DUST MODELS

Credit: *Rogelio Bernal Andreo*

Nathalie Ysard
Institut d’Astrophysique Spatiale, CNRS (France)

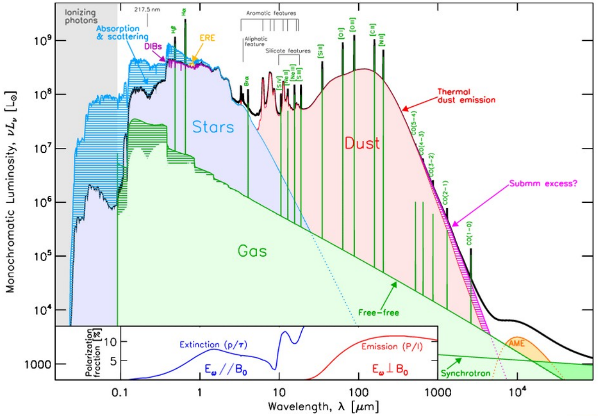
Dust everywhere

NGC 3190, VLT credit: ESO

- Interstellar medium less than 10% of the Milky Way mass
  Dust grains make only ~1 % of that mass
  Dust grains are tiny from a few Å to about 1 μm

- So why bother ? Because dust is everywhere !
  → extinction of UV and visible starlight
  → emission from near-IR to microwave

- An excellent tracer of matter in galaxies
  but also a major actor of its evolution



Galliano et al. (2018)

A major actor of matter evolution at all scales

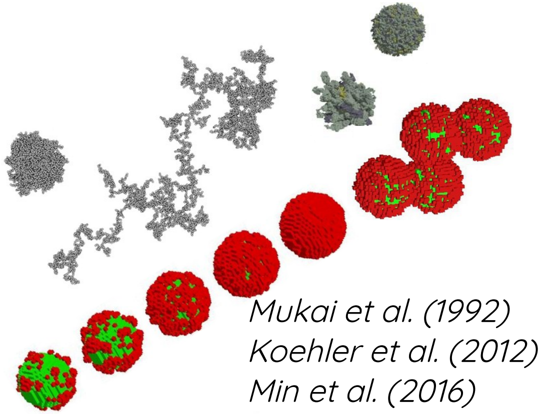
- Heating of the gas by photoelectic effect
  diffuse ISM ($A_V < 1$) & photon-dominated regions (PDRs)

- H_2 formation only possible on the grain surfaces
  intitiates all interstellar chemistry

- Determines if a cloud is optically thin or thick
  Molecules protected from photodissociation
  Reduced ionisation fraction
  Gas cooling through collisions

  } star formation

- Tracer for cloud masses & magnetic field

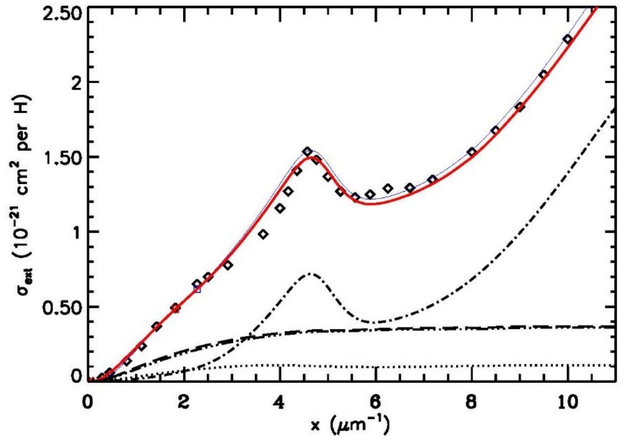


Mukai et al. (1992)
Koehler et al. (2012)
Min et al. (2016)

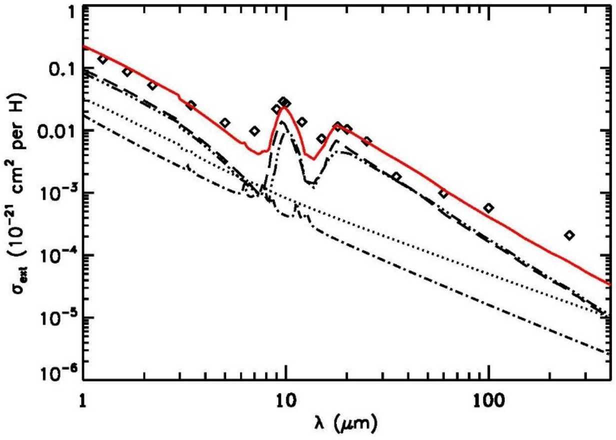
➡ ***All the above processes depend upon the exact grain size, structure, composition, shape and mass***

Dust basics: extinction & emission

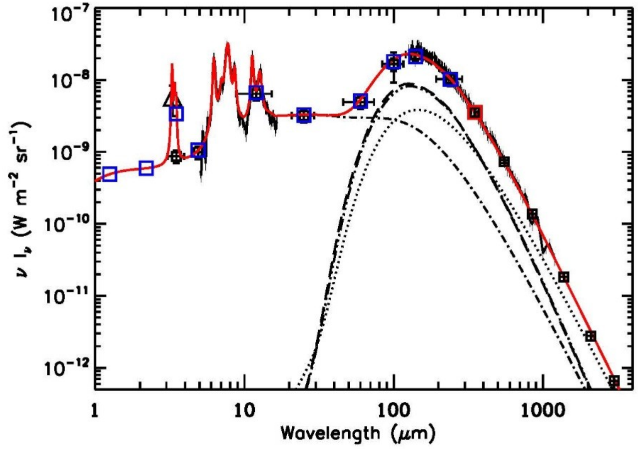
IR-vis-UV extinction



NIR-FIR extinction

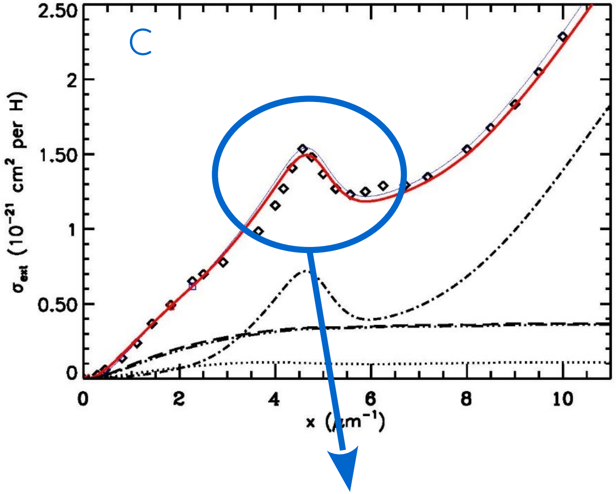


NIR-submm SED



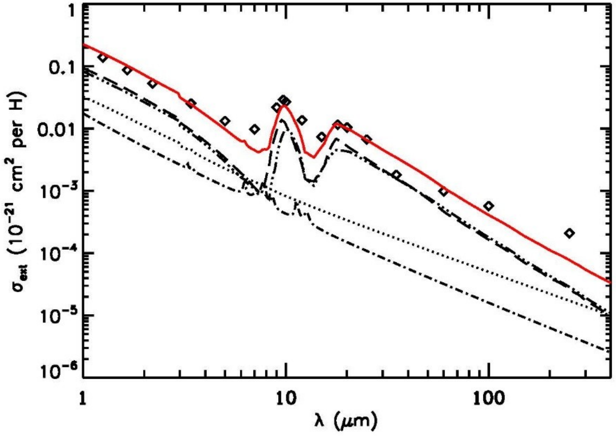
Dust basics: extinction & emission

IR-vis-UV extinction

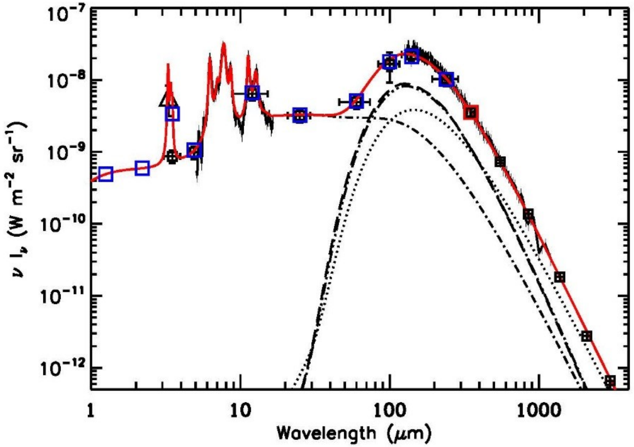


small carbonaceous particles

NIR-FIR extinction

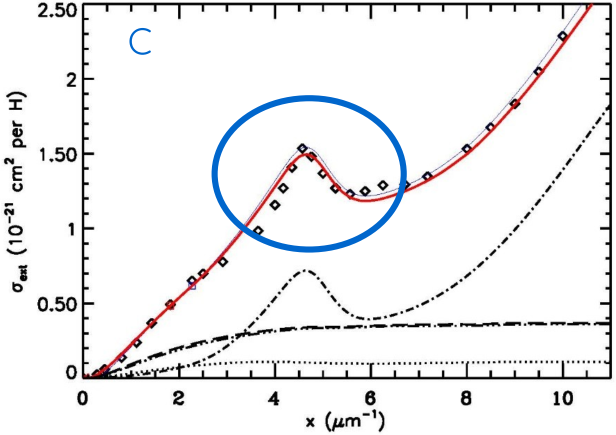


NIR-submm SED

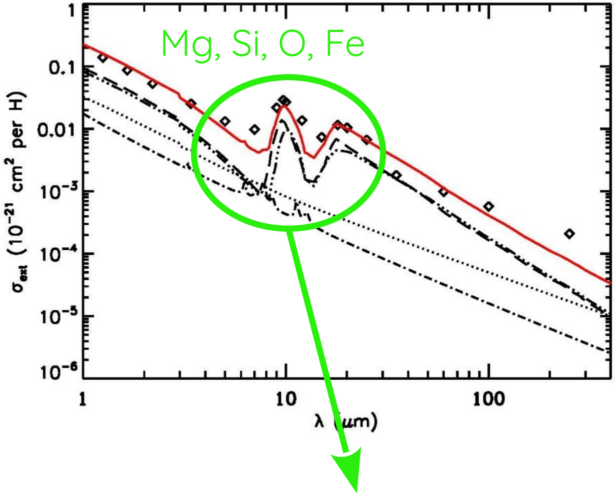


Dust basics: extinction & emission

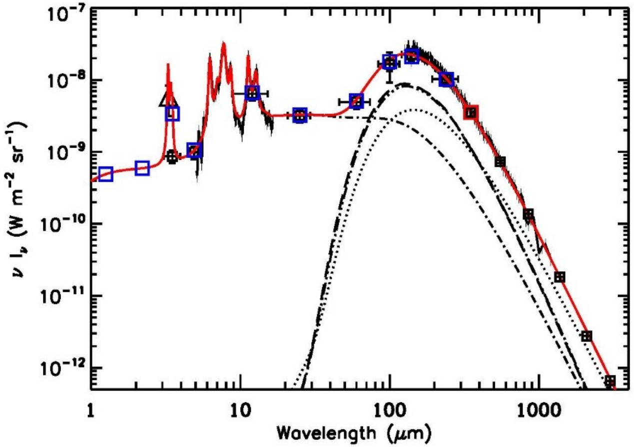
IR-vis-UV extinction



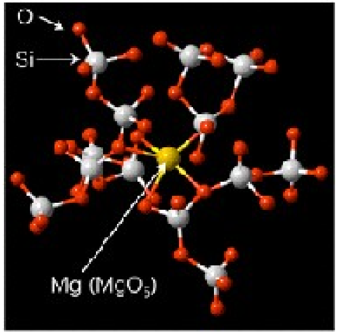
NIR-FIR extinction



NIR-submm SED



$MgSiO_3$ glass



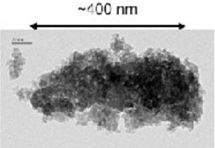
~ 9.7 and 18 microns features

amorphous silicates

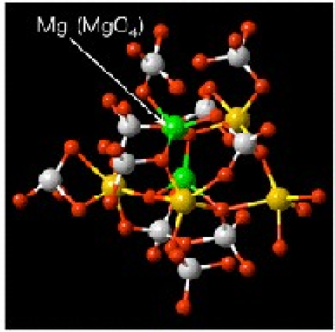
normative compositions of olivine & pyroxene

Mg_2SiO_4 & $MgSiO_3$

with metallic iron inclusions

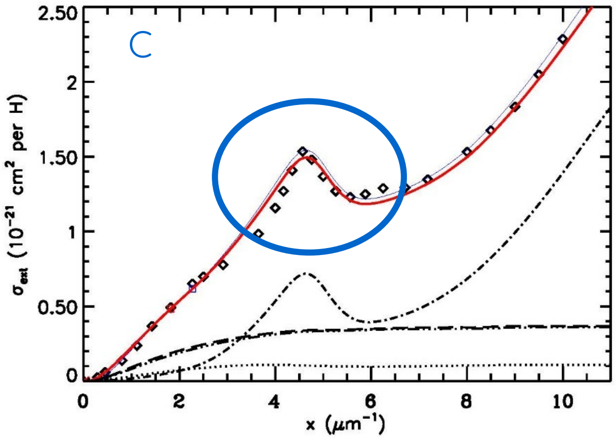


Mg_2SiO_4 glass

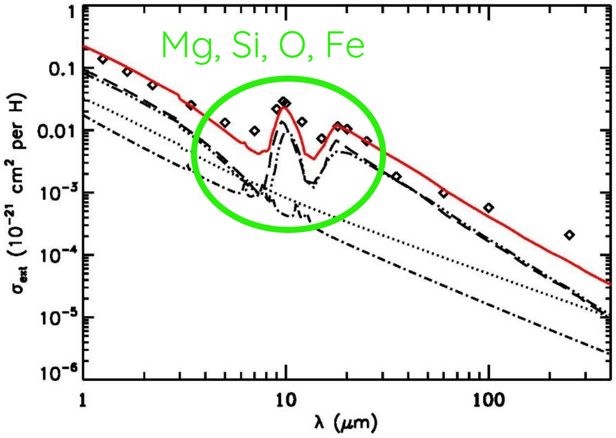


Dust basics: extinction & emission

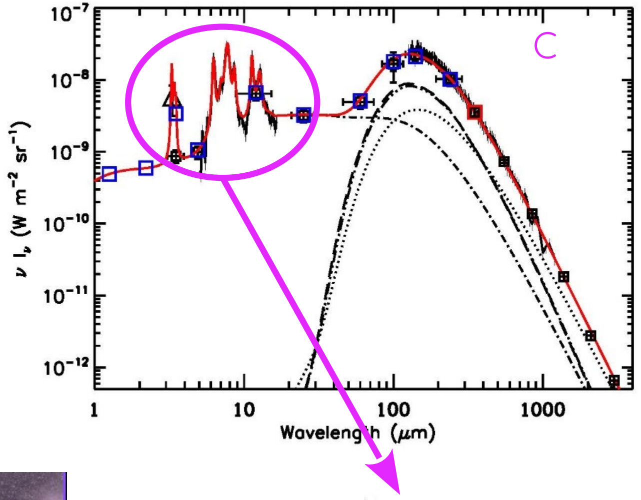
IR-vis-UV extinction

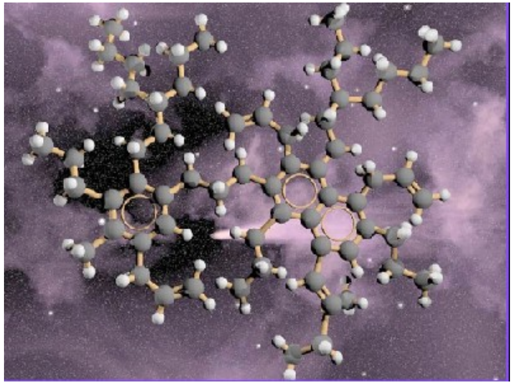


NIR-FIR extinction



NIR-submm SED

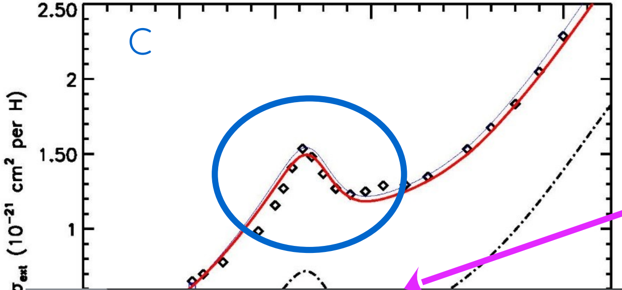




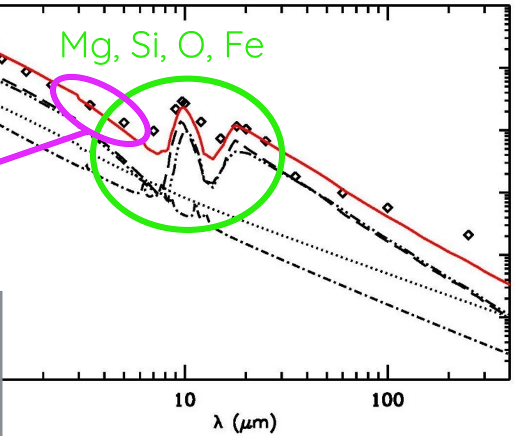
C-C and C-H on aromatic rings
on aliphatic chains
on olefinic bonds

Dust basics: extinction & emission

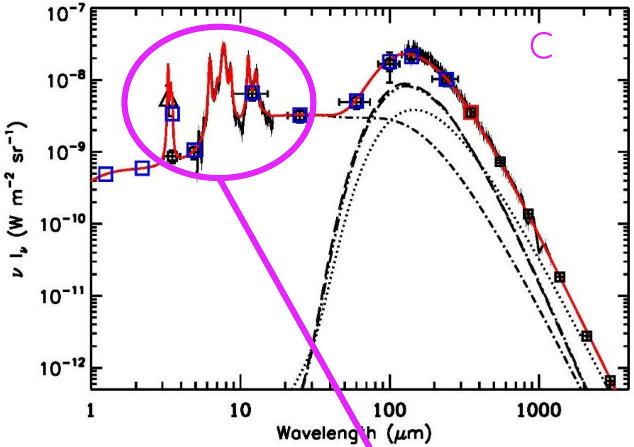
IR-vis-UV extinction



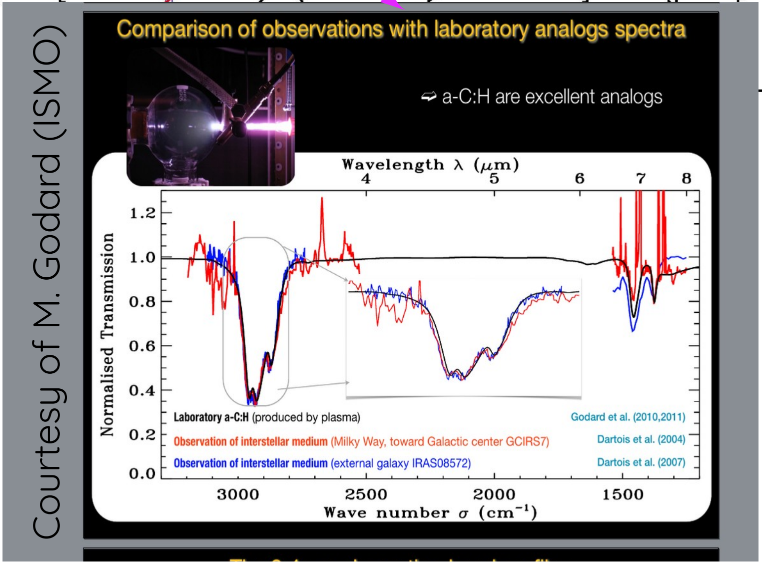
NIR-FIR extinction



NIR-submm SED



C-C and C-H on aromatic rings
on aliphatic chains
on olefinic bonds



Courtesy of M. Godard (ISMO)

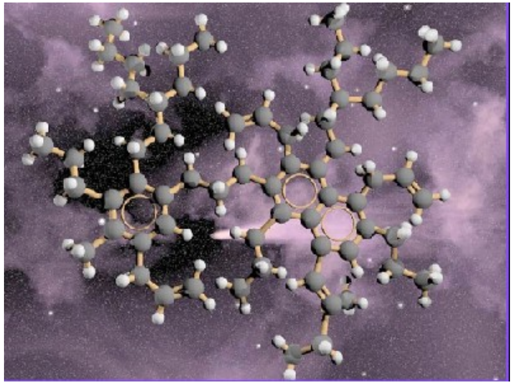
Comparison of observations with laboratory analogs spectra

➩ a-C:H are excellent analogs

Laboratory a-C:H (produced by plasma) Godard et al. (2010,2011)

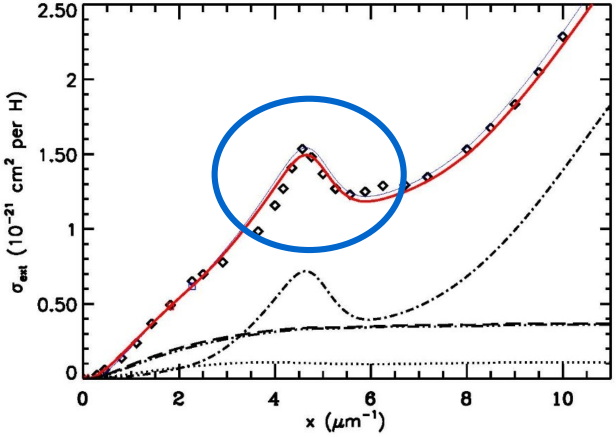
Observation of interstellar medium (Milky Way, toward Galactic center GCIRS7) Dartois et al. (2004)

Observation of interstellar medium (external galaxy IRAS08572) Dartois et al. (2007)

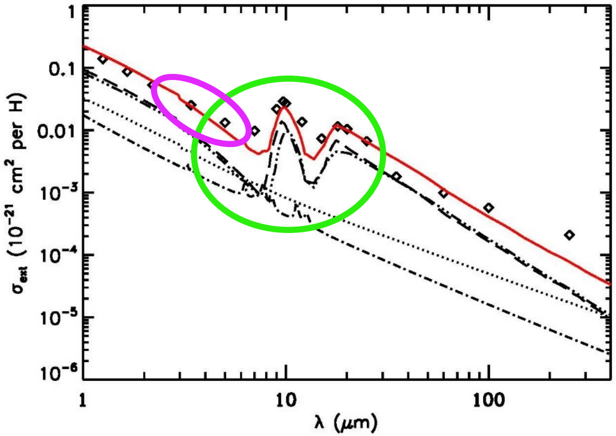


Dust basics: extinction & emission

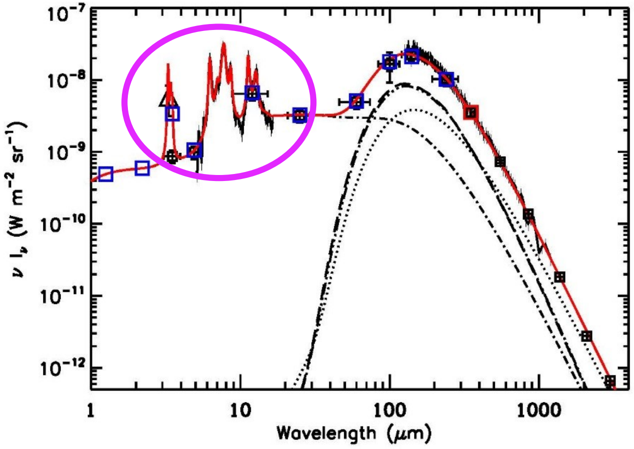
IR-vis-UV extinction



NIR-FIR extinction



NIR-submm SED

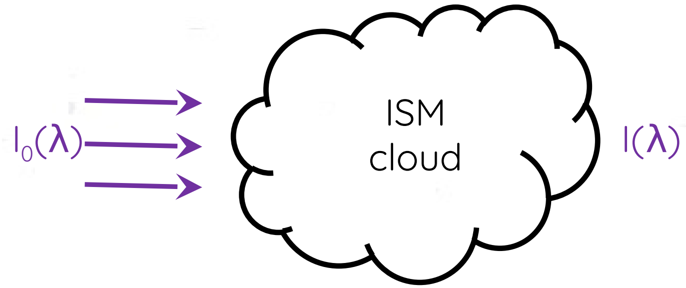


emission from NIR to submm

grains have different temperatures

grains have different sizes

Dust basics: extinction & emission



$I(\lambda) = I_0(\lambda)\, e^{-\tau_\lambda}$ $A(\lambda) = 1.086\, \tau_\lambda$

optical depth extinction

↳ depends on the grain composition, structure, and size

For spherical particles with radius *a*, one can define extinction cross-sections:

$\sigma_{ext} = \sigma_{abs} + \sigma_{sca}$

$\sigma_{abs} = \pi a^2\, Q_{abs}$ & $\sigma_{sca} = \pi a^2\, Q_{sca}$

absorption & scattering efficiencies

complex refractive index ←

Mie theory
Effective medium theory
Discrete dipole approximation, etc.

