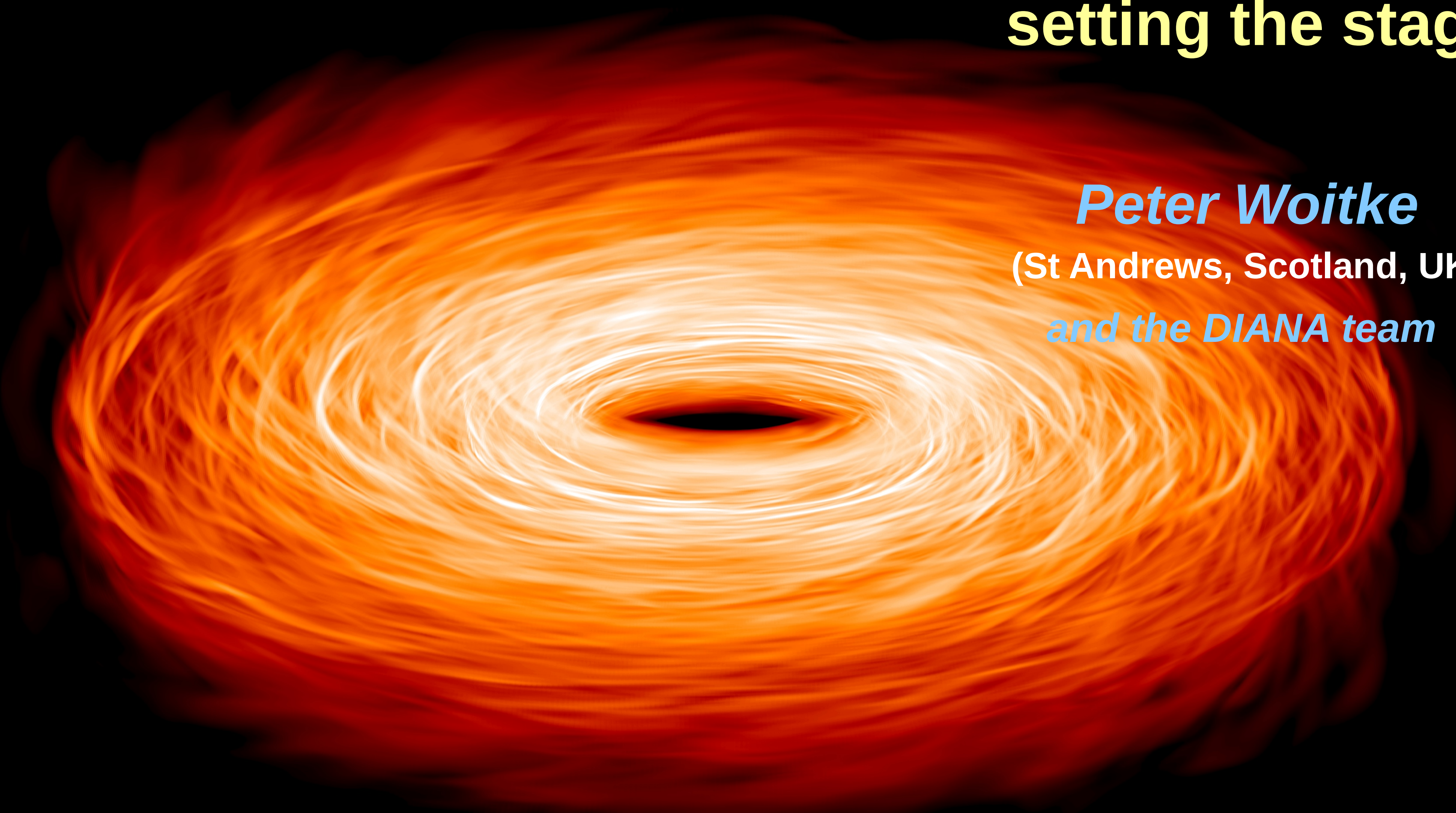
Astrochemistry in protoplanetary discs: disk shape and dust properties setting the stage



Peter Woitke

(St Andrews, Scotland, UK)

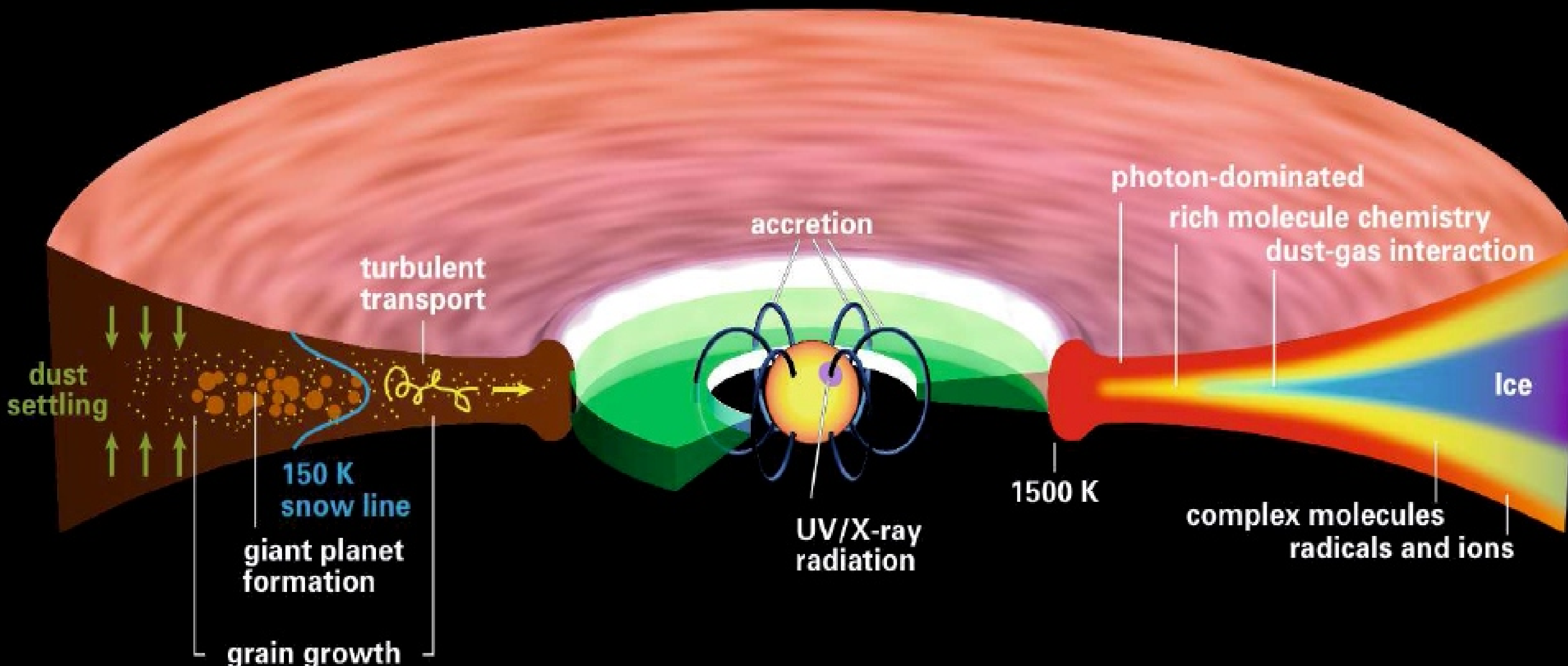
and the DIANA team

DiscAnalysis DIANA

University of St Andrews / universität wien / Astronomical Institute Anton Pannekoek / IPAG Institut de Planétologie et d'Astrophysique de Grenoble / cnes / university of groningen / kapteyn astronomical institute / Seventh Framework Programme

International Symposium and Workshop on Astrochemistry
July 3-8, 2016 - Campinas, SP - Brazil

Protoplanetary Disks



IS chemistry ≠ disk chemistry

- **larger densities** ≈ **10^4 … 10^{16} cm^{-3}**
- **higher temperatures** ≈ **10 … 10000 K** ($T_{gas} \geq T_{dust}$)
- **central star** = **strong UV and X-ray source**
- **2D/3D structure**

  → strongly irradiated and strongly shadowed regions

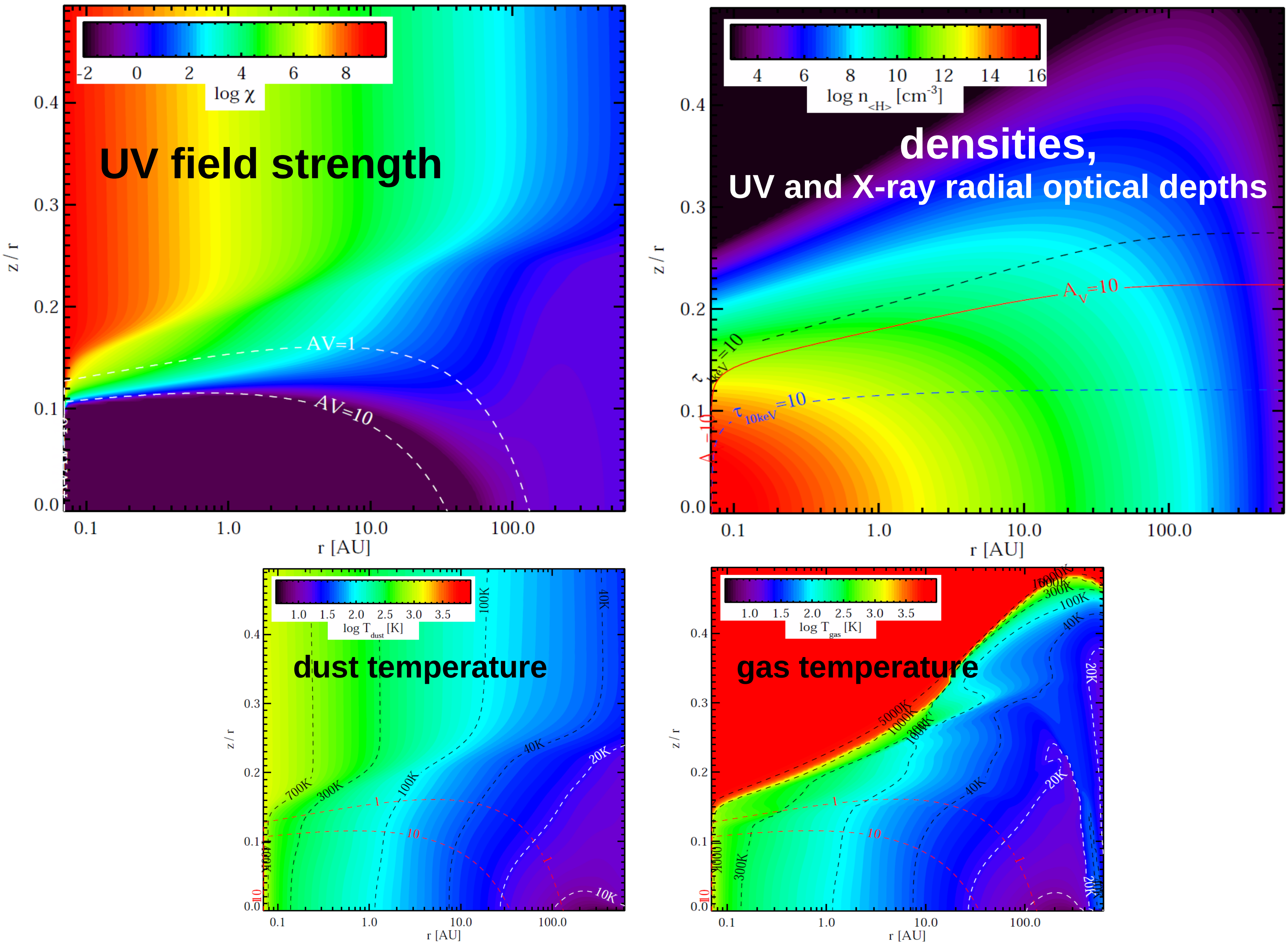
- **much larger dust grains** ≈ **0.1 µm … 1 mm** *(or even larger)*

  → reduction of UV dust opacity & total dust surface by factor ~100 (!)

  → penetration depths: UV ≈ X-ray « CR

  → important for chemistry and heating/cooling balance

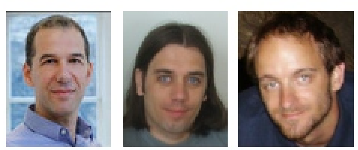
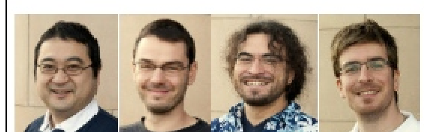
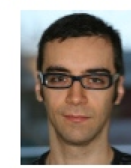
IS chemistry ≠ disk chemistry



DiscAnalysis DIANA

FP7-SPACE 2011 collaboration

Analysis and Modelling of Multi-wavelength Observational Data from Protoplanetary Discs

St Andrews	Vienna	Amsterdam	Grenoble	Groningen
				
P. Woitke	*M. Güdel*	*R. Waters*	*F. Ménard*	*I. Kamp*
				
Greaves Ilee Rigon	*Dionatos Rab Liebhart*	*Min Dominik*	*Thi Pinte Carmona Anthonioz*	*Antonellini*
sub-mm to cm	**X-rays**	**near-mid IR**	**near-far IR**	**near IR - mm**
coordination	obs./mod.	mod./obs.	obs./mod.	mod./obs.
JCMT, eMERLIN	XMM, Herschel	VLT, JWST	HST, Herschel	Herschel, JWST
astrobiology	high energy	dust mod.	interferometry	gas mod.

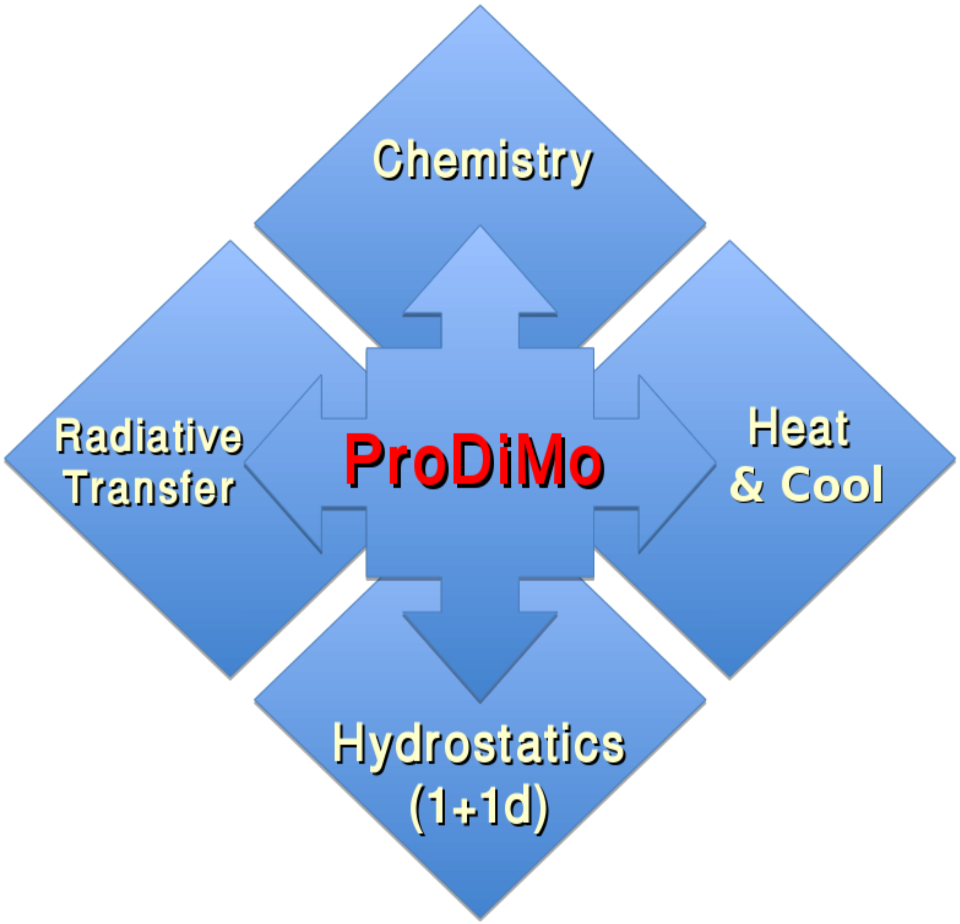
multi-λ data collection X-ray to cm (archival and proprietary)

coherent, detailed modelling of gas & dust throughout the disc

using disk modelling software ProDiMo, MCMax, MCFOST

aim: disc shape, temperatures, dust properties, chemistry in the birth-places of exoplanets

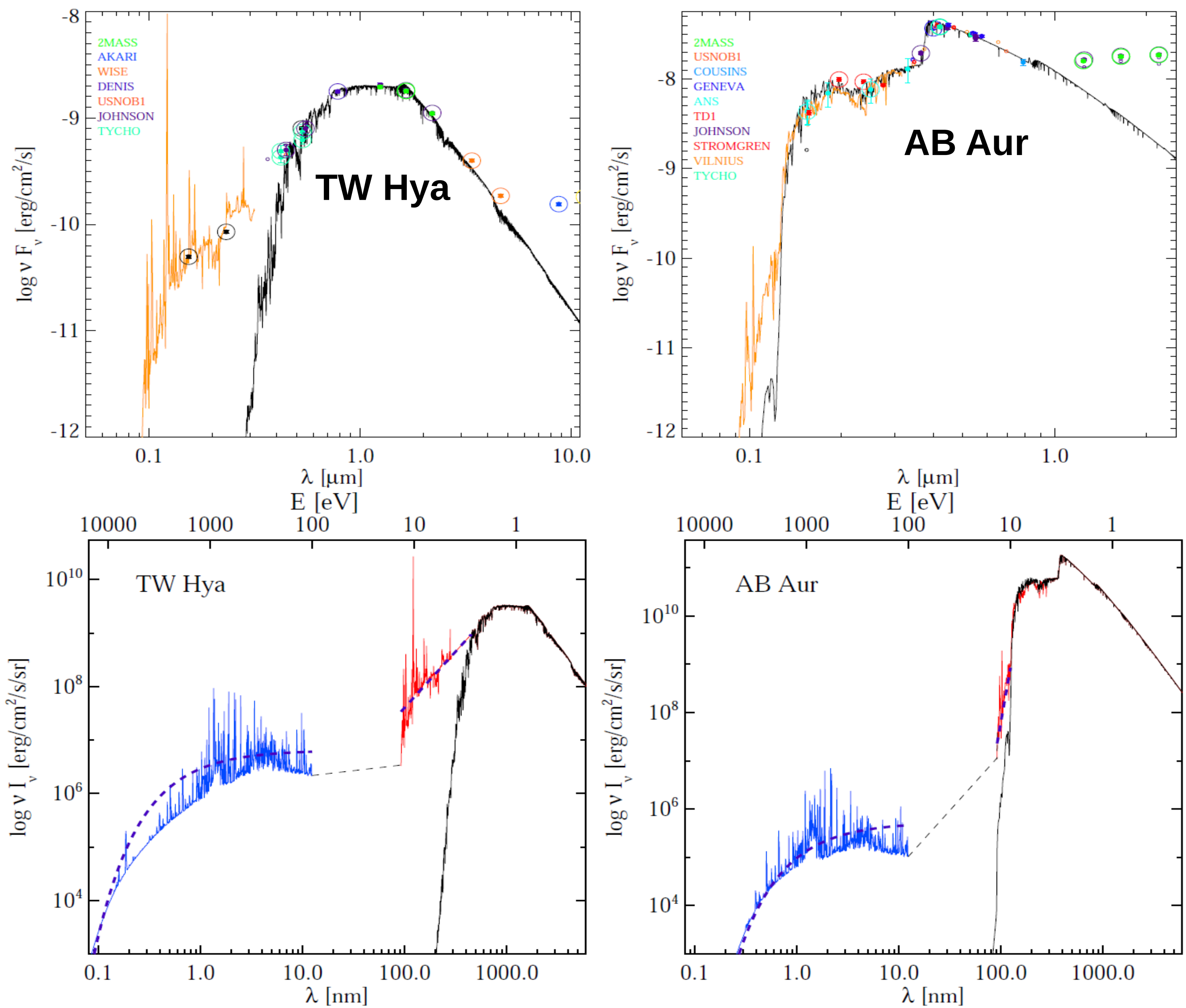
ProDiMo: a modular framework for *your* disc research



main papers: Woitke, Kamp, Thi (2009),
Kamp et al. (2010),
Thi et al. (2011),
Woitke et al. (2016)

