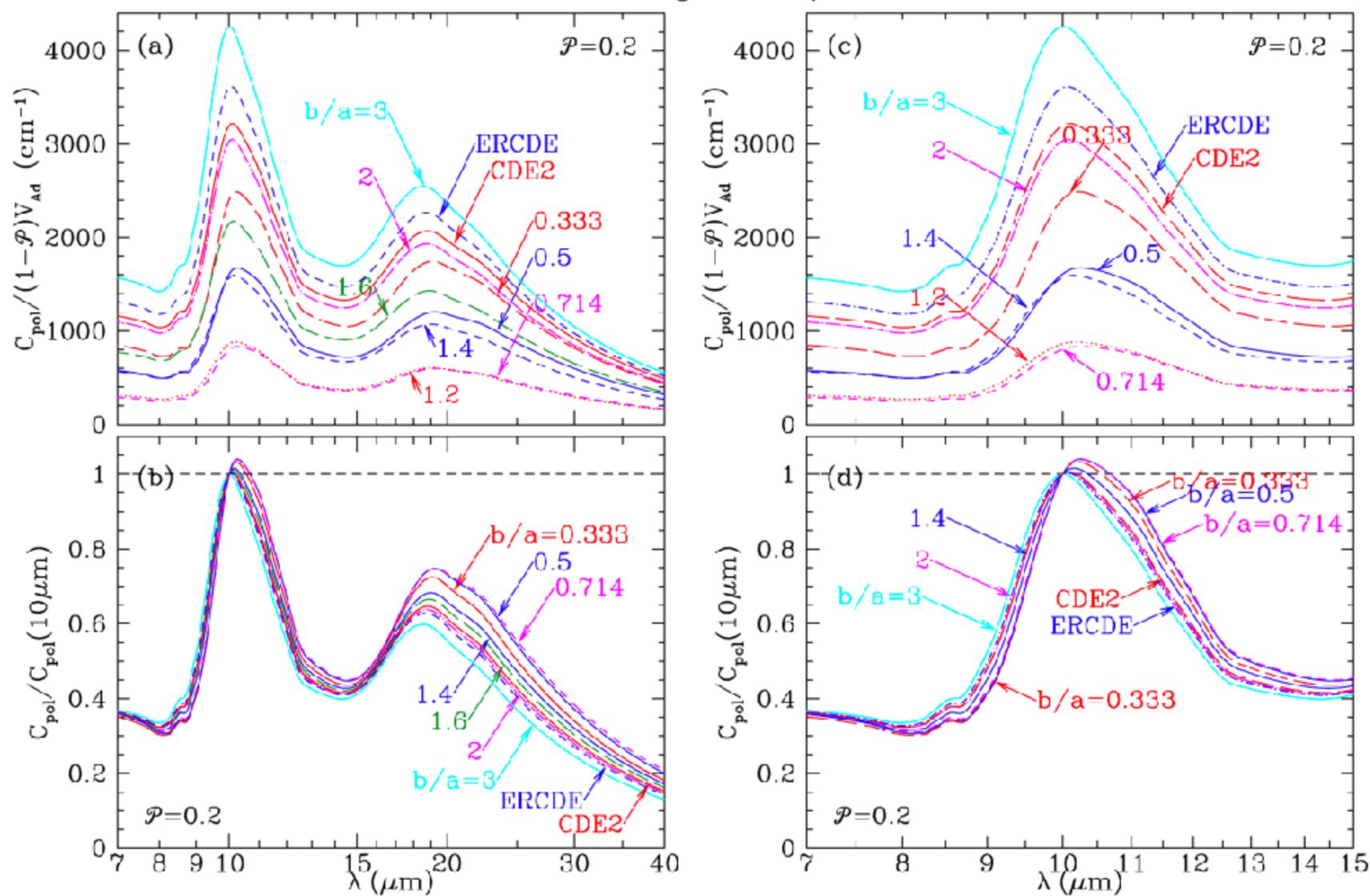


Cosmic dust models for the DISM

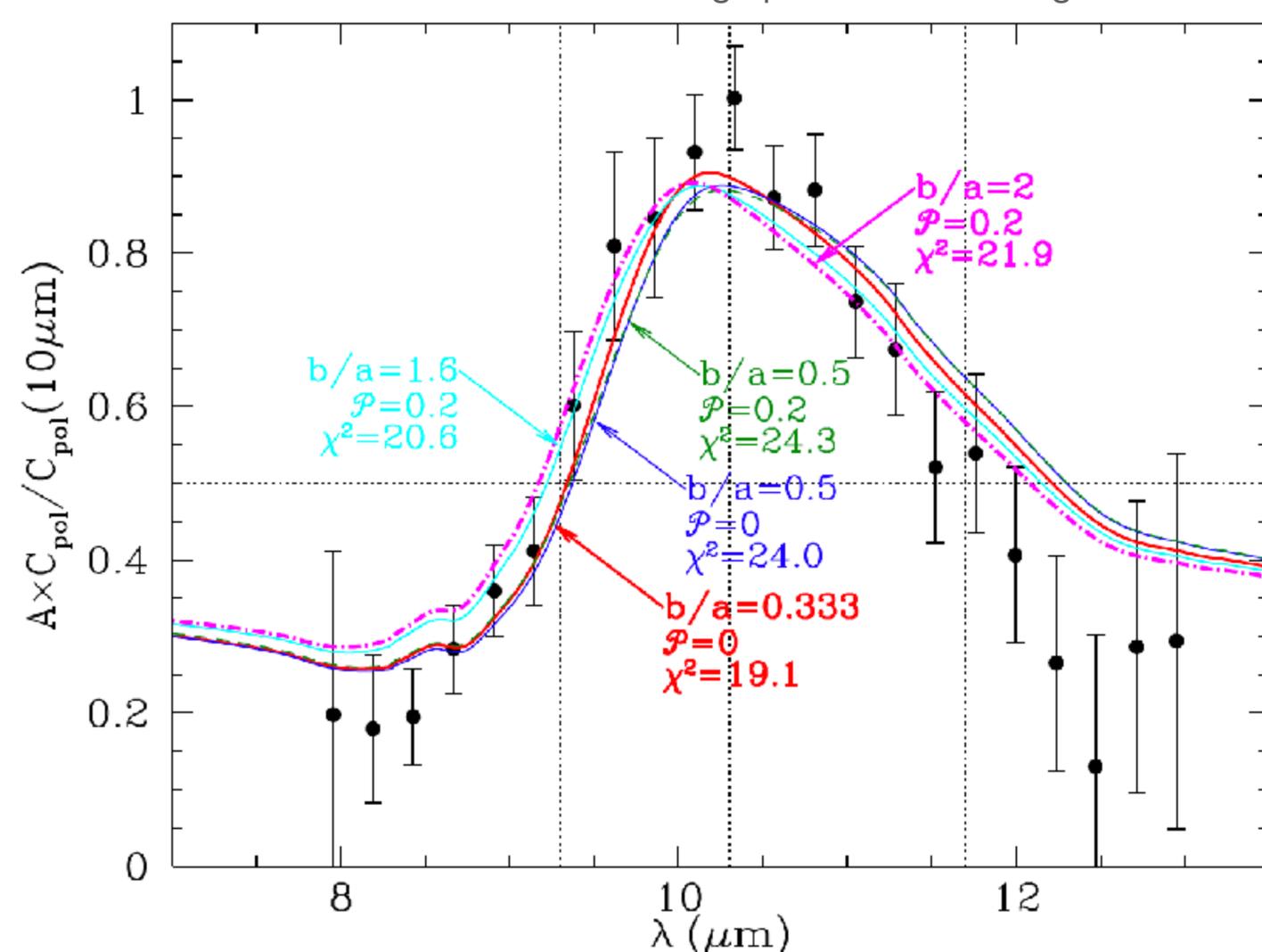
Model from Draine & Hensley (2021) (1/2):

- Spheroidal grains to reproduce polarisation observations
- Explore various shape, size distribution and porosity \rightarrow more data is needed to lift degeneracy

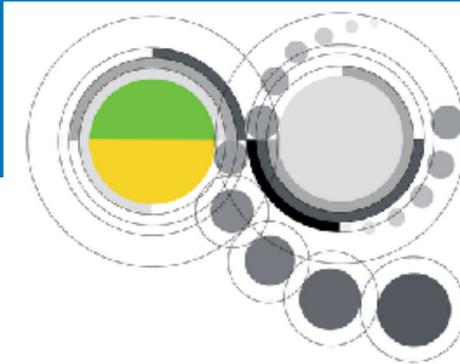
Polarisation cross section for various grain shape and size distribution