🔎 Tazaki & Tanaka (2018)
🔎 Ysard et al. (2018)

Dust basics: extinction & emission

Grain heating: absorption of UV/visible photons
Grain cooling: thermal emission of IR photons

Spherical grains of radius a illuminated by a radiation field density u_ν

$$E_{abs} = \int_0^\infty 4\pi a^2 \; Q_{abs}(\nu)\pi \; \frac{c u_\nu}{4\pi} \; d\nu$$

Dust basics: extinction & emission

Grain heating: absorption of UV/visible photons
Grain cooling: thermal emission of IR photons

Spherical grains of radius a illuminated by a radiation field density u_ν

$$E_{abs} = \int_0^\infty \underbrace{4\pi a^2}_{\text{grain surface}} \underbrace{Q_{abs}(\nu)\pi \underbrace{\frac{cu_\nu}{4\pi}}_{\text{flux per steradian}}}_{\text{energy absorbed per surface unit}} d\nu$$

Dust basics: extinction & emission

Grain heating: absorption of UV/visible photons
Grain cooling: thermal emission of IR photons

Spherical grains of radius *a* illuminated by a radiation field density u_ν

$$E_{abs} = \int_0^\infty \underbrace{4\pi a^2}_{\text{grain surface}} \underbrace{Q_{abs}(\nu)\pi \underbrace{\frac{cu_\nu}{4\pi}}_{\text{flux per steradian}}}_{\text{energy absorbed per surface unit}} d\nu$$

Emitted energy by a grain at temperature T

$$E_{\text{ém}} = \int_0^\infty 4\pi a^2 \; Q_{abs}(\nu) \; \pi B_\nu(T) \; d\nu$$

Dust basics: extinction & emission

Grain heating: absorption of UV/visible photons
Grain cooling: thermal emission of IR photons

Spherical grains of radius *a* illuminated by a radiation field density u_ν

$$E_{abs} = \int_0^\infty 4\pi a^2 \, Q_{abs}(\nu)\pi \, \frac{c u_\nu}{4\pi} \, d\nu$$

grain surface

energy absorbed
per surface unit

flux per
steradian

Emitted energy by a grain at temperature T

$$E_{\text{ém}} = \int_0^\infty 4\pi a^2 \, Q_{abs}(\nu) \, \pi B_\nu(T) \, d\nu$$

power emitted
per frequency unit

Planck function

$$E_{abs} = E_{\text{ém}} \longrightarrow T_{\text{éq}}$$

- Lèger et al. (1989)
- Draine & Li (2001)
- Krügel (2002)
- Lequeux (2002, 2005)

Dust basics: extinction & emission

small grains → weak heat capacity

at first order $E_{therm} \sim 3N_{at}k_BT$

$C(T) \sim 3N_{at}k_B$

one UV photon → quick and high T increase

$T \sim h\nu / 3N_{at}k_B$

30 atoms (~0.5nm) + $\langle h\nu \rangle = 8\text{eV} \Rightarrow \sim 1000\text{K}$!

quick cooling until the next absorption event

strong temperature fluctuations if $h\nu_m > \int_0^{T_{éq}} C(T)\,dT$

starting from T_0 $h\nu = \int_{T_0}^{T} C(T)\,dT$

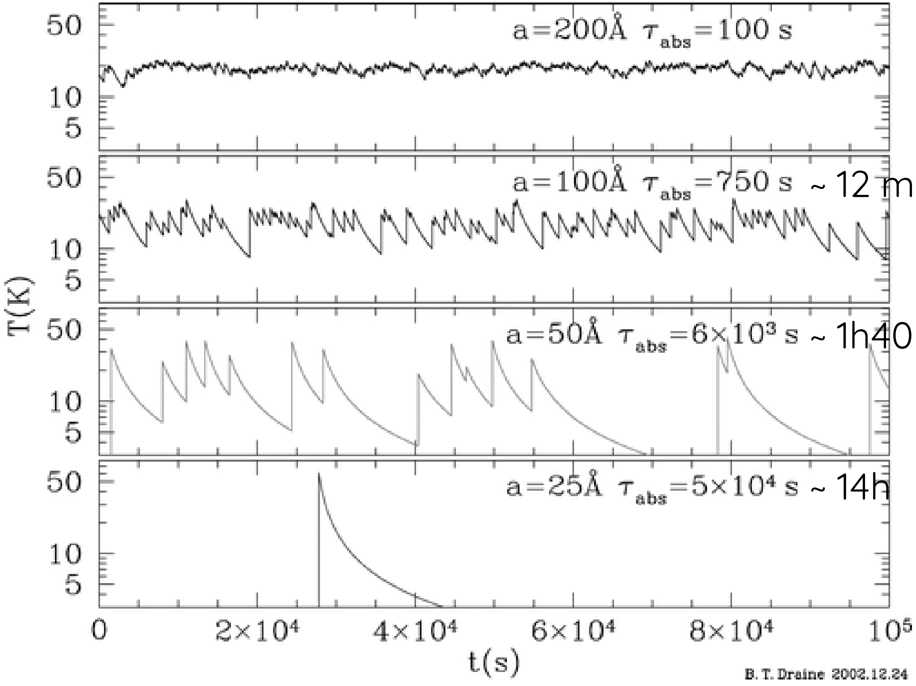
cooling as $\frac{dT}{dt} = \frac{1}{C(T)} \int_0^{\infty} 4\pi a^2\; Q_{abs}(\nu)\; \pi B_\nu(T)\; d\nu$

Dust basics: extinction & emission

small grains → weak heat capacity
at first order $E_{therm} \sim 3N_{at}k_BT$
$C(T) \sim 3N_{at}k_B$

one UV photon → quick and high T increase
$T \sim h\nu / 3N_{at}k_B$
30 atoms (~0.5nm) + $\langle h\nu \rangle$ = 8eV => ~ 1000K!

quick cooling until the next absorption event



~ 12 min

~ 1h40 min

~ 14h

smallest hydrocarbons ~ 1 year

Dust basics: extinction & emission

small grains → weak heat capacity

at first order $E_{therm} \sim 3N_{at}k_BT$

$C(T) \sim 3N_{at}k_B$

one UV photon → quick and high T increase

$T \sim h\nu / 3N_{at}k_B$

30 atoms (~0.5nm) + $\langle h\nu \rangle = 8$eV => ~ 1000K!

quick cooling until the next absorption event

strong temperature fluctuations if $h\nu_m > \int_0^{T_{éq}} C(T)\,dT$

starting from T_0 $h\nu = \int_0^{T} C(T)\,dT$

cooling as $\frac{dT}{dt} = \frac{1}{C(T)} \int_0^{\infty} 4\pi a^2\; Q_{abs}(\nu)\; \pi B_\nu(T)\; d\nu$

small grain emission

$$E_{ém}(\nu) = \int_0^{\infty} 4\pi a^2\; Q_{abs}(\nu)\; \pi B_\nu(T)\,\frac{dP}{dT}\,dT$$

Lèger et al. (1989)

Draine & Li (2001)

Krügel (2002)

Lequeux (2002, 2005)

Basics of all dust models

- Chemical composition
  - → $m = n + ik$: from the lab ? empirical ?
  - → composite grains ?
  - → inclusions, ice mantles ?
- Structure
  - → compact vs. porous
  - → core/mantle
  - → single grains vs. aggregates
  - → spheres vs. spheroids vs. irregular grains

Absorption efficiency $Q_{abs}(a, \lambda, T?)$
Scattering efficiency $Q_{sca}(a, \lambda)$
Scattering phase function $g(a, \lambda)$
Heat capacity $C(a, T)$

non-trivial step

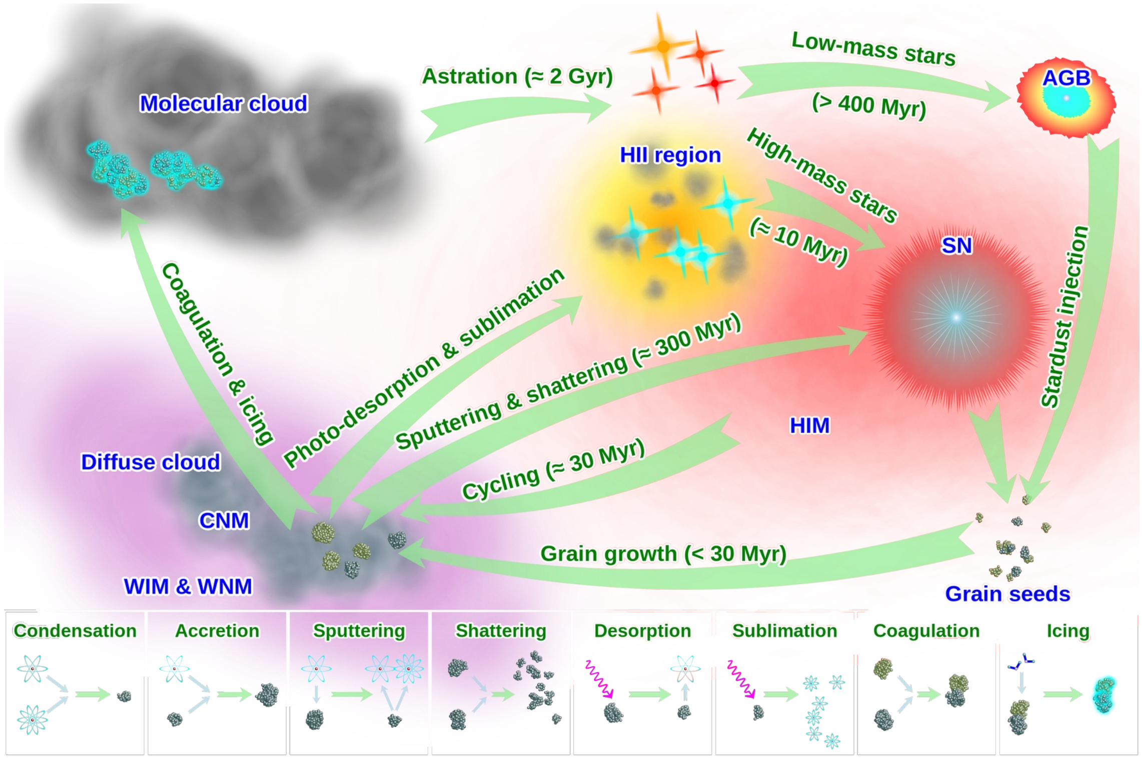
- Size distribution
  - → a_{min}, a_{max}
  - → log-normal, power-law, MRN, weird ?

Calculation of the optical properties: how ?

• Compact spherical grains Compact spherical grains with mantles	Mie: BHMIE BHCOAT 🔎 Van de Hulst (1957), Bohren & Huffman (1983)
• Porous grains Composite grains → random distribution	Effective Medium Theory (EMT) Maxwell Garnett or Bruggeman 🔎 Van de Hulst (1957), Bohren & Huffman (1983)
• Aggregates with one-point contact	T-MATRIX 🔎 Mishenko (2000)
• Aggregates with contact surface area Grains of any shape Composite/porous grains → controlled distribution	Discrete Dipole Approximation (DDA) 🔎 Draine & Flatau (1994), Yurkin & Hoekstra (2011)
• Spheroidal grains with or without mantles	DDA, T-MATRIX Analytical function in the Rayleigh limit Geometric limit in the UV 🔎 Van de Hulst (1957), Bohren & Huffman (1983)

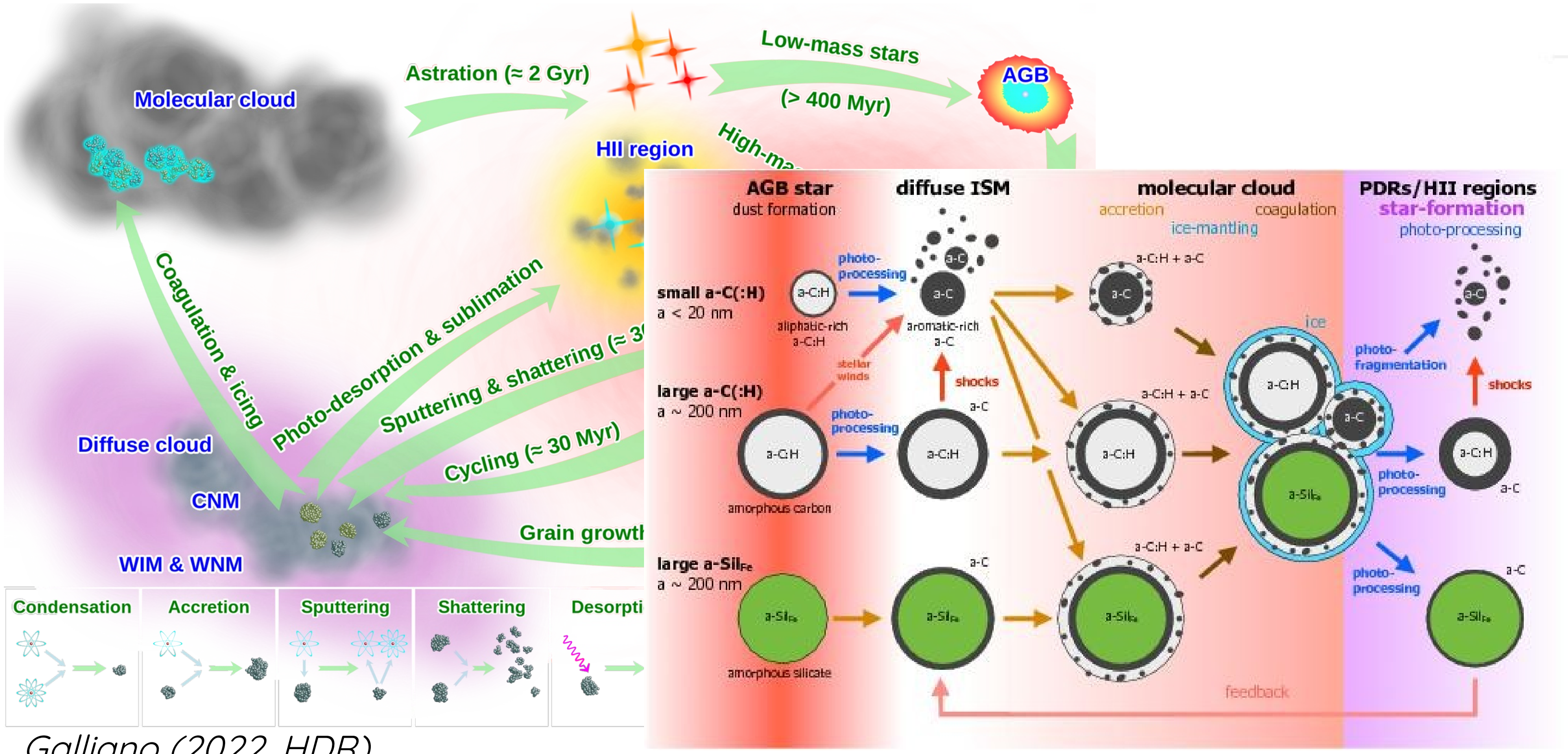
Comparison of methods
in Tazaki & Tanaka (2018)

Lifecycle of interstellar dust: a restless journey



Galliano (2022, HDR)

Lifecycle of interstellar dust: a restless journey



Galliano (2022, HDR)

Jones et al. (2013)

Summary

- What should a Galactic dust model fit ?
  - → observations of the diffuse ISM
  - → observations of the dense ISM
  - → observations of PDRs

- Dust models: 2 public examples
  - → an empirical model
  - → a lab-based model

- A few points to bear in mind when using dust models
  - → uncertainties in models
  - → grain size determination
  - → cloud mass estimate

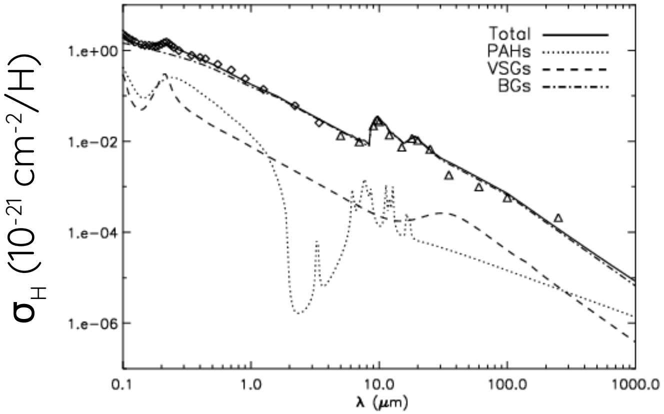
Summary

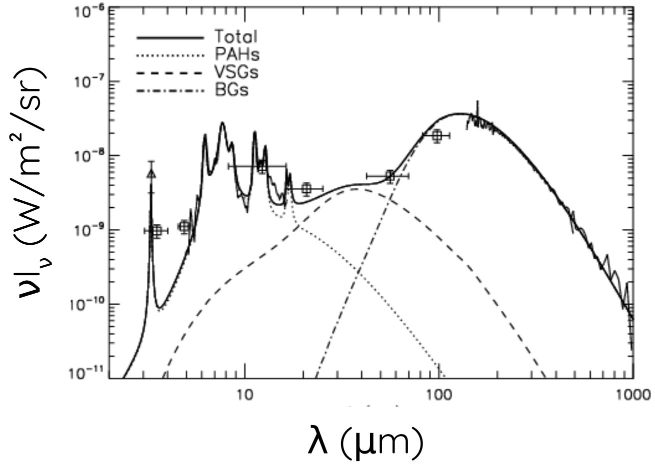
- **What should a Galactic dust model fit ?**
  - **→ observations of the diffuse ISM**
  - → observations of the dense ISM
  - → observations of PDRs

- Dust models: 2 public examples
  - → an empirical model
  - → a lab-based model

- A few points to bear in mind when using dust models
  - → uncertainties in models
  - → grain size determination
  - → cloud mass estimate

What do we have to constrain the grain properties ?





- Depletion measurements + X-ray → composition
- Extinction

  $E(B-V) = A_B - A_V$ & $R_V = A_V / E(B-V)$

  mid-IR silicate bands at ~ 10 and 18 μm
- Emission

  mid-IR to far-IR ratio

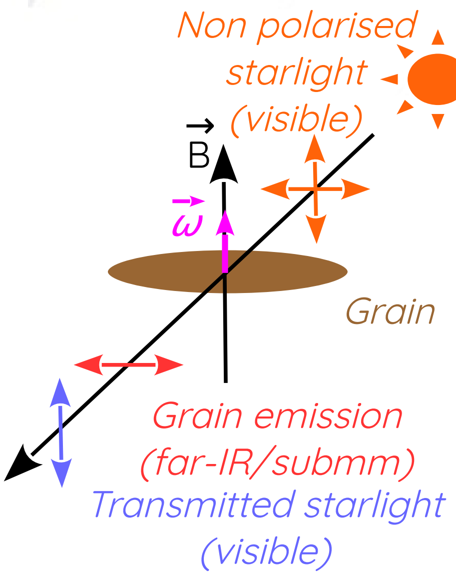
  modified BB fit → $I_\nu = N_H\, \sigma_{\nu 0}\, B_\nu(T)\, (\nu/\nu_0)^\beta$

  optical depth → $\tau_{\nu 0} = N_H\, \sigma_{\nu 0}$
- Scattered light from visible to mid-IR → size
- Polarisation

  λ_{max} → peak wavelength of starlight polarisation

  P/I → polarisation fraction in far-IR/submm

What do we have to constrain the grain properties ?



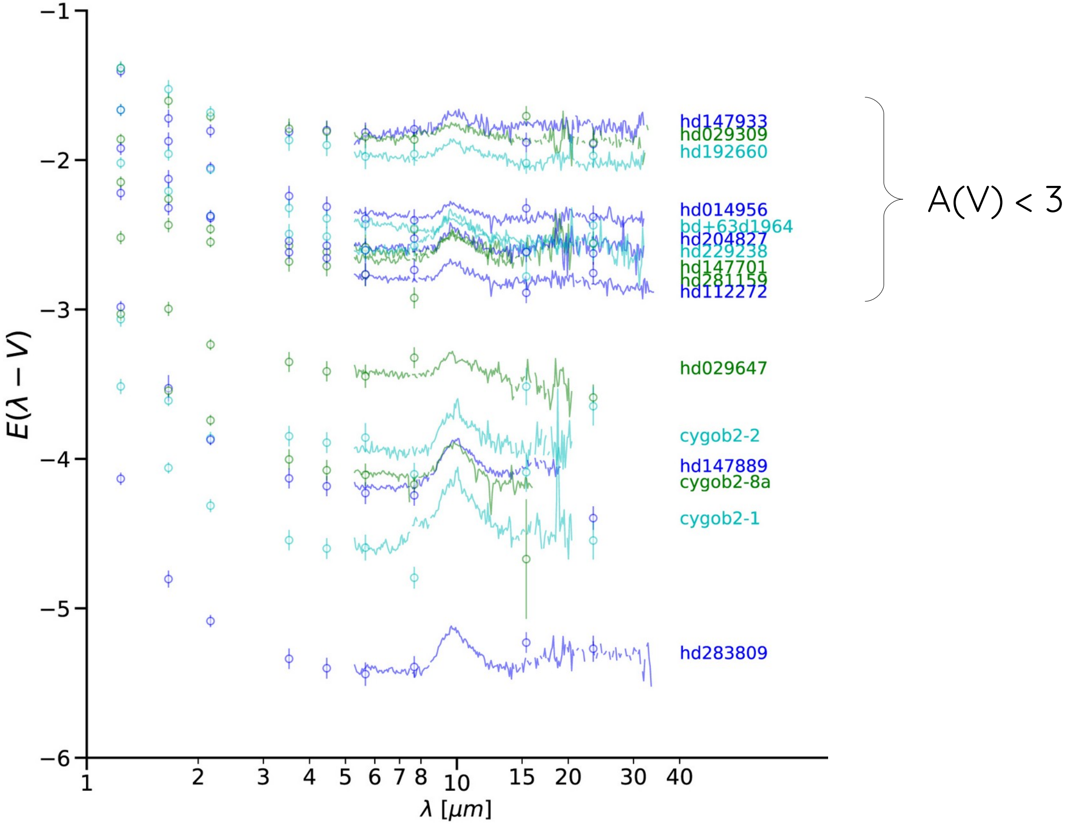
- Depletion measurements + X-ray → composition
- Extinction
  - $E(B-V) = A_B - A_V$ & $R_V = A_V / E(B-V)$
  - mid-IR silicate bands at ~ 10 and 18 μm
- Emission
  - mid-IR to far-IR ratio
  - modified BB fit → $I_\nu = N_H \, \sigma_{\nu 0} \, B_\nu(T) \, (\nu/\nu_0)^\beta$
  - optical depth → $\tau_{\nu 0} = N_H \, \sigma_{\nu 0}$
- Scattered light from visible to mid-IR → size
- Polarisation
  - λ_{max} → peak wavelength of starlight polarisation
  - P/I → polarisation fraction in far-IR/submm

→ ***Grain composition, abundance, size, shape, structure…***

What should a dust model fit for the diffuse ISM ?

Variations in the extinction curve

Gordon et al. (2021), Decleir et al. (2022)



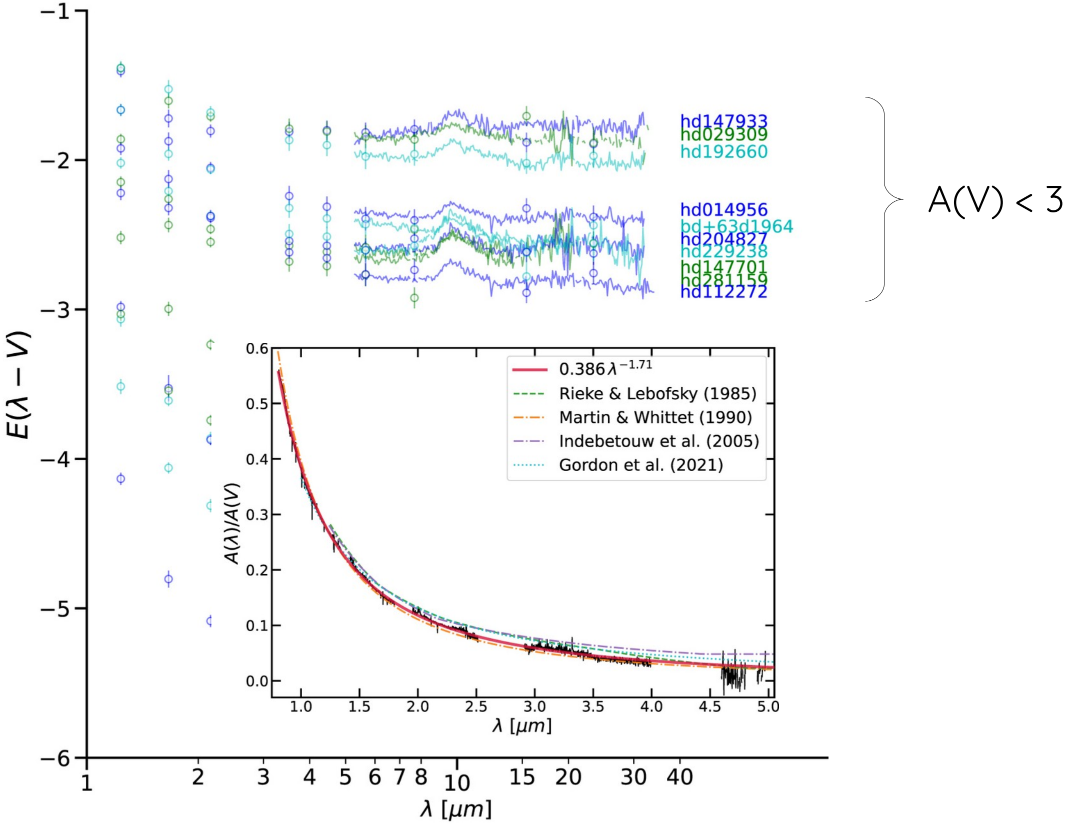
- 16 reddened stars Spitzer IRS spectra
- Silicate band-to-continuum ratio increases with increasing A(V)
- Small variations in the near-IR (IRTF SpeX)

Variation in grain size distributions ?
Iron nano-inclusions vs. Fe^{2+} in the silicate matrix ?
Different silicate/carbon mixing ?
Different grain shapes ?

What should a dust model fit for the diffuse ISM ?

Variations in the extinction curve

Gordon et al. (2021), Decleir et al. (2022)



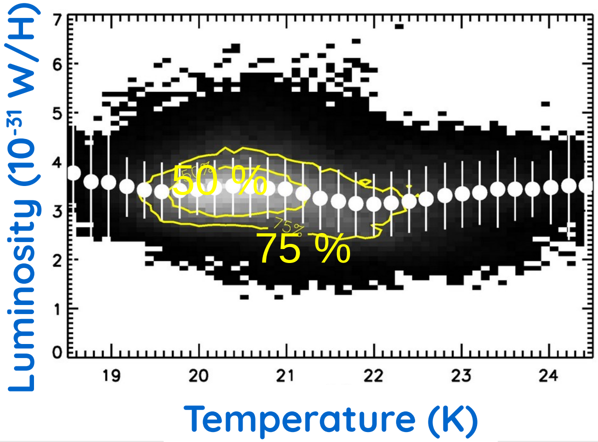
- 16 reddened stars Spitzer IRS spectra
- Silicate band-to-continuum ratio increases with increasing A(V)
- Small variations in the near-IR (IRTF SpeX)

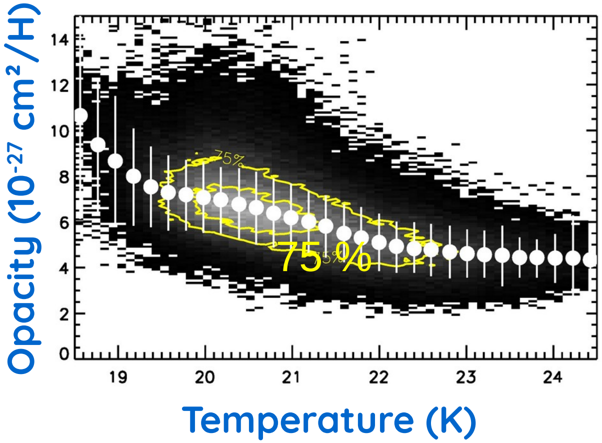
Variation in grain size distributions ?
Iron nano-inclusions vs. Fe^{2+} in the silicate matrix ?
Different silicate/carbon mixing ?
Different grain shapes ?