- select ***your chemical species***
- compile ***your chemical rates***
  (or use UMIST or OSU or KIDA)
- set stellar ***UV & X-rays*** properties
- ***grain material & size distribution***
- ***column density & disc zones***
- **options:**
  - parametric / hydrostatic ***vertical extension*** ?
  - ***dust settling*** ?
  - ***PAHs*** ? (RT / chemistry / heating)
  - ***X-ray radiative transfer*** ?
  - ***time-dependent chemistry*** ?
  - ***grain charges*** ? (in development)
  - ***surface chemistry*** ? (in development)

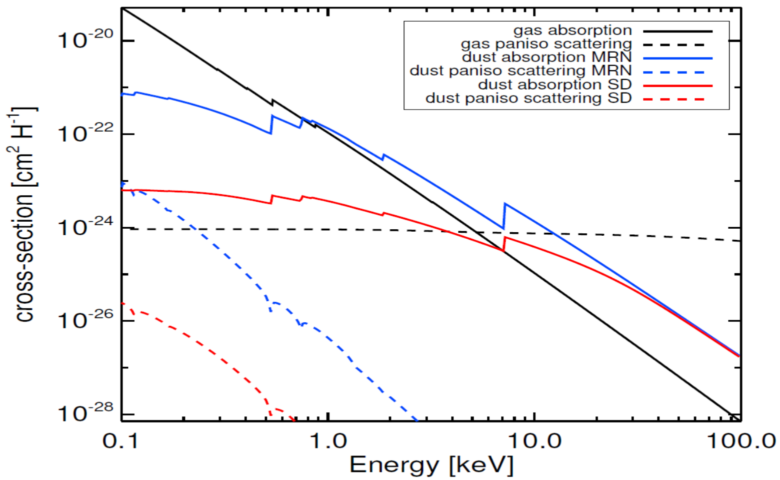
usage of UV and X-ray data



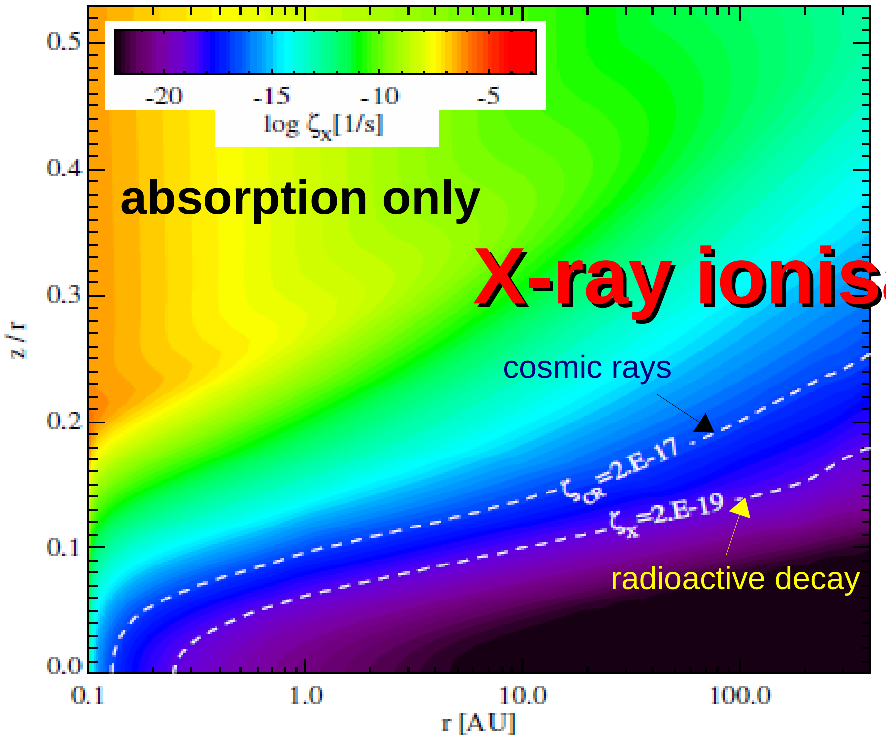
X-ray radiative transfer

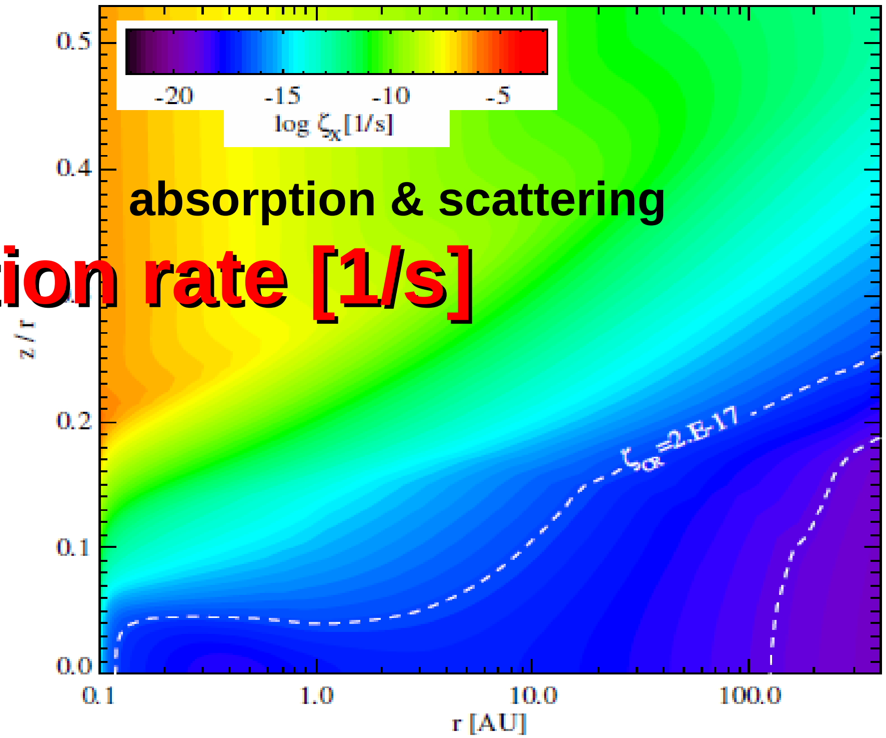
→ *Christian Rab, University of Vienna, Austria*

X-ray gas & dust opacities



X-ray ionisation rate [1/s]





Charged Grain Chemistry

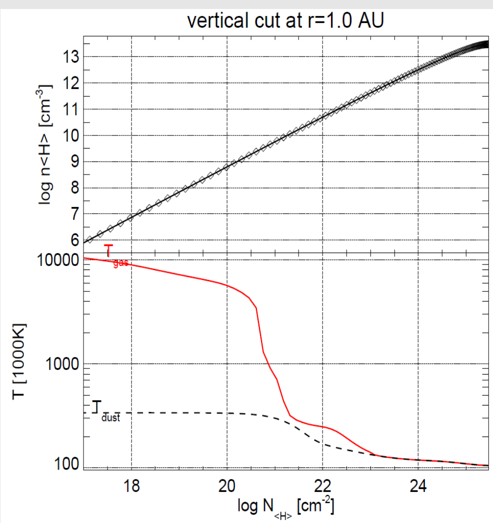
$Z + h\nu \rightarrow Z^+ + e^-$	photoelectric / photodetachment
$Z + e^- \rightarrow Z^-$	electron attachment
$Z + A^+ \rightarrow Z^+ + A$	charge exchange
$Z + AB^+ \rightarrow Z^+ + A + B$	dissociative charge exchange
$Z \rightarrow Z^+ + e^-$	thermionic emission
$Z + M \rightarrow Z^+ + e^- + M$	collisional electron detachment

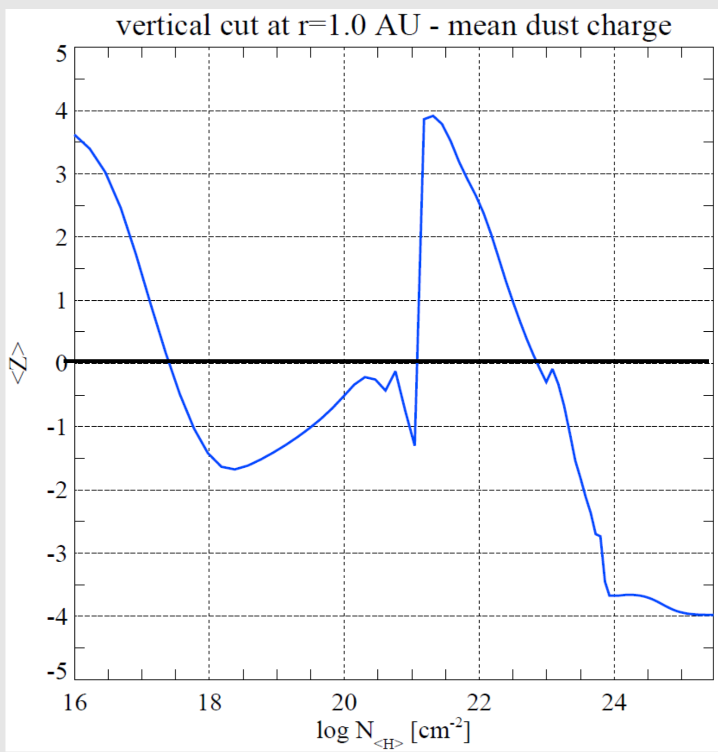
included species

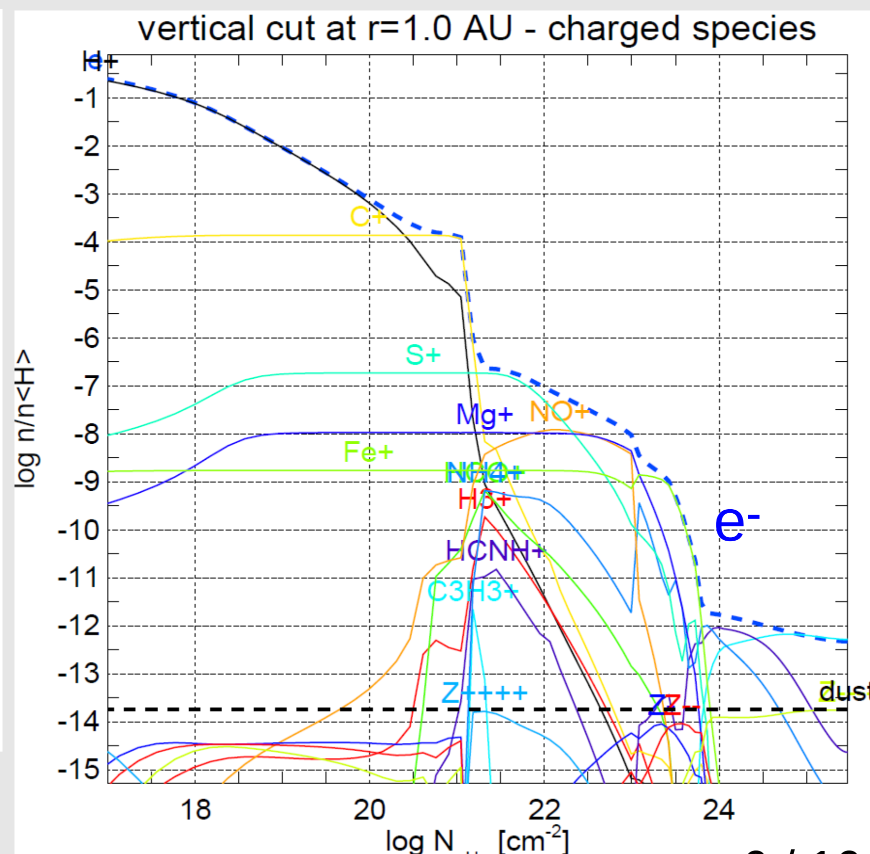
Z^{----}, Z^{---}, Z^{--}, Z^{-},

Z,

Z^{+}, Z^{++}, Z^{+++}, Z^{++++}

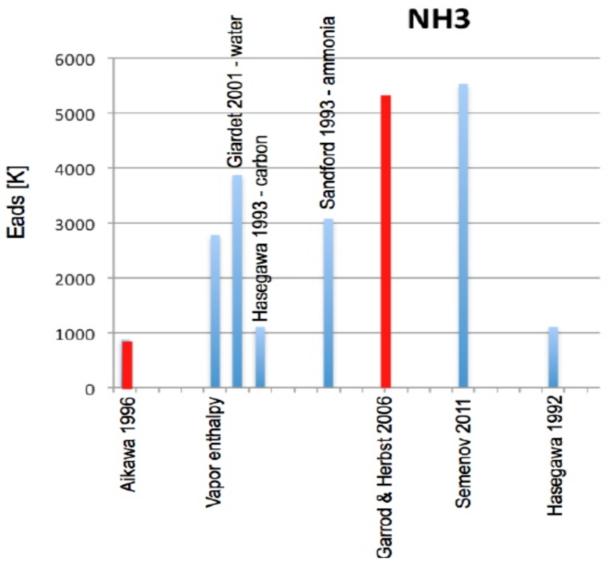


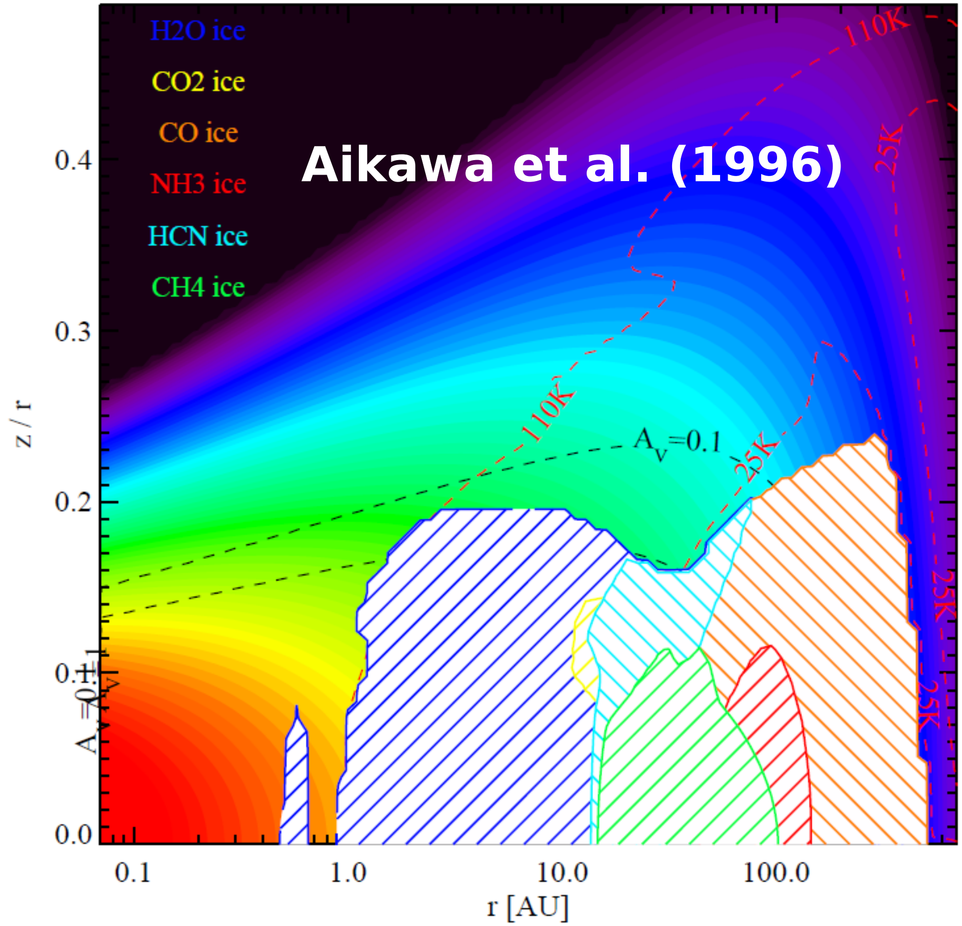


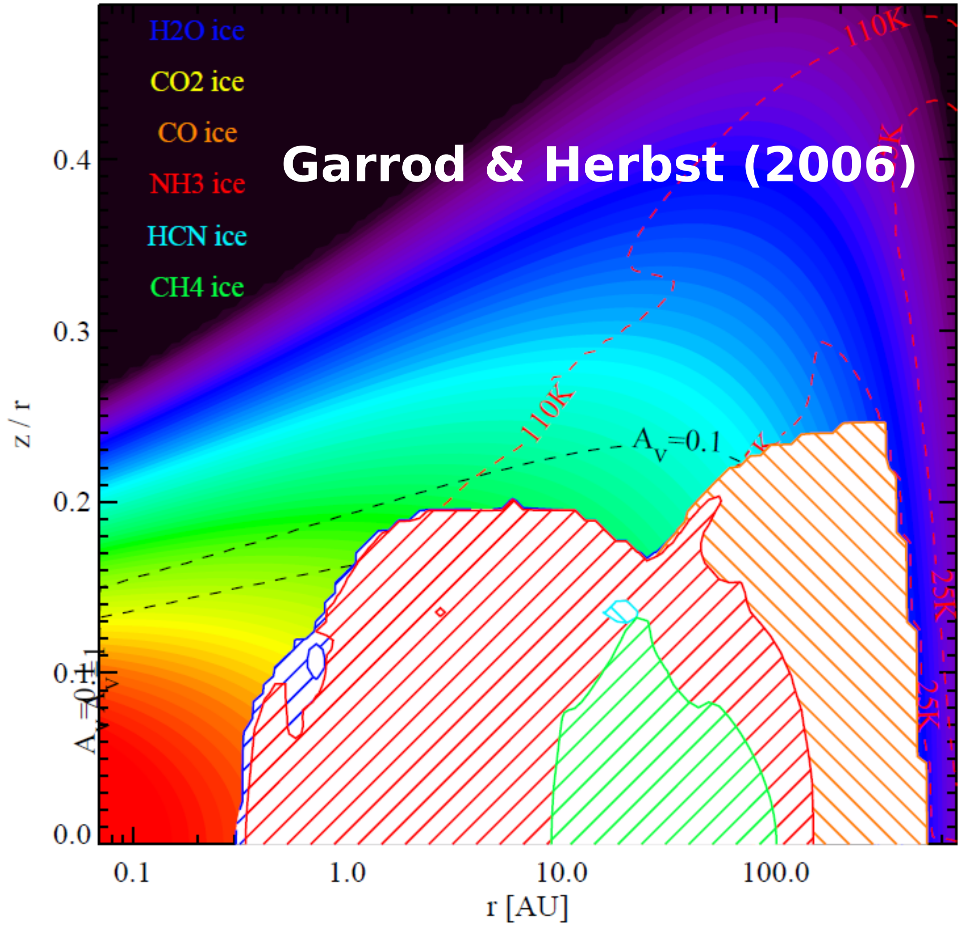


ice abundances

→ *impact of adsorption energies*



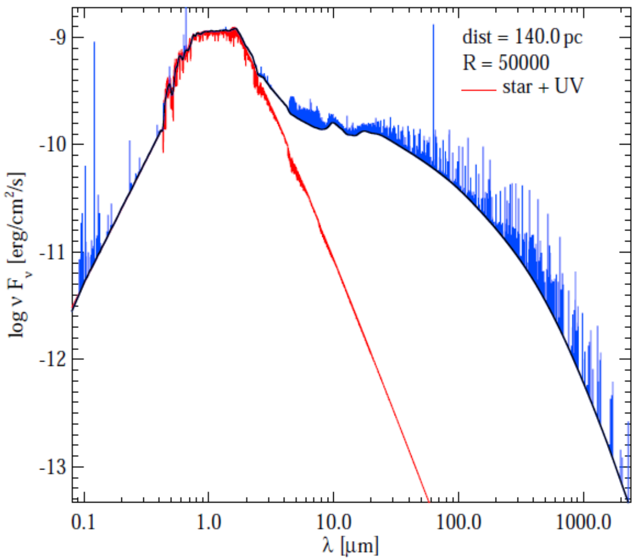




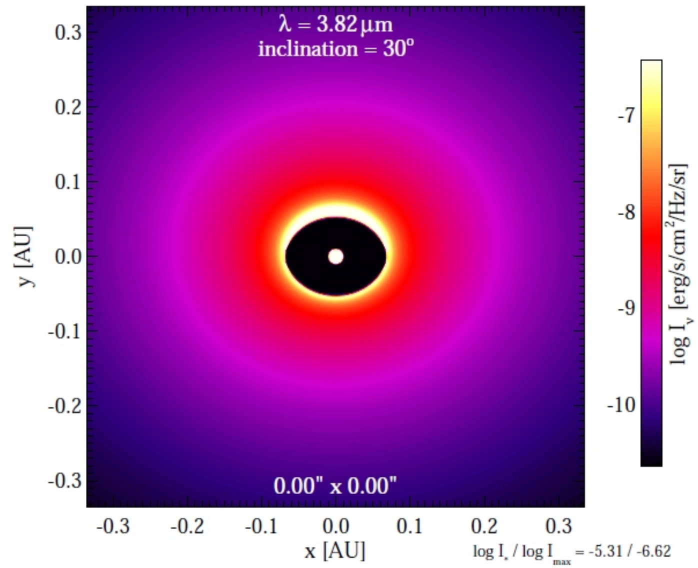
Kamp et al. (2016, in prep.)