Average polarisation through the DISM



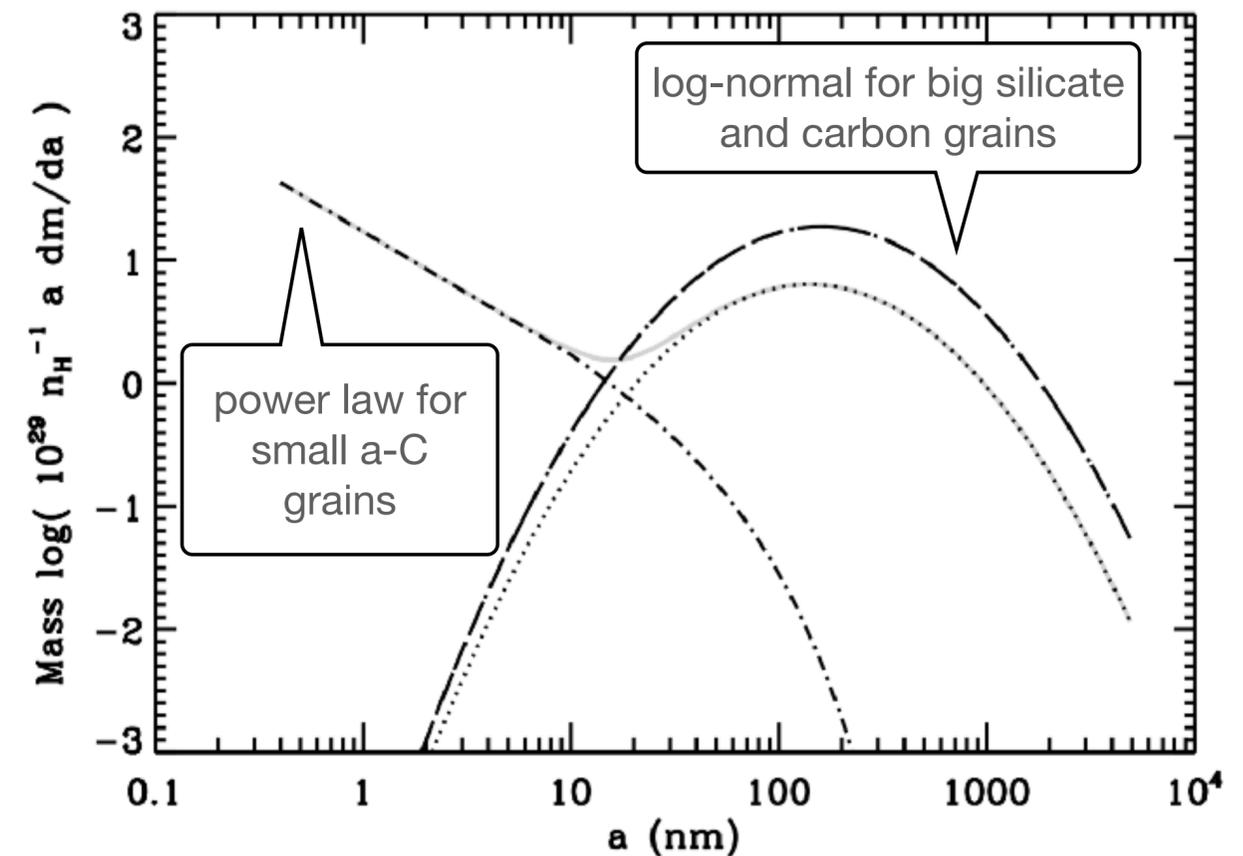
Cosmic dust models for the DISM



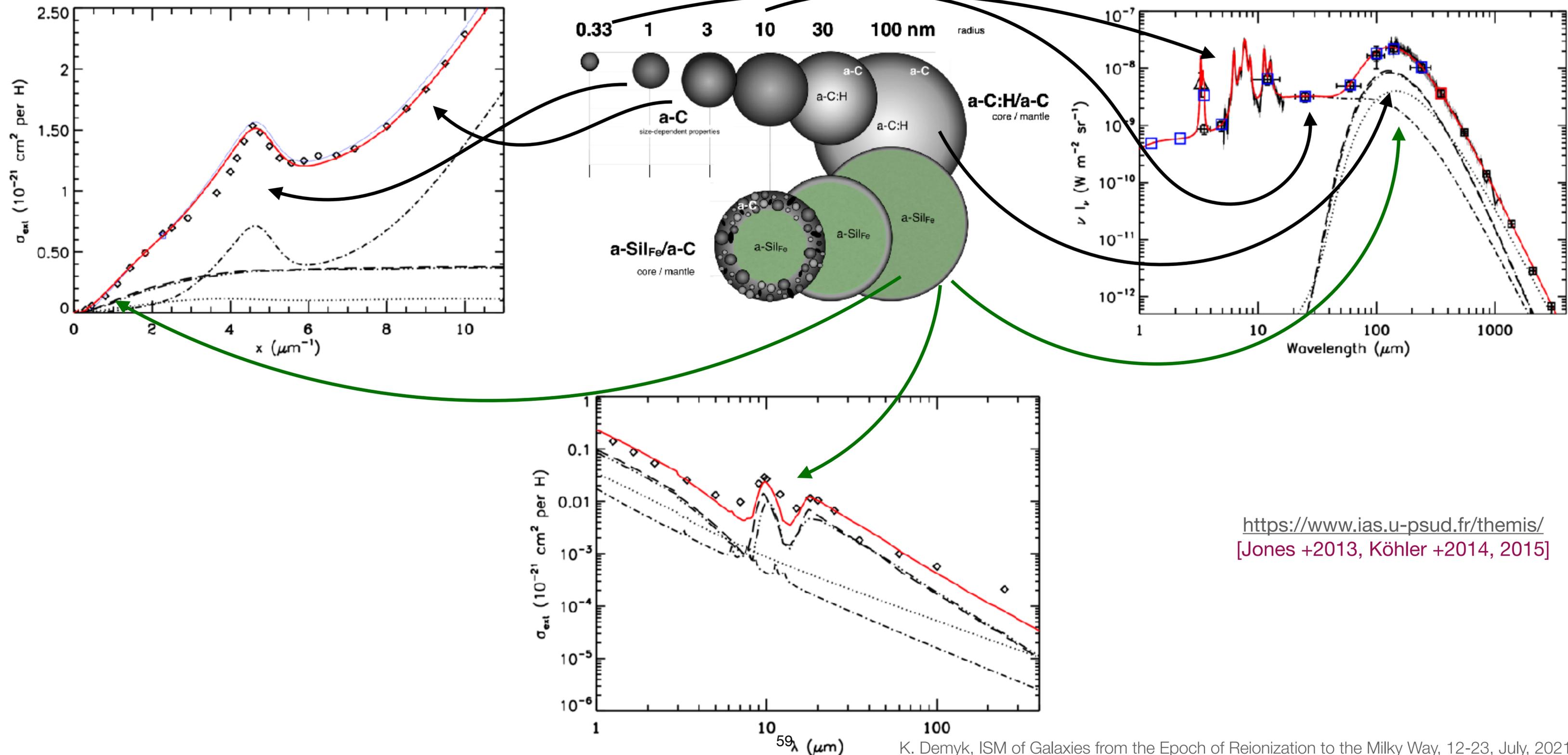
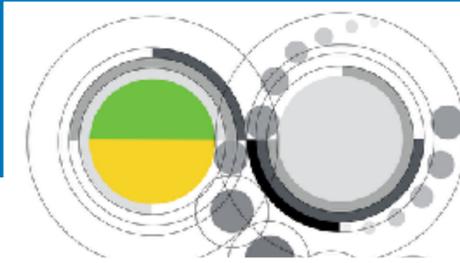
THEMIS: The Heterogeneous Evolution Model of ISM Solids