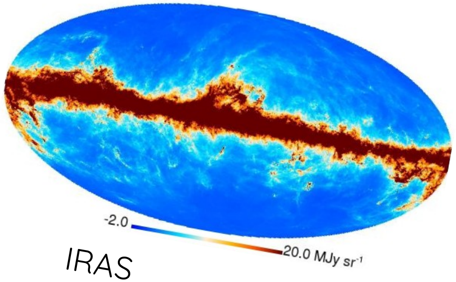
What should a dust model fit for the diffuse ISM ?

All-diffuse-sky variations in the dust properties

Planck Collaboration XI (2014): $N_H < 3\times10^{20}$ H/cm²







IRAS

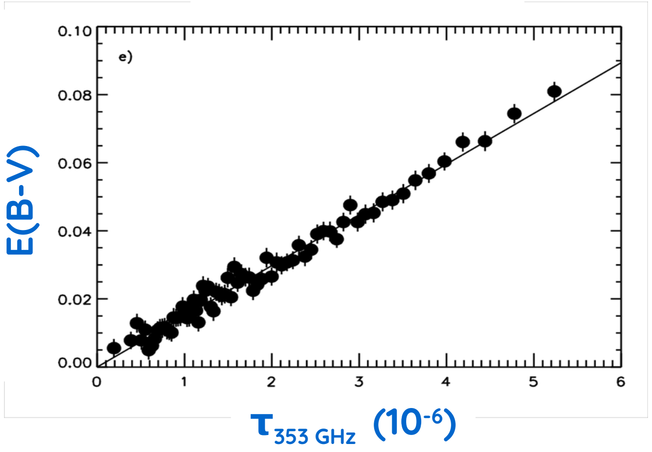
Planck-HFI

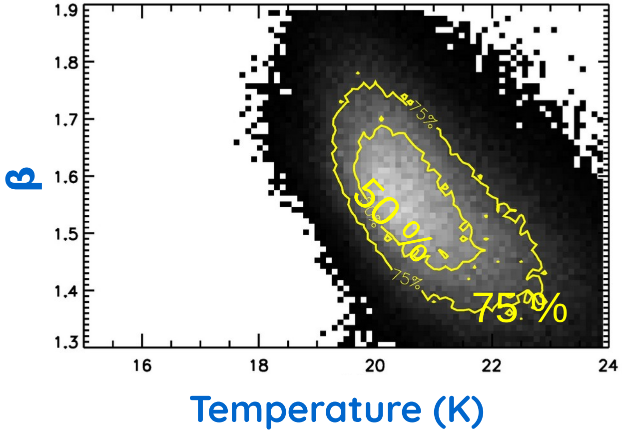
- 100 µm
- 350 µm
- 550 µm
- 850 µm

$$I_\nu = N_H\, \sigma_{\nu 0}\, B_\nu(T)\, (\nu/\nu_0)^\beta$$

$$L_H = \int I_\nu\, d\nu \,/\, N_H$$

$$\tau_{\nu 0} = N_H\, \sigma_{\nu 0}$$

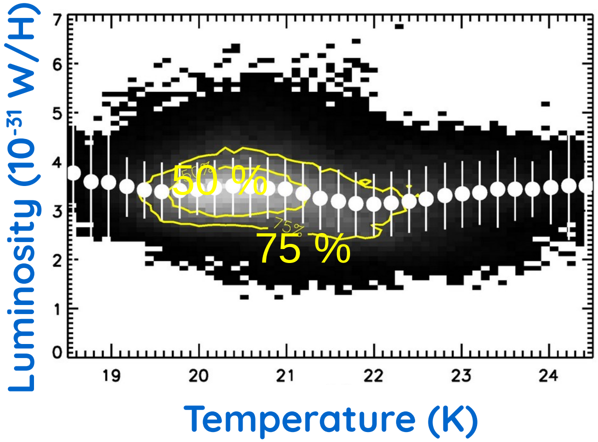


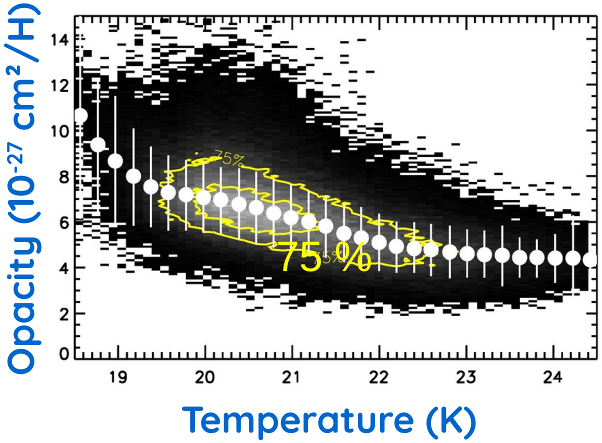


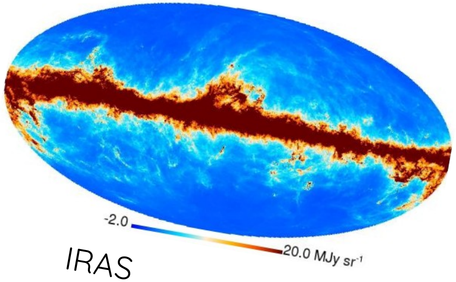
What should a dust model fit for the diffuse ISM ?

All-diffuse-sky variations in the dust properties

Planck Collaboration XI (2014): $N_H < 3\times10^{20}$ H/cm^2







IRAS

Planck-HFI

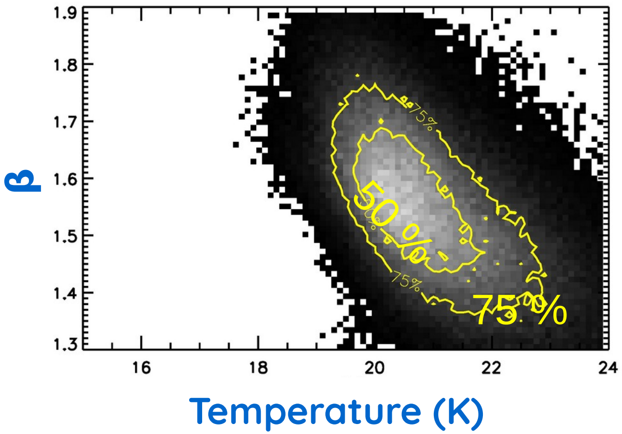
- 100 µm
- 350 µm
- 550 µm
- 850 µm

$$I_\nu = N_H\, \sigma_{\nu 0}\, B_\nu(T)\, (\nu/\nu_0)^\beta$$

$$L_H = \int I_\nu\, d\nu \,/\, N_H$$

$$\tau_{\nu 0} = N_H\, \sigma_{\nu 0}$$

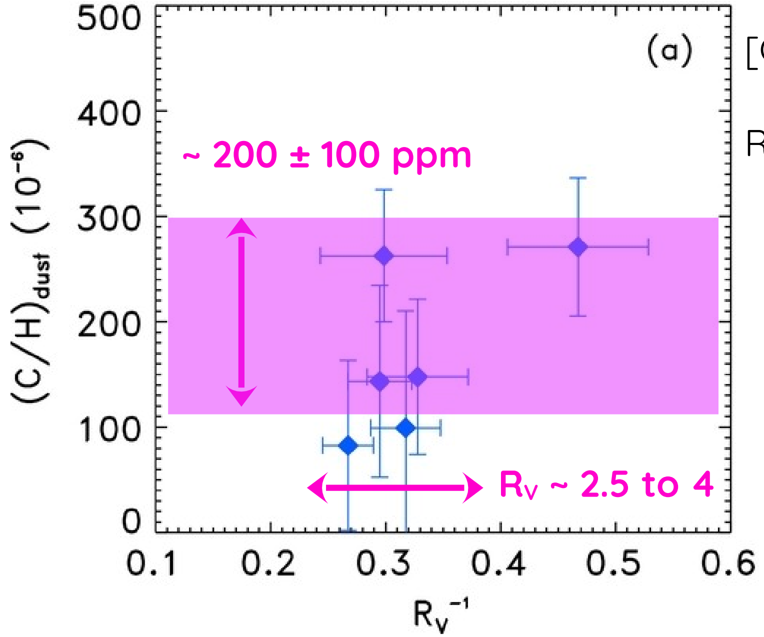
- $N_H < 3\times10^{20}$ H/cm^2
- E(B-V) from SDSS data towards quasars
- Observational results
  → β-T variations
  → luminosity independent of T
  → hotter grains = less emissive grains



Carbon depletion in the diffuse ISM

Parvathi et al. (2012)

- 21 Galactic sightlines toward neutral medium
  - CII measurements from the 1334 Å transition
  - local variations in the total carbon abundance gas+dust
  - local variations in the carbon depletion



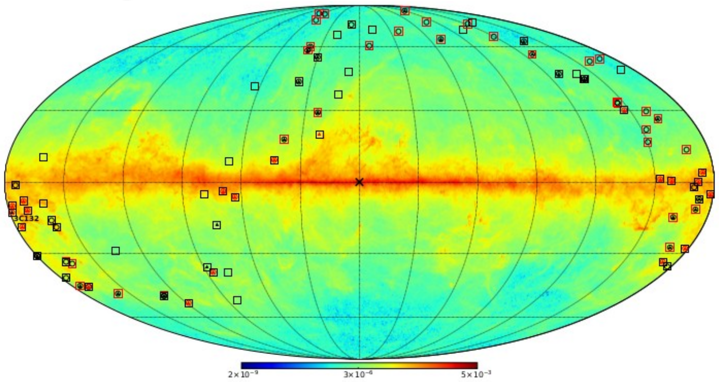
$[C/H]_{dust}$ for $N_H < 10^{21}$ cm²

$R_V = A_V / E(B-V)$

What should a dust model fit for the diffuse ISM ?

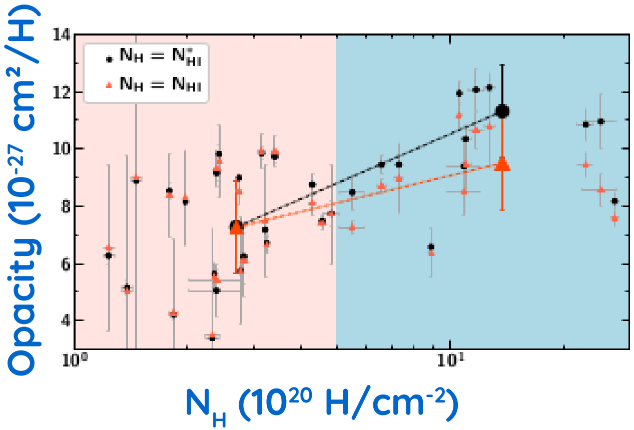
Variations in the dust opacity

Nguyen et al. (2018): 93 LOS with $10^{20} \leq N_H \leq 3\times10^{21}$ H/cm^2



Optical depth

- 34 atomic lines of sight
  +40 % in opacity when $N_H > 5\times10^{20}$ H/cm^2
- Very little variations in $E(B-V)/N_H$
  $E(B-V) = A_B - A_V$
- Increase in dust mass or change in dust properties ?



What should a dust model fit for the diffuse ISM ?

Is the canonical Bohlin's ratio still canonical ? No.

Used to normalise dust models

- Bohlin et al. (1978) → $N_H/E(B-V) = 5.8\times10^{21}$ cm^2/mag
- Liszt (2014) → $N_H/E(B-V) = 8.3\times10^{21}$ cm^2/mag
- Planck Collaboration XI (2014) → $N_H/E(B-V) = 7\times10^{21}$ cm^2/mag
- Lenz et al. (2017) → $N_H/E(B-V) = 8.8\times10^{21}$ cm^2/mag
- Rémy et al. (2018) → $N_H/E(B-V) = 3.9$ to 6.2×10^{21} cm^2/mag
- Nguyen et al. (2018) → $N_H/E(B-V) = 9.4\times10^{21}$ cm^2/mag

Most recent studies find ratios 20 to 60 % higher
Be careful when comparing dust models to what ratio they are normalised

Remember that variations in the dust properties are expected in the diffuse ISM

Summary

- **What should a Galactic dust model fit ?**
  - → observations of the diffuse ISM
  - **→ observations of the dense ISM**
  - → observations of PDRs

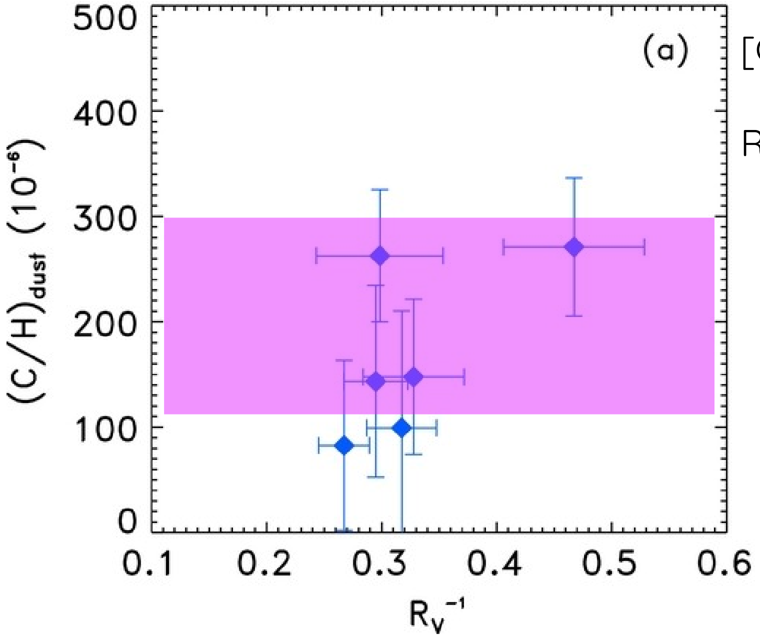
- Dust models: 2 public examples
  - → an empirical model
  - → a lab-based model

- A few points to bear in mind when using dust models
  - → uncertainties in models
  - → grain size determination
  - → cloud mass estimate

Carbon depletion in the diffuse ISM

Parvathi et al. (2012)

- 21 Galactic sightlines toward neutral medium
  - CII measurements from the 1334 Å transition
  - local variations in the total carbon abundance gas+dust
  - local variations in the carbon depletion



$[C/H]_{dust}$ for $N_H < 10^{21}$ cm²

$R_V = A_V / E(B-V)$

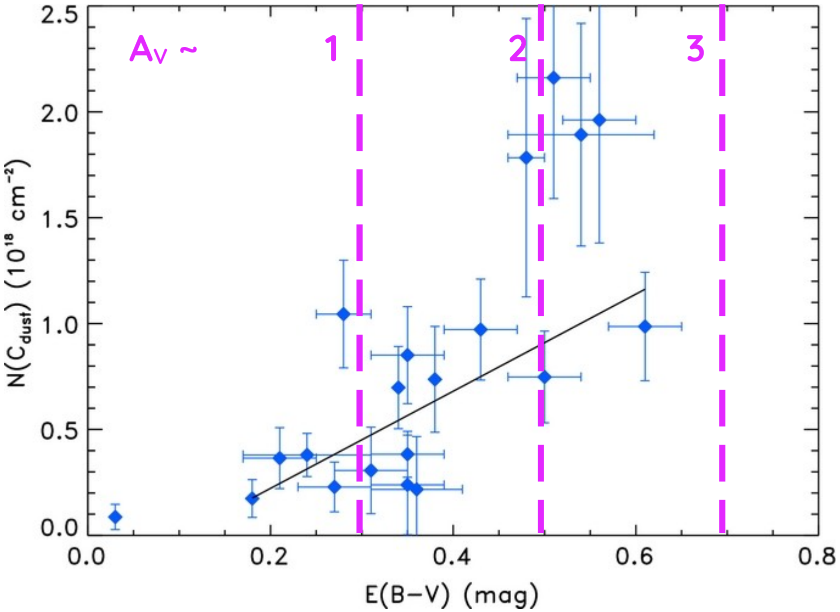
What should a dust model fit for the dense ISM ?

Carbon depletion in the dense ISM

Parvathi et al. (2012)

- What can happen to a grain when the local density increases?

  Accretion of gas phase carbon (A_V > 1-2) ?
  Grain-grain coagulation (A_V > 2-3) ?
  Ice mantle formation (A_V > 3) ?



Column density of C in dust

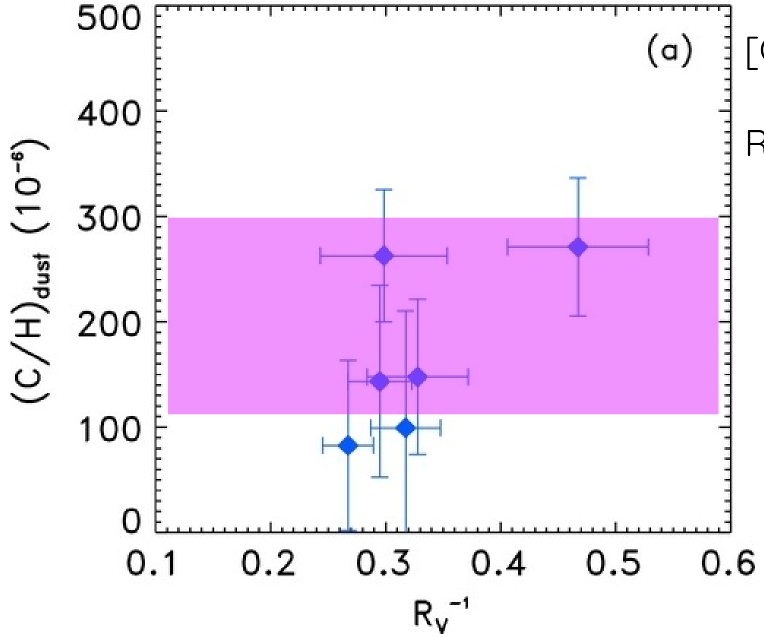
What should a dust model fit for the dense ISM ?

Carbon depletion in the dense ISM

Parvathi et al. (2012)

- What can happen to a grain when the local density increases?

  Accretion of gas phase carbon ($A_V > 1\text{-}2$) ?
  Grain-grain coagulation ($A_V > 2\text{-}3$) ?
  Ice mantle formation ($A_V > 3$) ?



$[C/H]_{dust}$ for $N_H < 10^{21}$ cm²

$R_V = A_V / E(B\text{-}V)$

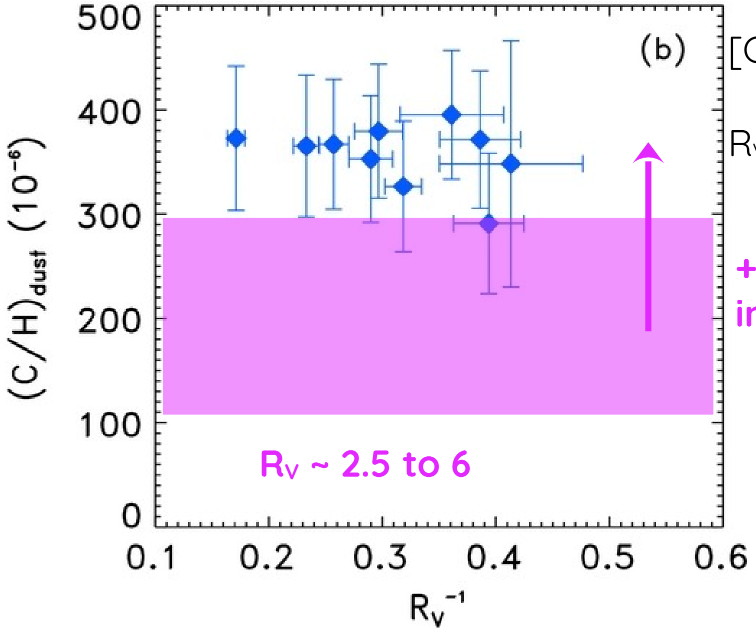
What should a dust model fit for the dense ISM ?

Carbon depletion in the dense ISM

Parvathi et al. (2012)

- What can happen to a grain when the local density increases?

  Accretion of gas phase carbon ($A_V > 1\text{-}2$) ?
  Grain-grain coagulation ($A_V > 2\text{-}3$) ?
  Ice mantle formation ($A_V > 3$) ?



$[C/H]_{dust}$ for $N_H > 10^{21}$ cm²

$R_V = A_V / E(B\text{-}V)$

+100-200 ppm of C in dense clouds

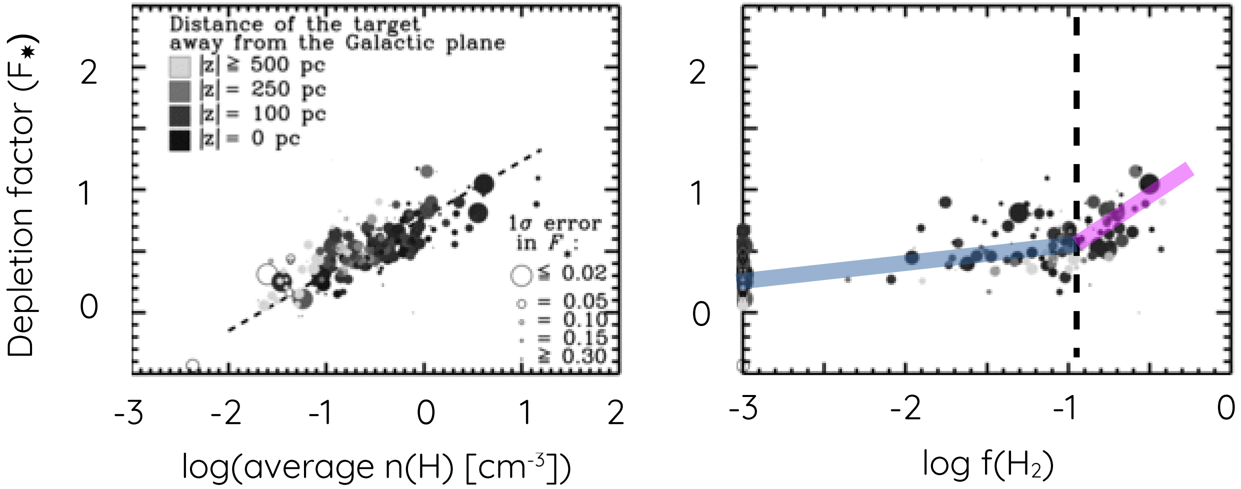
What should a dust model fit for the dense ISM ?

Depletion of heavier elements

Jenkins (2009)

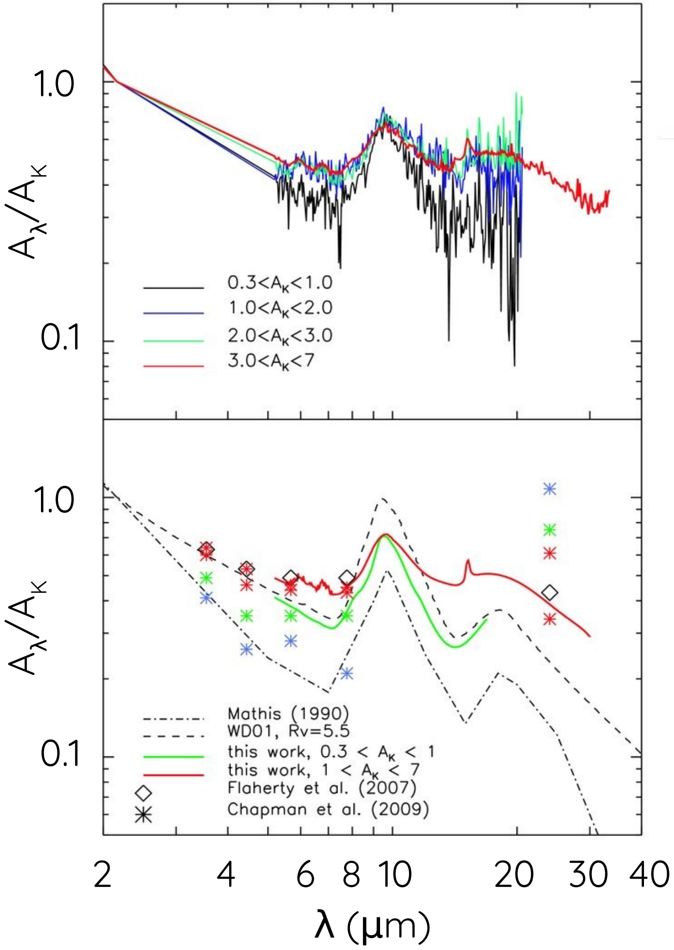
- Depletion of heavier elements
  Mg, Si, O, Fe, Cr, Ni, Ti, S...

- Depletion of 17 elements on 243 sightlines
  Local variations in [X_{gas}/H] strengths
  Linear relation between the various log. of [X_{gas}/H]



Variations in the silicate mid-IR features

McClure (2009)



- Sample
  24 G0-M4 III stars behind dark clouds
  Chameleon, Serpens, Taurus
  Barnard 68, Barnard 59, IC 5146

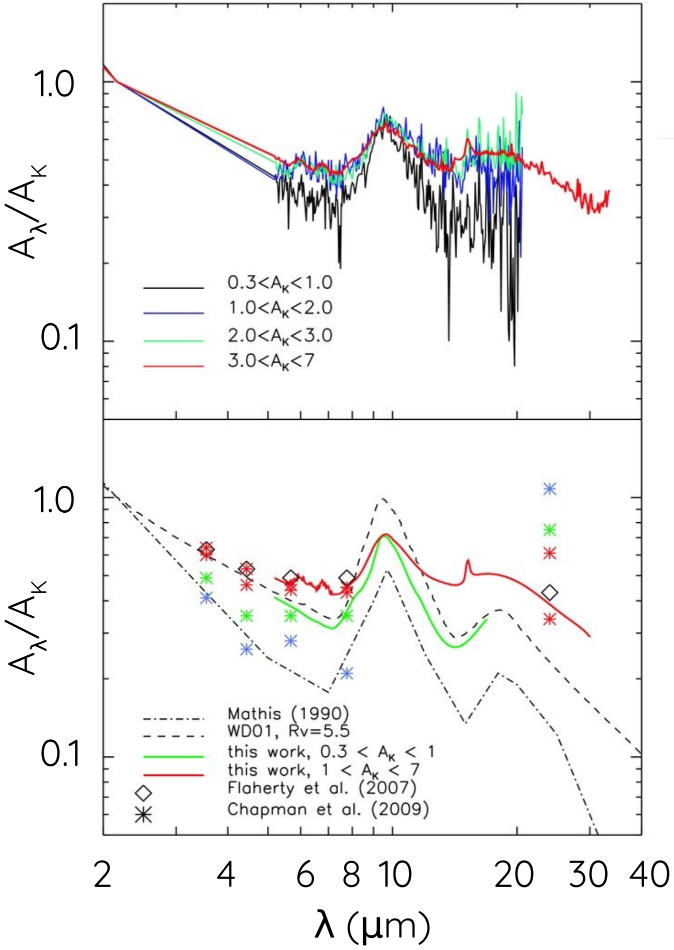
- Normalisation to K band at 2.2 μm (2MASS)

- Observational results for $A_K > 0.5$ (⇔ $A_V \sim 4$)
  extinction curve flattening
  widening of both bands
  BUT peak positions unchanged
  variations correlated with ice features

What should a dust model fit for the dense ISM ?