simulated observations

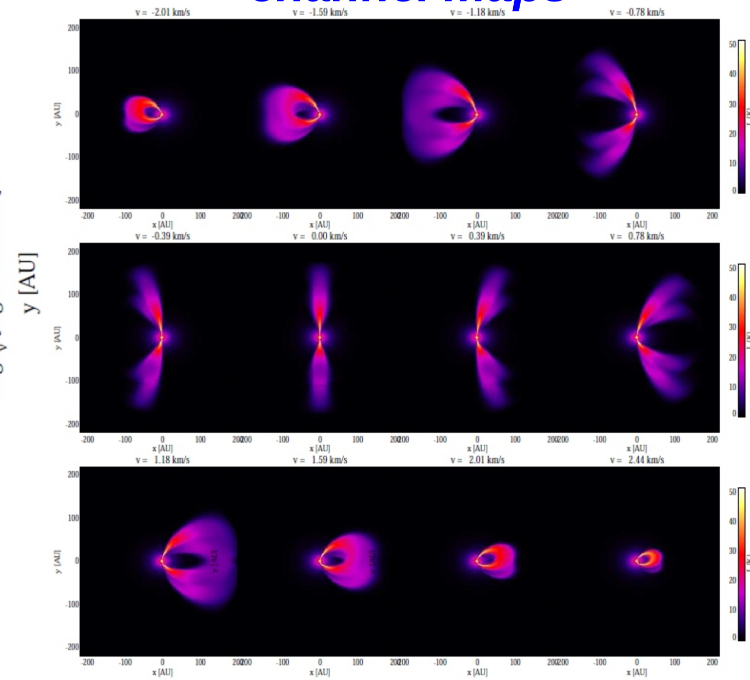
SED and line fluxes



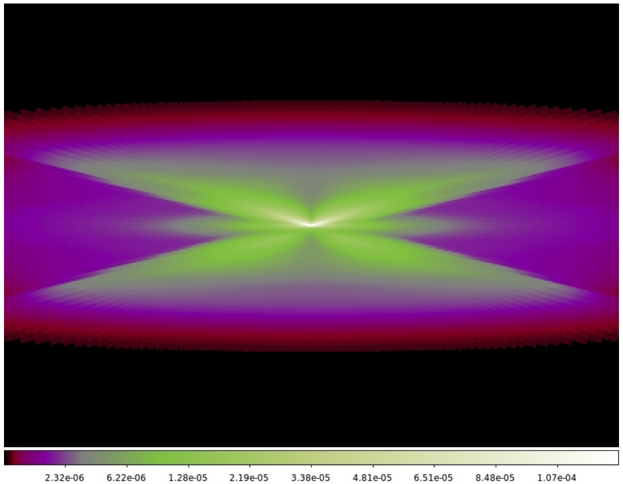
continnum images



channel maps

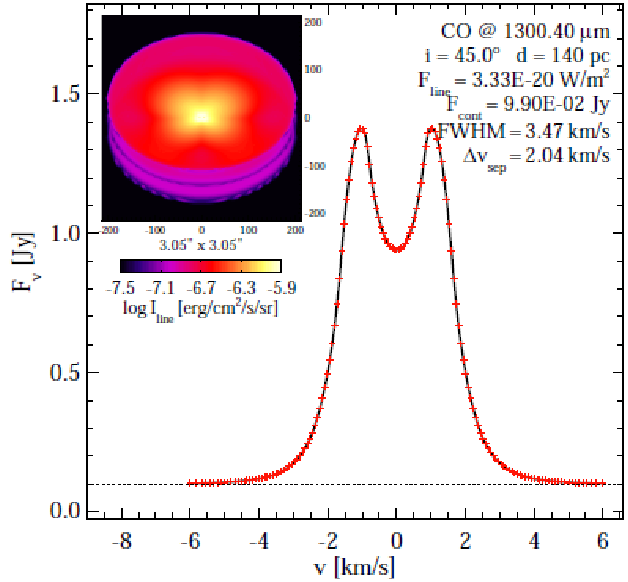


emission line maps



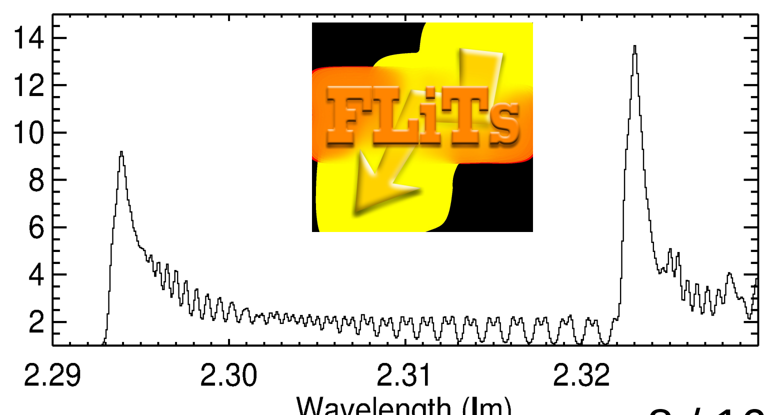
^{13}CO line @ 220.399 GHz from an edge-on disk

velocity profile



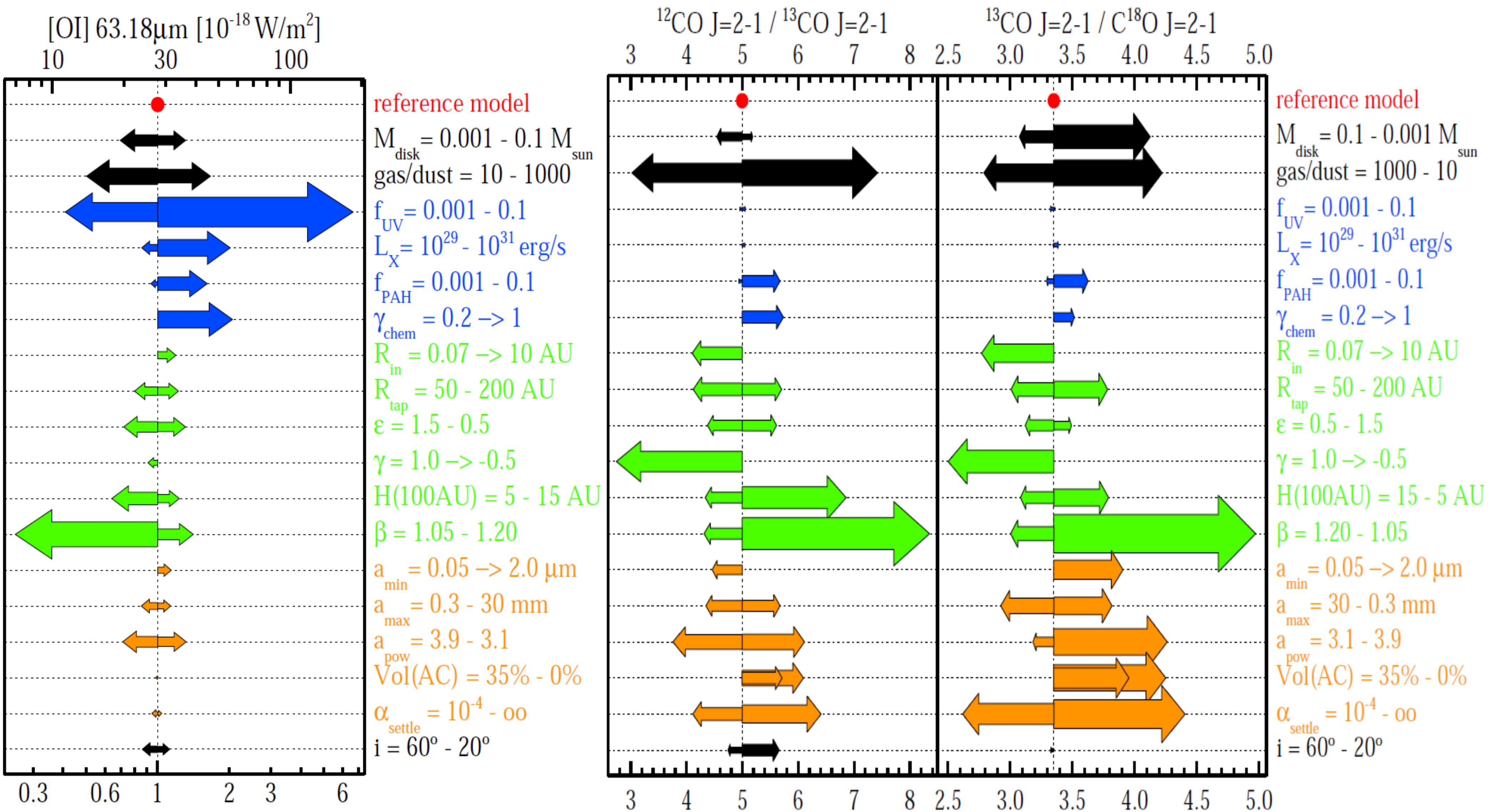
new: *high-res IR spectrum*

ProDiMo model + FLiTs



"Impactograms"