<https://www.ias.u-psud.fr/themis/>
[Jones +2013, Köhler +2014, 2015]

- Reproduces grain evolution in the ISM: mantle accretion and dust coagulation
- Core/mantle grain model
- Mixed solid phases of aromatic carbon (a-C), hydrogenated hydrocarbons (a-C:H) and silicates
- Two silicates dust component: amorphous enstatite (MgSiO_3) and forsterite (Mg_2SiO_4) with Fe and FeS inclusions
- a-C(:H) : hydrogenated amorphous carbon grains with varying optical properties with size and surface, calculated from physical models [see Jones 2012]

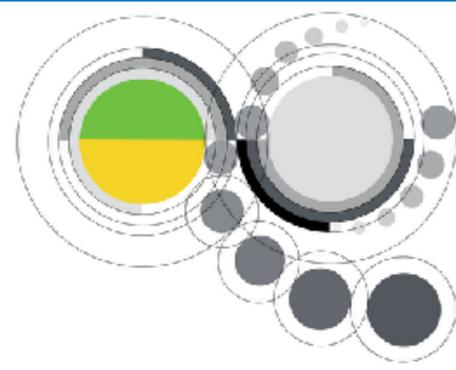


Cosmic dust models for the DISM



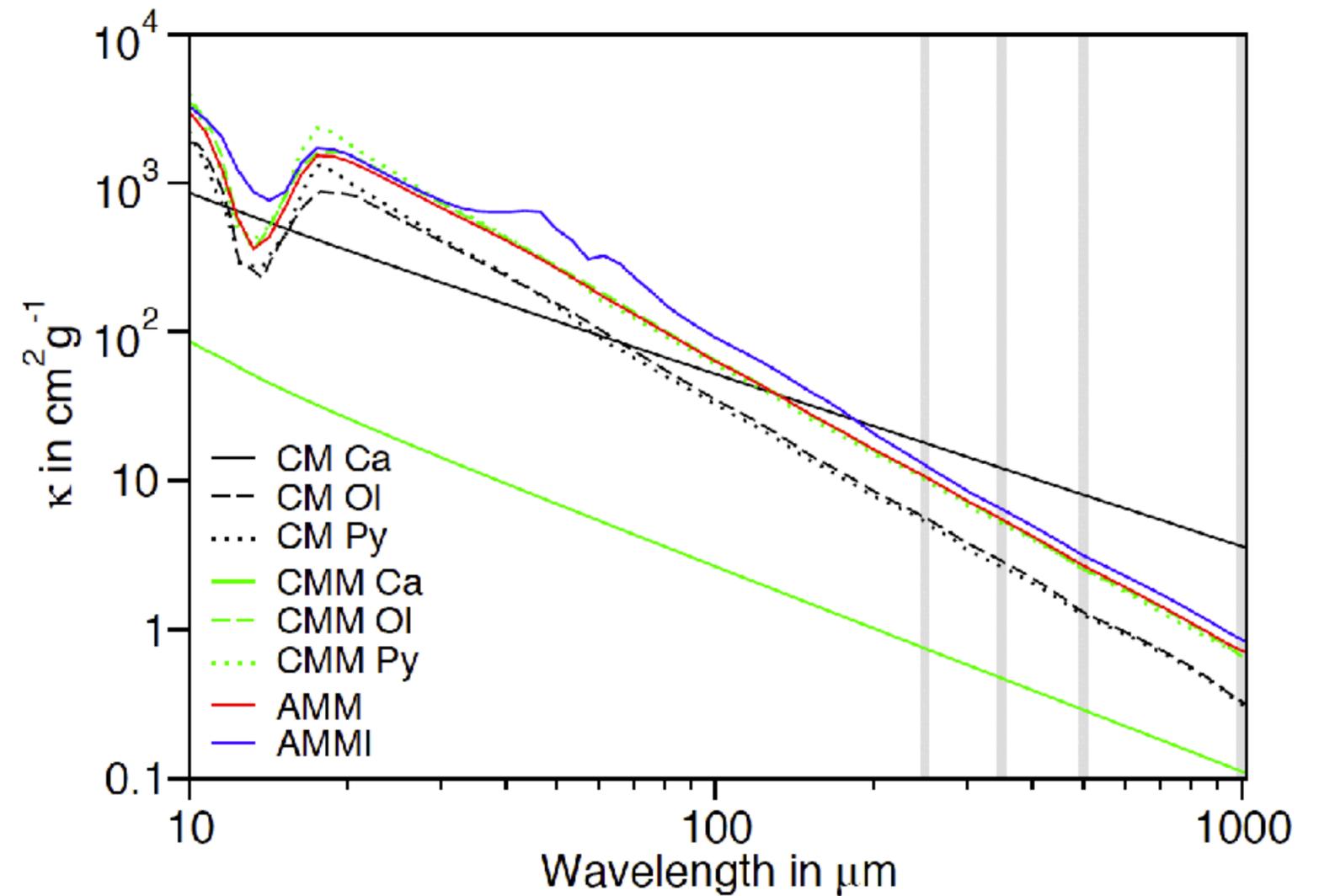
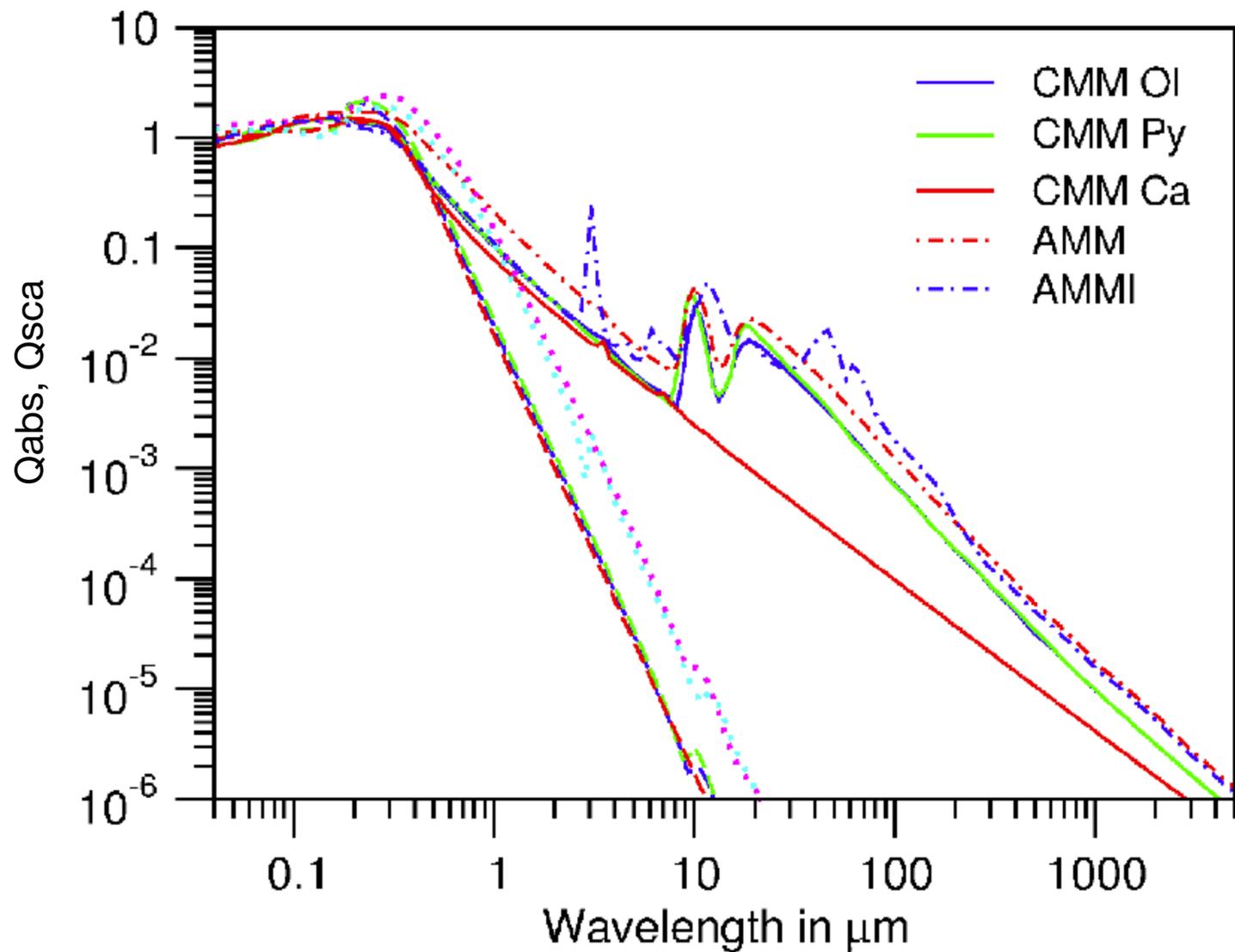
<https://www.ias.u-psud.fr/themis/>
 [Jones +2013, Köhler +2014, 2015]

Cosmic dust models for the dense ISM



THEMIS adaptation for the dense ISM:

<https://www.ias.u-psud.fr/themis/>
[Jones +2013, Köhler +2014, 2015]