Variations in the silicate mid-IR features

McClure (2009)



- Sample

  24 G0-M4 III stars behind dark clouds
  Chameleon, Serpens, Taurus
  Barnard 68, Barnard 59, IC 5146

- Normalisation to K band at 2.2 µm (2MASS)

- Observational results for $A_K > 0.5$ (⇔ $A_V \sim 4$)

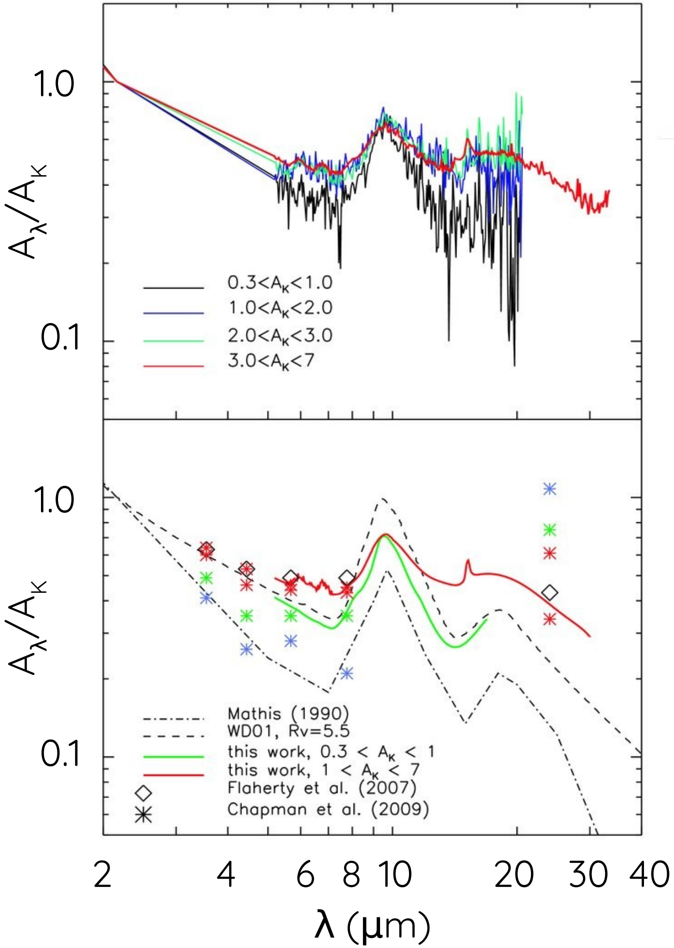
  extinction curve flattening
  widening of both bands
  BUT **peak positions unchanged**
  variations correlated with ice features

Grain size cannot exceed ~ 1 µm

What should a dust model fit for the dense ISM ?

Variations in the silicate mid-IR features

McClure (2009)



- Sample

  24 G0-M4 III stars behind dark clouds
  Chameleon, Serpens, Taurus
  Barnard 68, Barnard 59, IC 5146

- Normalisation to K band at 2.2 μm (2MASS)

- Observational results for $A_K > 0.5$ (⇔ $A_V \sim 4$)

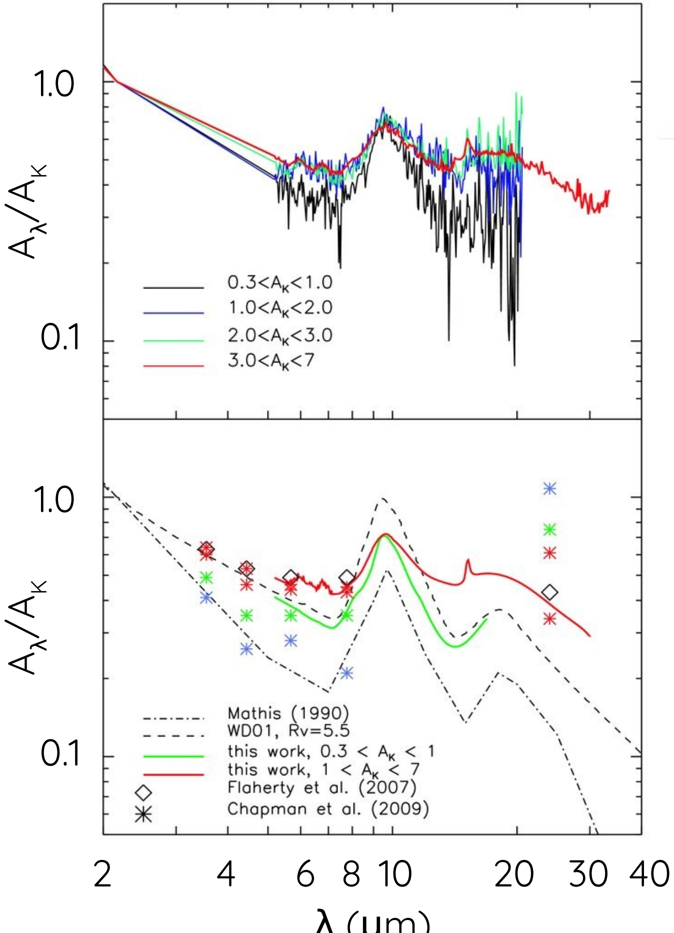
  extinction curve flattening
  widening of both bands
  BUT **peak positions unchanged**
  variations correlated with ice features

Grain size cannot exceed ~ 1 μm
Carbon accretion ?

What should a dust model fit for the dense ISM ?

Variations in the silicate mid-IR features

McClure (2009)



- Sample
  24 G0-M4 III stars behind dark clouds
  Chameleon, Serpens, Taurus
  Barnard 68, Barnard 59, IC 5146

- Normalisation to K band at 2.2 μm (2MASS)

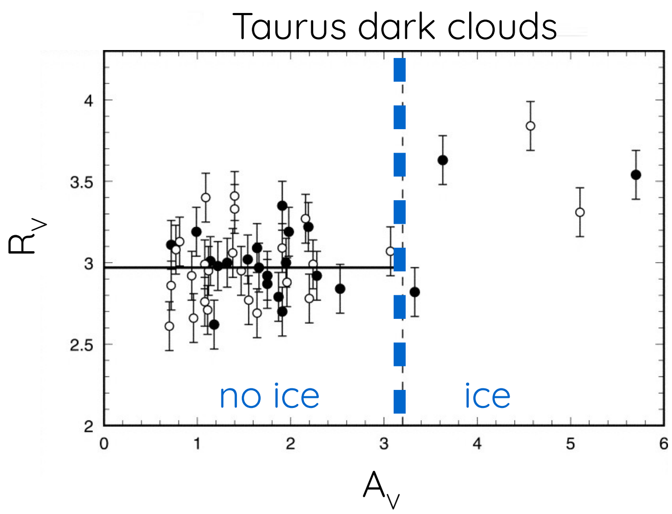
- Observational results for $A_K > 0.5$ (⇔ $A_V \sim 4$)
  extinction curve flattening
  widening of both bands
  BUT **peak positions unchanged**
  variations correlated with ice features

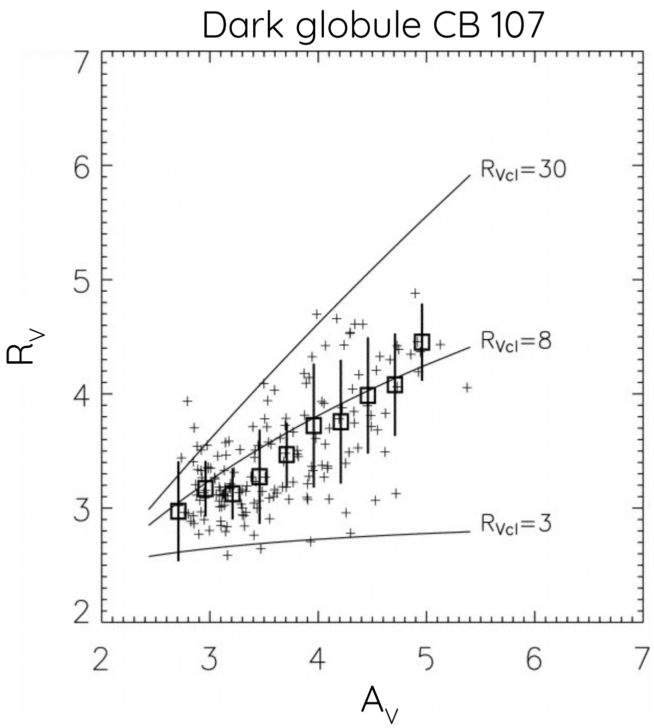
Grain size cannot exceed ~ 1 μm
Carbon accretion ?
Carbon and ice accretion ?
From isolated grains to icy aggegates ?
→ widening only of the 18 μm band

What should a dust model fit for the dense ISM ?

Variations in total-to-selective extinction R_V

Whittet et al. (2001) & Campeggio et al. (2007)





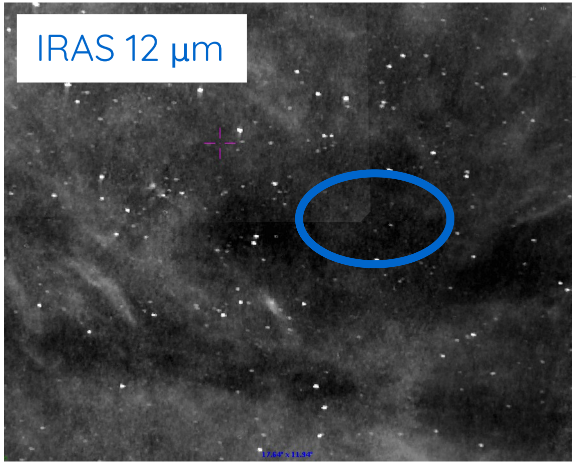
- Increase in R_V with A_V
- Increase when water ice features are detected

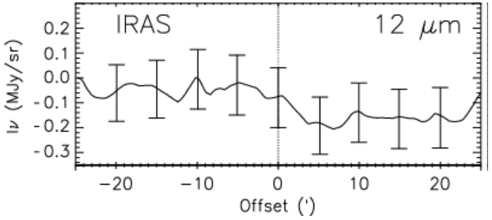
↳ **Grain growth** associated to ice accretion

What should a dust model fit for the dense ISM ?

Variations in the mid- to far-IR SED

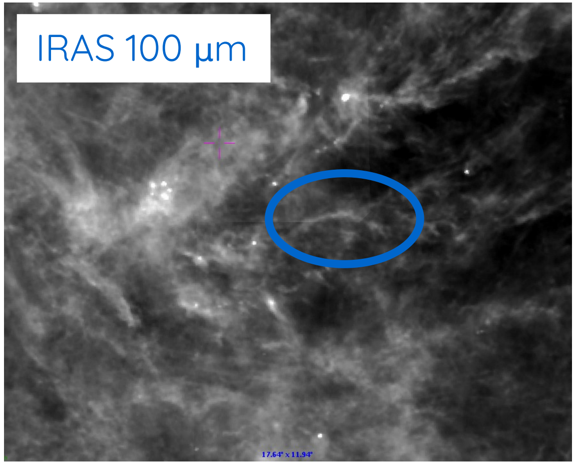
Stepnik et al. (2003)

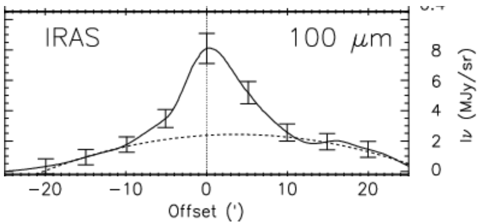




Taurus
molecular
cloud

L1506
filament





Not an effect of radiative transfer !

Bernard et al. (1993)

Ysard et al. (2012, 2013)

- No emission in from the mid-IR to ~ 70 µm
  → small grains disappear from the diffuse to the dense ISM

↳ **Small grain accretion onto larger grains → grain growth**

What should a dust model fit for the dense ISM ?

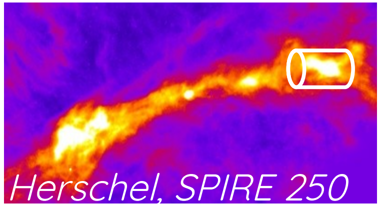
Visible extinction vs. far-IR SED

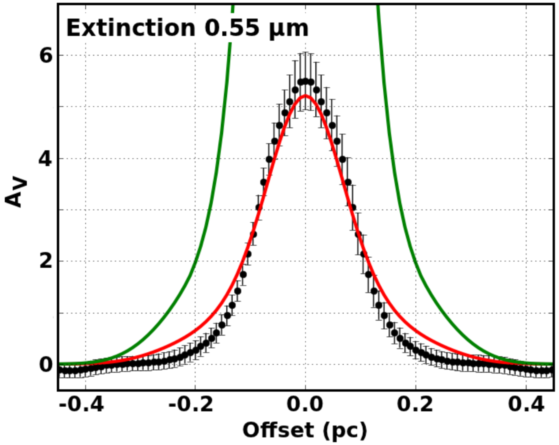
Ysard et al. (2013)

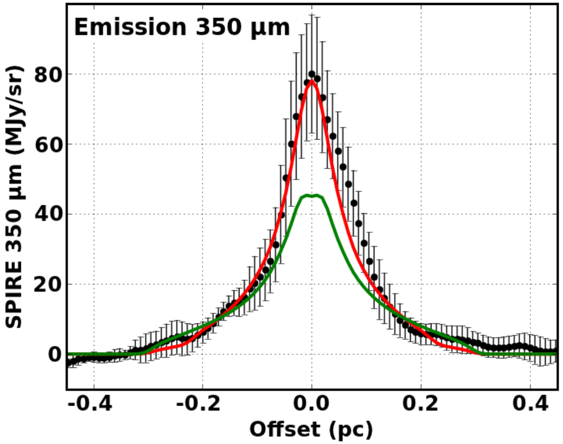
- Aggregates for $1000 < n_H < 2000$ H/cm^3
  → $A_V \sim 2$ to 4
- Same as increase in R_V, ice features, mid-IR silicate bands

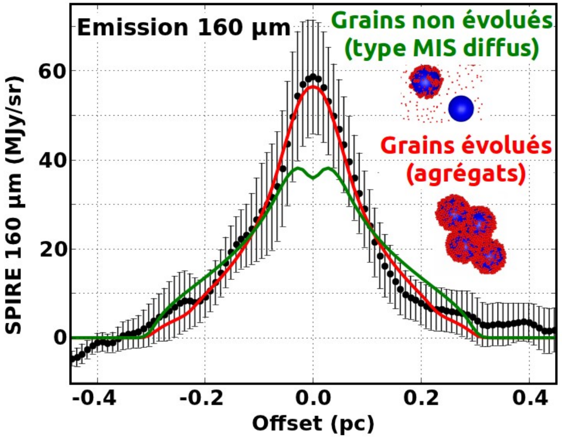
→ Grain growth
→ From isolated grains to aggregates

Ysard et al. (2013)





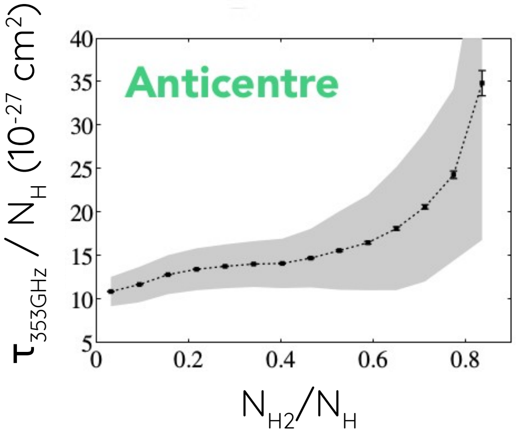




What should a dust model fit for the dense ISM ?

Variations in the far-IR SED

Rémy et al. (2017, 2018)



- Observations of 6 nearby anti-centre clouds
- Usual behaviour of dense clouds
  - → T_{dust} ↘
  - → $\tau_{submm/FIR}$ and β ↗

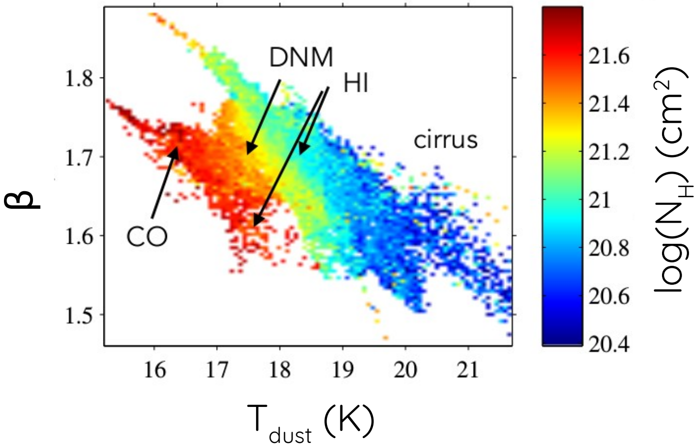
Grain growth

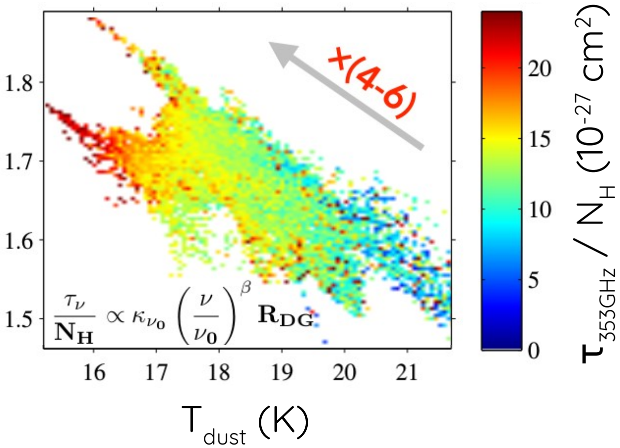
From isolated grains to aggregates

Carbon accretion ? DCD-TLS ?

🔎 Mény et al. (2007)

🔎 Koehler et al. (2015)

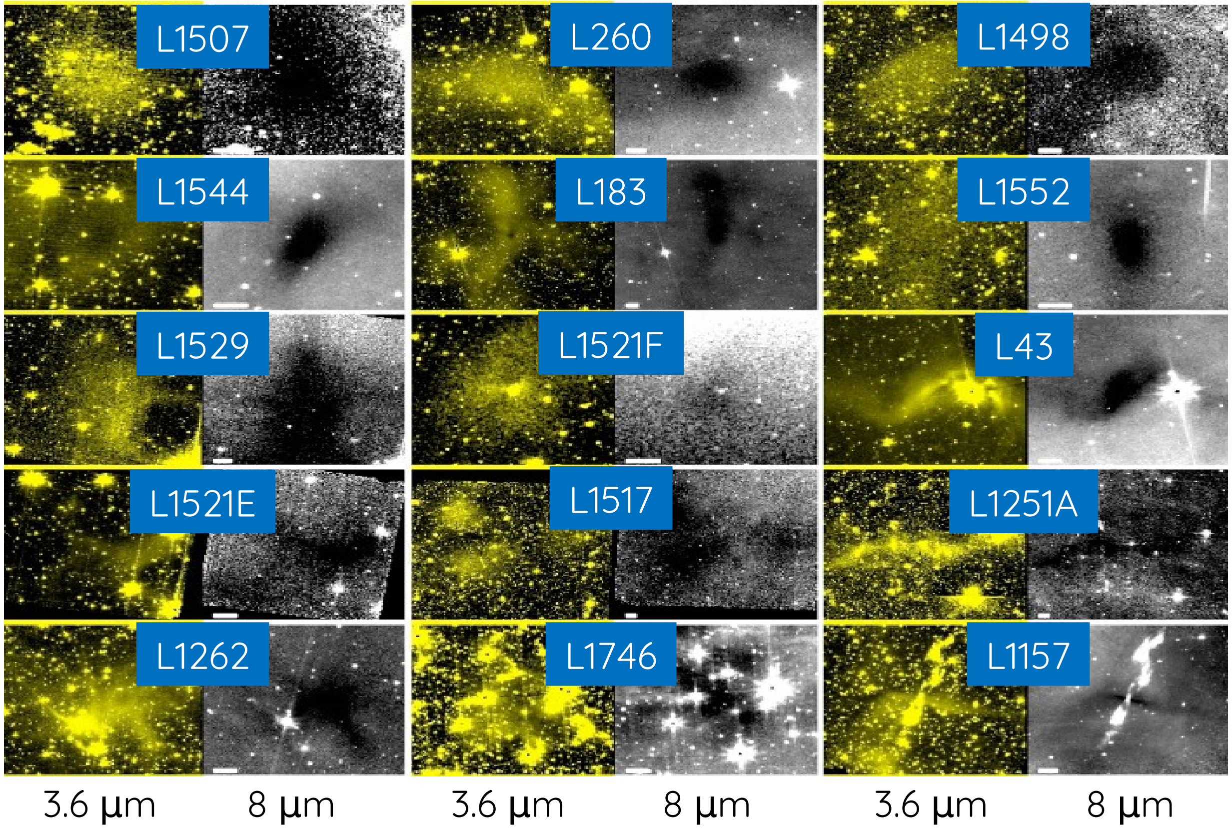




- Gradual evolution across phases
  - significant in DNM
  - stronger in CO

Variations in the dust scattering efficiency

Cloud- & Core-shine



- In the visible: 30’s
  Struve & Elvey (1936)
- In the near-IR: 90’s
  Witt et al. (1994)
- In the mid-IR: 2010
  Pagani et al. (2010)
- Albedo and asymmetry parameter
  Mattila (1970ab, 2018)
- Scattering by bigger grains than in the diffuse ISM
  Steinacker et al. (2010)
  Lefèvre et al. (2014)

Grain growth

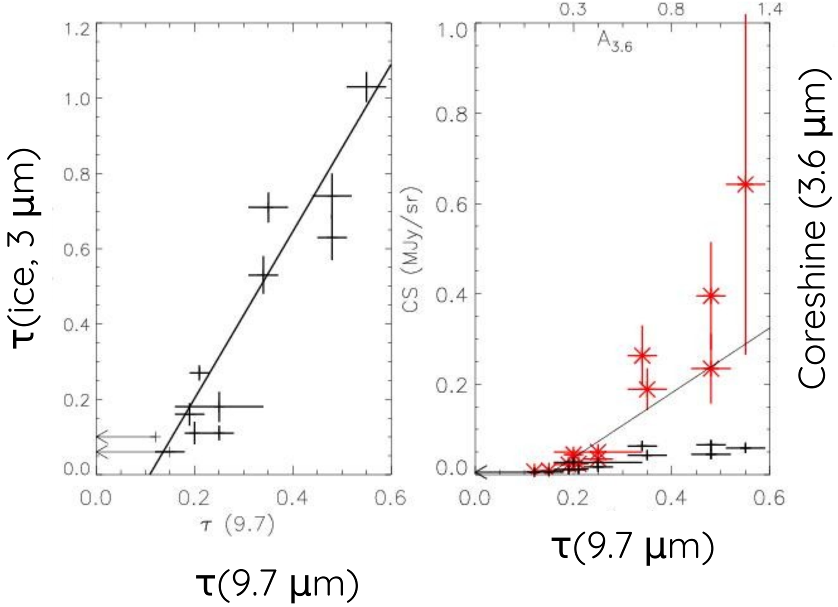
What should a dust model fit for the dense ISM ?

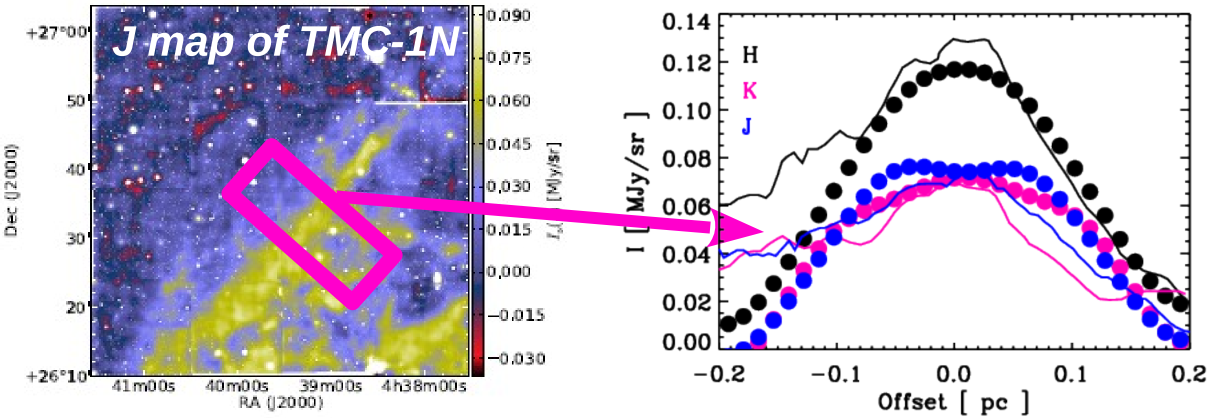
Variations in the dust scattering efficiency

Andersen et al. (2014) & Ysard et al. (2016)

- Andersen et al. (2014)
  → common density threshold for
  coreshine & ice feature at 3 μm

- Ysard et al. (2016)
  need for aggregates when 1000 < n_H < 2000 H/cm^3
  → A_V ~ 2 to 4





Malinen's data

●●●●●● THEMIS model

Grain growth

Aggregates?

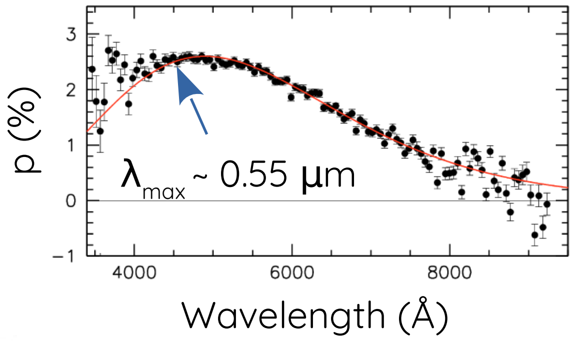
Ice accretion ?

Carbon accretion ?

What should a dust model fit for the dense ISM ?