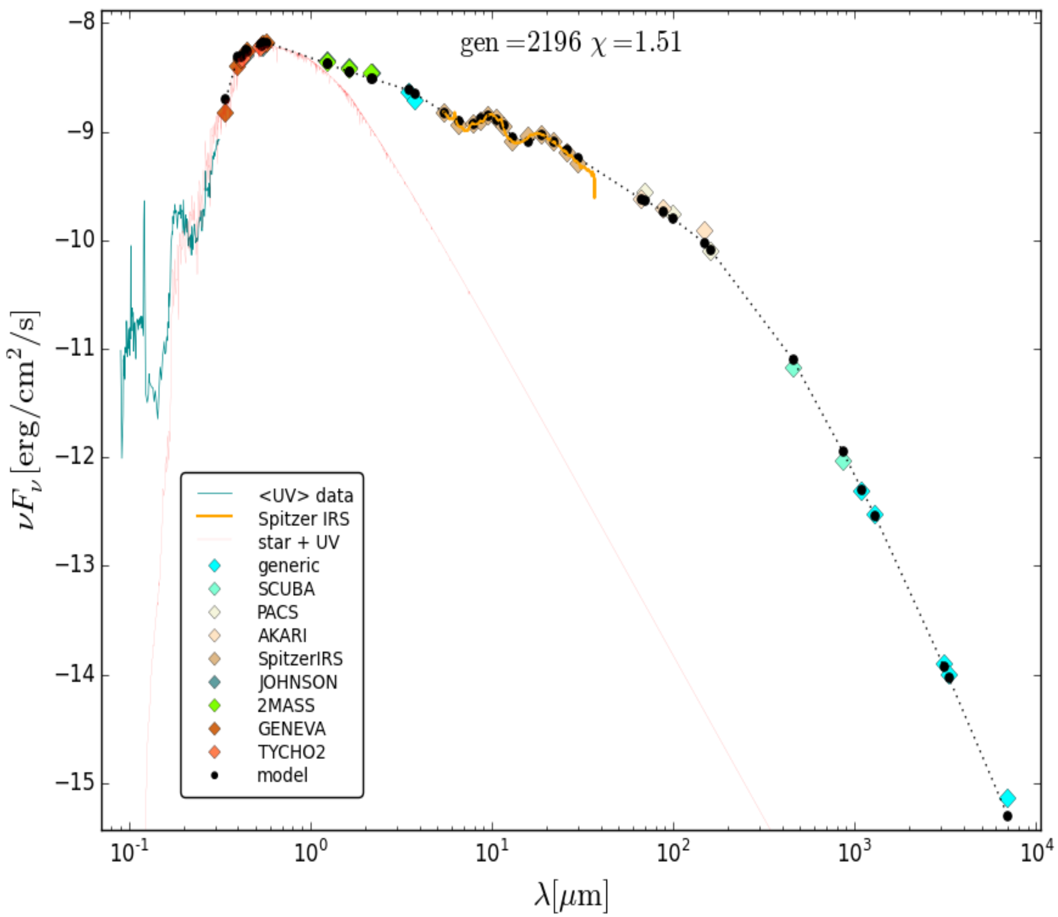
→ *Woitke et al. 2016, A&A 585, 61*



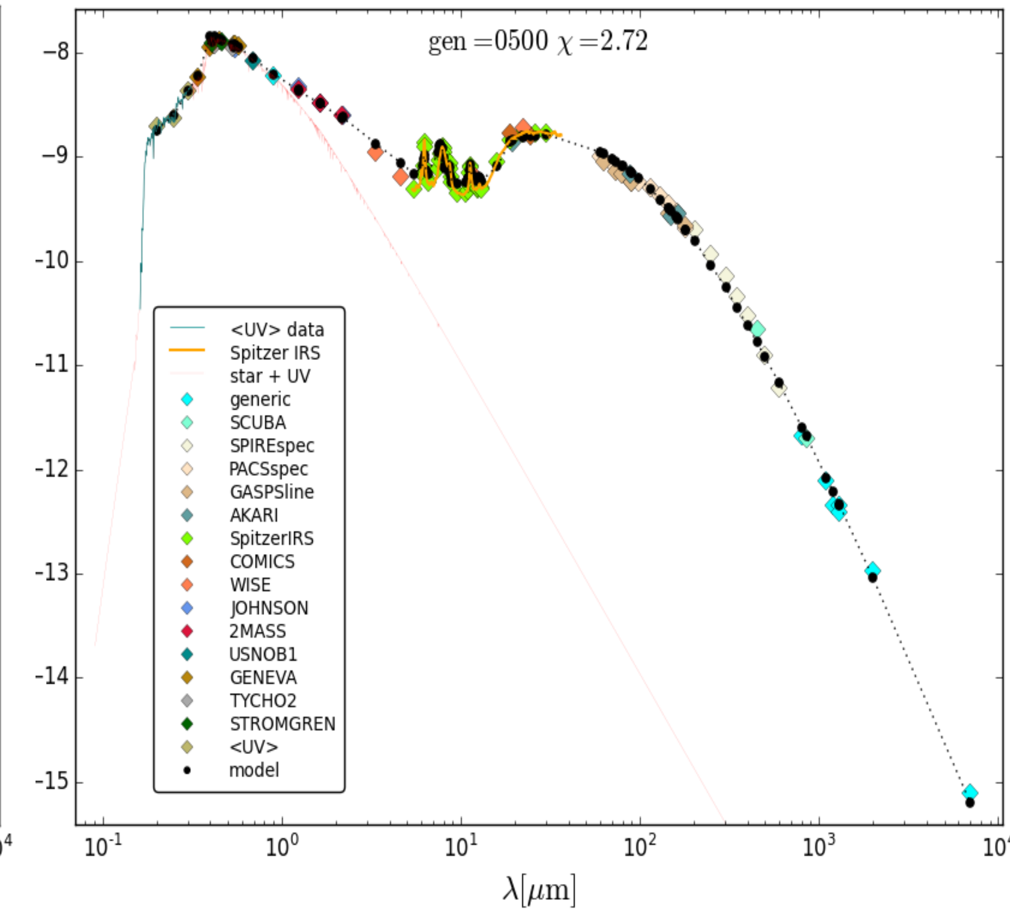
Impact of PAHs

→ *Woitke et al. 2015, submitted to A&A*

HD 142666

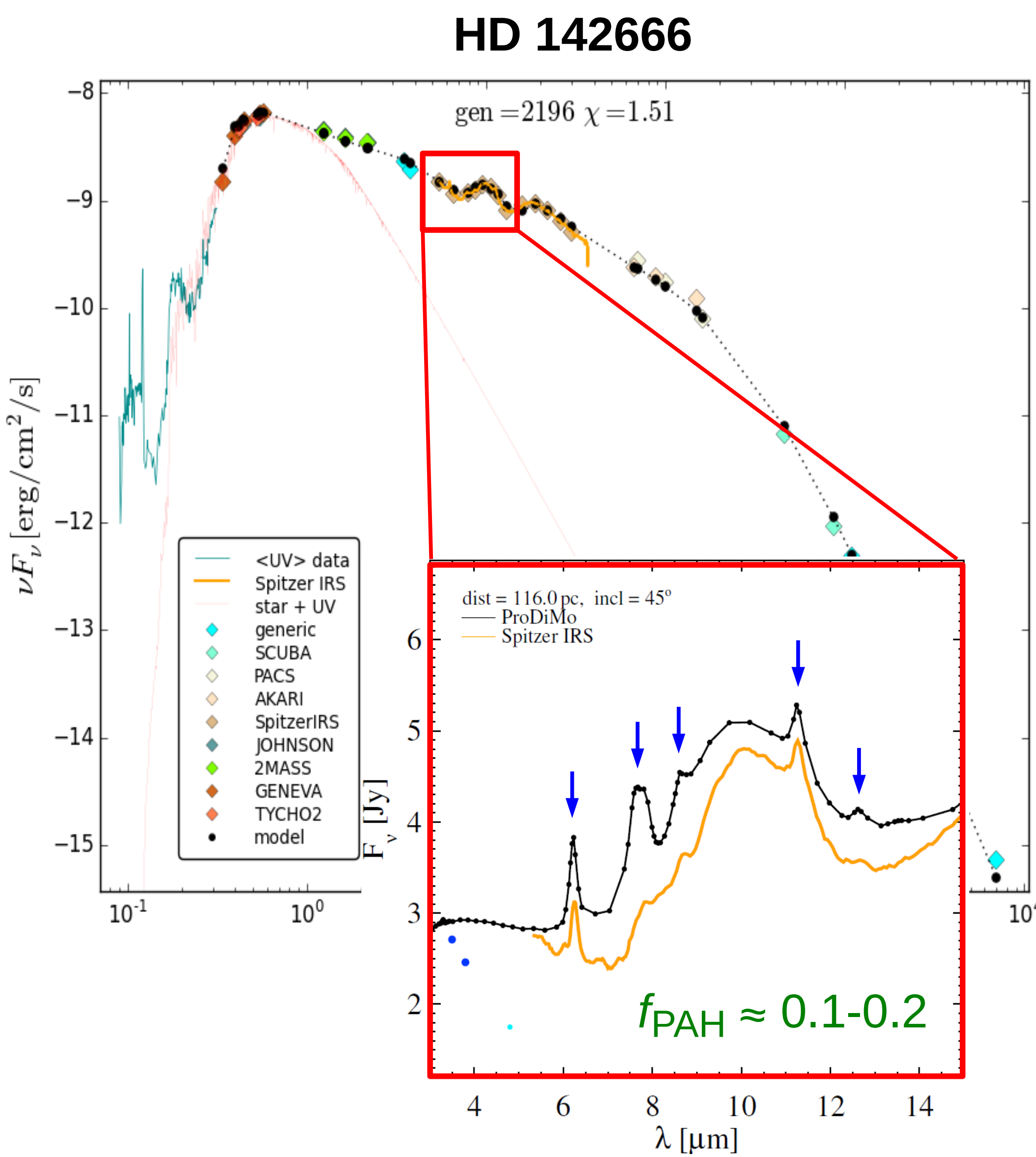


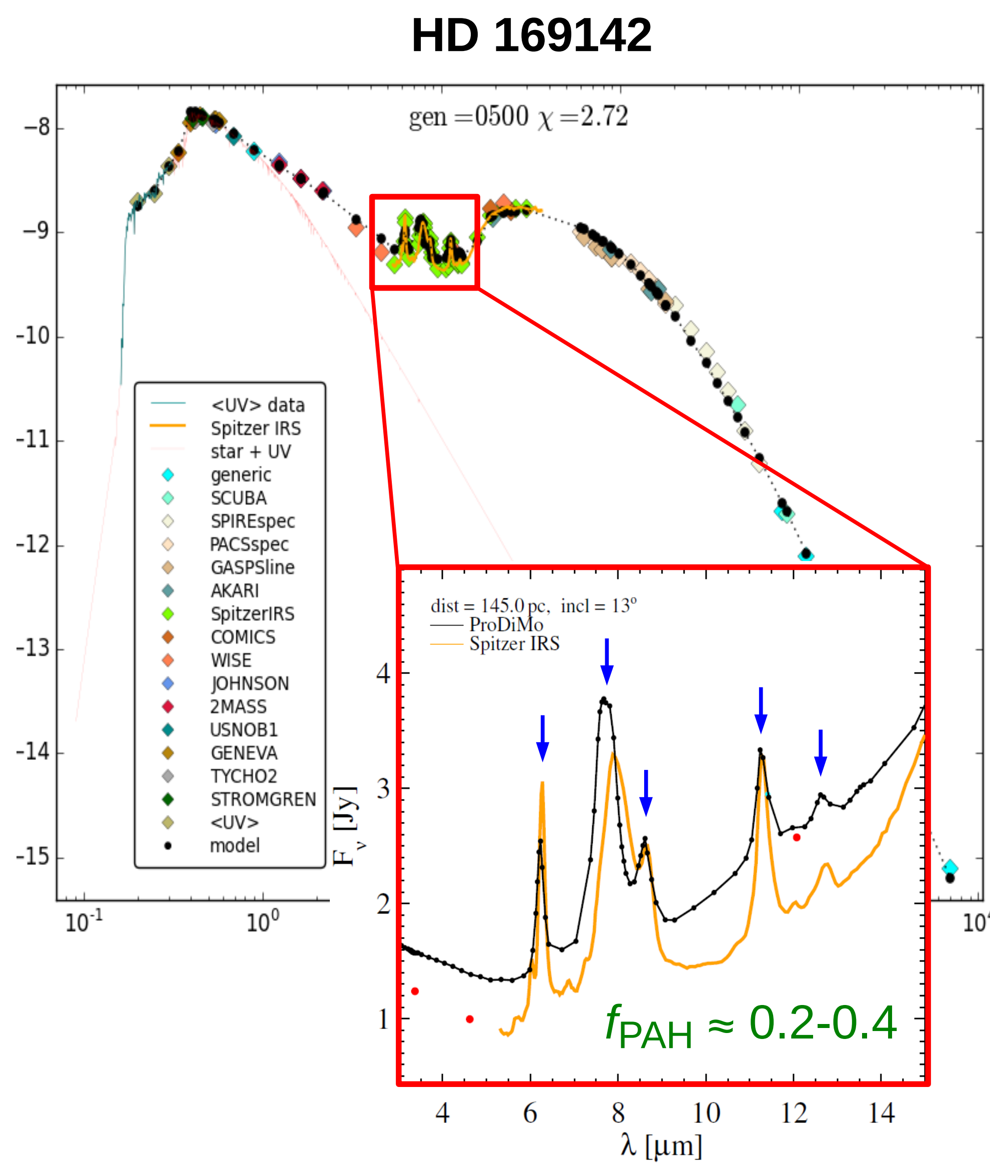
HD 169142



Impact of PAHs

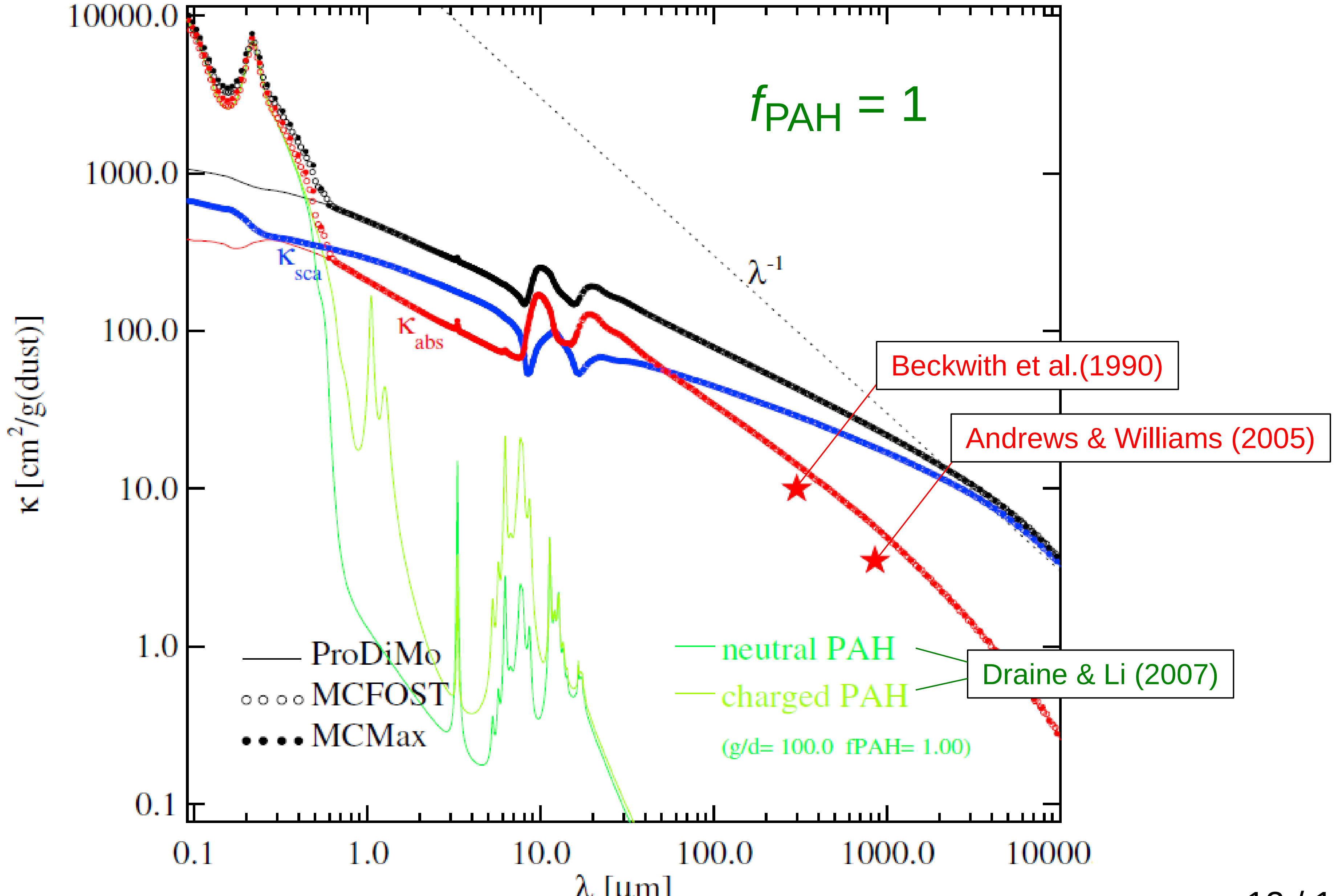
→ *Woitke et al. 2015, submitted to A&A*



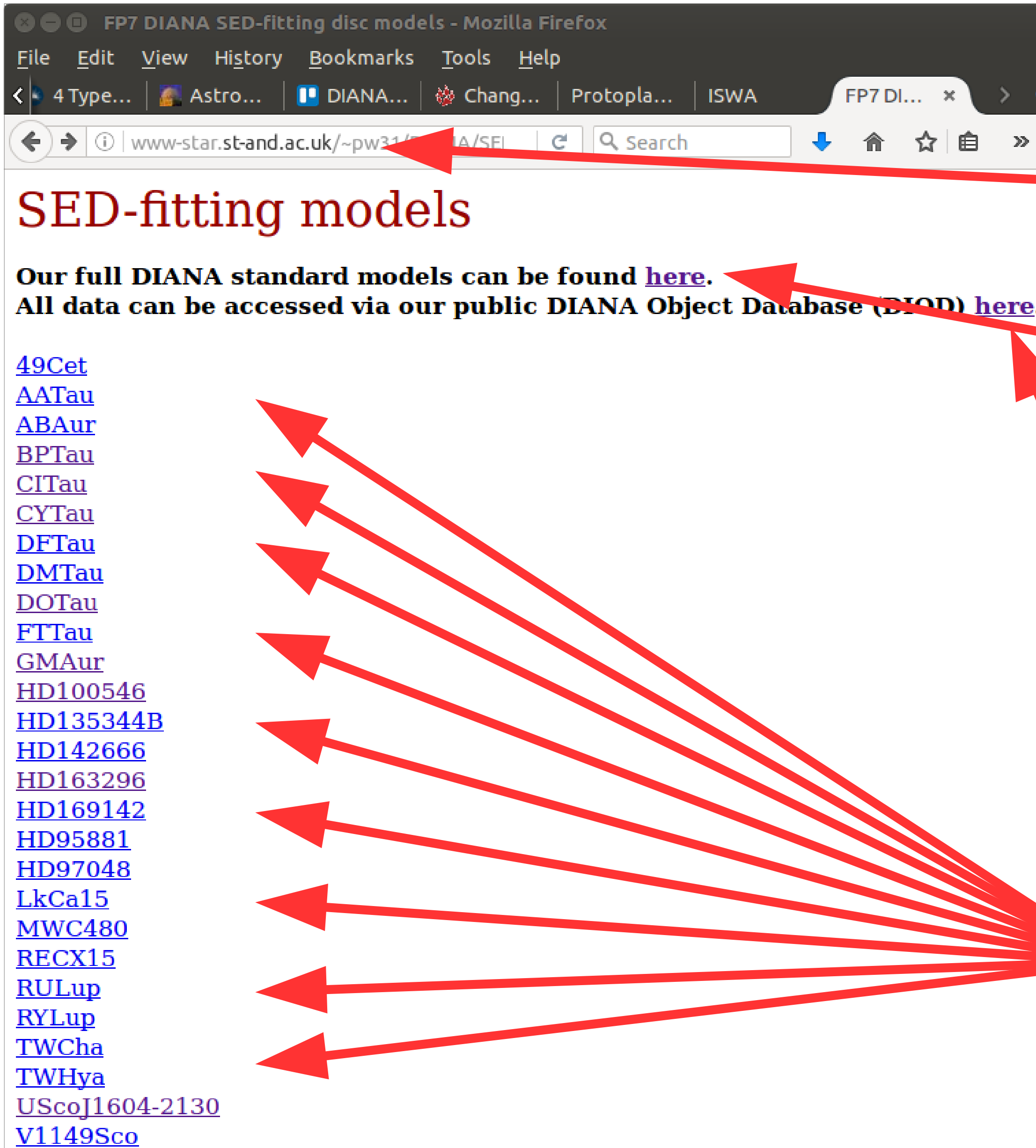


PAH and dust opacities

→ *Woitke et al. (2016, A&A 586, 103)*



All results are public



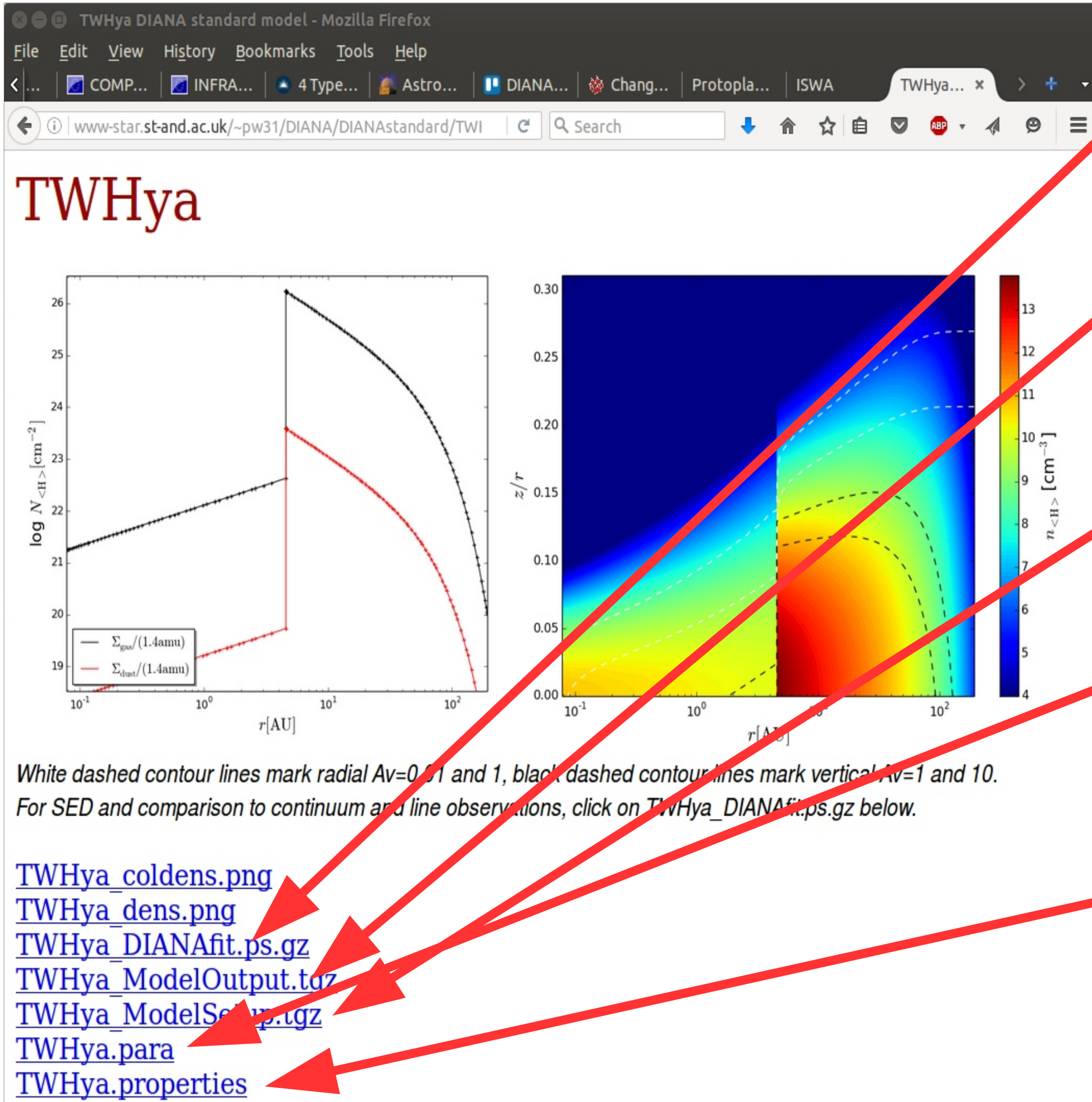
google *"DIANA SED-fit"*

find the DIANA standard models here

access our public database DIOD here (complete data collection)

27 well-studied discs, host star = single star, spectral type M3 … B9

All results are public



281 plots! (physico-chemical structure, dust properties, SED, images, line results ...)

detailed 2D model output

complete model setup:
input parameter, observational data files, … → **reproducible model** (ProDiMo / MCFOST / MCMax)

human-friendly model parameter

selection of derived properties (IR-excess, SED-fluxes, apparent sizes, mm-slope, line fluxes and FWHM vs. observations, predicted line fluxes, ...)

Conclusions

astrochemistry in protoplanetary disks ...

- **at least 2D with wide range of conditions**

  → *densities*
  → *dust and gas temperatures*
  → *radiation fields*
  → *disc shape → shielding*
  → *different lines come from different disc regions*
  → *"nebula analysis" highly questionable (for example rot. diagrams)*

- **large grains need to be included to fit SED**

  → ***reduction of UV dust opacity & total dust surface*** *by factor ~100*
  → ***deeper warm, chemically active disk surface layer***
  → ***stronger emission lines*** *(e.g. far-IR lines, CO ro-vib)*
  → ***less ice***
  → ***fewer charged grains****, larger electron concentration in midplane*

a word on lab chemistry ...

ProDiMo uses ~ 530 physical/chemical input data files (!)

- **non-LTE data for atoms and molecules**

  → *energy states & degeneracies (rotational, vibrational, some electronic)*
  → *line data (level indices, wavelengths, Einstein coefficients)*
  → *collisional data (!), specific pumping processes, ...*

- **ice data**

  → *adsorption energies (!)*
  → *photodesorption efficiencies,*
  → *optical constants, ...*

- **dust data**

  → *optical constants*
  → *photoelectric effect efficiencies, threshold energies, ...*

- **cross sections, cross sections, cross sections ...**

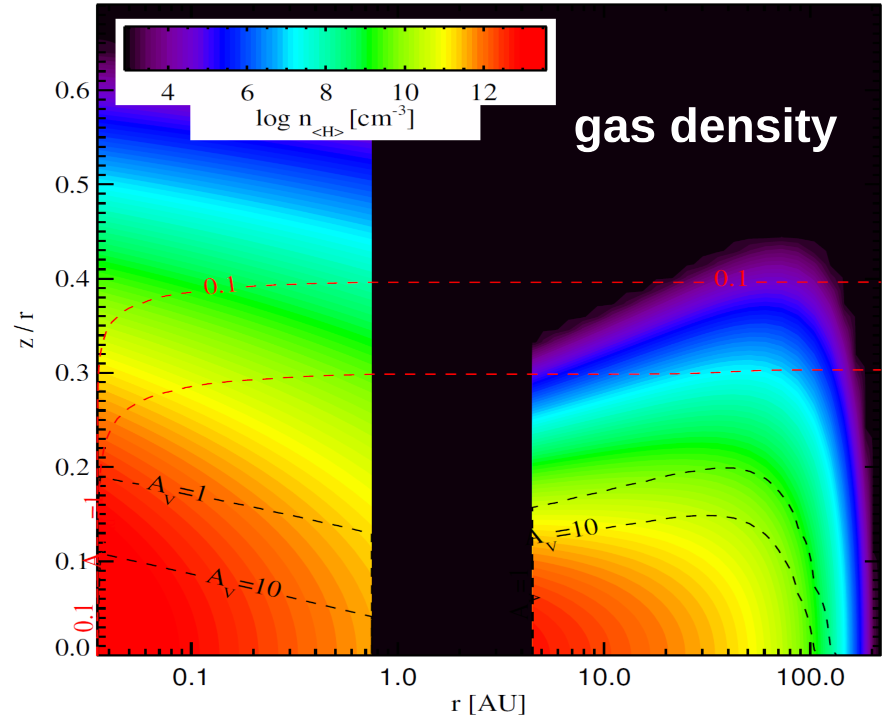
  → *e.g. UV-photodissociation, X-ray processes, PAHs, ...*

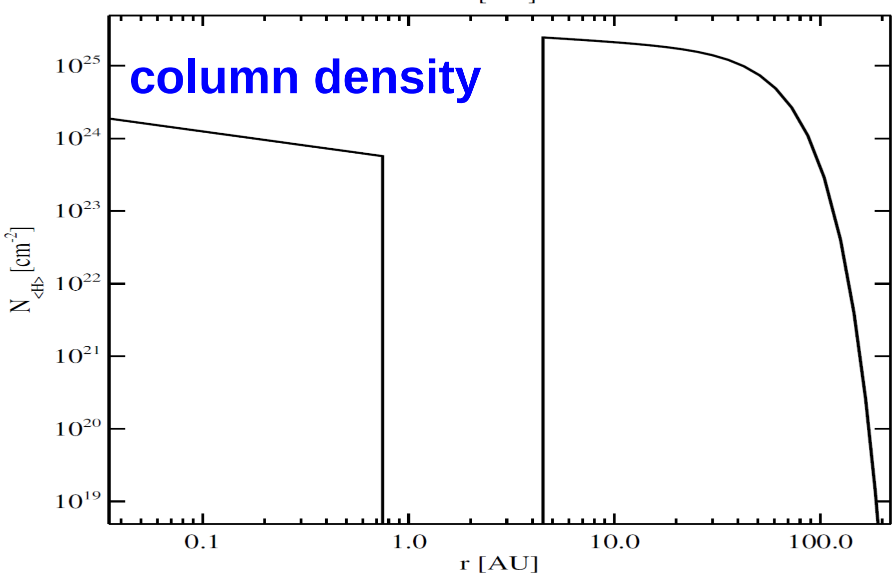
- **chemical rates**

  → *Arrhenius parameters*
  → *self-shielding factors*
  → *special processes (H_2-formation on grains, excited H_2, surface chemistry, ...)*