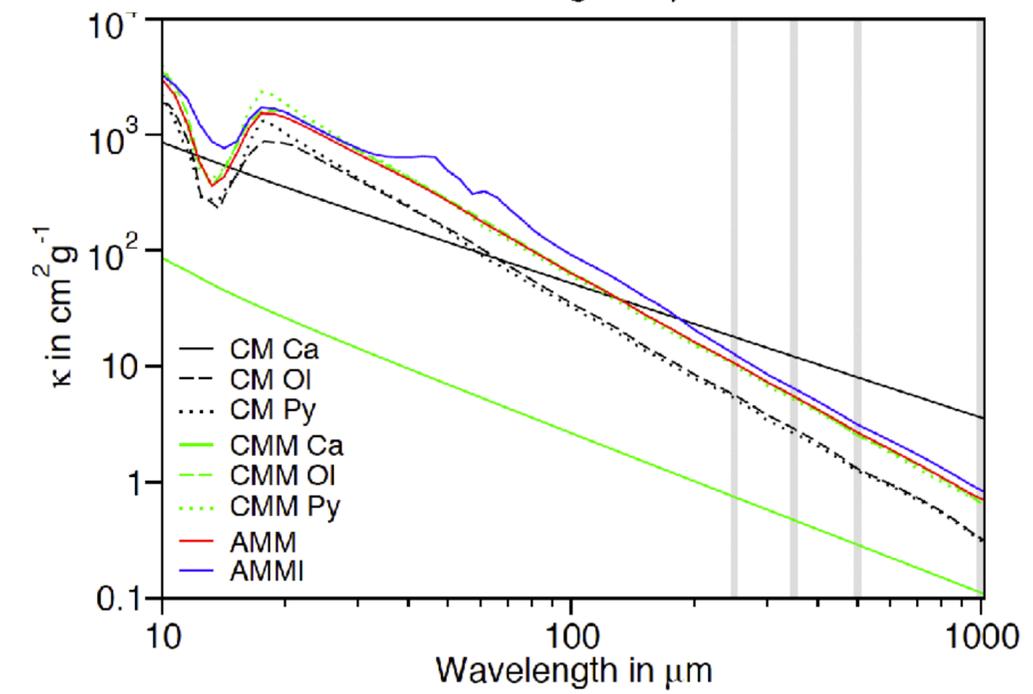
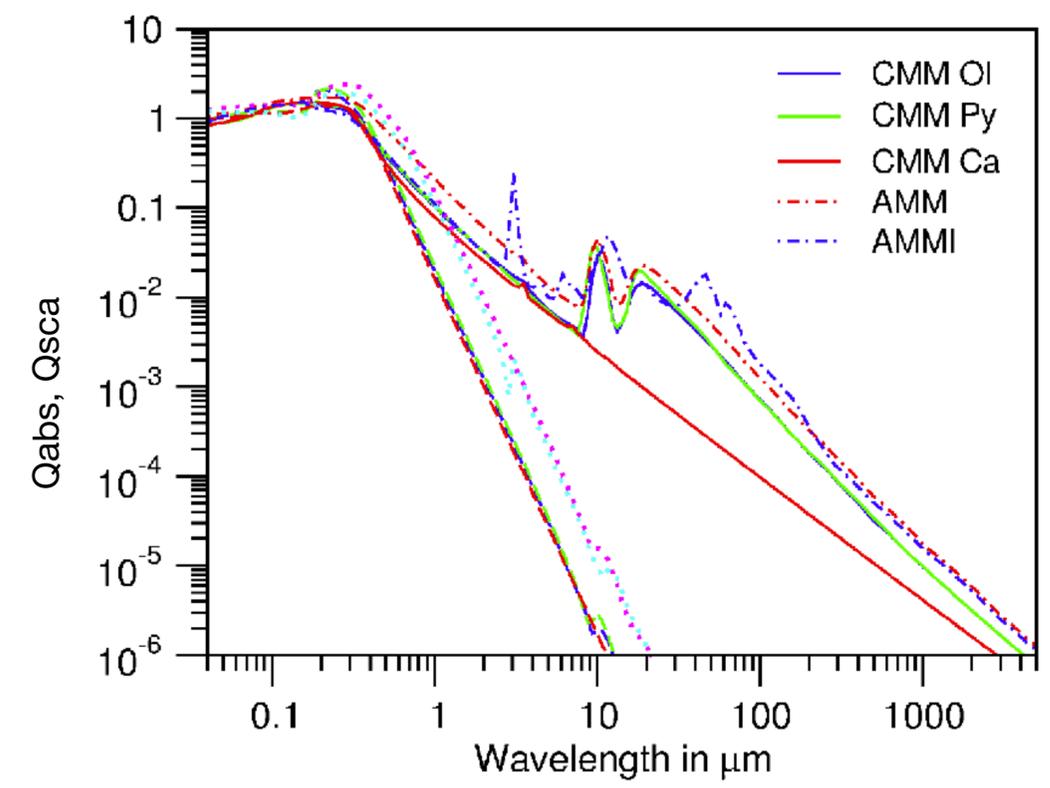