Variations in the visible starlight polarisation

Patat et al. (2010): diffuse ISM

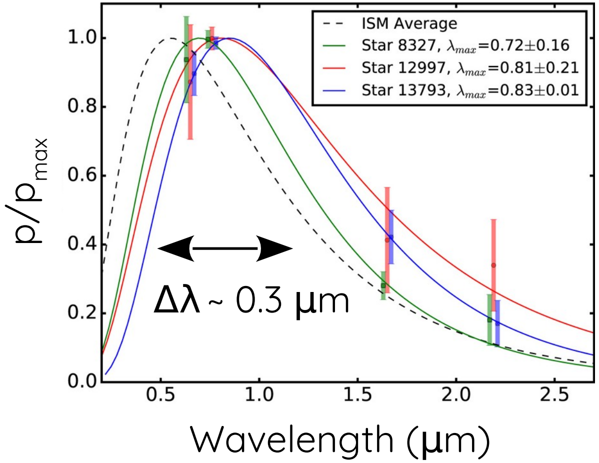


- Linear polarisation of starlight in the visible
  → λ_{max} proportional to aligned <grain size>
- Increase in λ_{max} & decrease in p_{max}/E(B-V) in dense clouds
  → threshold around A_V = 3-4

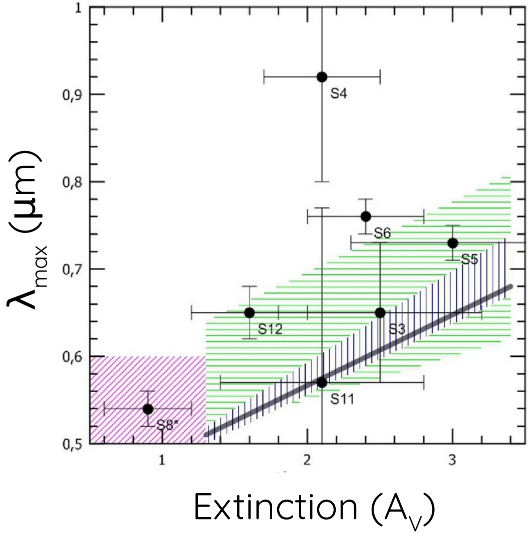
↳ Grain growth

Fanciullo et al. (2017)

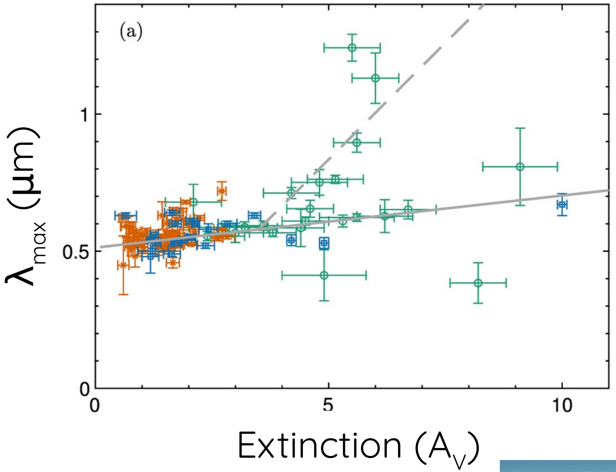
Wang et al. (2017): dark cloud IC5146



Il'in et al. (2018): Barnard 5



Vaillancourt et al. (2020): Taurus MC



Summary

- **What should a Galactic dust model fit ?**
  - → observations of the diffuse ISM
  - → observations of the dense ISM
  - **→ observations of PDRs**

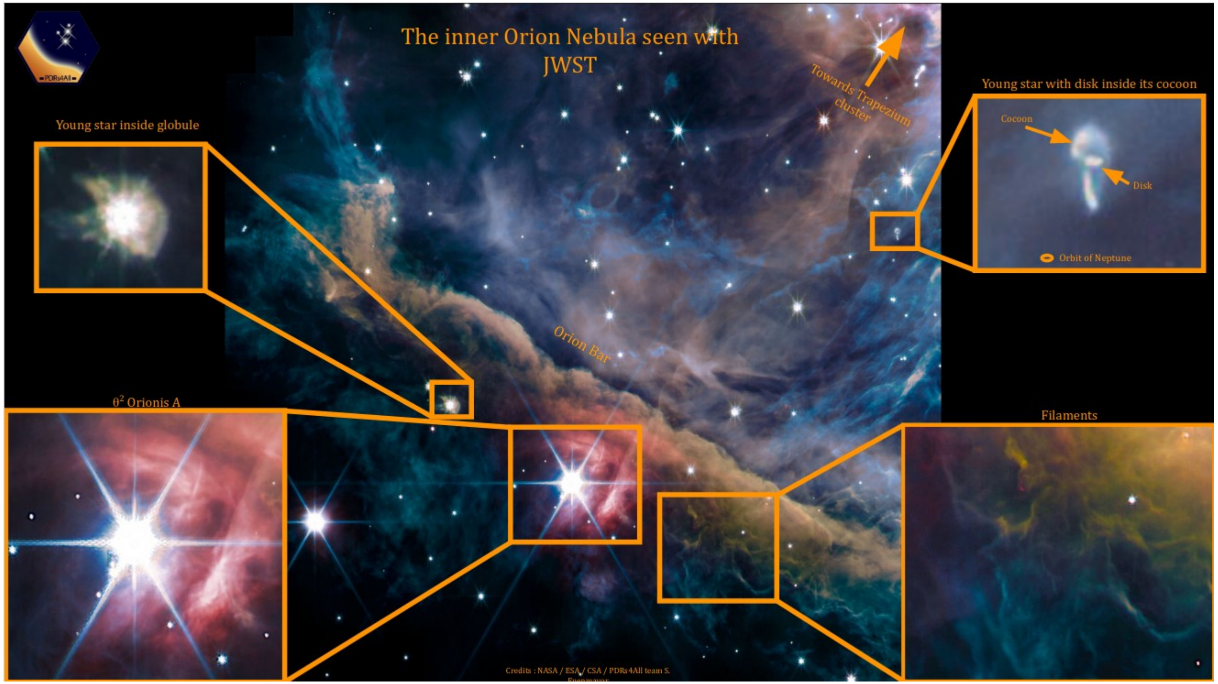
- Dust models: 2 public examples
  - → an empirical model
  - → a lab-based model

- A few points to bear in mind when using dust models
  - → uncertainties in models
  - → grain size determination
  - → cloud mass estimate

What should a dust model fit for PDRs ?

The Orion Bar seen by the JWST (ERS PDR4All)

PI: O. Berné, E. Habart, E. Peeters

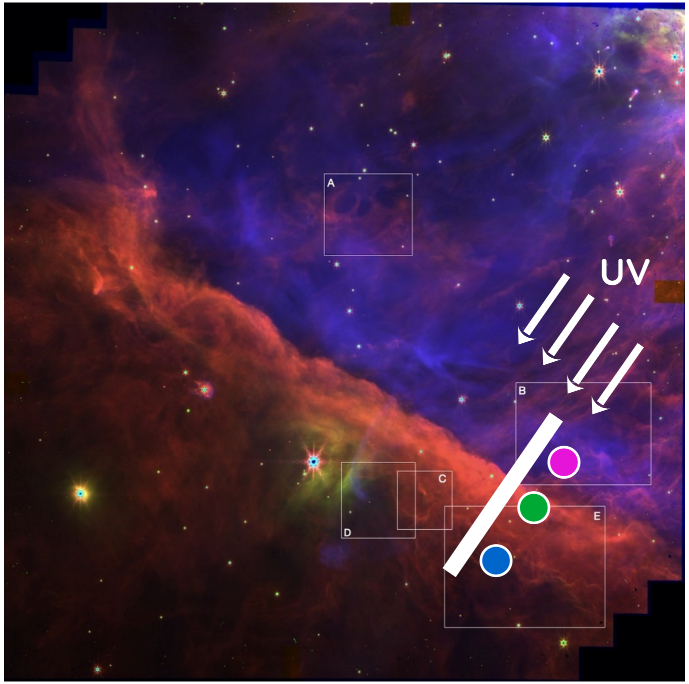


Credits : NASA / ESA / CSA / PDRs4All team S. Fuenmayor

What should a dust model fit for PDRs ?

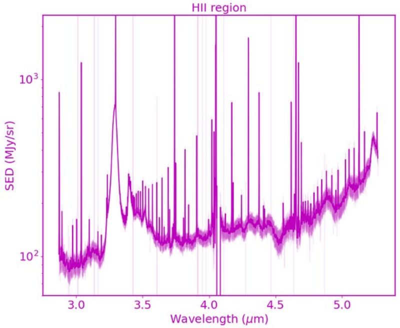
Dust evolution across the Orion Bar

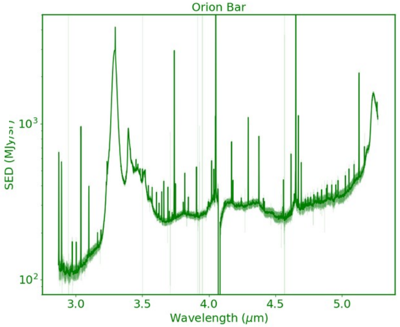
Elyajouri et al. (in prep)

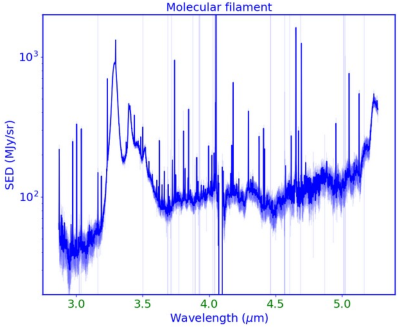


Adapted from Habart et al. (subm.)
Peeters et al. (in prep)

- Variations in
  - band-to-continuum ratio
  - 3.3 to 3.4 band ratio



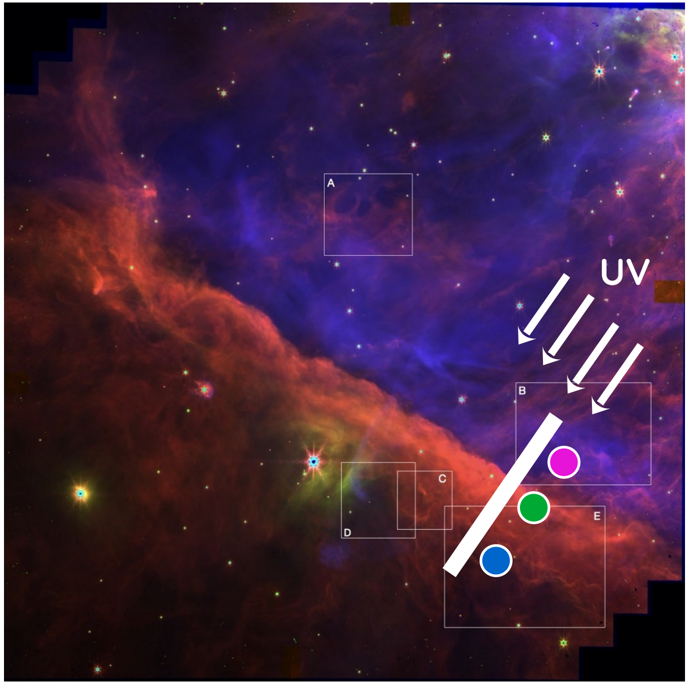




What should a dust model fit for PDRs ?

Dust evolution across the Orion Bar

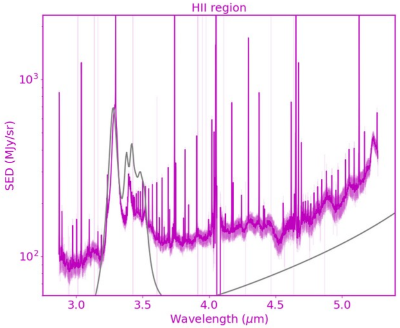
Nano-grain sizes & hydrogenation

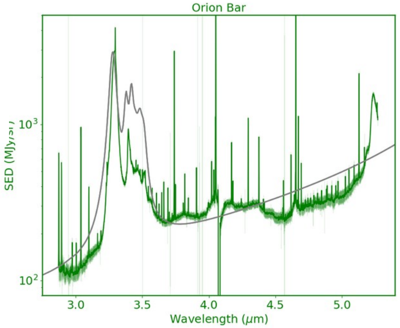


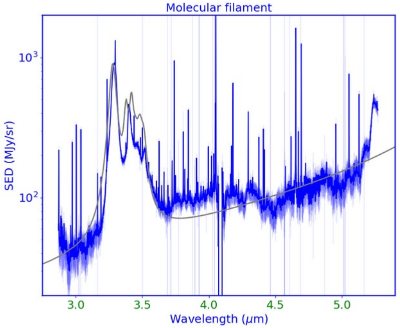
Adapted from Habart et al. (subm.)
Peeters et al. (in prep)

- Variations in band-to-continuum ratio
  3.3 to 3.4 band ratio

  → minimum grain size & hydrogenation (E_g)





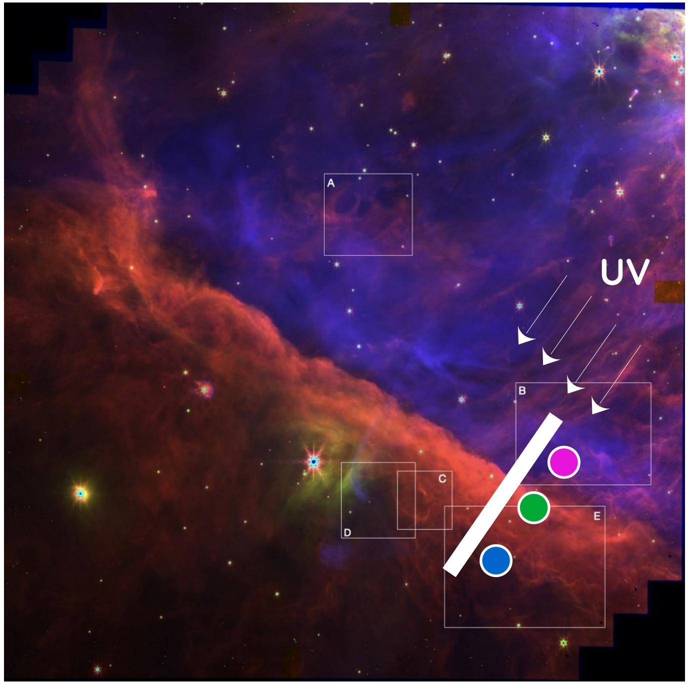


as in DISM
a_{min} = 0.4 nm
E_g = 0.1 eV ⇔ X_H ~ 0.02

What should a dust model fit for PDRs ?

Dust evolution across the Orion Bar

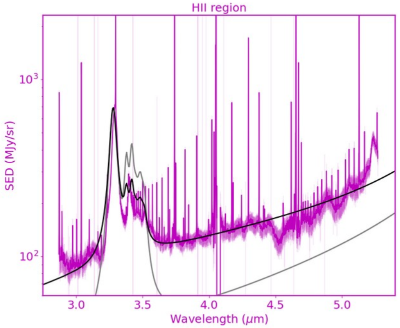
Nano-grain sizes & hydrogenation

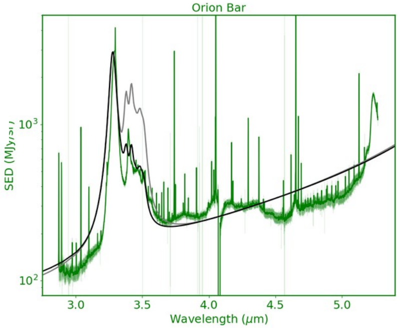


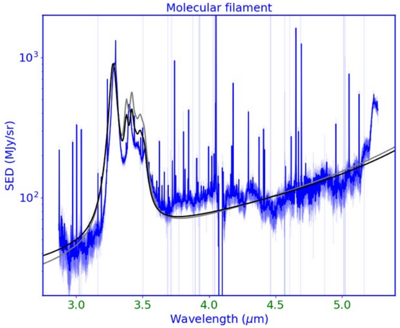
Adapted from Habart et al. (subm.)
Peeters et al. (in prep)

- Variations in | band-to-continuum ratio
  | 3.3 to 3.4 band ratio

  → minimum grain size & hydrogenation (E_g)



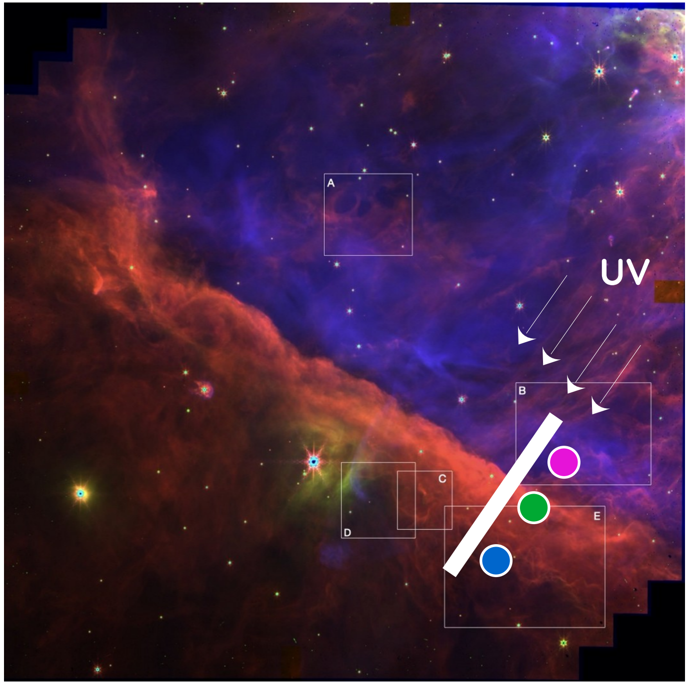




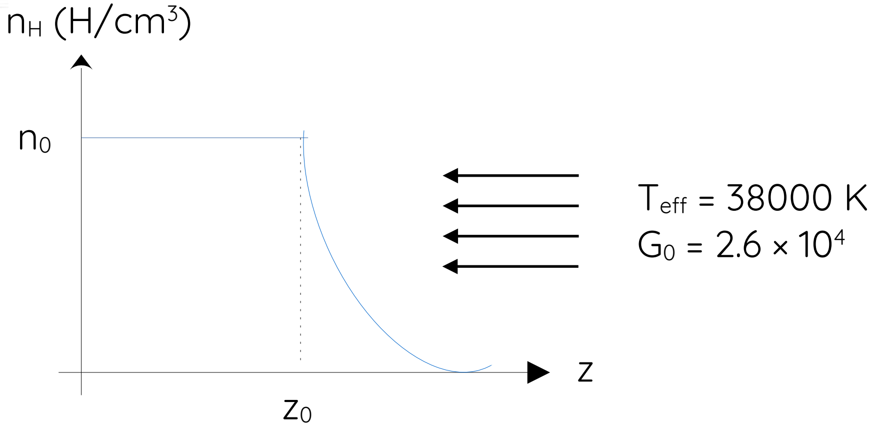
increasing number of UV photons
decreasing E_g from ~ 0.08 to 0.03 eV
increasing a_{min} from ~ 0.4 to 0.5 nm

Dust evolution across the Orion Bar

Radiative transfer model (plane parallel)



Adapted from Habart et al. (subm.)

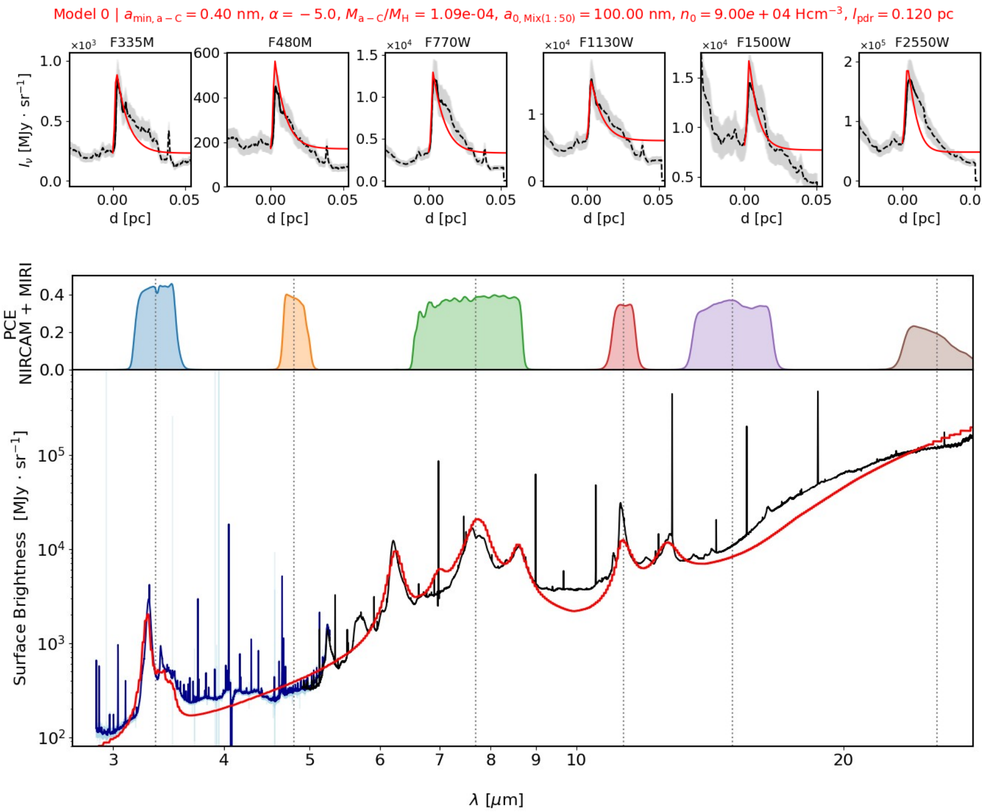


T_{eff} = 38000 K
$G_0 = 2.6 \times 10^4$

same methodology as in Schirmer et al. (2020, 2022)
THEMIS + DustEM + SOC
nano-grains with Eg = 0.03 eV
pseudo-aggregates from Ysard et al. (2019)

What should a dust model fit for PDRs ?

Dust evolution across the Orion Bar



- Fit emission profiles in 6 NIRCam + MIRI filters
  A posteriori comparison with NIRSpec and MRS spectra

- 15 times less abundant nano-grains than in the diffuse ISM

- Consequences for estimates of the gas temperature, H_2 formation and intensities of the H_2 pure rotational lines
  - Meshaka et al. (in prep.)
  - Murga et al. (2023)
  - Schirmer et al. (2021)
  - Jones & Habart (2015)

Summary

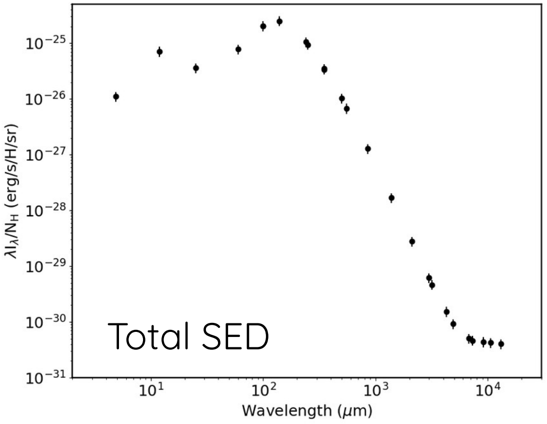
- What should a Galactic dust model fit ?
  - → observations of the diffuse ISM
  - → observations of the dense ISM
  - → observations of PDRs

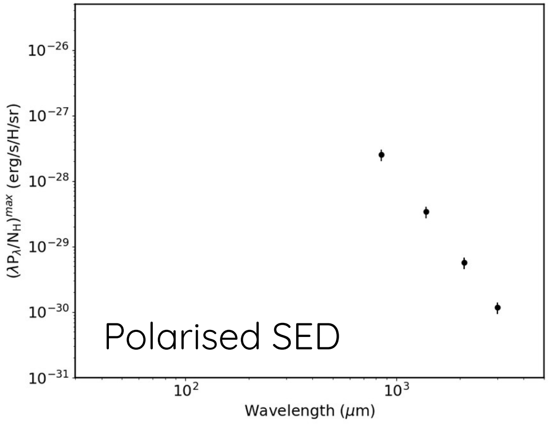
- **Dust models: 2 public examples**
  - → an empirical model
  - → a lab-based model

- A few points to bear in mind when using dust models
  - → uncertainties in models
  - → grain size determination
  - → cloud mass estimate

Observational constraints [sky]

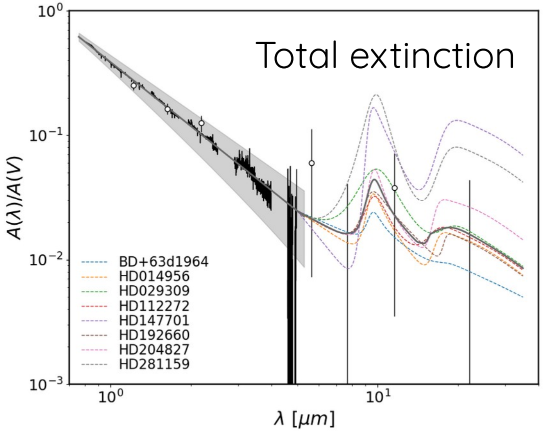
Compiègne et al. (2011)
Planck collab. XVII (2014)
Planck collab. XXII (2015)
Bianchi et al. (2017)
Planck collab. XI (2020)

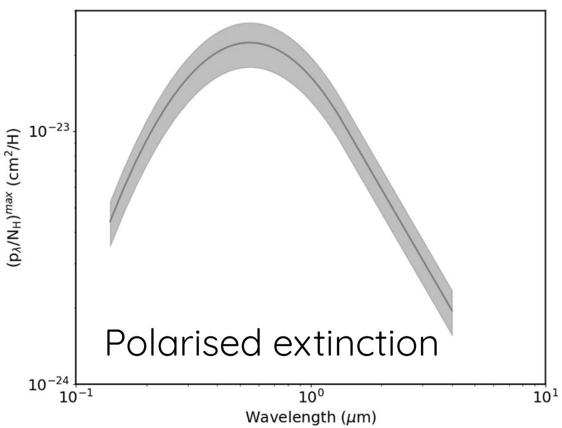




Planck collab. XXII (2015)
Planck collab. XI (2020)

Gordon et al. (2021)
Decleir et al. (2022)





Panopoulou et al. (2019)
Planck collab. XII (2020)

Summary

- What should a Galactic dust model fit ?
  - → observations of the diffuse ISM
  - → observations of the dense ISM
  - → observations of PDRs

- **Dust models: 2 public examples**
  - **→ an empirical model**
  - → a lab-based model

- A few points to bear in mind when using dust models
  - → uncertainties in models
  - → grain size determination
  - → cloud mass estimate

An empirical model: astrodust + astroPAHs

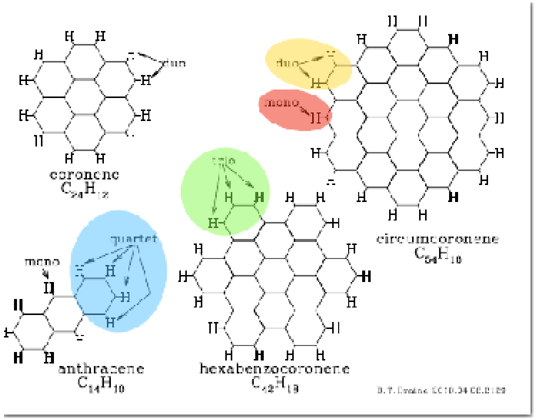
Dust components

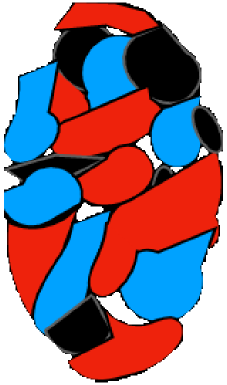
Draine & Hensley (2021 a)

astroPAHs
Draine & Li (2007)

\+

astrodust





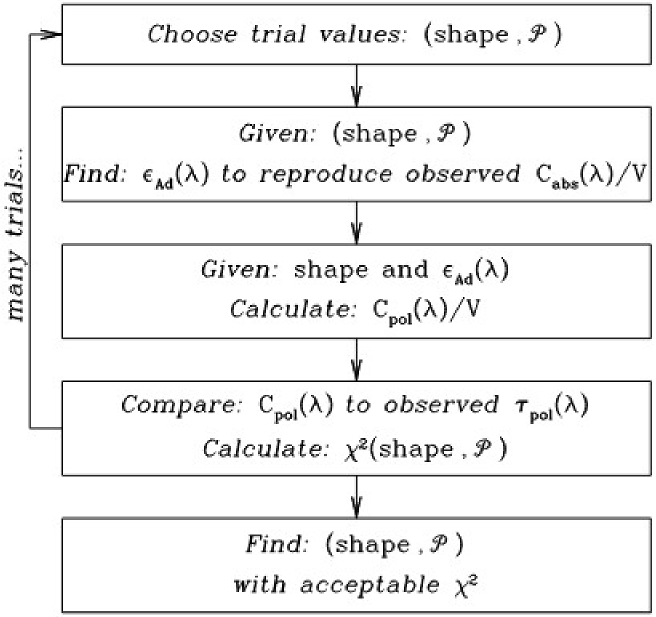
Assumption about composition:

amorphous silicate
hydrocarbon material
other materials (e.g. Fe oxides, Al_2O_3, $CaCO_3$)

An empirical model: astrodust + astroPAHs

Definition of the astrodust properties

Draine & Hensley (2021 a, b, c)



Choose trial values: (shape , $\mathcal{P}$)

Given: (shape , $\mathcal{P}$)
Find: $\epsilon_{\rm Ad}(\lambda)$ *to reproduce observed* $C_{\rm abs}(\lambda)/V$

Given: shape and $\epsilon_{\rm Ad}(\lambda)$
Calculate: $C_{\rm pol}(\lambda)/V$

Compare: $C_{\rm pol}(\lambda)$ *to observed* $\tau_{\rm pol}(\lambda)$
Calculate: χ^2(shape , $\mathcal{P}$)

Find: (shape , $\mathcal{P}$)
with acceptable χ^2

Figure 1. Approach used to determine the shape and dielectric function $\epsilon_{\rm Ad}$ of the silicate-bearing "astrodust" grains. $\mathcal{P}$ is the porosity of the astrodust grains (see text).