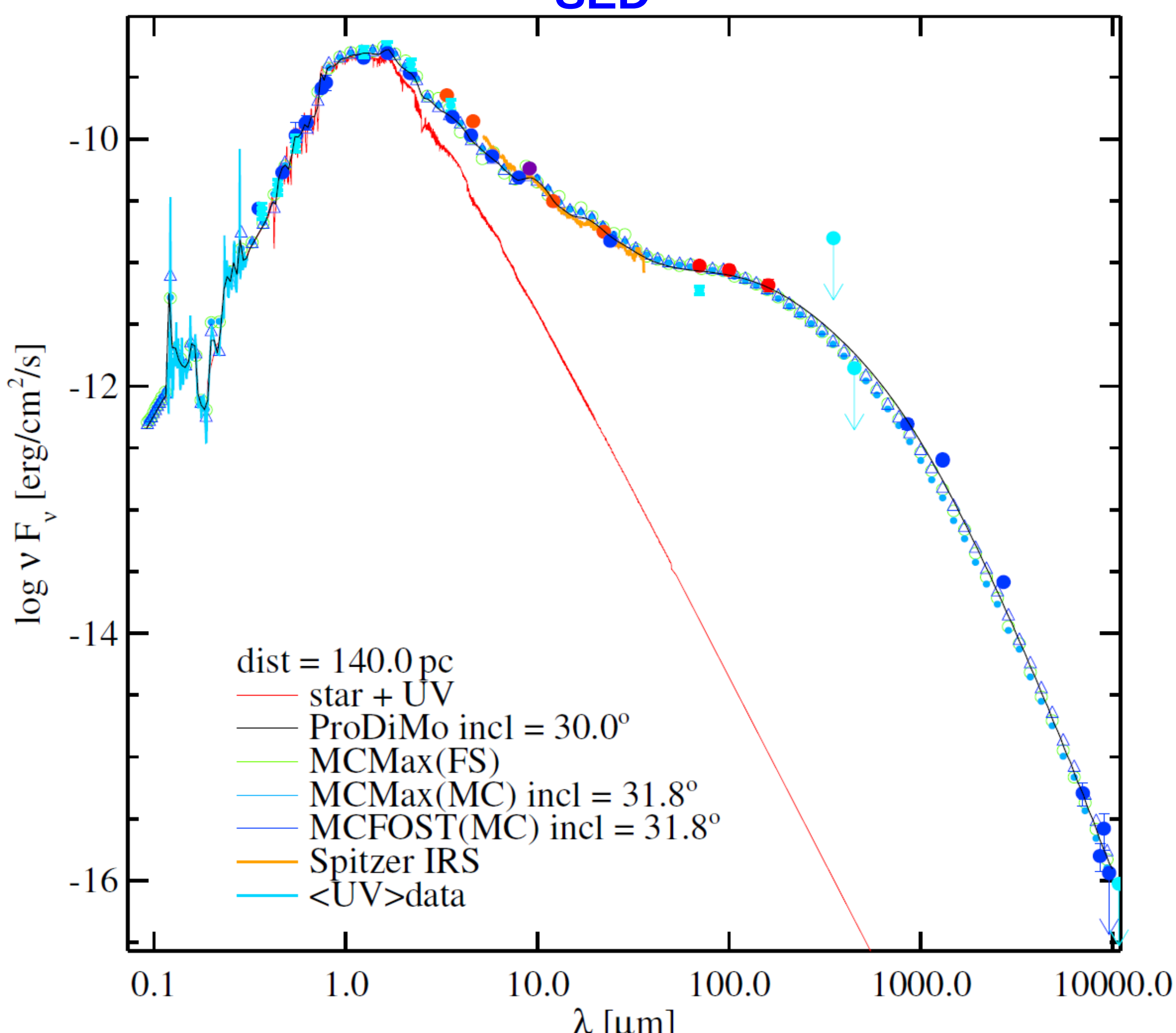
standard model CY Tau

CTTS, M1, A_V = 0.1, T_{eff} = 3640 K, L_* = 0.36 L_{sun},
M_* = 0.42 M_{sun}, M_{acc} ~ 7 x 10^{-9} M_{sun}/yr, age ~ 2.2 Myr



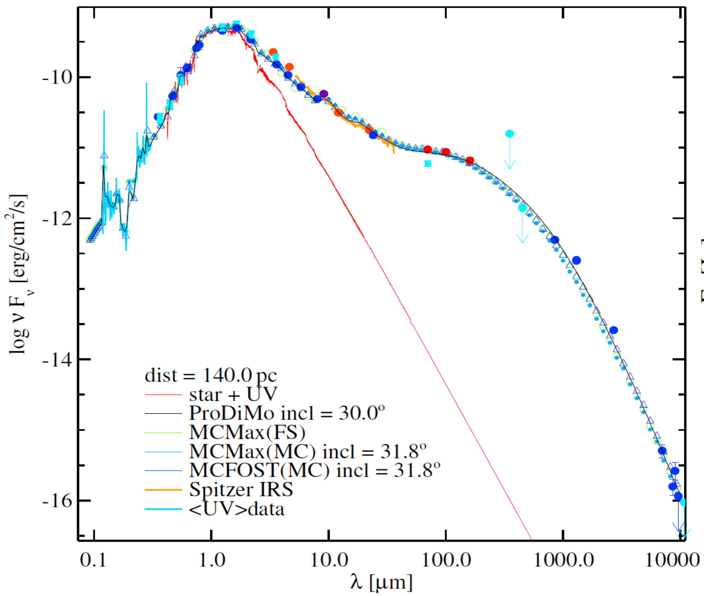


SED

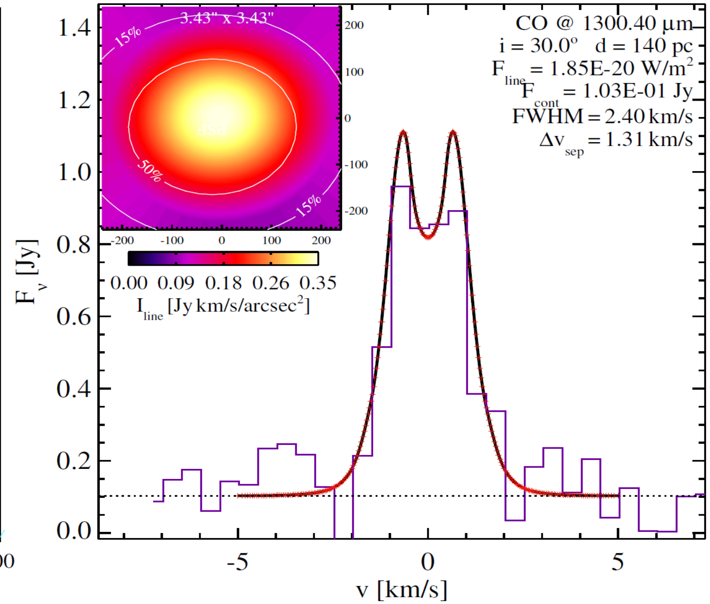


standard model CY Tau

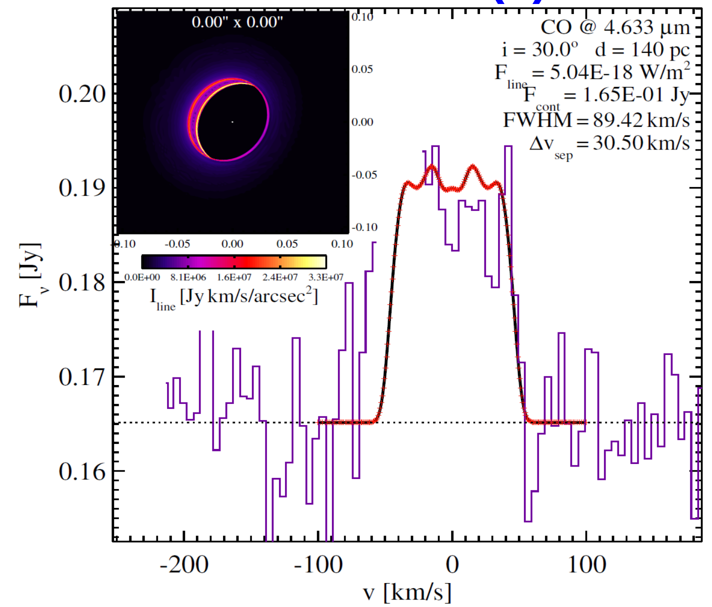
SED



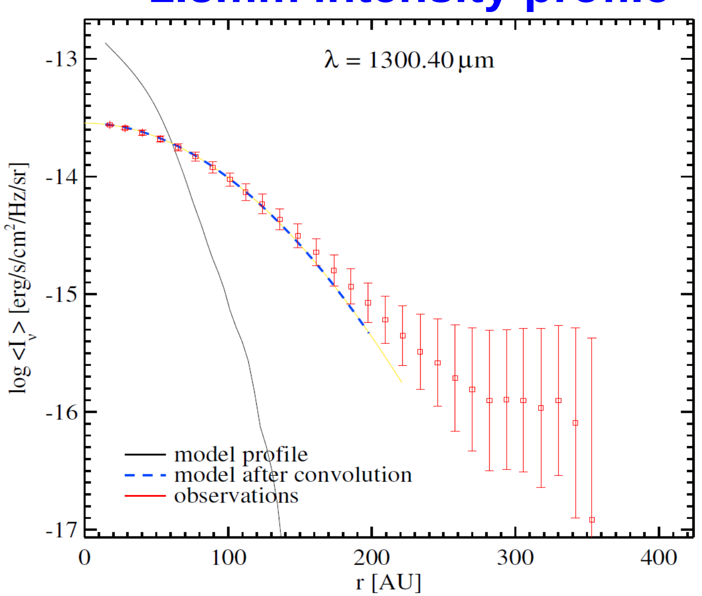
^{12}CO J=2-1



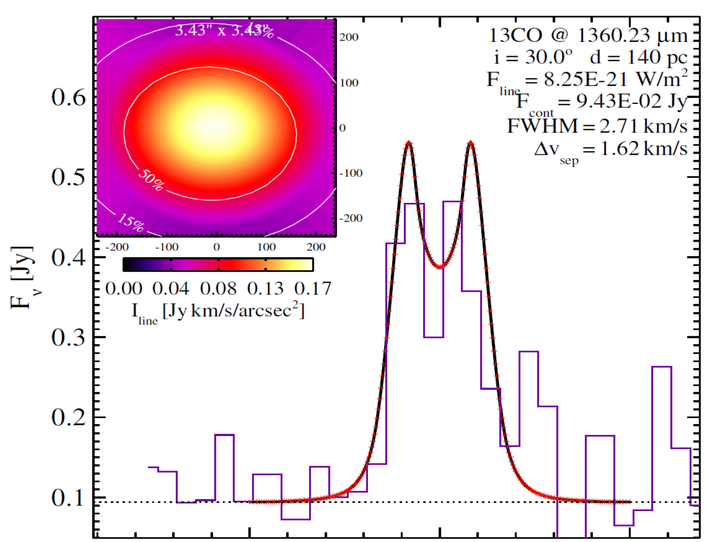
^{12}CO v=1-0 R(3)



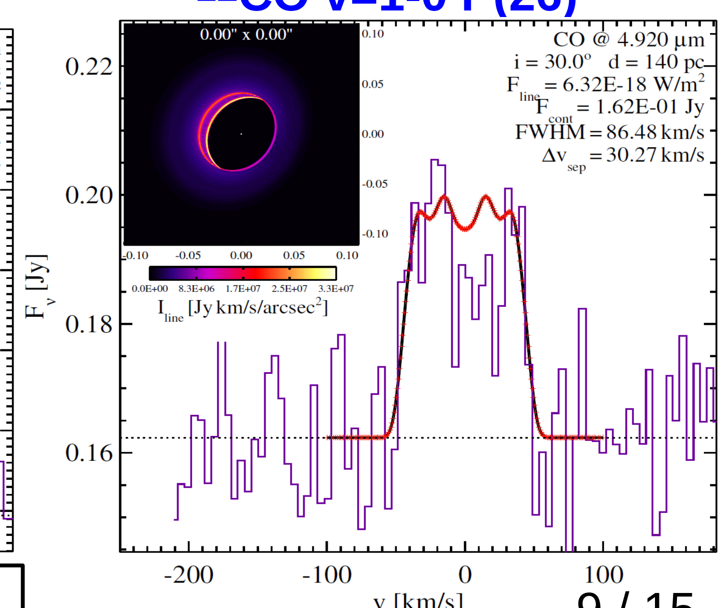
1.3mm intensity profile



^{13}CO J=2-1

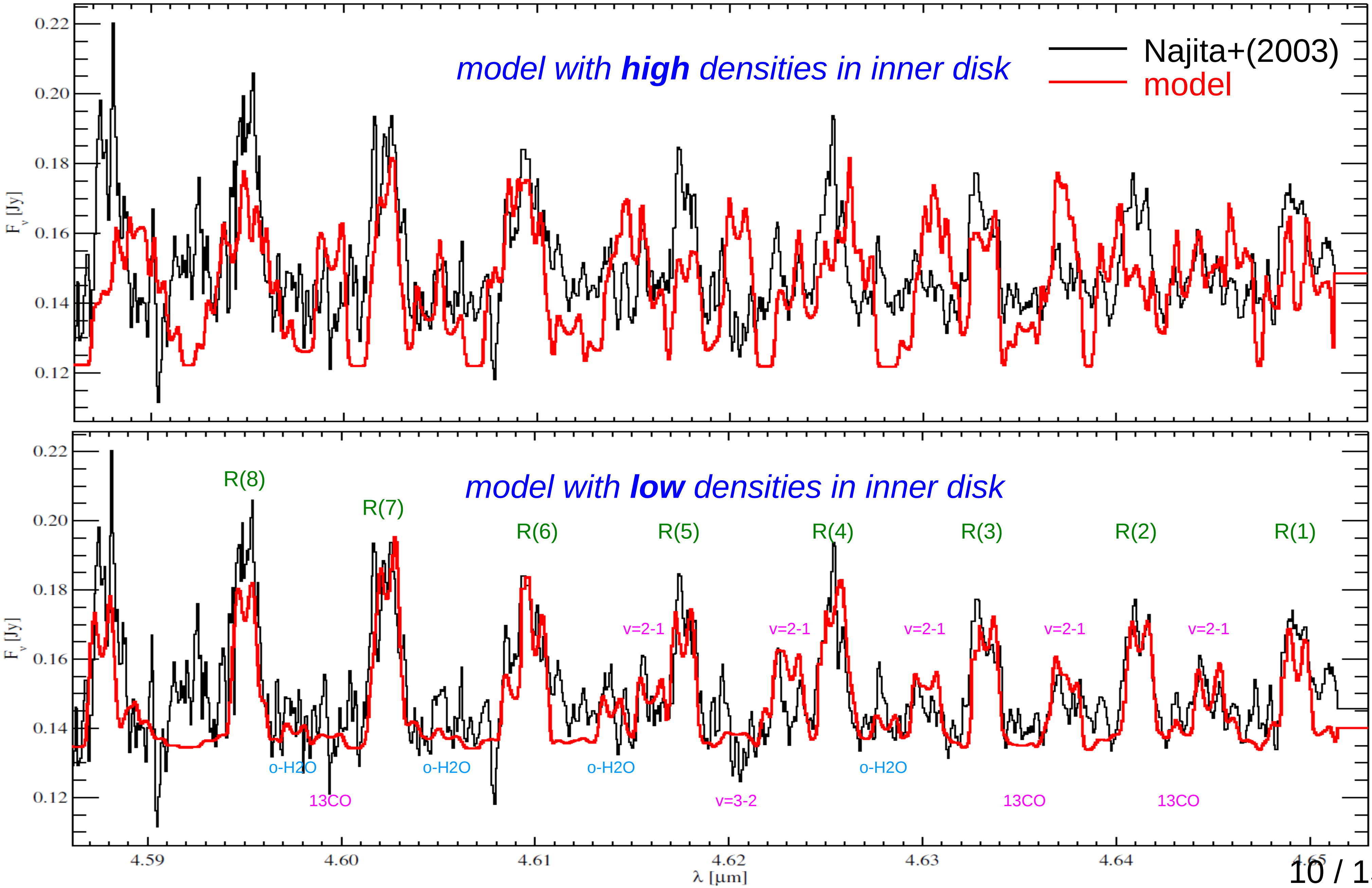


^{12}CO v=1-0 P(26)

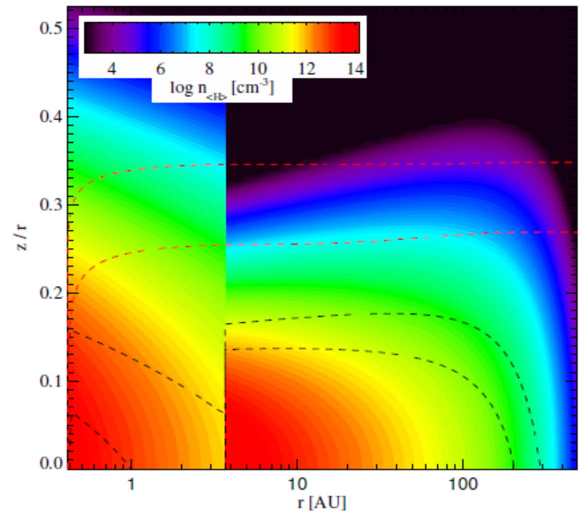


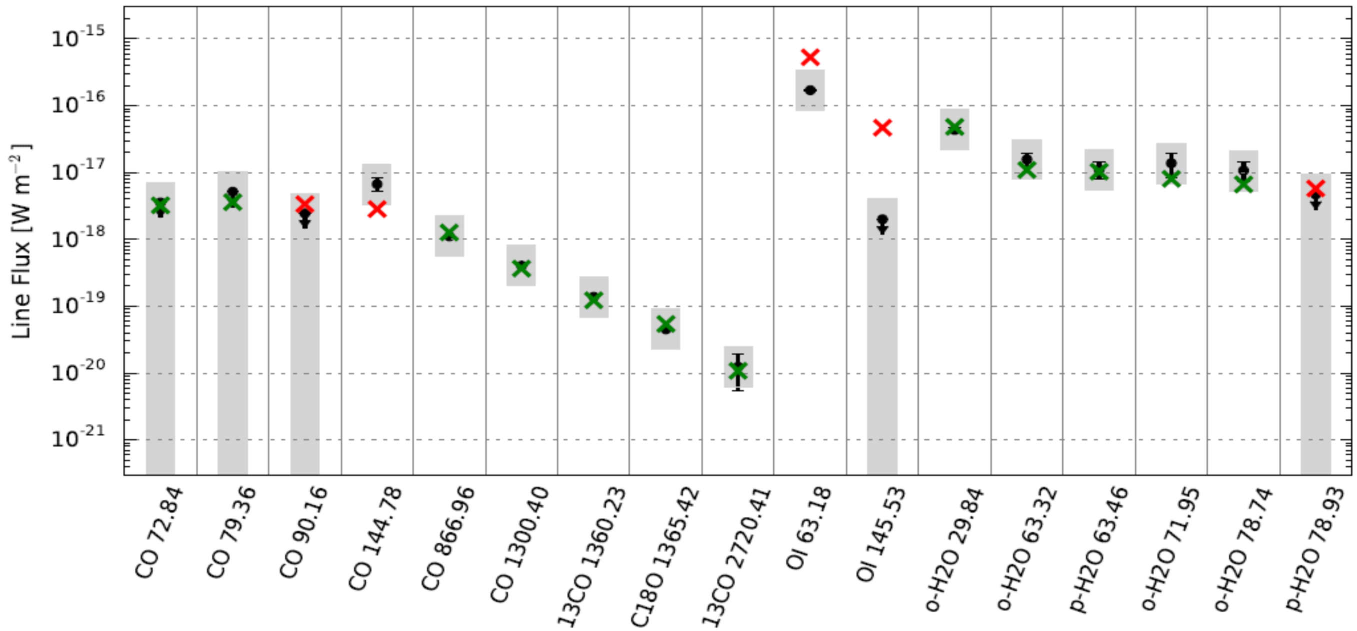
also [OI] 63μm, [OI] 6300A

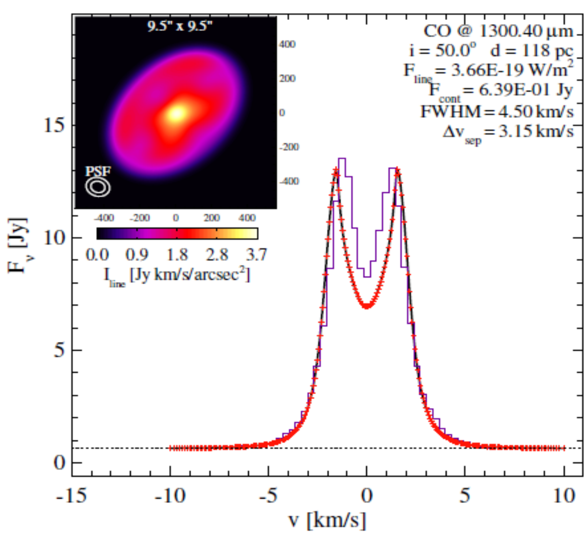
The R-branch CO fundamental with FLiTs ...