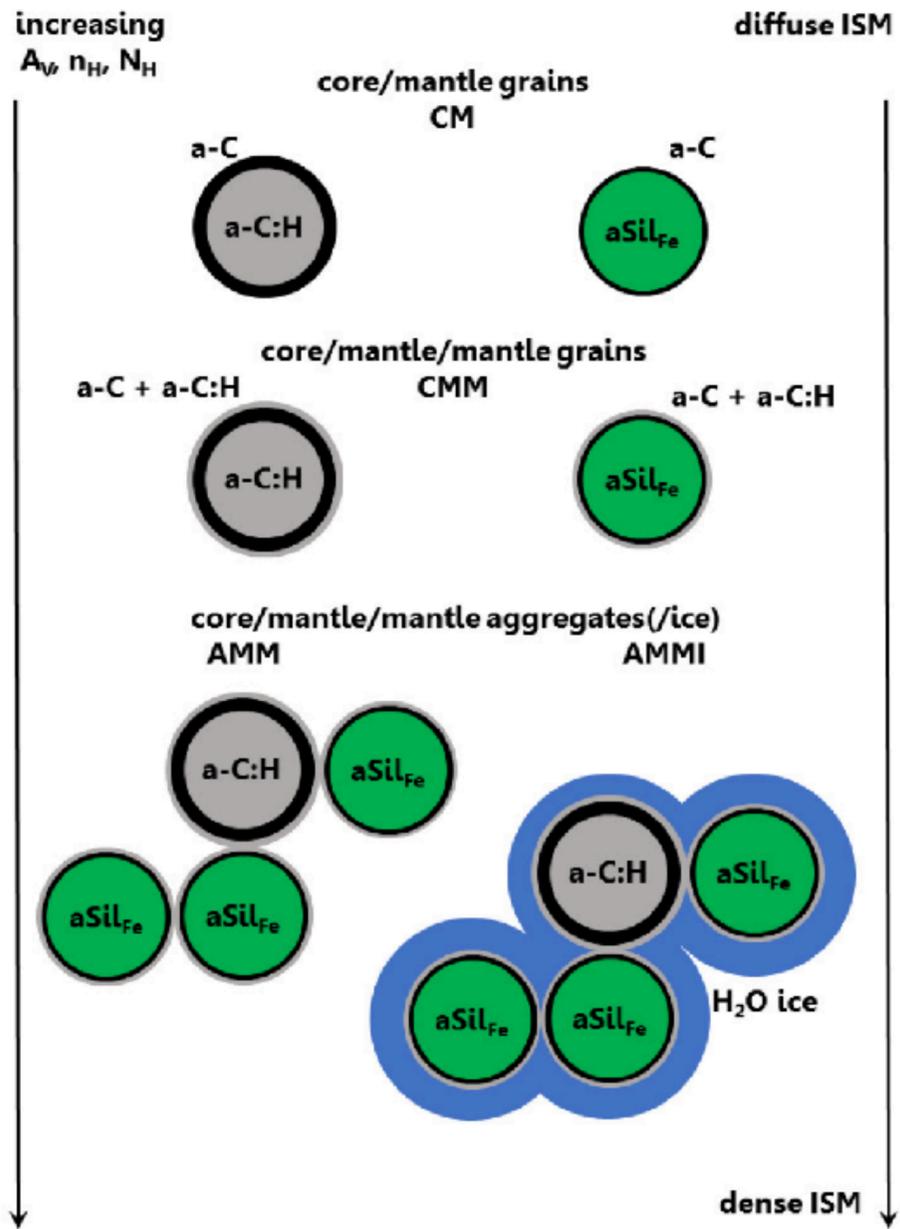