- Use of IR absorption to empirically derive a complex dielectric function for "astrodust" that fits perfectly the observations (in the Rayleigh limit, $a \ll \lambda$, extinction dominated by absorption and C_{abs}/V is directly related to ε_{ad} and independent of a)

$$< \kappa_{\rm abs} >= \frac{2\pi N}{3\rho\lambda}{\rm Im}\left(\frac{\epsilon-\epsilon_m}{\epsilon_m + L(\epsilon-\epsilon_m)} + \frac{4(\epsilon-\epsilon_m)}{2\epsilon_m + (1-L)(\epsilon-\epsilon_m)}\right)$$

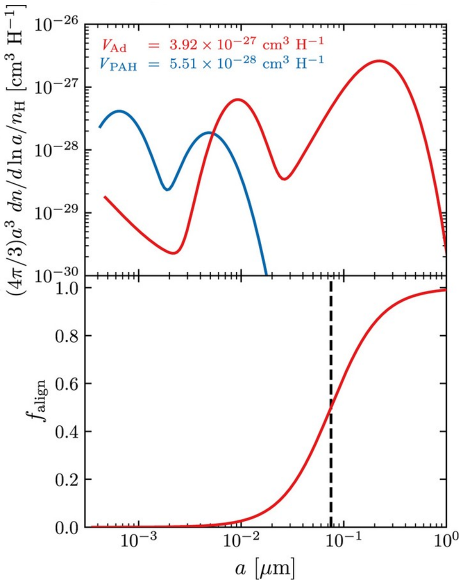
- Check if consistent with polarised extinction

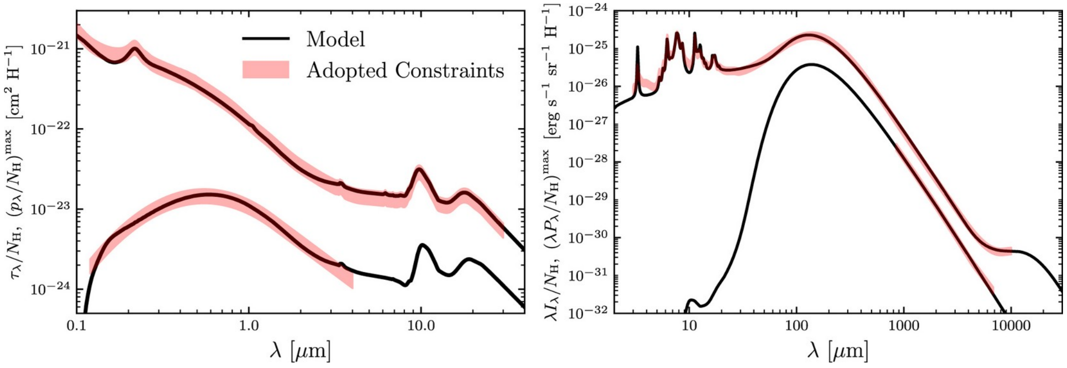
$\longrightarrow$ Gets optical properties associated with shape and porosity

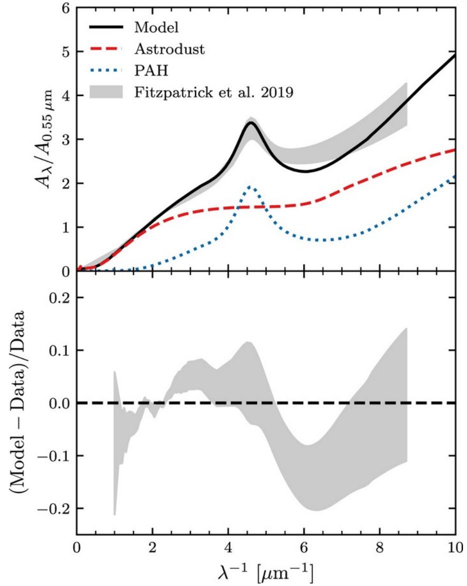
An empirical model: astrodust + astroPAHs

Fitting results

Hensley & Draine (2022)







- Draine & Hensley (2021 a, b, c)
- Hensley & Draine (2020, 2022)
- Draine (2016)
- Draine & Li (2007)

Dust model available here:
https://dataverse.harvard.edu/dataverse/astrodust

Summary

- What should a Galactic dust model fit ?
  - → observations of the diffuse ISM
  - → observations of the dense ISM
  - → observations of PDRs

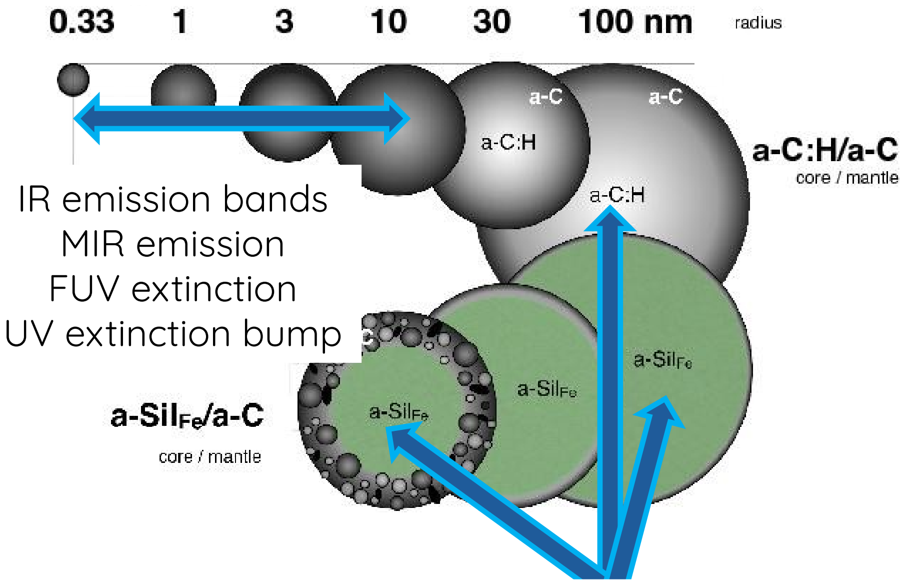
- **Dust models: 2 public examples**
  - → an empirical model
  - **→ a lab-based model**

- A few points to bear in mind when using dust models
  - → uncertainties in models
  - → grain size determination
  - → cloud mass estimate

A lab based model: THEMIS

Dust components

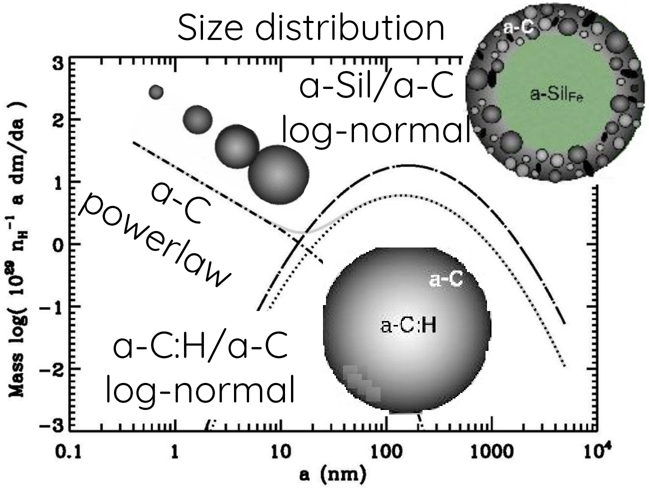
Jones et al. (2013)



IR emission bands
MIR emission
FUV extinction
UV extinction bump

IR absorption bands
visible/MIR extinction
FIR/submm emission

Size distribution



Dust model available here:
https://www.ias.u-psud.fr/themis/
https://www.ias.u-psud.fr/DUSTEM/

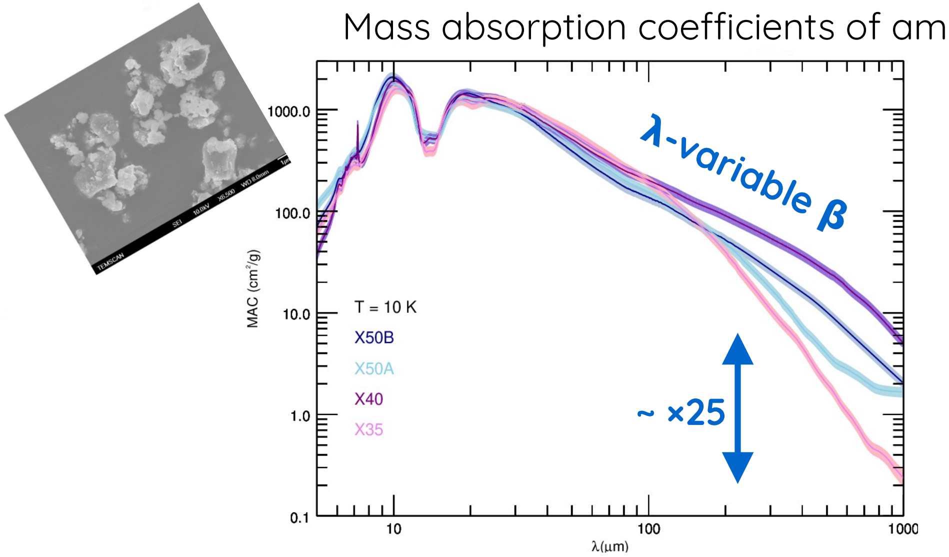
- Jones, Köhler, Ysard et al. (2017)
- Ysard, Köhler, Jones et al. (2015)
- Köhler, Jones & Ysard (2014)
- Jones et al. (2013)

A lab based model: THEMIS

Observational constraints [lab]

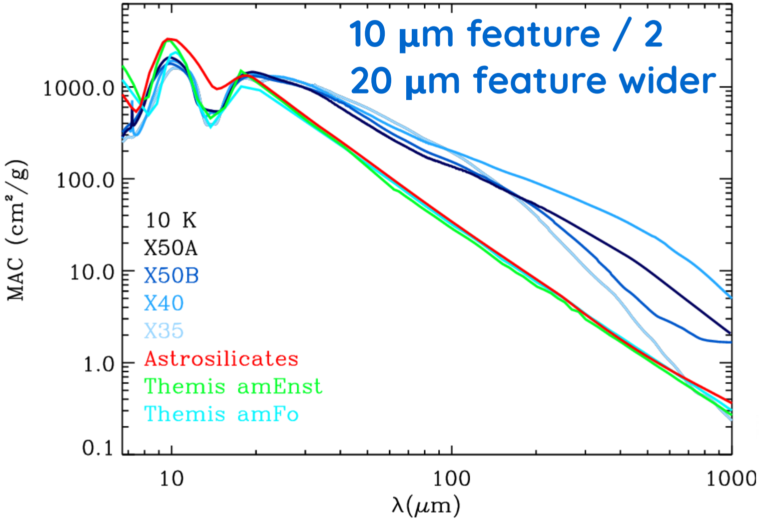
Demyk et al. (2017, 2022)

Mass absorption coefficients of amorphous Mg-rich silicates from 5 µm to 1 mm



λ-variable β

~ ×25



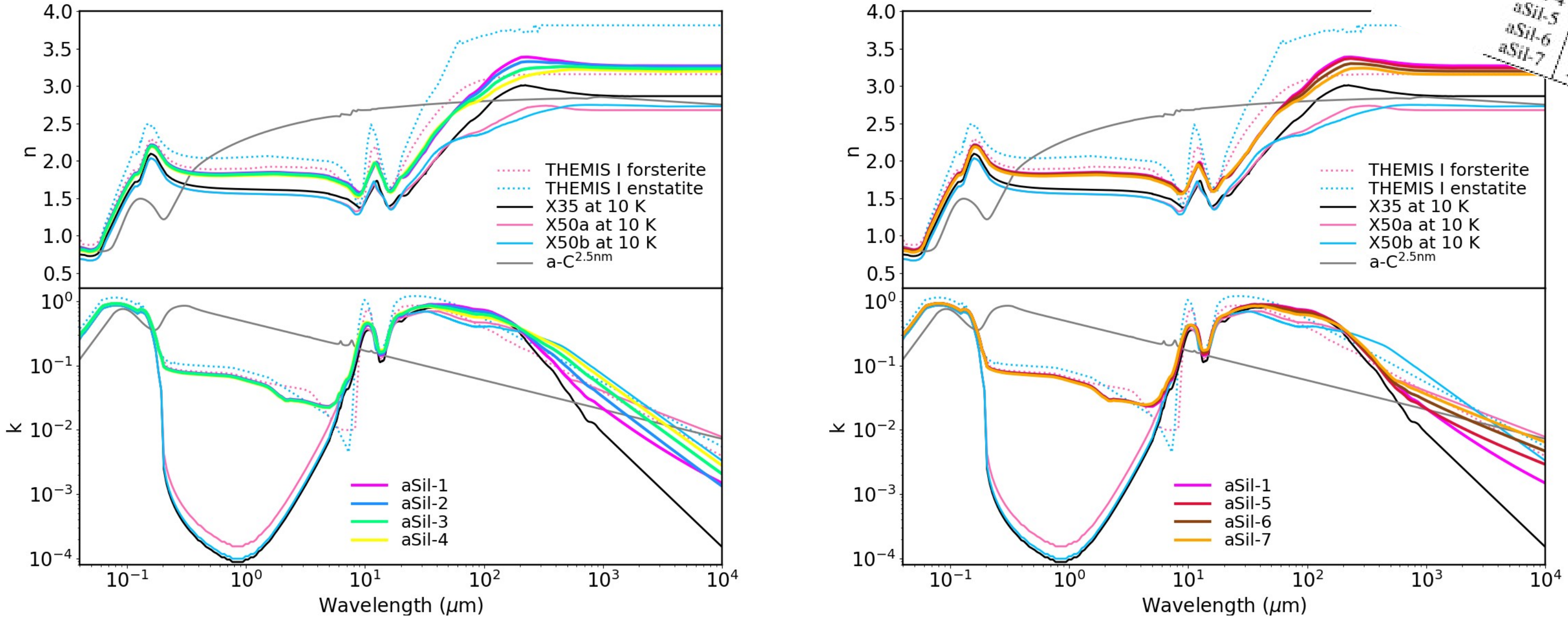
10 µm feature / 2
20 µm feature wider

- X35 → stoechiometry of forsterite
  X50a, X50b → stoechiometry of enstatite
  X40 → in-between
- Major differences at all wavelengths, high variability with wavelength and composition

A lab based model: THEMIS

Optical constants → silicate grains

Ysard et al. (to be subm.)



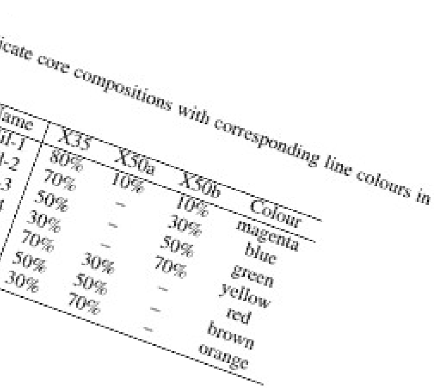


Table 1. Silicate core compositions with corresponding line colours in the figures.

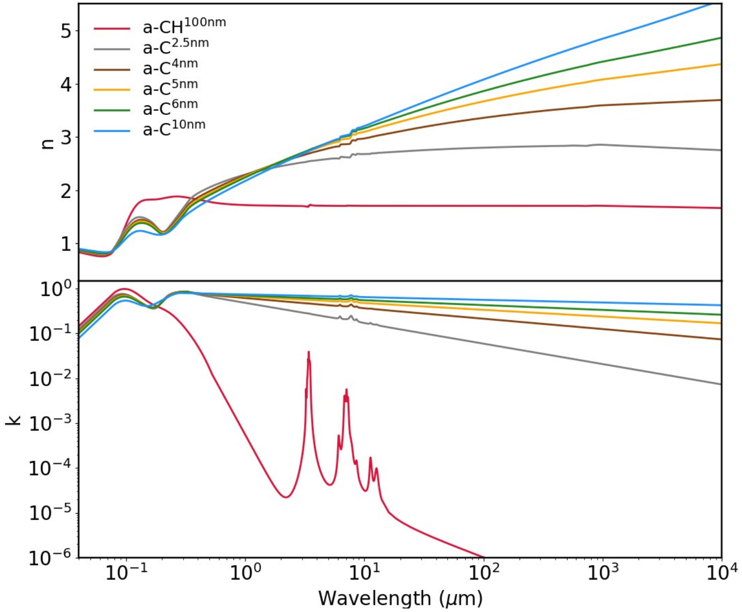
Name	X35	X50a	X50b	Colour
aSil-1	80%	10%	10%	magenta
aSil-2	70%	–	30%	blue
aSil-3	50%	–	50%	green
aSil-4	30%	–	70%	yellow
aSil-5	70%	30%	–	red
aSil-6	50%	50%	–	brown
aSil-7	30%	70%	–	orange

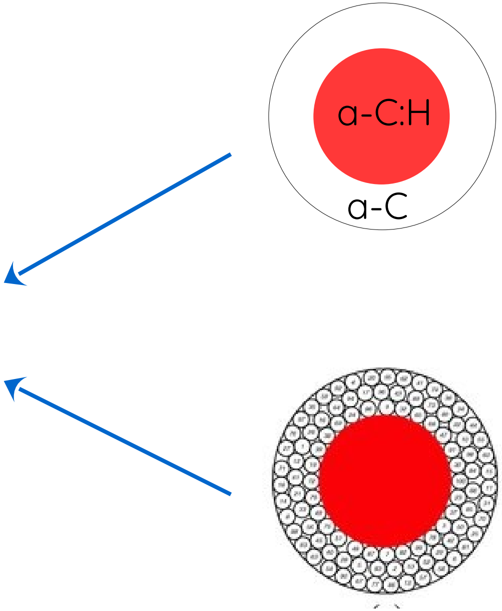
- Spectral index variations from 2.5-3.0 to 1.7-2.5 from far-IR to mm
- Submm absorption efficiencies × 1.5
- Mid-IR silicate features shift by a few 0.1 µm

A lab based model: THEMIS

Optical constants → carbonaceous grains

Description of the mantle

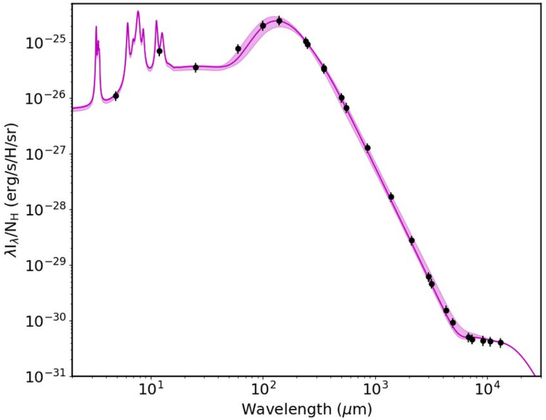


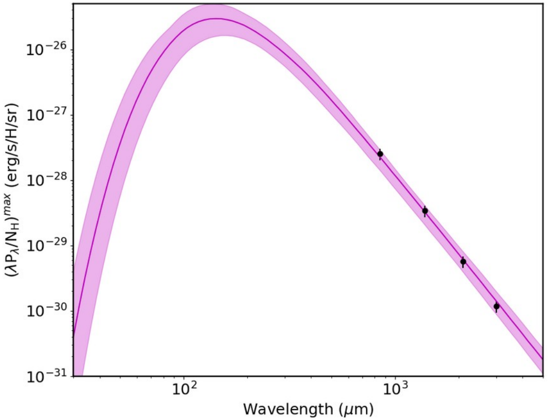


- From a-C:H/a-C$^{2.5nm}$ to a-C:H/a-C^{10nm}
  → far-IR/submm Q_{abs} × 4
  → **β** = 1.35 to 1.12
  → T decrease by ~ 5 K

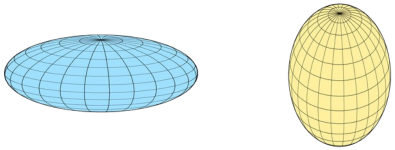
A lab based model: THEMIS

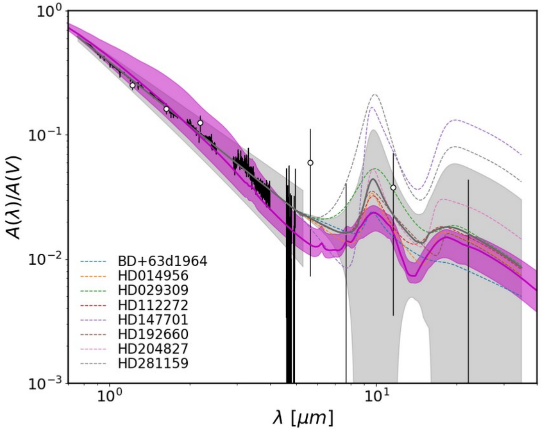
Fitting results

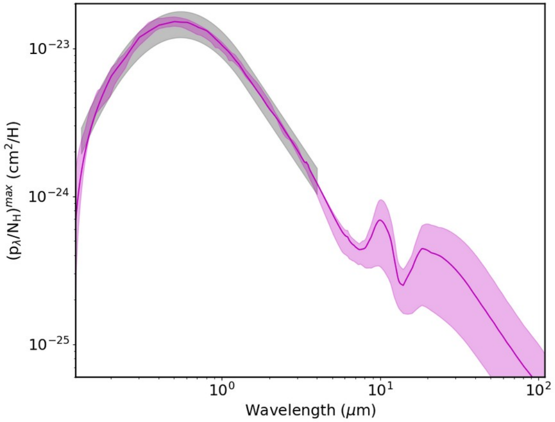




- Core/mantle spheroidal grains with e = 1.3 & 2
  - → oblates
  - → prolates



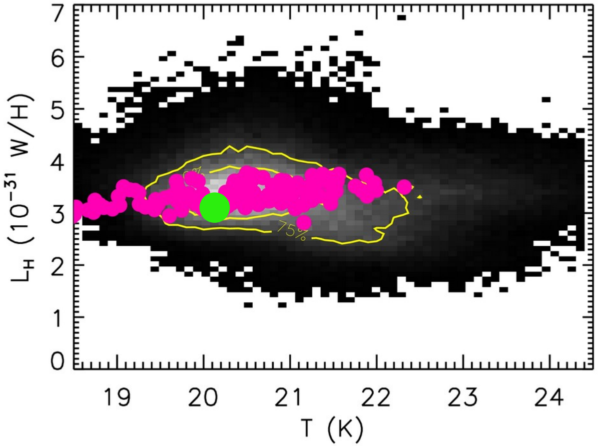


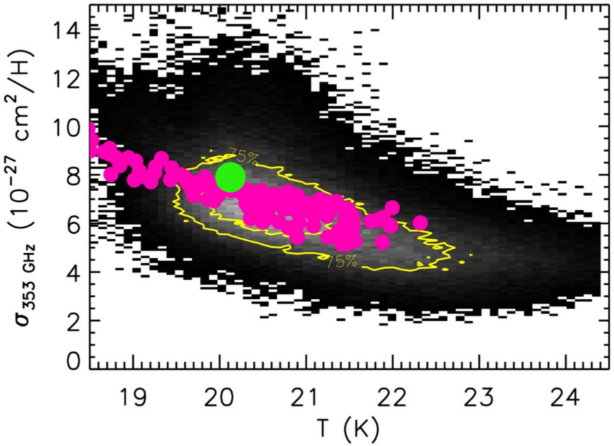


- All shapes yield acceptable solutions
- All silicate compositions too
- $0.9 \leq G_0 \leq 1.2$