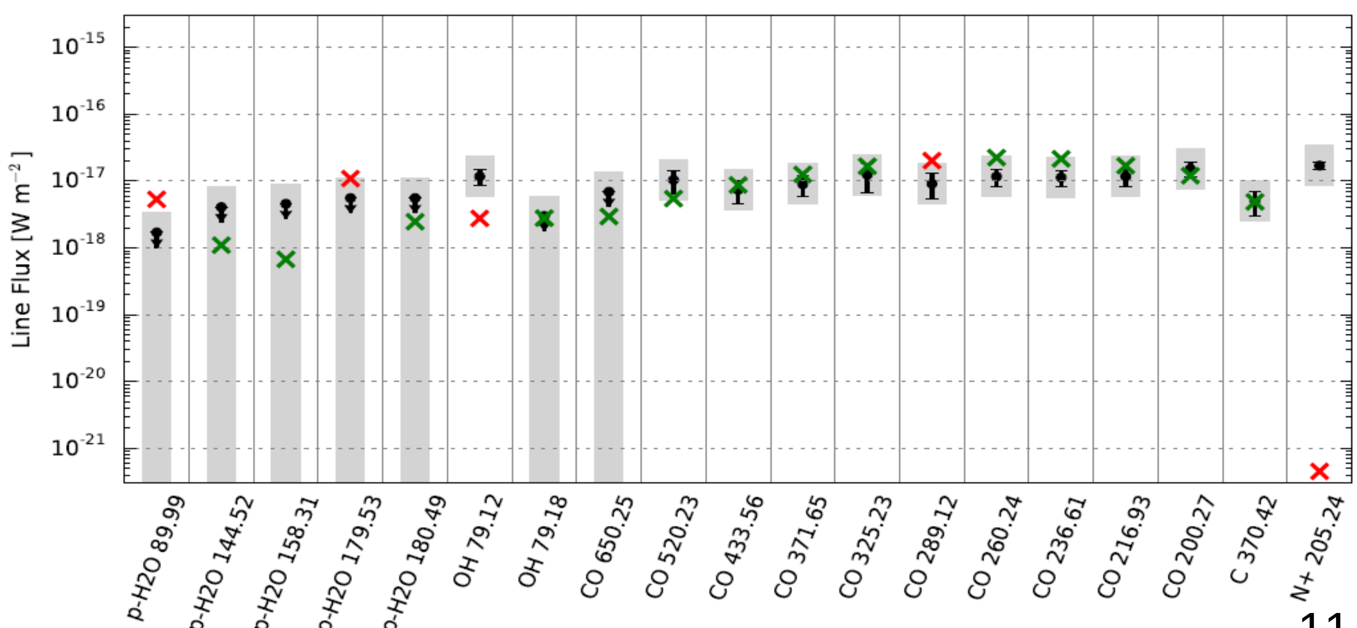


standard model HD 163296



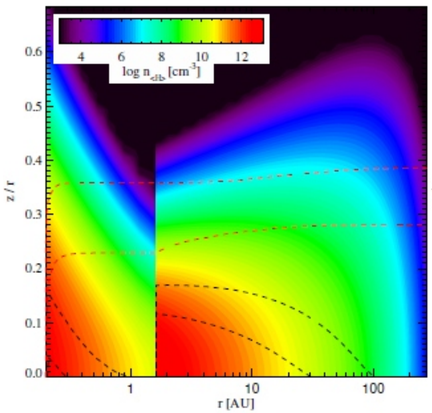




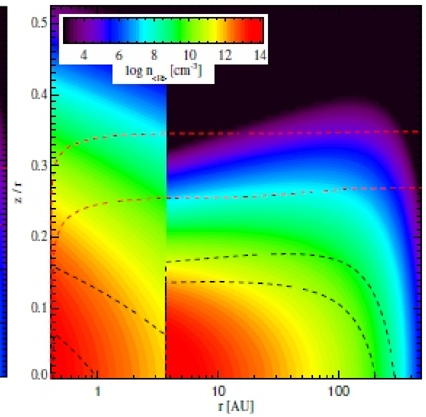


A massive outer disc in the shadow of a tall tenuous inner disc?

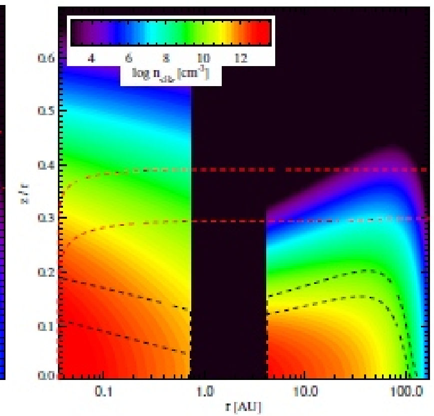
HD 142666*



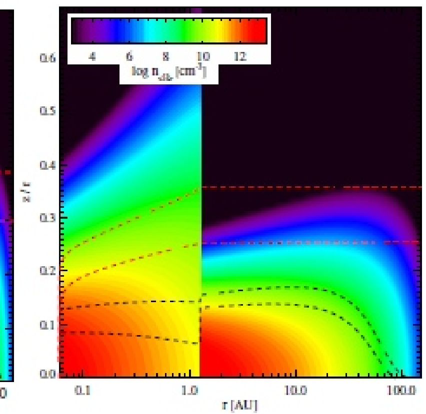
HD 163296



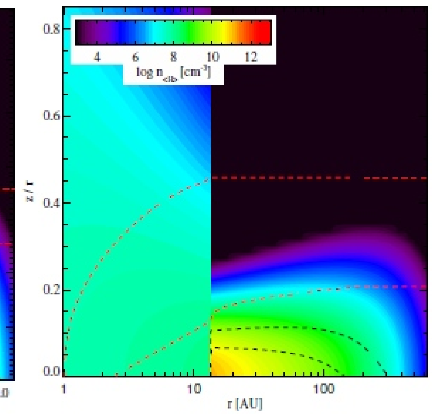
CY Tau*



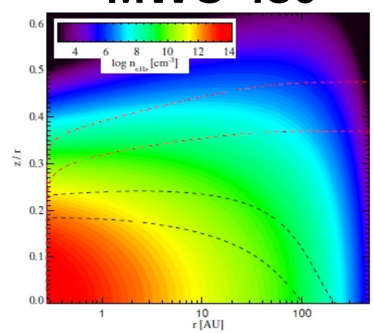
BP Tau*



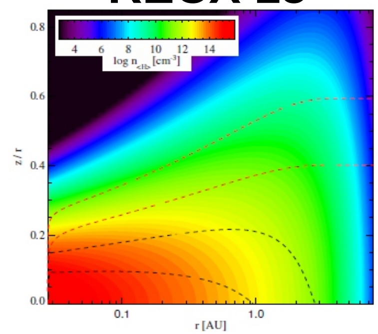
DM Tau



MWC 480*



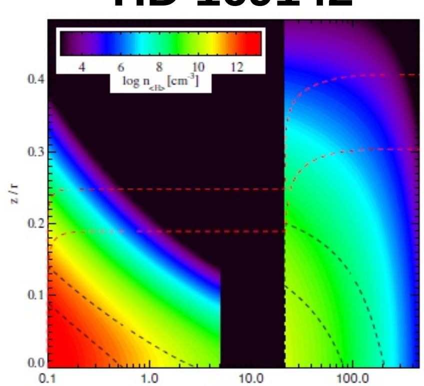
RECX 15



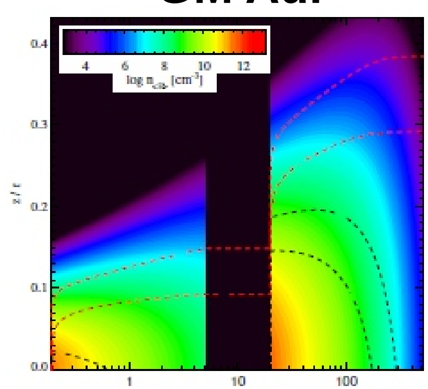
*: CO ro-vib lines fit (green)

*: CO ro-vib lines do not fit (red)

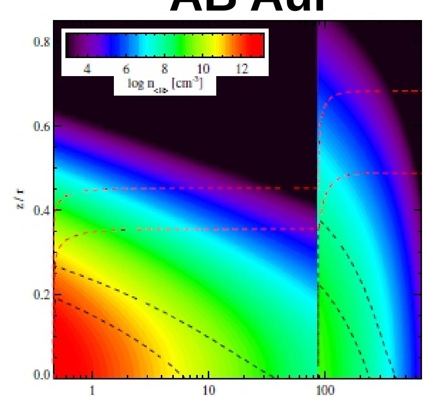
HD 169142*



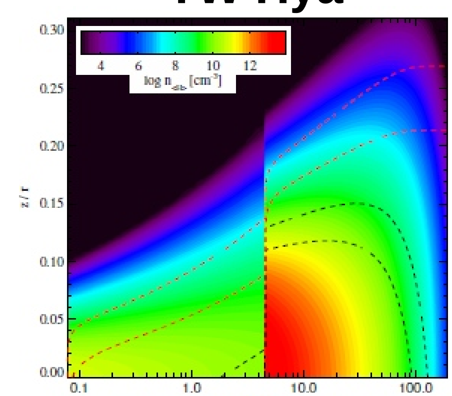
GM Aur*



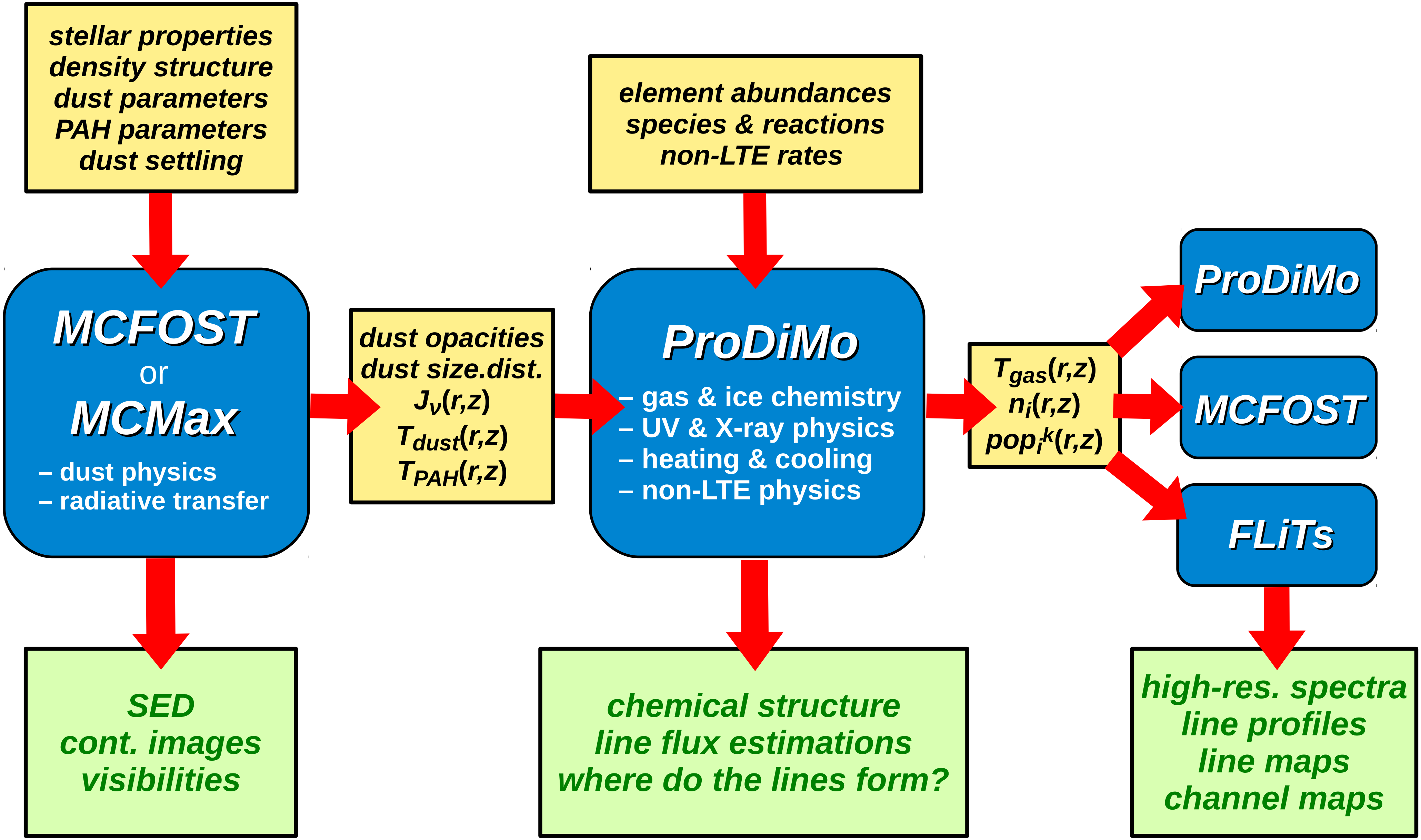
AB Aur*



TW Hya*



"*holistic*" modelling approach

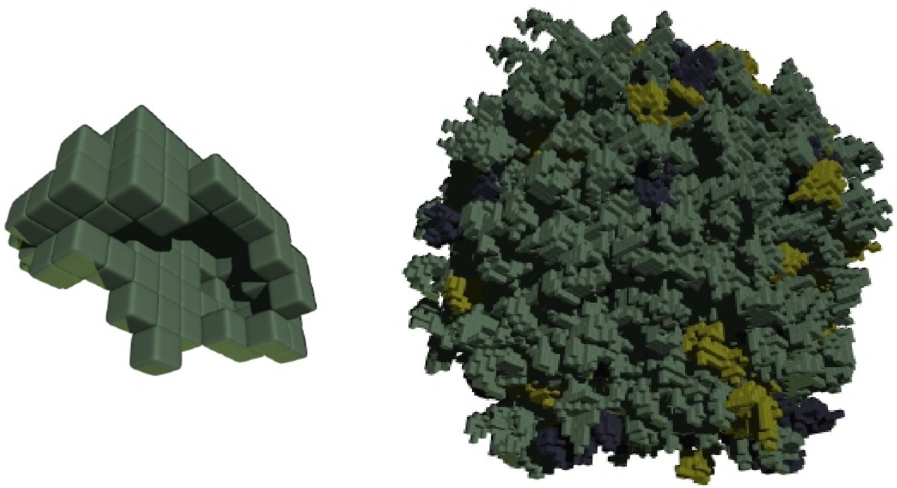


“Standard” dust opacities for disks

→ *Min et al. 2015, University of Amsterdam, NL, A&A accepted*

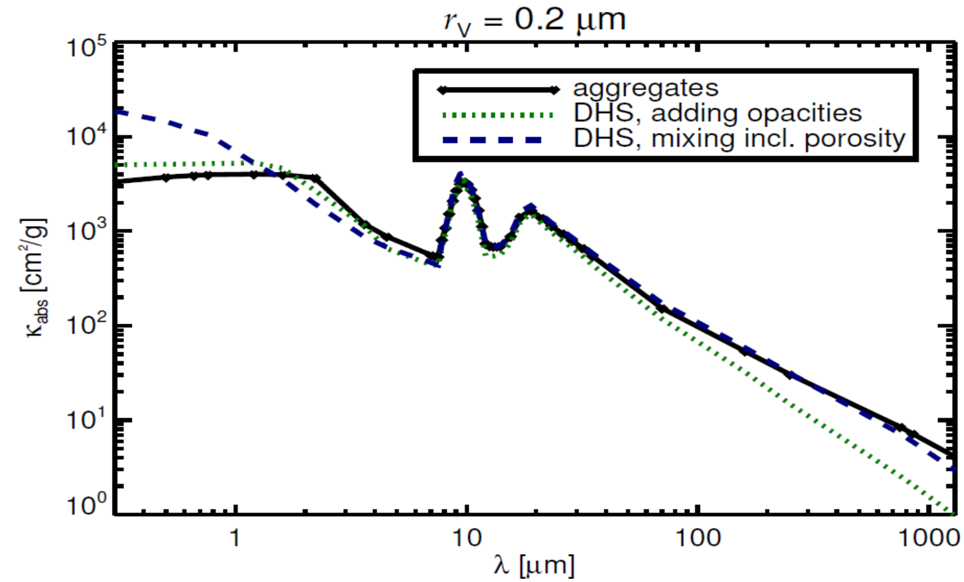
Opacities of aggregates

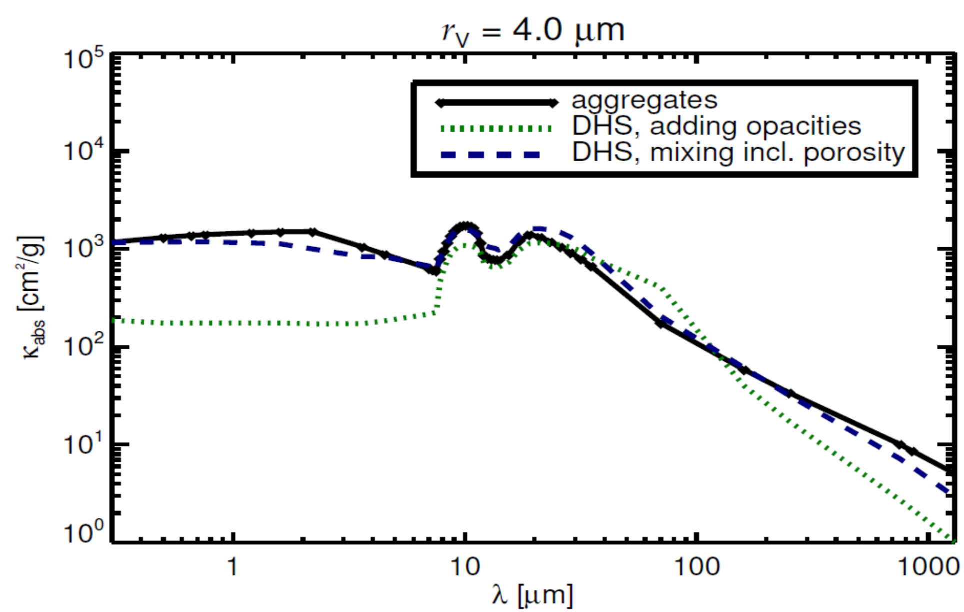
– DDA, 100 dipoles/GRF, up to 8000 GRFs (4μm)
– results include phase function, polarisation, ...



Fit with “simple” methods

(effective medium, porosity, DHS)





DIANA dust opacity standard

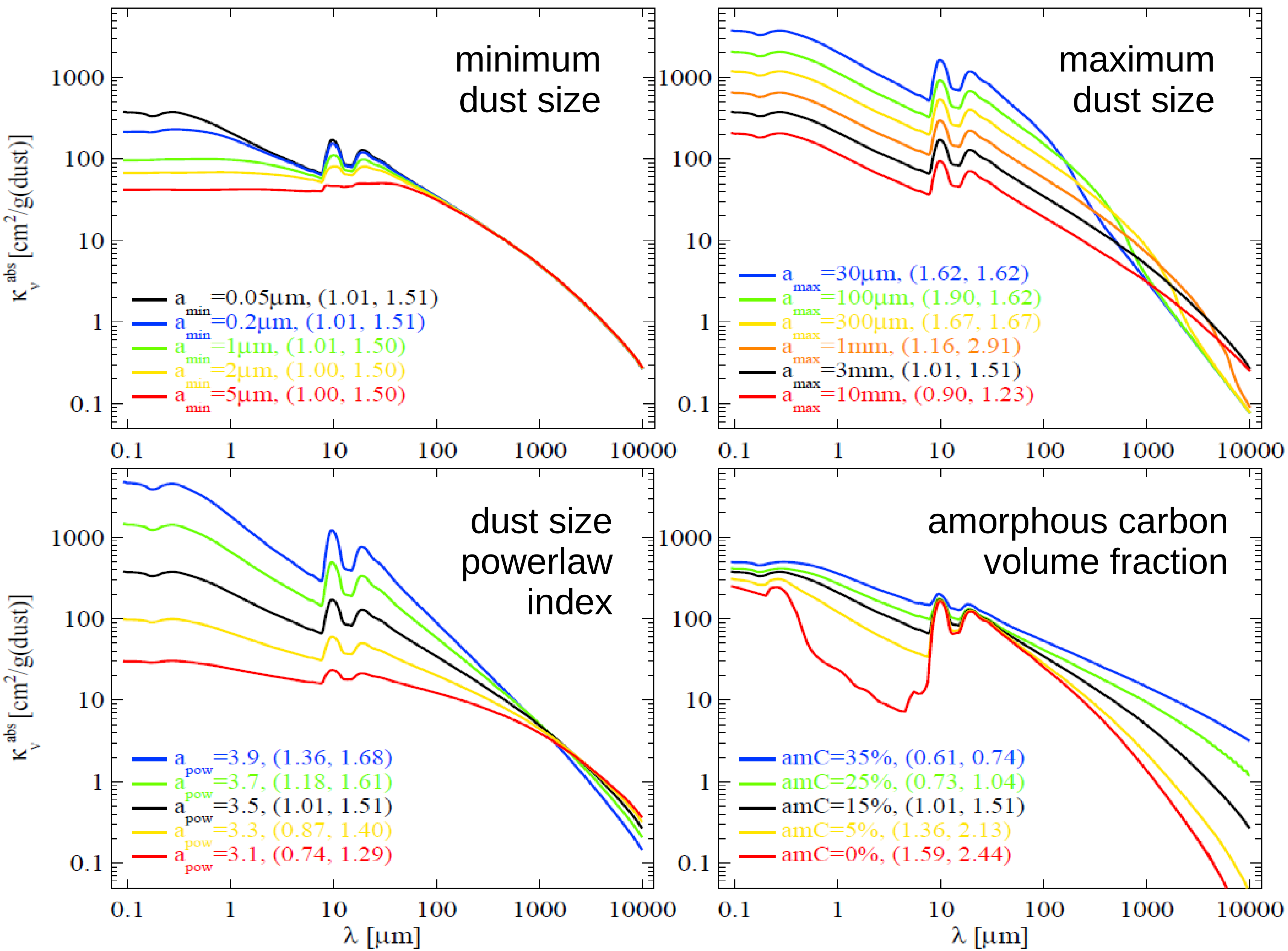
- ***effective mixture of***
  ~60% laboratory amorphous silicates
  ($Mg_{0.7}Fe_{0.3}SiO_3$, Dorschner+1995)