Cosmic dust models for the dense ISM

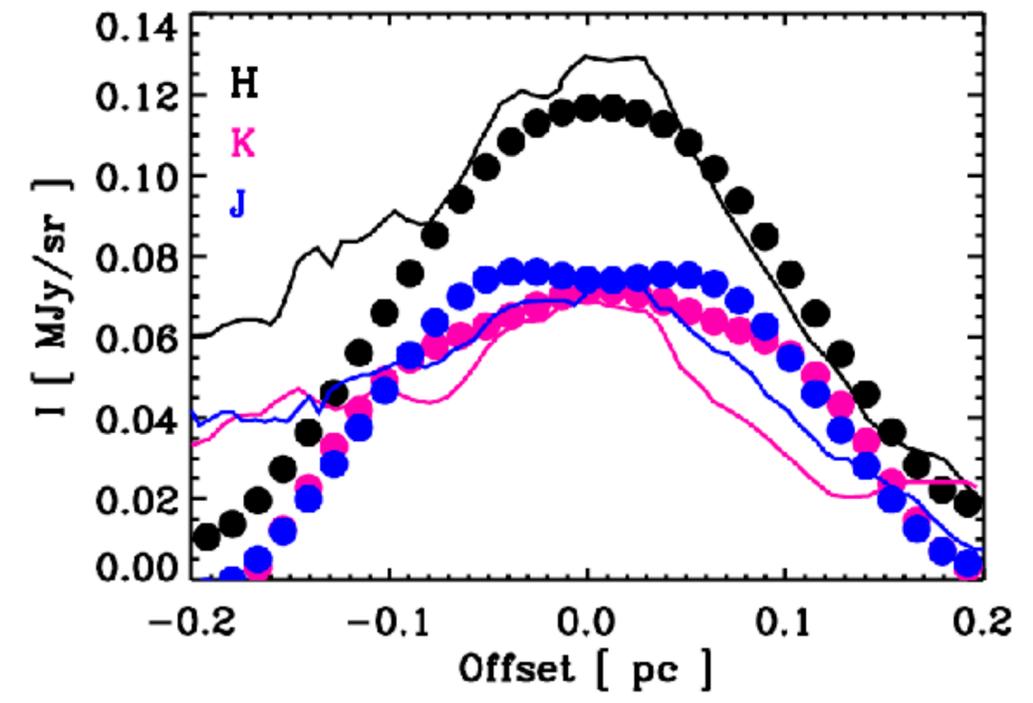
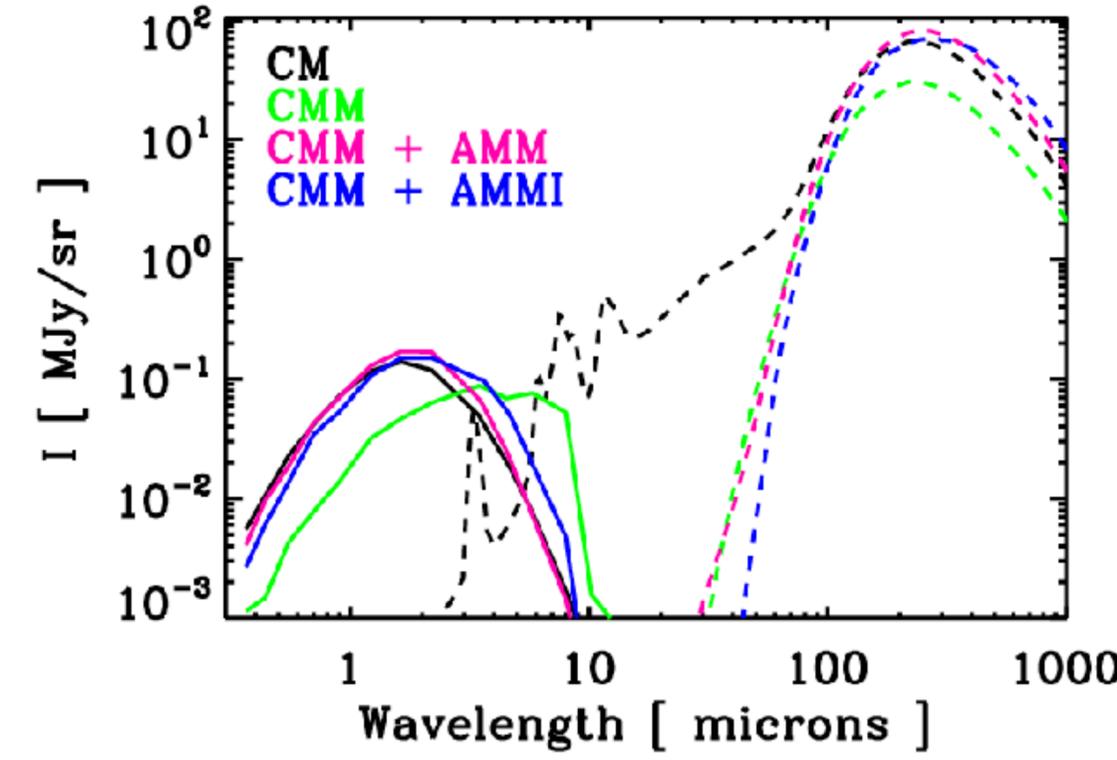


THEMIS adaptation for the dense ISM:

<https://www.ias.u-psud.fr/themis/>
 [Jones +2013, Köhler +2014, 2015]



Coreshine effect [Ysard+2016]



Some dust models for the DISM

Constraints from extinction & emission:

- Draine & Lee (1984) and later versions [eg. Weingartner & Draine 2001, Draine & Fraisse 2009...]: astrosilicates & graphite & PAHs
- Compiègne et al. 2011: astrosilicates & amorphous carbon & PAHs & PAHs⁺
- Zubko et al. 2004: astrosilicates & graphite or amorphous carbon & PAHs & H₂O ice and organic refractory
- The THEMIS model [Jones et al. 2013, 2017, Koehler et al. 2015]: lab silicates & a-C(:H)

Constraints from extinction, emission & polarisation:

- Siebenmorgen et al. 2014, 2017: astrosilicates & amorphous carbon & PAHs — *polarised extinction*
- Guillet et al. 2018: astrosilicates & amorphous carbon & PAHs — *polarised extinction and emission*
- Draine & Hensley (2021): *Astrodust* + PAHs — *polarised extinction*
- The THEMIS II model [Ysard et al. 2022]: lab silicates at low T & a-C(:H) — *polarised extinction and emission*

Some dust models for the dense ISM

Constraints from extinction & emission:

- Pollack (1994) model: lab silicates, Fe, organic C — molecular clouds and transition disks — extinction & emission
- Ossenkopf et al (1994): lab silicate and amorphous carbon grains, ices - dense protostellar cores — extinction & emission
- Zubko et al. 2004: astrosilicates & graphite or amorphous carbon & PAHs & H₂O ice and organic refractory
- The THEMIS model [Jones et al. 2013, 2017, Koehler et al. 2015]: lab silicates & a-C(:H) — extinction & emission

Cosmic dust models : summary

- There are many cosmic dust models
- Their differences are sometimes subtle because many models use the same or partly the same observational constraints and dust components.
- Some criteria to classify dust models:
 - The environment they are supposed to represent: diffuse vs dense medium
 - The observational constraints they consider
 - The adopted description of the dust: empirical (observational) vs physical (measurements on cosmic dust analogues or theory)
 - Their capacity to follow grain evolution and to adapt to other astrophysical environments
- No dust model is unique or perfect
- But they improve little by little as new observational constraints are available and as new results are obtained on dust analogues