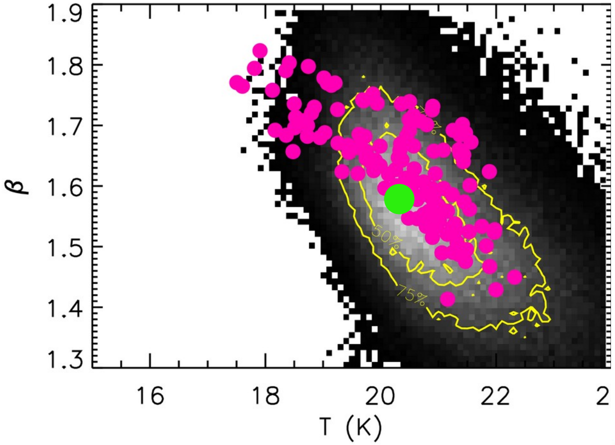
↳ No unique solution

Comparison with Planck collaboration XI (2014)





- ● astrodust + astroPAHs
- ● various lab silicates + a-C



Laboratory data in agreement with:
- → average high latitude SED & extinction
- → dispersion in the derived dust parameters

Summary

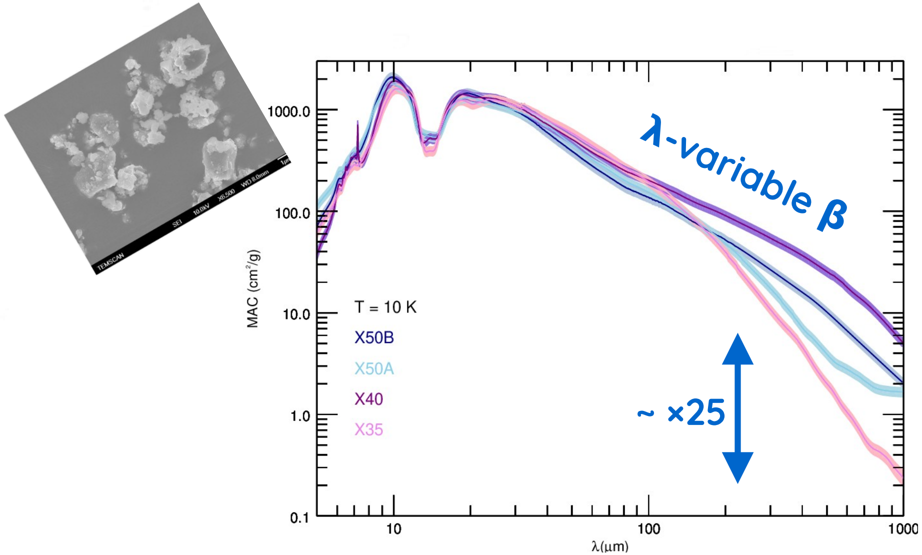
- What should a Galactic dust model fit ?
  - → observations of the diffuse ISM
  - → observations of the dense ISM
  - → observations of PDRs

- Dust models: 2 public examples
  - → an empirical model
  - → a lab-based model

- **A few points to bear in mind when using dust models**
  - → uncertainties in models
  - → grain size determination
  - → cloud mass estimate

Uncertainties in the optical constants

Demyk et al. (2017, 2022)



λ-variable β

~ ×25

Uncertainties on size distribution
shape distribution
visible optical properties

$\Delta n < 10\ \%$
$5\ \% < \Delta k < 20\ \%$

$$\epsilon = m^2$$

$$n = \sqrt{\frac{\sqrt{\epsilon'^2 + \epsilon''^2} + \epsilon'}{2}}$$

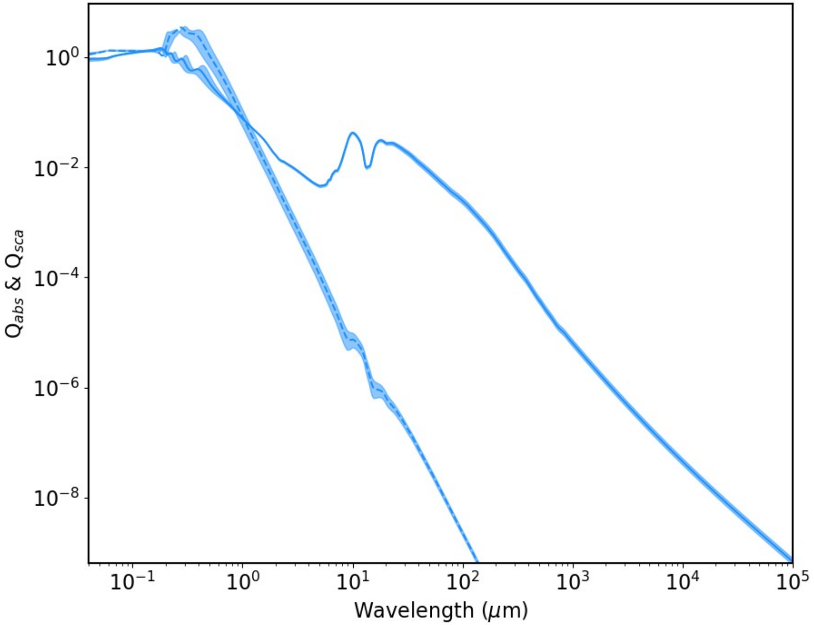
$$k = \sqrt{\frac{\sqrt{\epsilon'^2 + \epsilon''^2} - \epsilon'}{2}}.$$

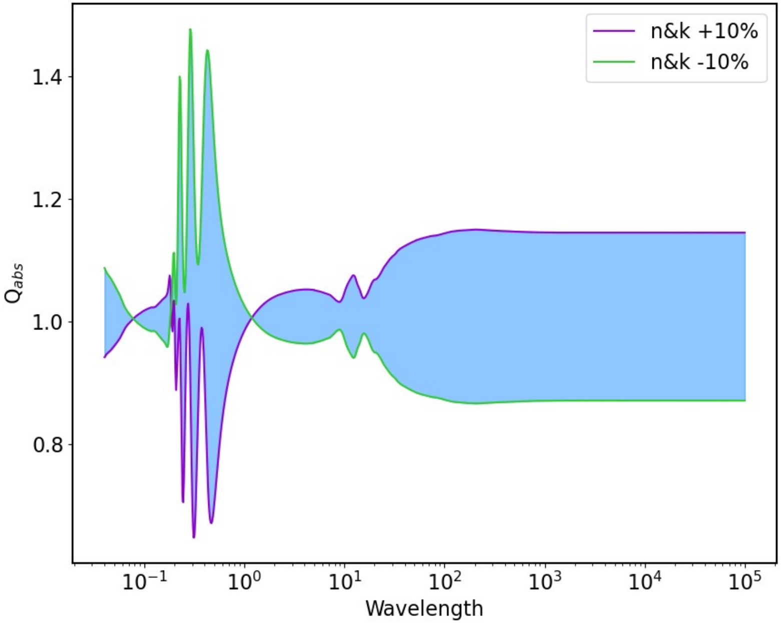
$$< \kappa_{\rm abs} >= \frac{2\pi N}{3\rho\lambda} \mathrm{Im}\left(\frac{\epsilon - \epsilon_m}{\epsilon_m + L(\epsilon - \epsilon_m)} + \frac{4(\epsilon - \epsilon_m)}{2\epsilon_m + (1 - L)(\epsilon - \epsilon_m)} \right)$$

Uncertainties in the optical constants

→ translation in the Q_{abs} & Q_{sca}

Let’s assume that both n & k vary by +10 % or -10 % for silicates
a = 0.1 µm



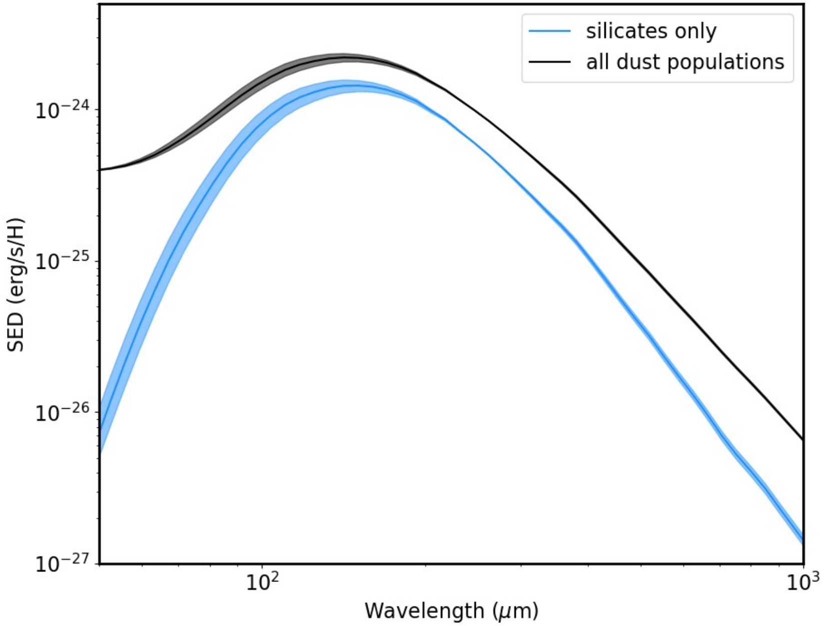


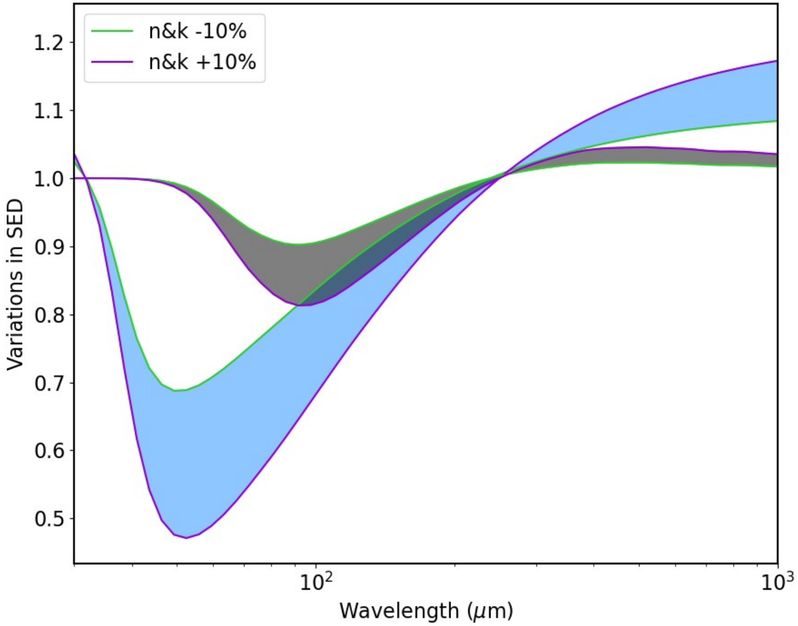
Uncertainties in models

Uncertainties in the optical constants

→ translation in the SED

Let’s assume that both n & k vary by +10 % or -10 % for silicates
→ silicates with a log-normal size distribution

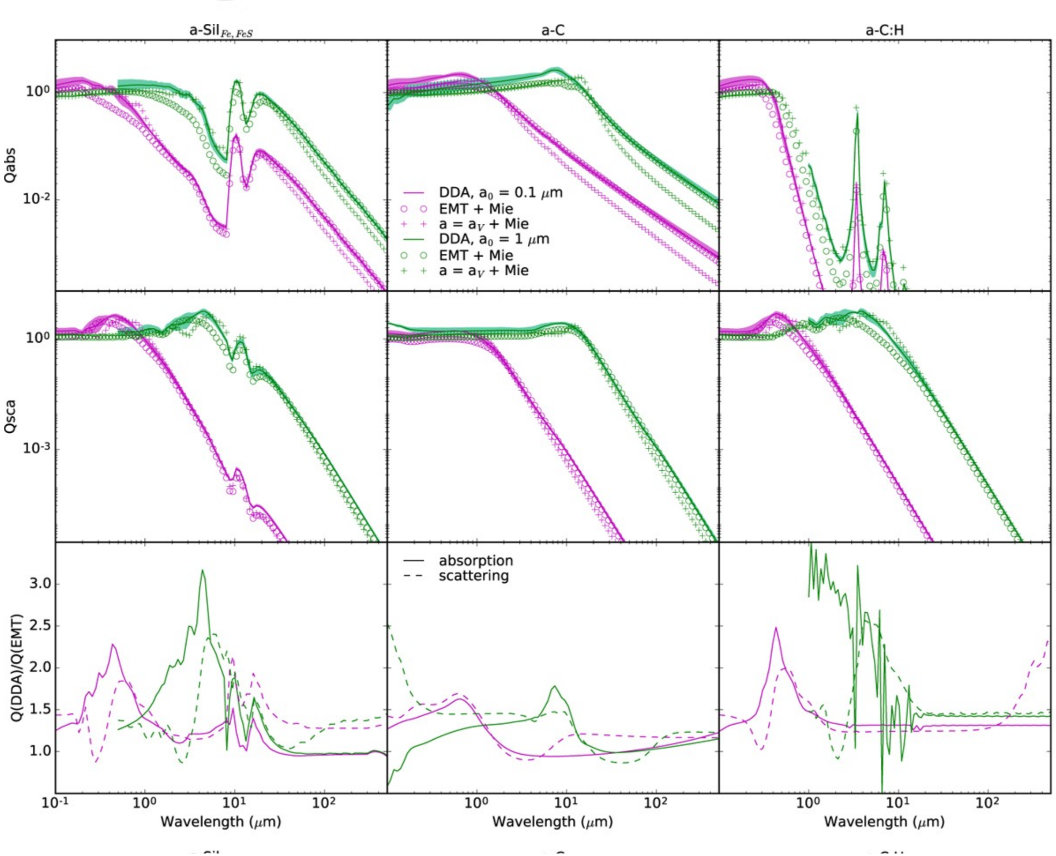


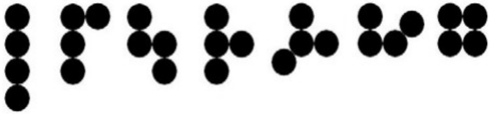


→ 10 % at long wavelength
→ more around the peak of the SED due to ≠ temperatures

Uncertainties in the models

Choice of the calculation method





Koehler et al. (2011)

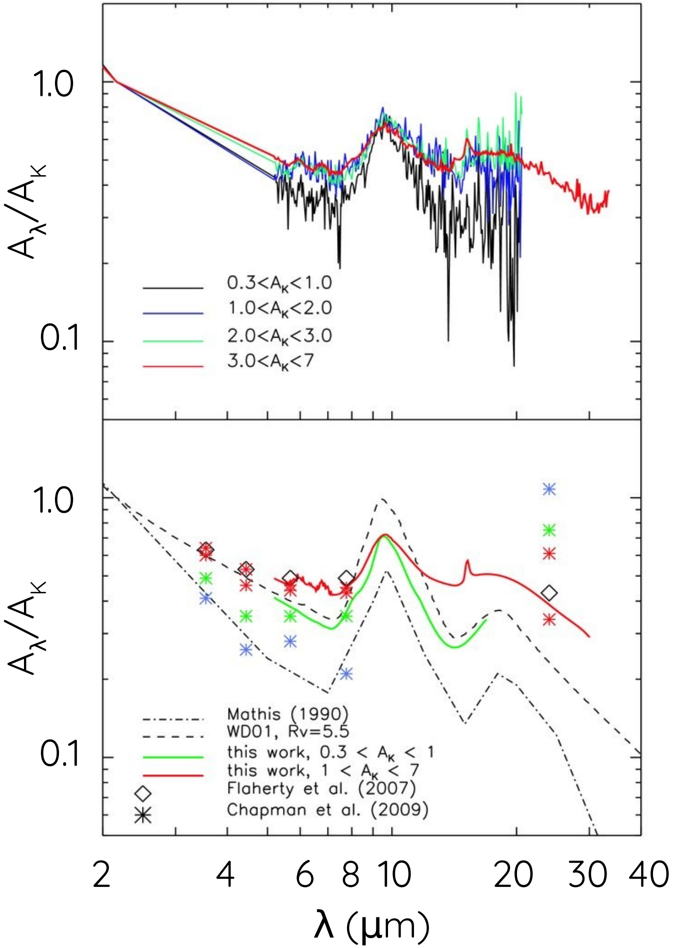
- Aggregates of 8 momoners
  monomer → 0.1 and 1 μm compact sphere

- Three types of calculations
  → DDA = "exact" method
  → Mie for a sphere of equivalent mass
  → EMT+Mie sphere with same radius of gyration $\mathcal{R}_g$ and $\mathcal{P}_{equivalent}$

- Significant differences
  → different grain temperatures
  → shifted SEDs
  → mid-IR silicate features ≠ size estimates

Example: silicate mid-IR features

McClure (2009) → observations



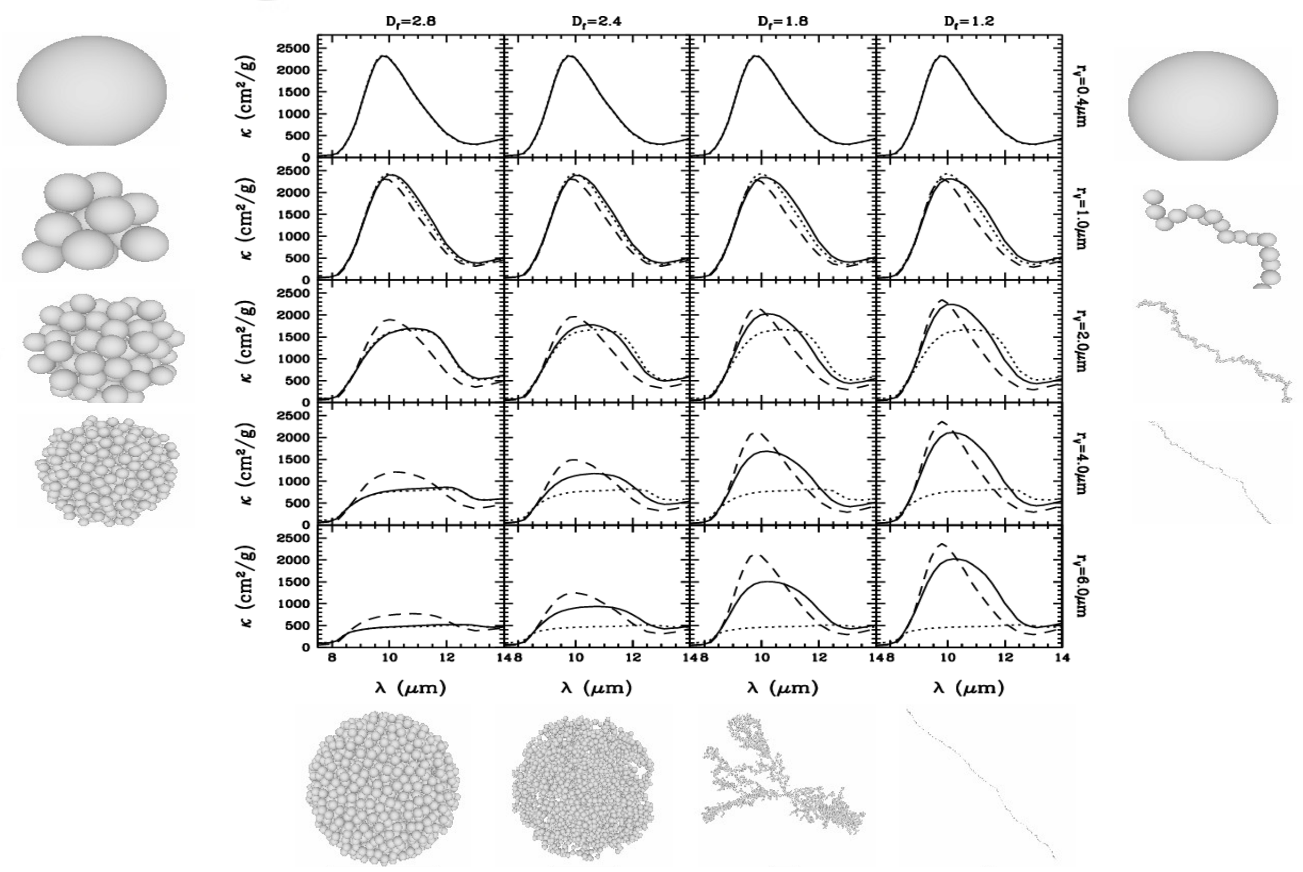
- Broader features in dense than diffuse ISM
- Lower constrast with continuum

⇨ significant grain growth ?

Grain size determination

Example: silicate mid-IR features

Min et al. (2016) → fractal dimension



—— aggregate

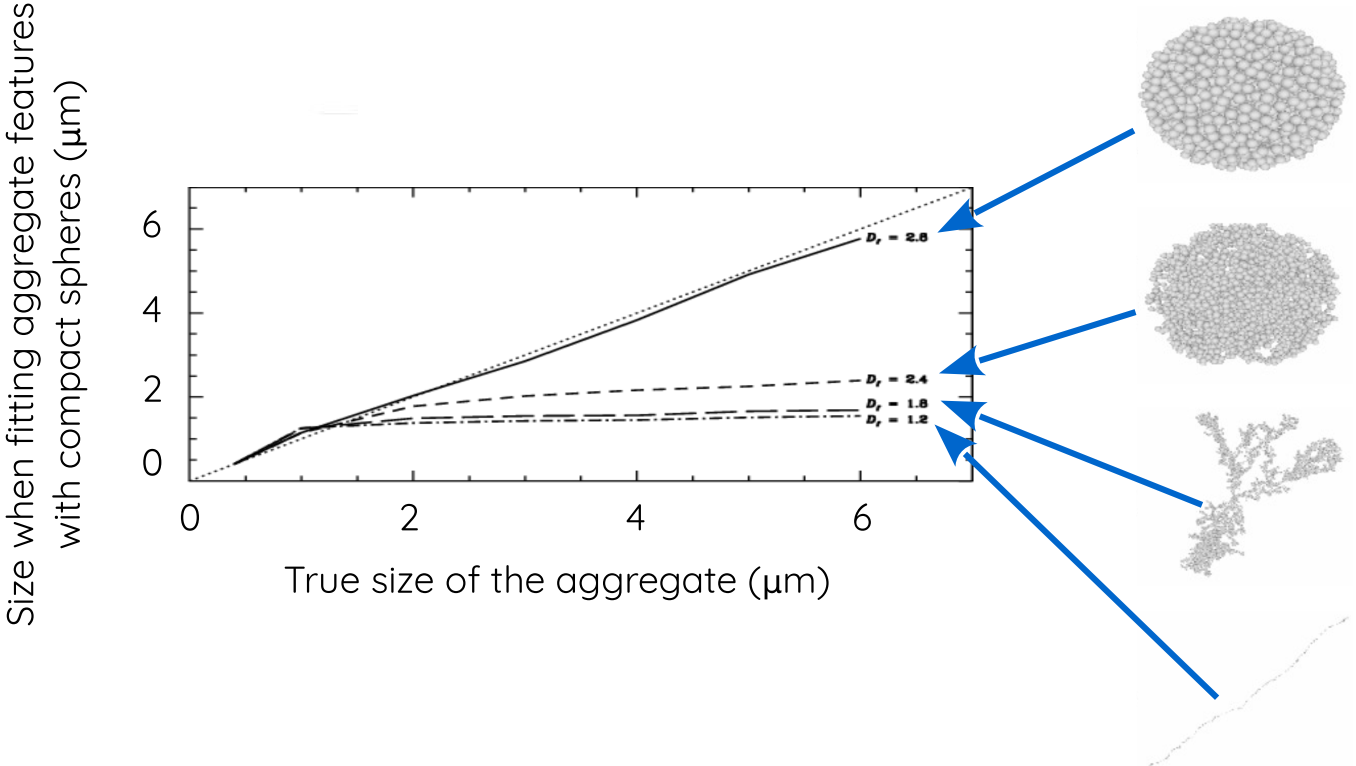
– – volume equivalent compact sphere

······ equivalent porous sphere

amorphous "olivine"
monomer radius a_0 = 0.4 µm

Example: silicate mid-IR features

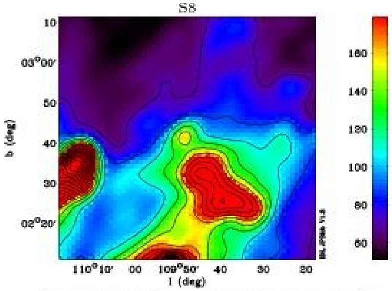
Min et al. (2016) → fractal dimension

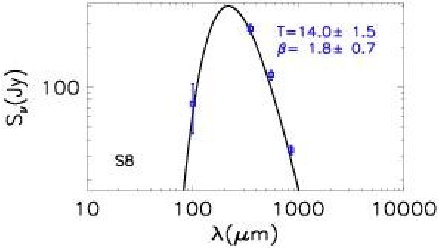


→ sizes UNDERestimated when using compact spheres
sizes OVERestimated when using porous spheres

Many mass estimates based on MBB fits

- Mass estimates based on modified blackbody fits for dense ISM regions
    - ↳ molecular clouds & prestellar cores (e.g. Planck Collaboration 2011 XXII)
    - ↳ young stellar objects & protoplanetary discs (e.g. Busquet et al. 2019)





- Assume a dust opacity at a given wavelength
    - ↳ pb. 1: depends on grain size distribution
    - ↳ pb. 2: depends on grain composition
    - ↳ pb. 3: depends on grain structure
    - ↳ pb. 4: depends on temperature distribution

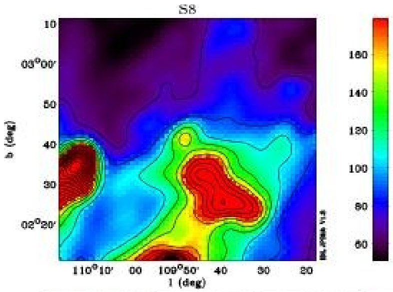
Why is it important to determine n(a) ?