  ~15% amorphous carbon
  (Zubko 1996, BE-sample)

  ~25% porosity
- ***powerlaw size distribution*** $f(a) \sim a^{-pow}$
  ($a_{min} \sim$ ***0.05 μm***, $a_{max} \sim$ ***3 mm***, $a_{pow} \sim$ ***3.5***)
- ***distribution of hollow spheres***
  (hollow volume ratio ***0.8***)

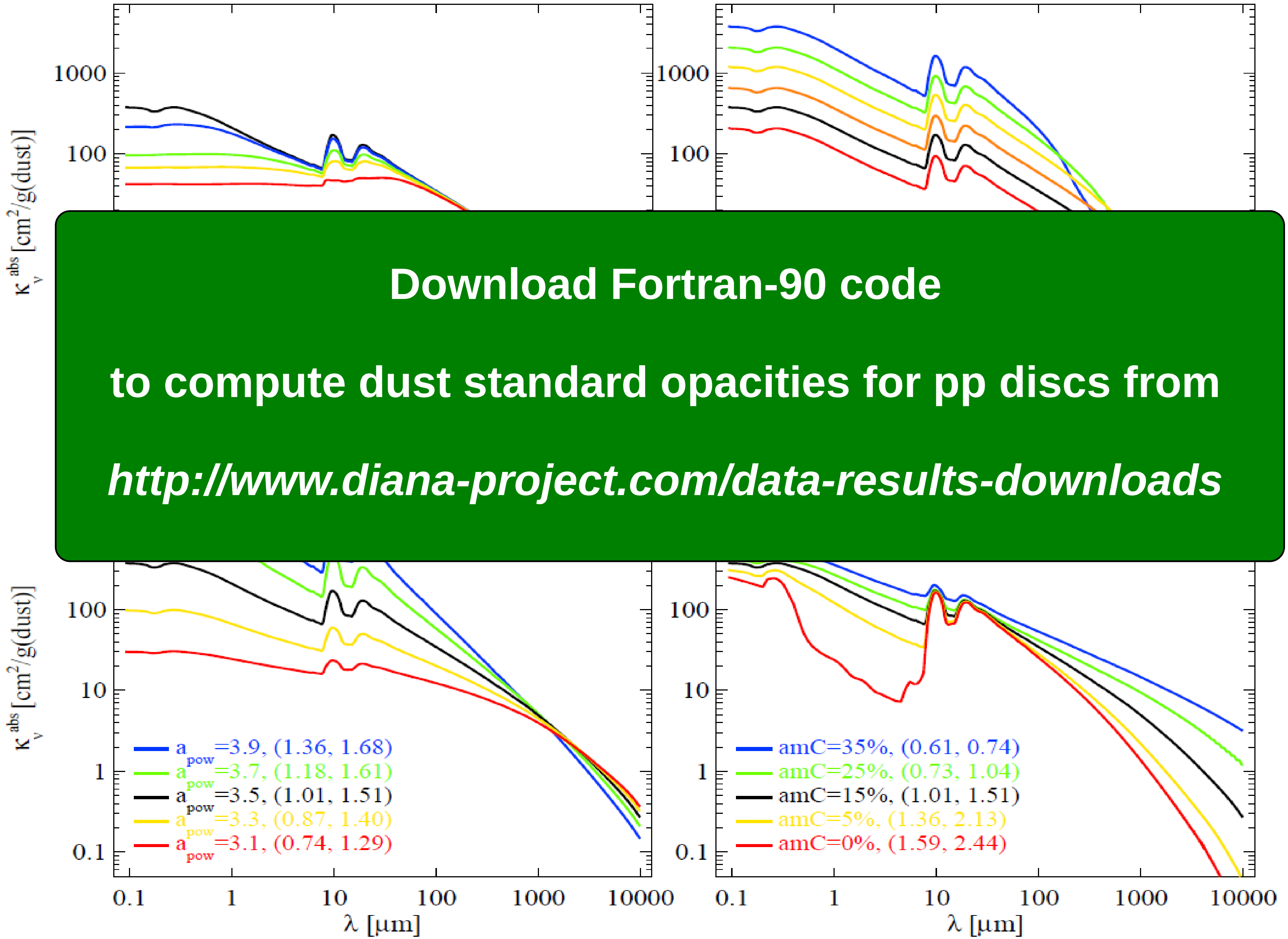
"Standard" dust opacities for disks

→ Min et al. 2015, University of Amsterdam, NL, A&A submitted



“Standard” dust opacities for disks

→ *Min et al. 2015, University of Amsterdam, NL, A&A submitted*



Download Fortran-90 code

to compute dust standard opacities for pp discs from

http://www.diana-project.com/data-results-downloads

DiscAnalysis DIANA

impact on gas modelling

→ *Woitke et al. 2015, submitted to A&A*

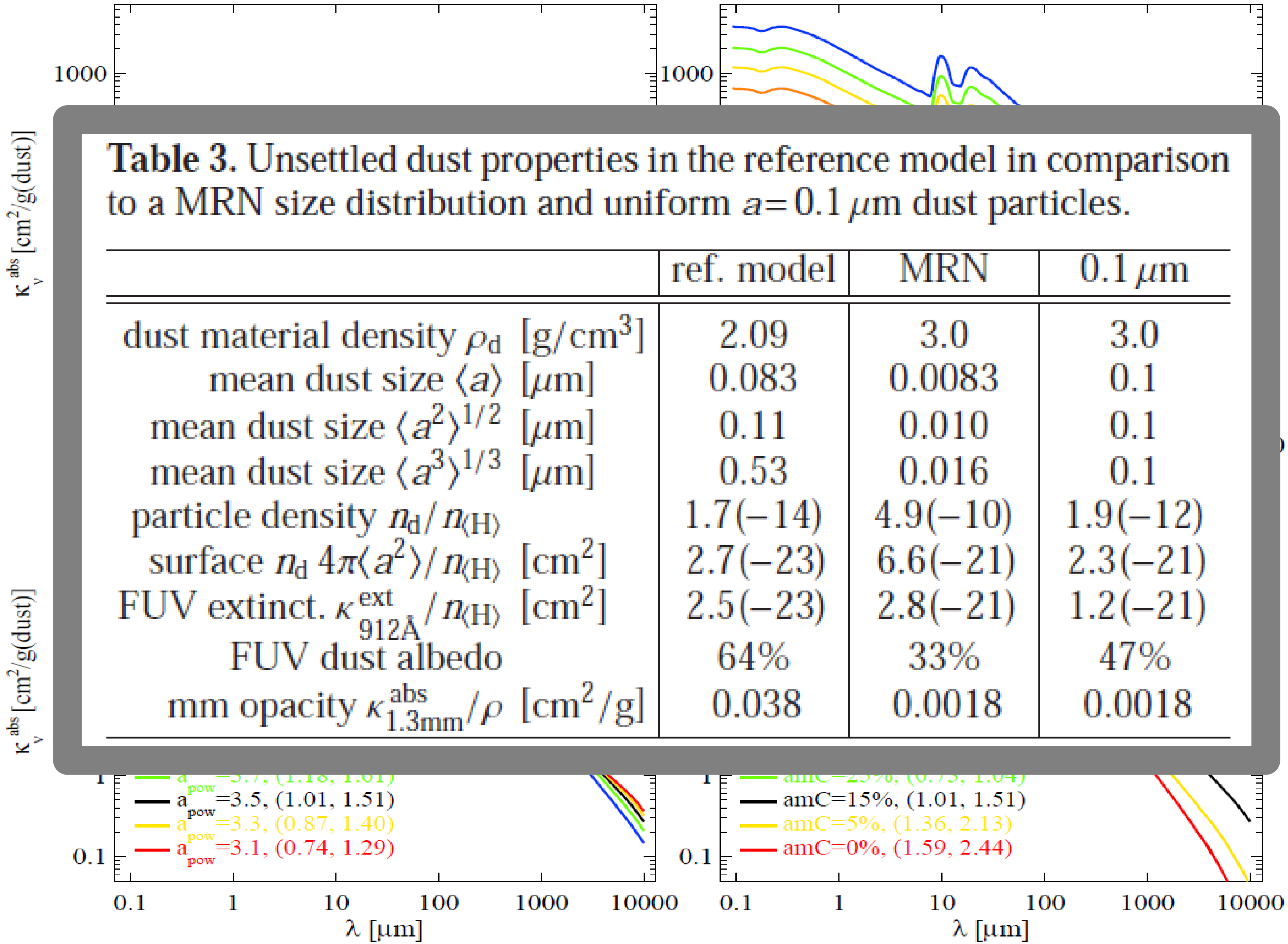
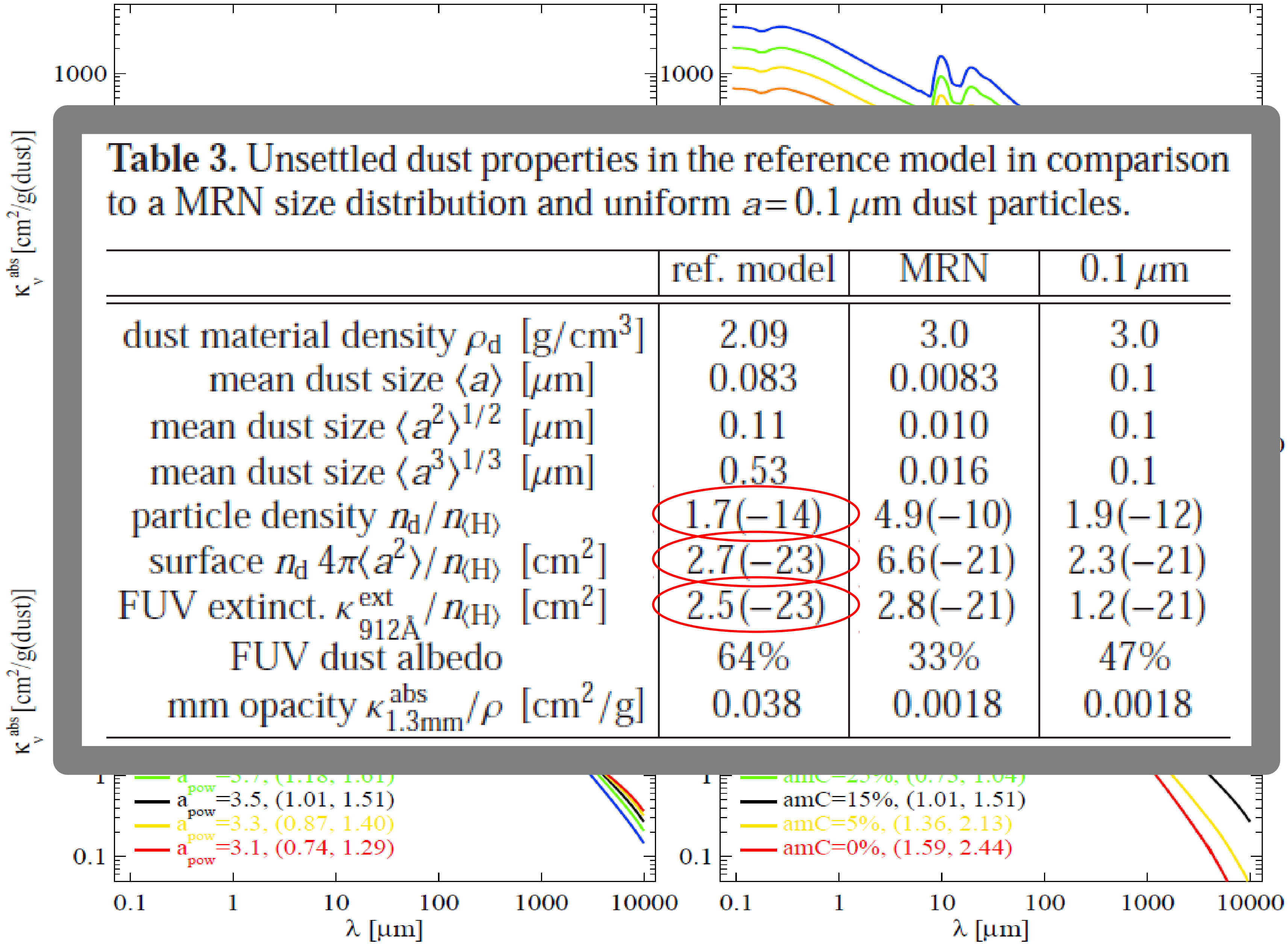


Table 3. Unsettled dust properties in the reference model in comparison to a MRN size distribution and uniform $a = 0.1\,\mu$m dust particles.

	ref. model	MRN	0.1 μm
dust material density ρ_d [g/cm^3]	2.09	3.0	3.0
mean dust size $\langle a \rangle$ [μm]	0.083	0.0083	0.1
mean dust size $\langle a^2 \rangle^{1/2}$ [μm]	0.11	0.010	0.1
mean dust size $\langle a^3 \rangle^{1/3}$ [μm]	0.53	0.016	0.1
particle density $n_d / n_{\langle H \rangle}$	1.7(−14)	4.9(−10)	1.9(−12)
surface $n_d\, 4\pi \langle a^2 \rangle / n_{\langle H \rangle}$ [cm^2]	2.7(−23)	6.6(−21)	2.3(−21)
FUV extinct. $\kappa^{ext}_{912\text{Å}} / n_{\langle H \rangle}$ [cm^2]	2.5(−23)	2.8(−21)	1.2(−21)
FUV dust albedo	64%	33%	47%
mm opacity $\kappa^{abs}_{1.3mm}/\rho$ [cm^2/g]	0.038	0.0018	0.0018

impact on gas modelling

→ *Woitke et al. 2015, submitted to A&A*



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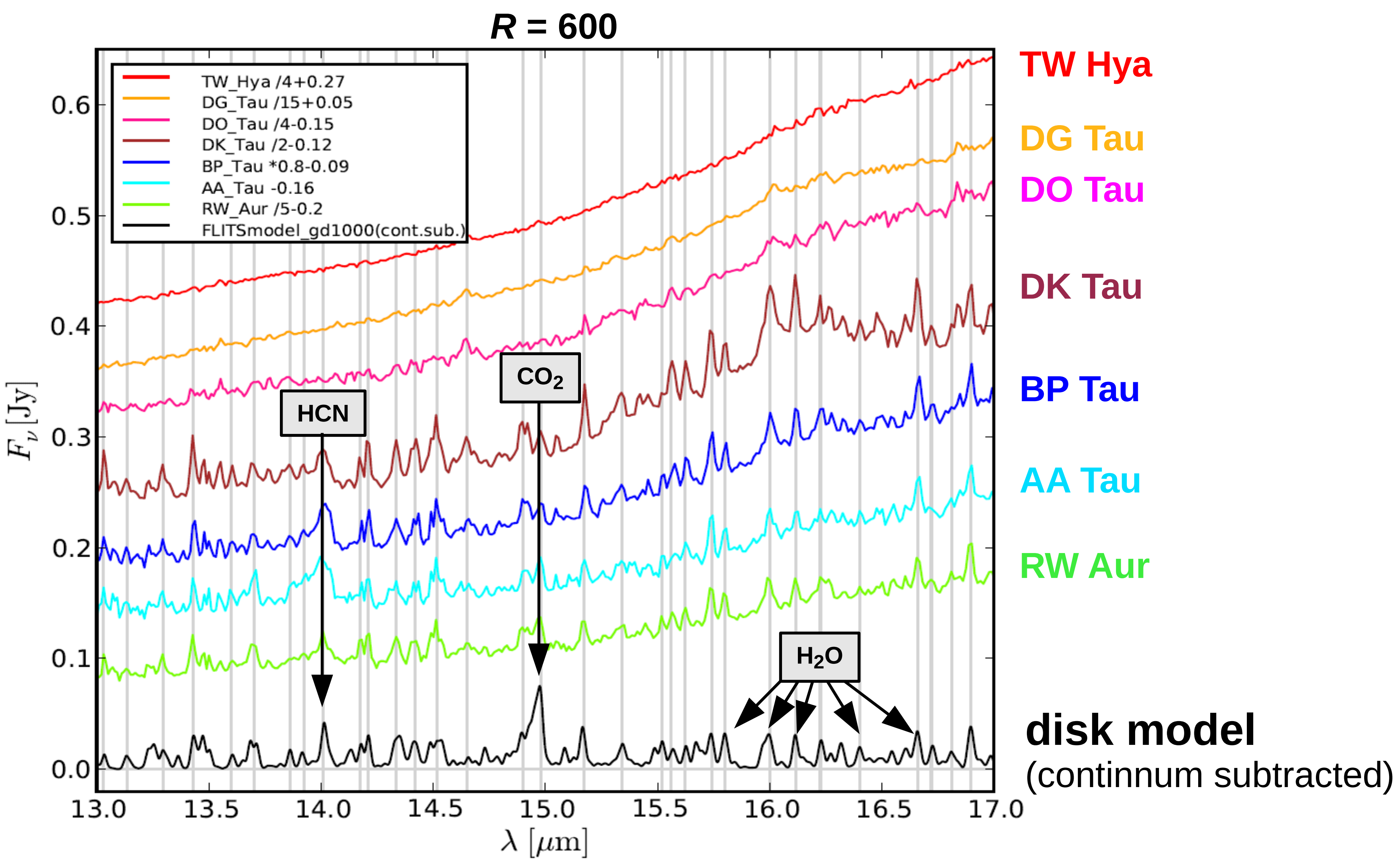
Spitzer molecular emission lines

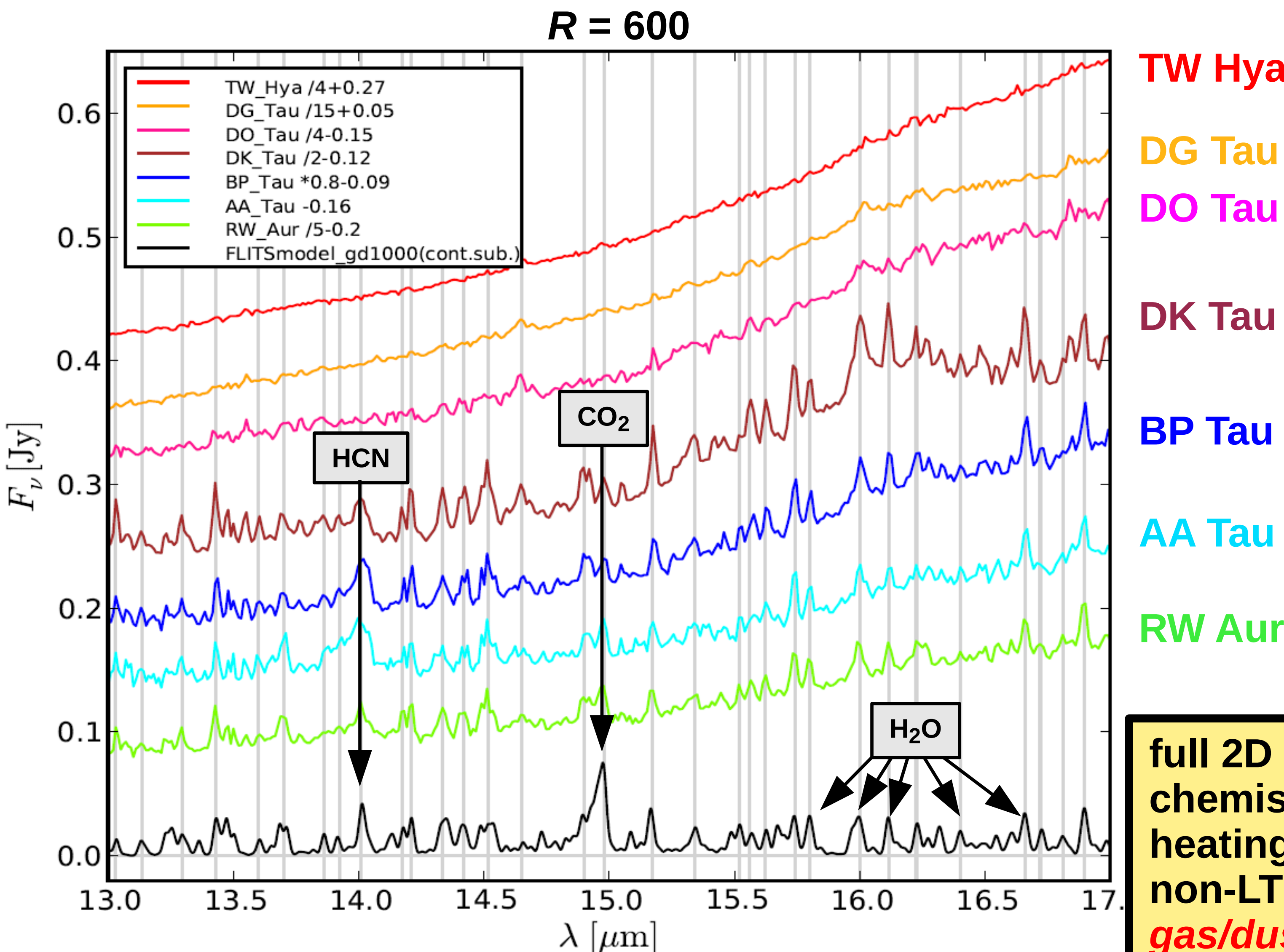
→ *Antonellini et al. 2015, A&A accepted*