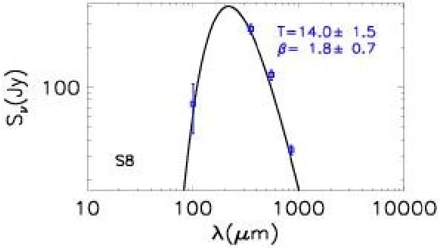
And not only a_{max}

- Mass estimates based on modified blackbody fits for dense ISM regions
  - ↳ molecular clouds & prestellar cores (e.g. Planck Collaboration 2011 XXII)
  - ↳ young stellar objects & protoplanetary discs (e.g. Busquet et al. 2019)

- Assume a dust opacity at a given wavelength
  - ↳ **pb. 1: depends on grain size distribution**
  - ↳ pb. 2: depends on grain composition
  - ↳ pb. 3: depends on grain structure
  - ↳ pb. 4: depends on temperature distribution

- Classical choice for pb. 1: power-law size distribution
  - ↳ Weidenschilling (1997)
  - ↳ Natta & Testi (2004)
  - ↳ Draine (2006)
  - ↳ …

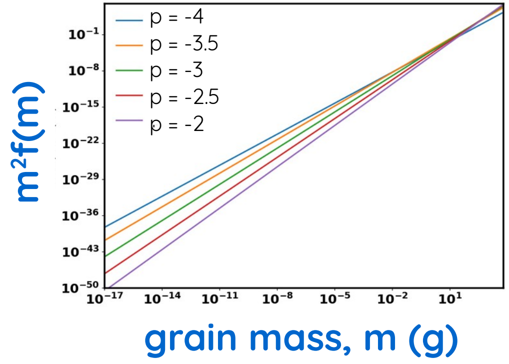




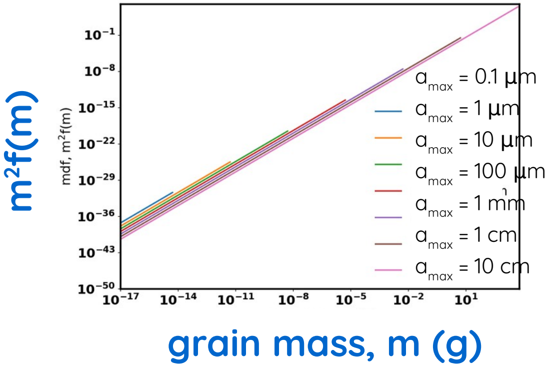
Cloud mass estimate

Influence on the dust opacity in the millimetre

Power-law size distribution

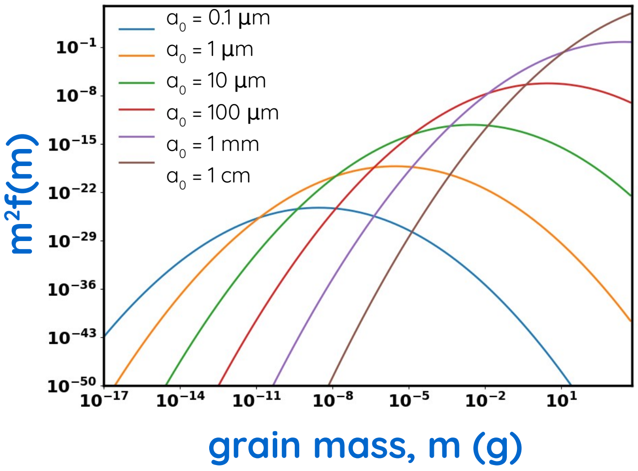


$$\frac{dm}{da} \propto a^{p}$$



$$\frac{dm}{da} \propto a^{-3.5}$$

Log-normal size distribution



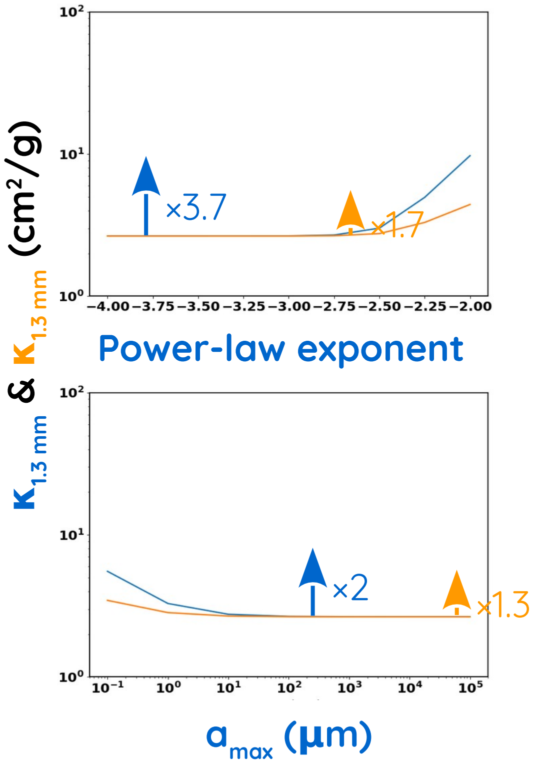
$$\frac{dm}{da} \propto \exp\left\{-\frac{1}{2}\left(\frac{\ln(a/a_0)}{\sigma}\right)^2\right\}$$

In all cases: a_{min} = 0.01 μm, a_{max}= 10 cm, M_{gas}/M_{dust} = 100

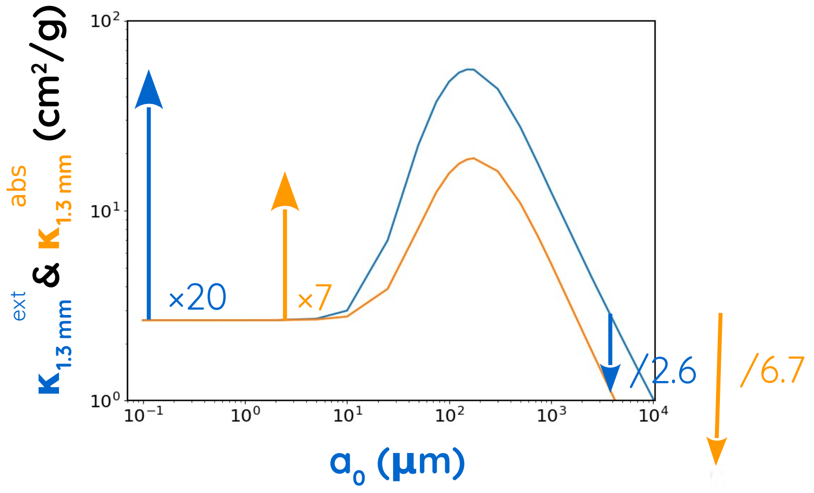
2/3 silicate + 1/3 amorphous carbon + 50% porosity → spherical grains

Influence on the dust opacity in the millimetre

Power-law size distribution



Log-normal size distribution



$$\kappa^{ext}\,[\mathrm{cm^2/g}] = \frac{3}{4\rho}\,\frac{Q_{abs}+Q_{sca}}{a}$$

$$\kappa^{abs}\,[\mathrm{cm^2/g}] = \frac{3}{4\rho}\,\frac{Q_{abs}}{a}$$

In all cases: a_{min} = 0.01 µm, a_{max} = 10 cm, M_{gas}/M_{dust} = 100

2/3 silicate + 1/3 amorphous carbon + 50% porosity → spherical grains

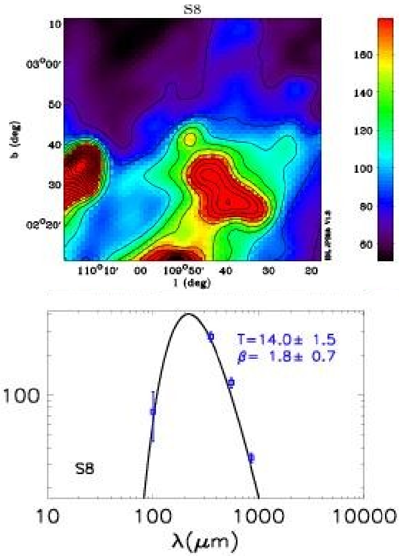
Why is it important to determine the grain composition ?

And not only their size

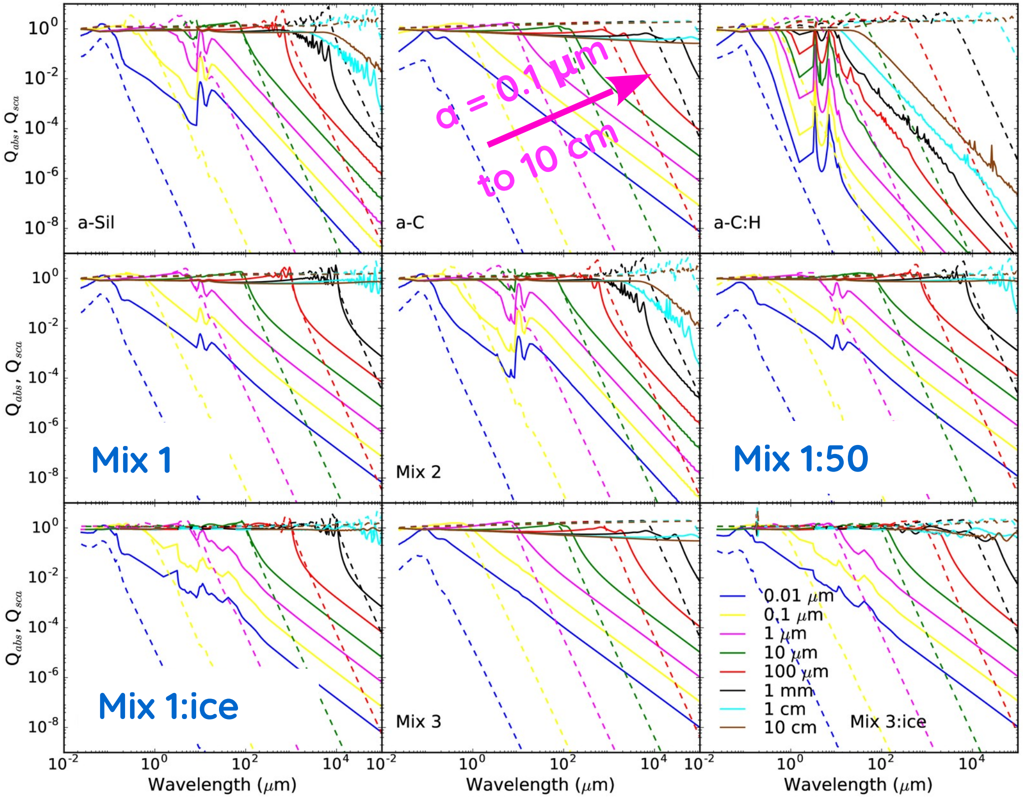
- Mass estimates based on modified blackbody fits for dense ISM regions
  - ↳ molecular clouds & prestellar cores (e.g. Planck Collaboration 2011 XXII)
  - ↳ young stellar objects & protoplanetary discs (e.g. Busquet et al. 2019)

- Assume a dust opacity at a given wavelength
  - ↳ pb. 1: depends on grain size distribution
  - ↳ **pb. 2: depends on grain composition**
  - ↳ pb. 3: depends on grain structure
  - ↳ pb. 4: depends on temperature distribution

- Classical choice for pb. 2: fixed κ value with fixed β
  - ↳ any dust model from the litterature



Absorption and scattering efficiencies



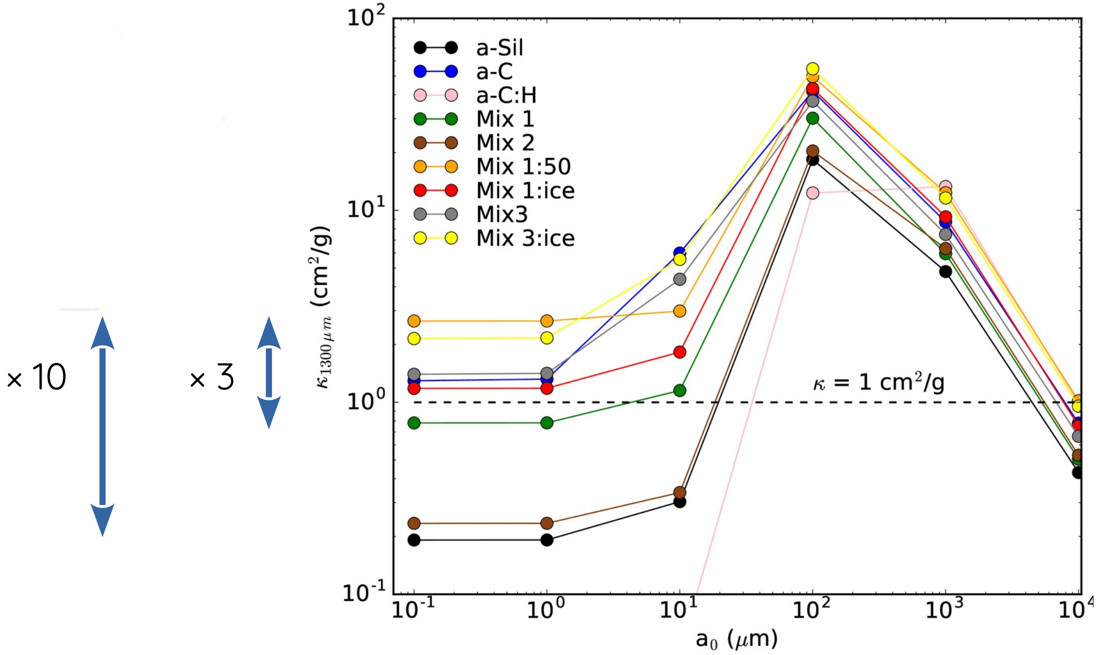
Mix 1 ~ compact AMM
Mix 1:50 ~ AMM
Mix 1:ice ~ compact AMMI

Mix 3 & Mix 3:ice ~ Pollack (1994)

a-Sil →THEMIS amorphous silicates
a-C→THEMIS E_g = 0.1 eV
a-C:H →THEMIS E_g = 2.5 eV
Mix 1 → 2/3 aSil + 1/3 a-C
Mix 2 → 2/3 aSil + 1/3 a-C:H
Mix 1:50 → porous Mix 1 ~ AMM
Mix 1:ice → Mix 1 with an ice mantle
Mix 3 → 20% a-Sil + 80% a-C
Mix 3:ice → Mix 3 with an ice mantle

Cloud mass estimate

Mass absorption coefficients at 1.3 mm



$$\frac{\text{Mgas}}{\text{Mdust}} = 100$$

$$\frac{dn}{da} \propto \exp\left\{-\frac{1}{2}\left[\frac{\ln(a/a_0)}{\sigma}\right]^2\right\}$$

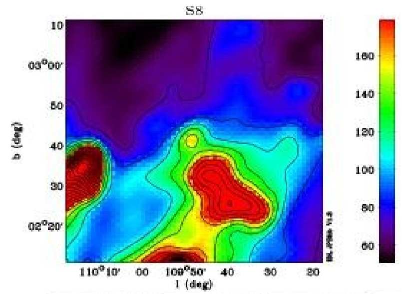
Why is it important to determine the grain composition ?

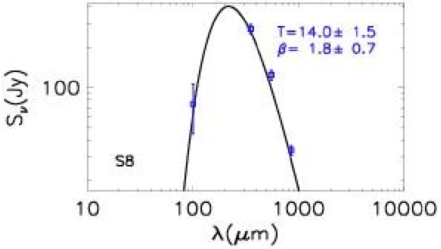
And not only their size and composition

- Mass estimates based on modified blackbody fits for dense ISM regions
  ↳ molecular clouds & prestellar cores (e.g. Planck Collaboration 2011 XXII)
  ↳ young stellar objects & protoplanetary discs (e.g. Busquet et al. 2019)

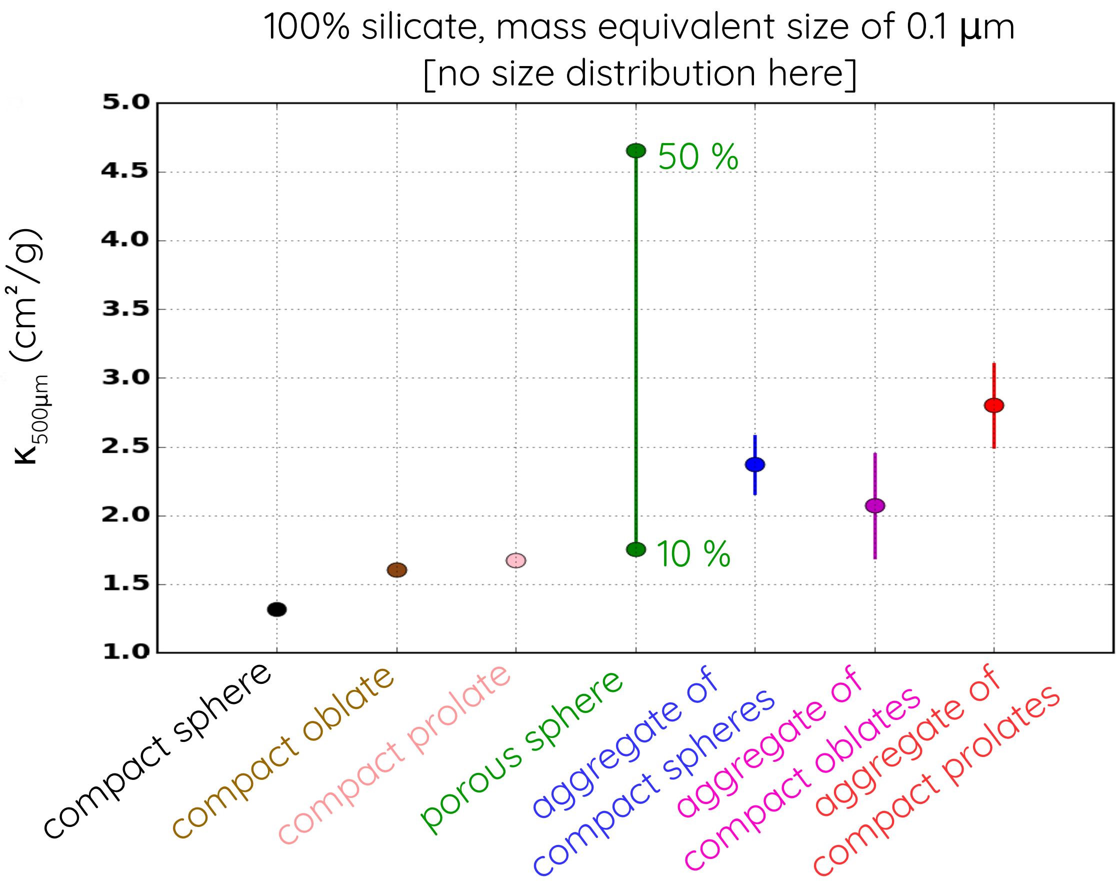
- Assume a dust opacity at a given wavelength
  ↳ pb. 1: depends on grain size distribution
  ↳ pb. 2: depends on grain composition
  ↳ **pb. 3: depends on grain structure**
  ↳ pb. 4: depends on temperature distribution

- Classical choice for pb. 3
  ↳ignore the problem



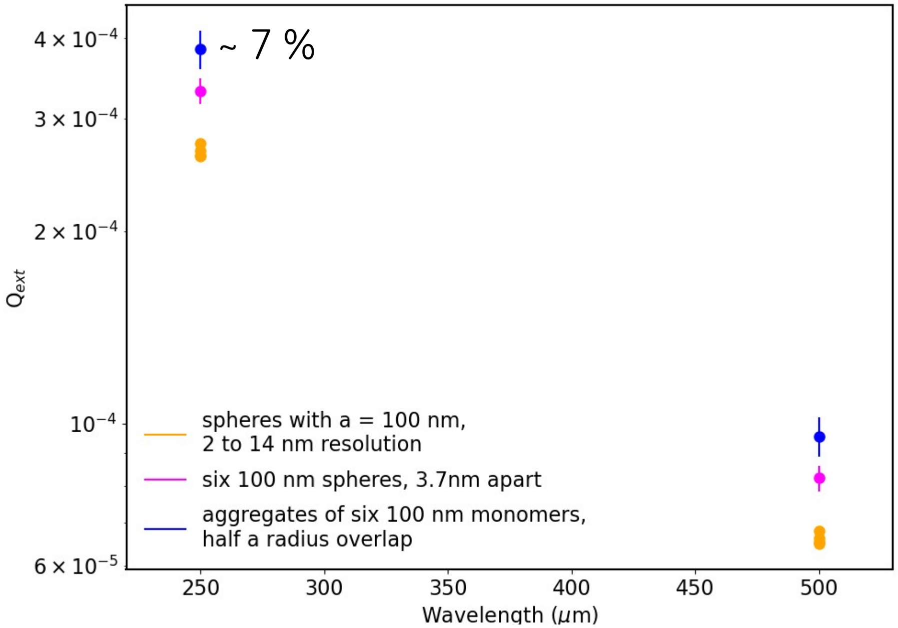


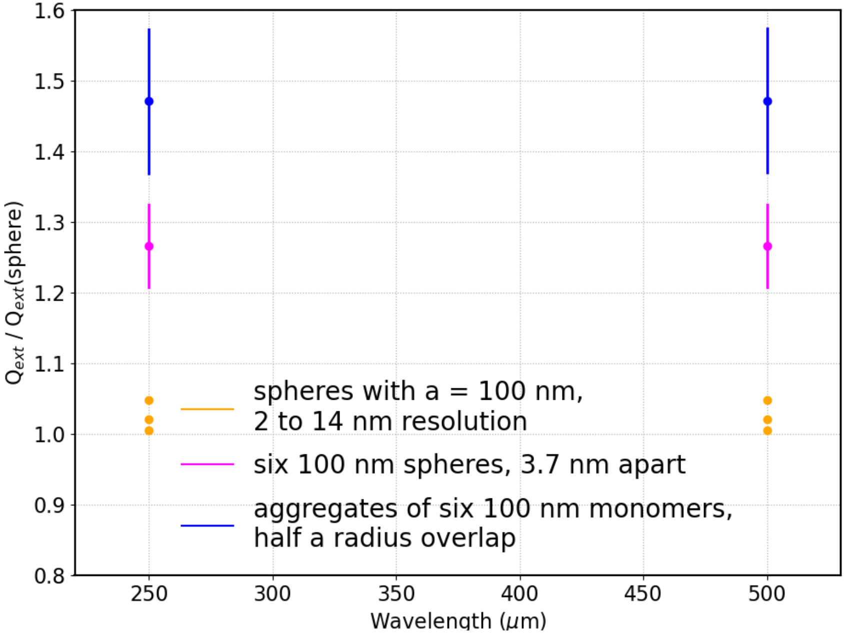
Mass absorption coefficients at 500 µm



Description of the grain surface

→ completely smooth vs. irregular





→ single grains: increase by ~ 5 % for highly irregular surface

→ aggregates: increase by ~ 20 % for large contact area

Cloud mass estimate

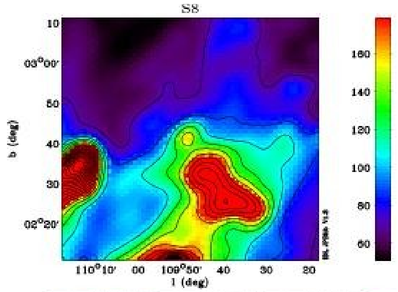
Why is it important to take into accound the radiative transfer ?

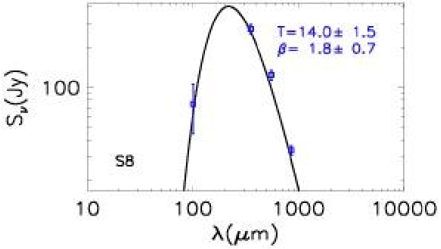
And not only the dust grain properties

- Mass estimates based on modified blackbody fits for dense ISM regions
  - ↳ molecular clouds & prestellar cores (e.g. Planck Collaboration 2011 XXII)
  - ↳ young stellar objects & protoplanetary discs (e.g. Busquet et al. 2019)

- Assume a dust opacity at a given wavelength
  - ↳ pb. 1: depends on grain size distribution
  - ↳ pb. 2: depends on grain composition
  - ↳ pb. 3: depends on grain structure
  - ↳ **pb. 4: depends on temperature distribution**

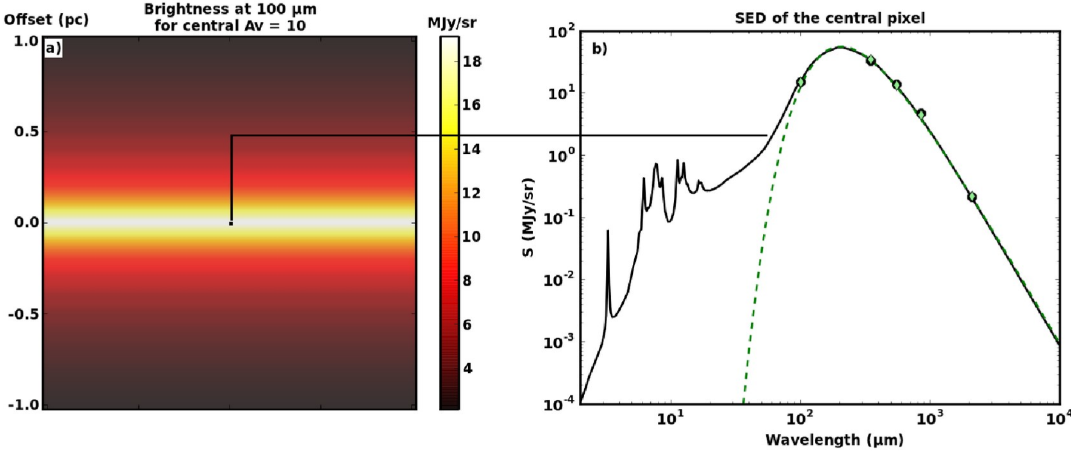
- Classical choice for pb. 4
  - ↳depends on the concerned community

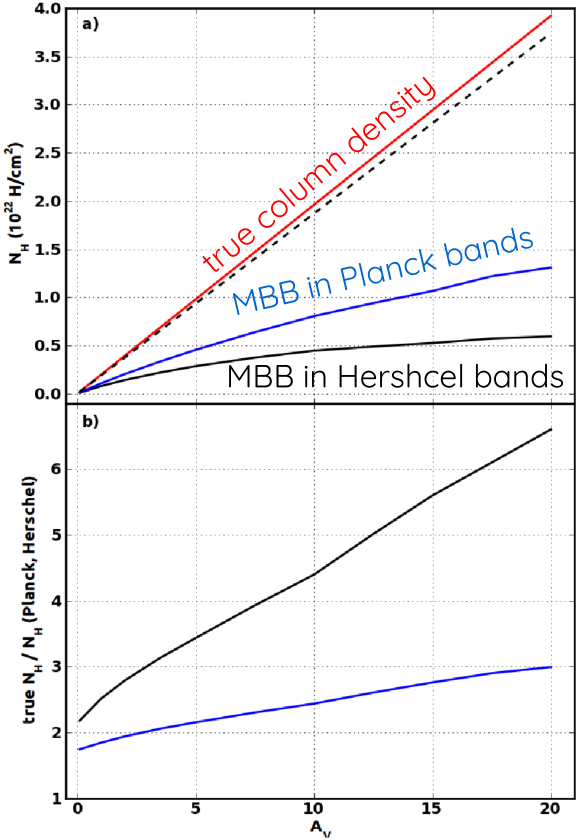




Cloud mass estimate

Column density as a function of cloud visual extinction





- Cylindrical clouds with $0.1 \leq A_V \leq 20$
- Depending on the dataset, mass can be strongly underestimated when using a MBB

Final words

- Dust properties vary both in the diffuse and the dense ISM
- Be careful to always know which dataset was used to define a dust model
  → comparison between different dust models does not always make sense
- Uncertainties in the dust models are probably always larger than uncertainties in your data
- Keep in mind what you are neglecting when fitting your data

Many dust models available in the DustEM numerical tool to calculate dust emission & extinction (polarised or not)
https://www.ias.u-psud.fr/DUSTEM/