→ *Spitzer IRS (R=600) data from Rigliaco et al. (2015)*

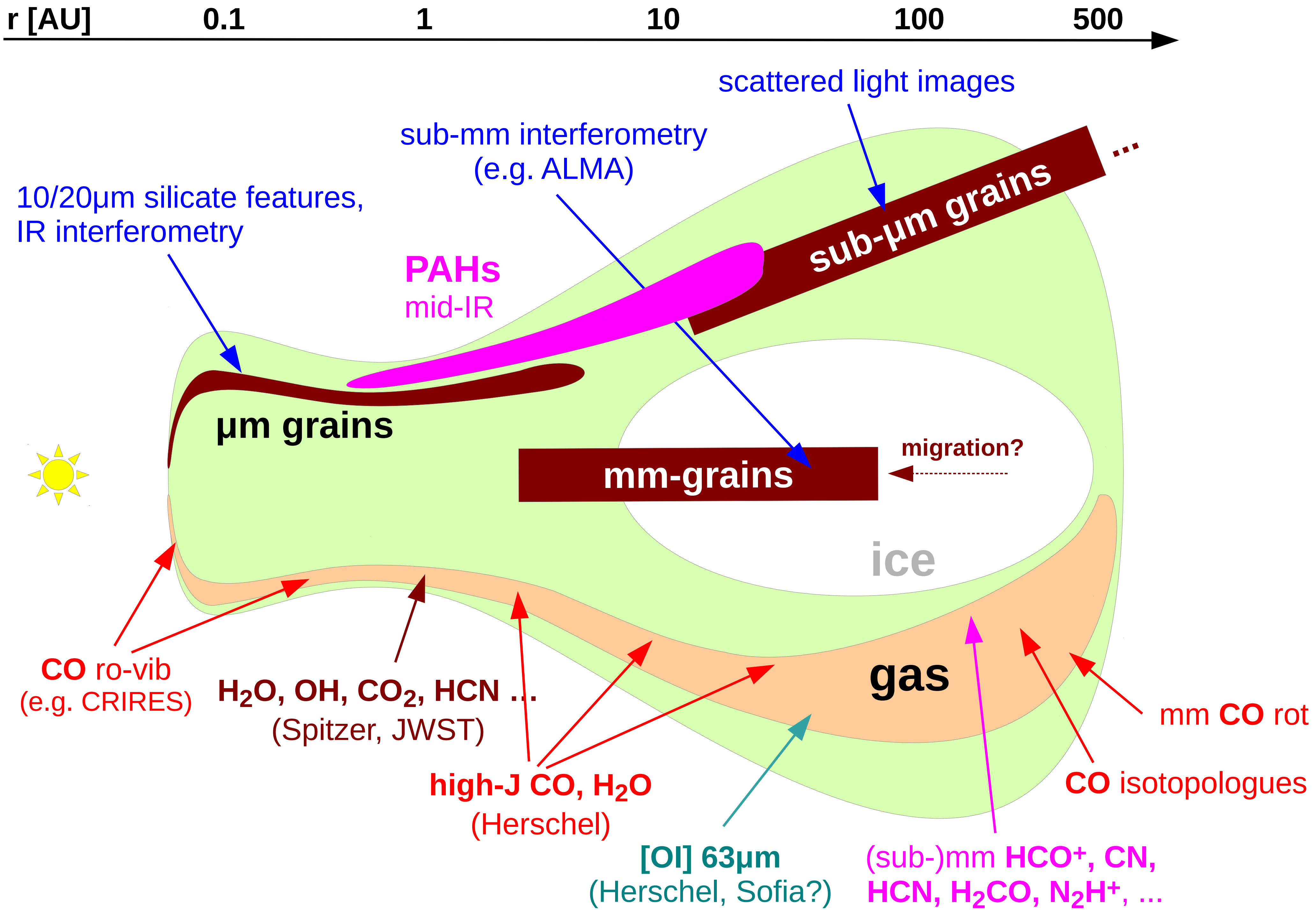
Spitzer molecular emission lines

→ *Antonellini et al. 2015, A&A accepted*



full 2D disk model chemistry, heating/cooling balance non-LTE pops
gas/dust = 1000

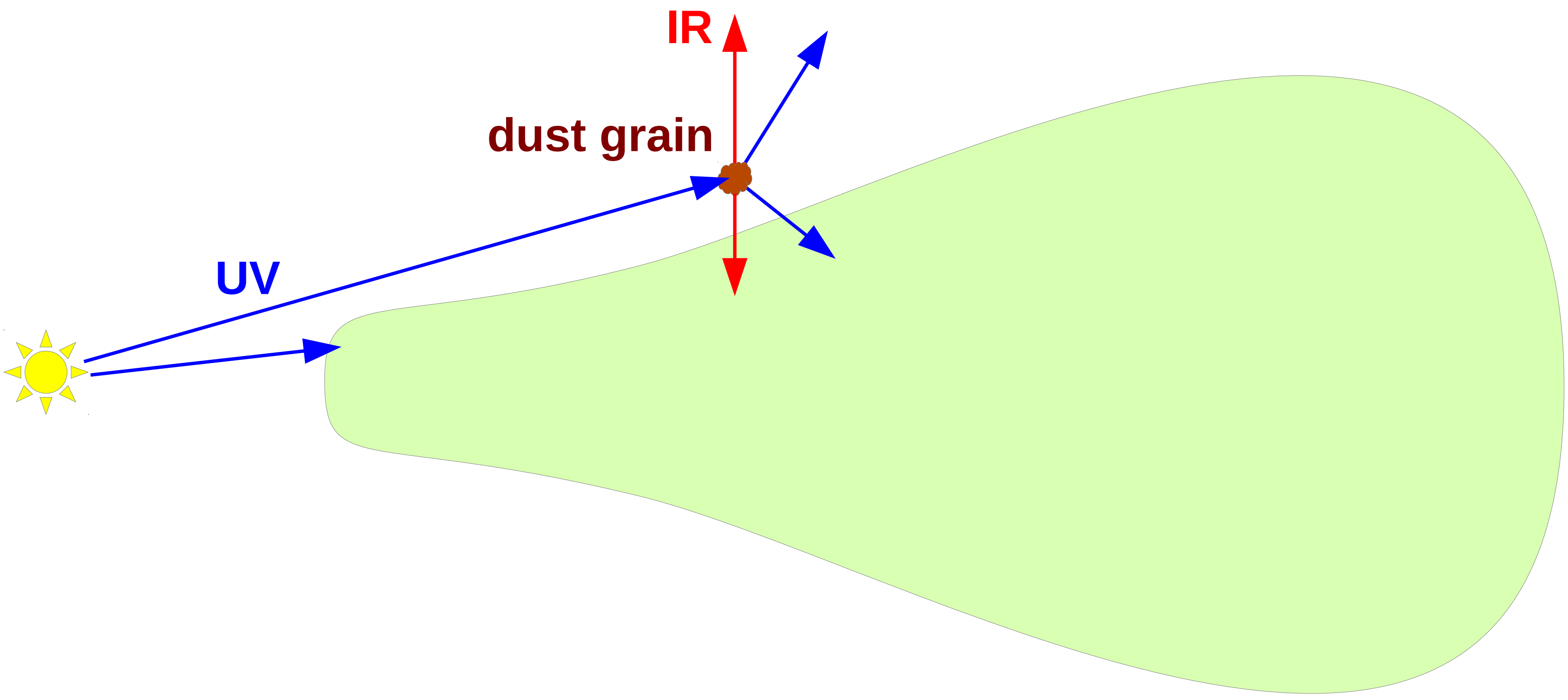
→ *Spitzer IRS (R=600) data from Rigliaco et al. (2015)*



r [AU]
0.1
1
10
100
500
scattered light images
sub-mm interferometry
(e.g. ALMA)
10/20μm silicate features,
IR interferometry
PAHs
mid-IR
sub-μm grains
...
μm grains
mm-grains
migration?
ice
gas
CO ro-vib
(e.g. CRIRES)
H2O, OH, CO2, HCN ...
(Spitzer, JWST)
high-J CO, H2O
(Herschel)
[OI] 63μm
(Herschel, Sofia?)
(sub-)mm HCO+, CN,
HCN, H2CO, N2H+, ...
mm CO rot
CO isotopologues

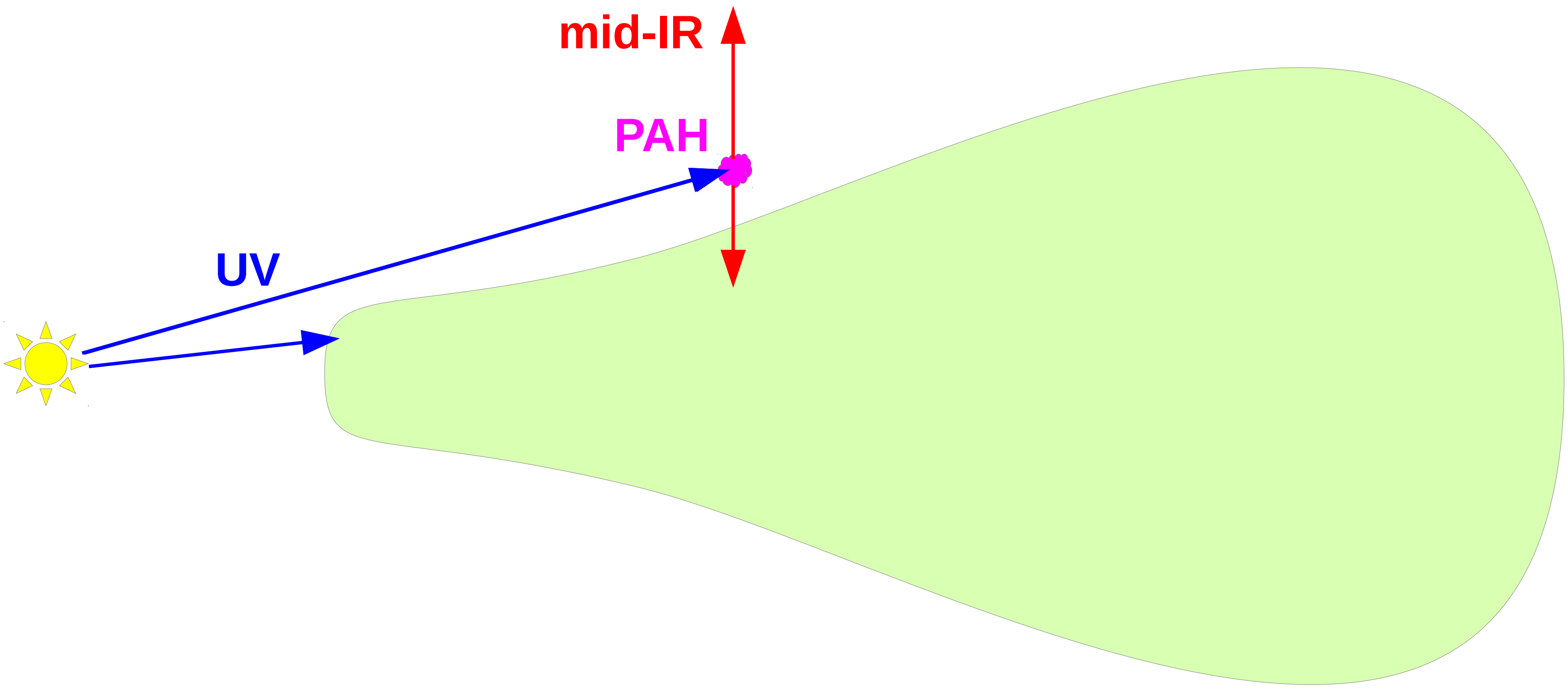
The PAH UV-shield

→ Woitke et al. 2015, submitted to A&A



The PAH UV-shield

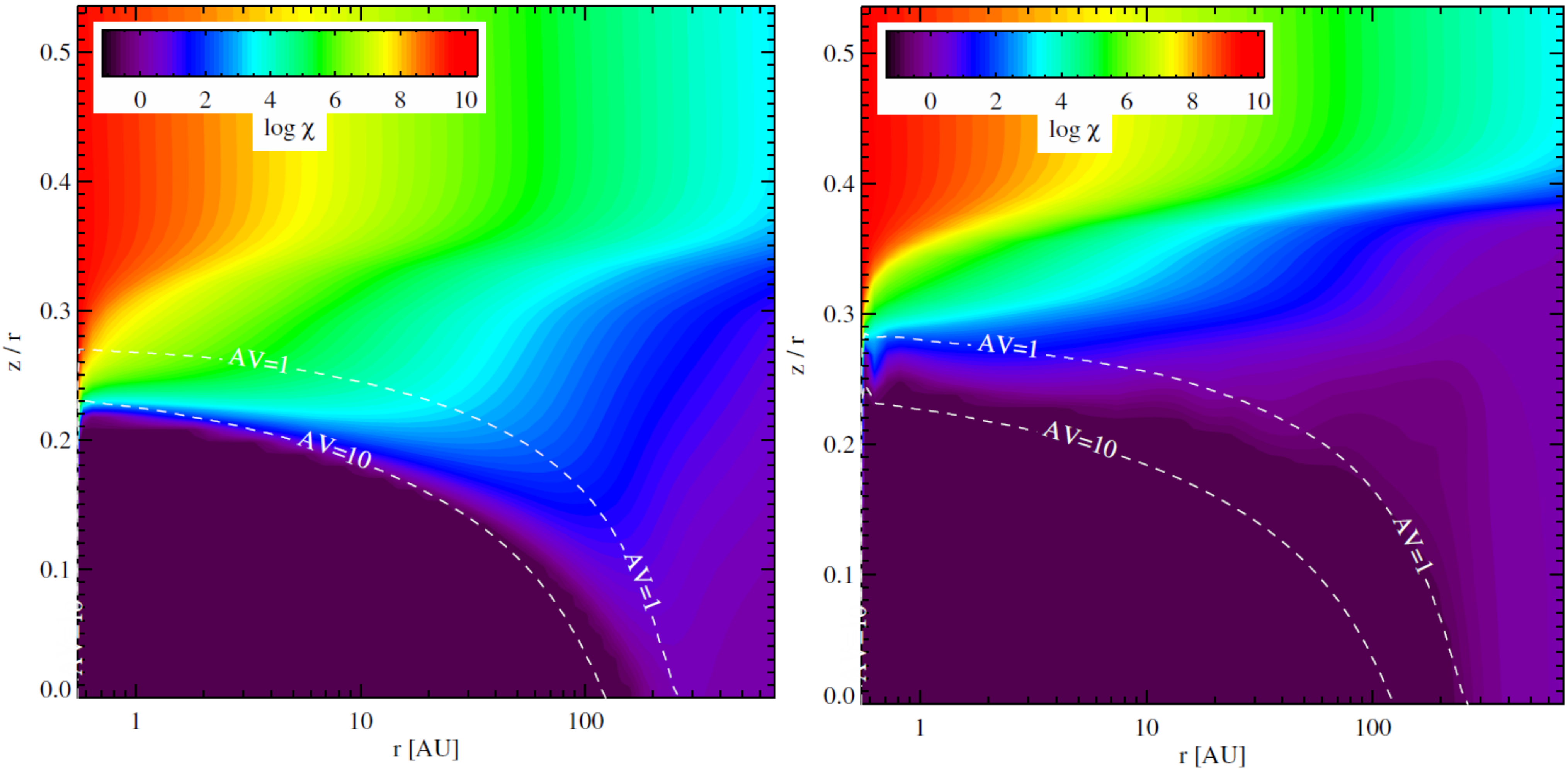
→ *Woitke et al. 2015, submitted to A&A*



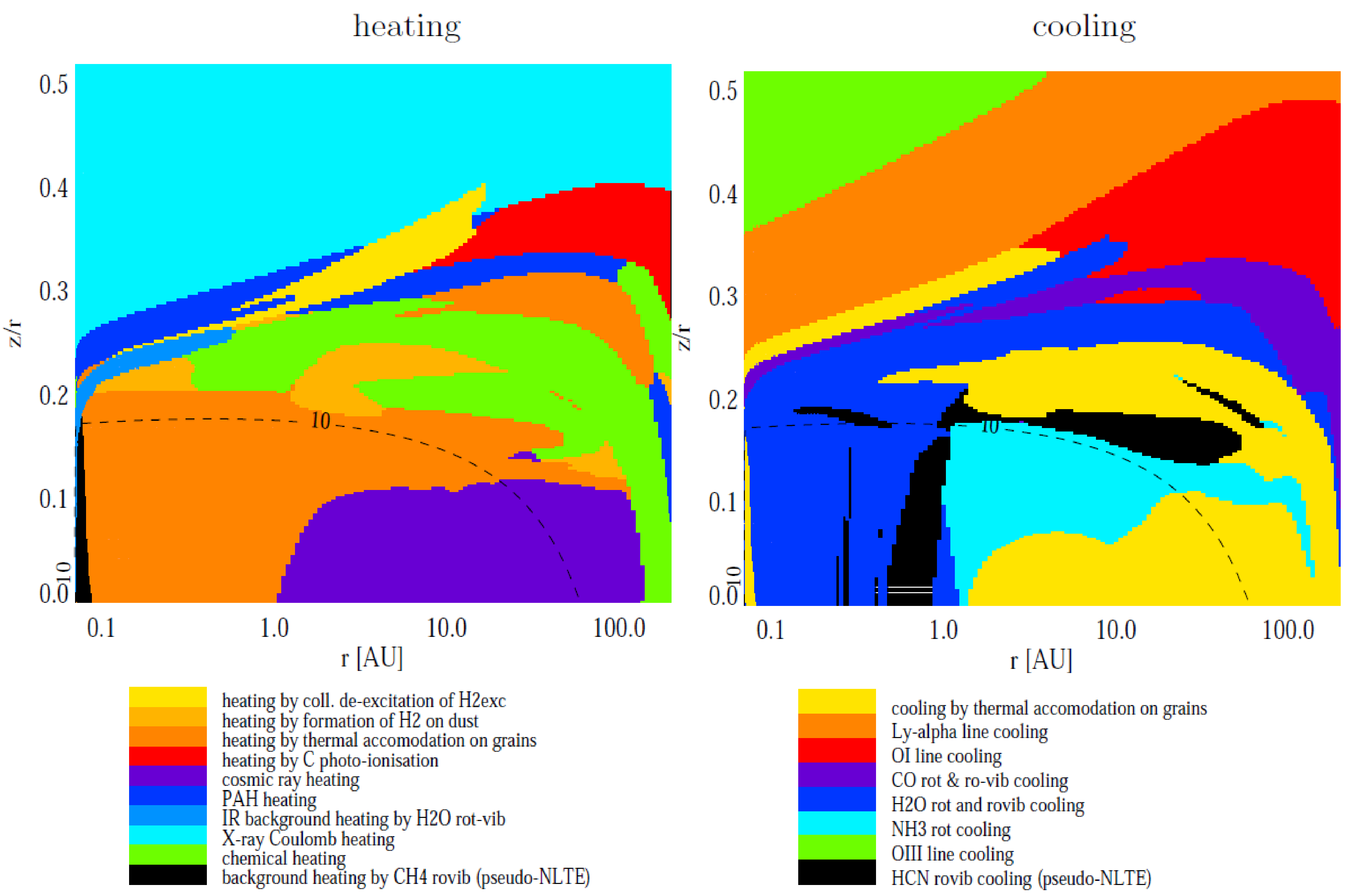
The PAH UV-shield

→ *Woitke et al. 2015, submitted to A&A*

fPAH=0 HD 163296 model fPAH=1

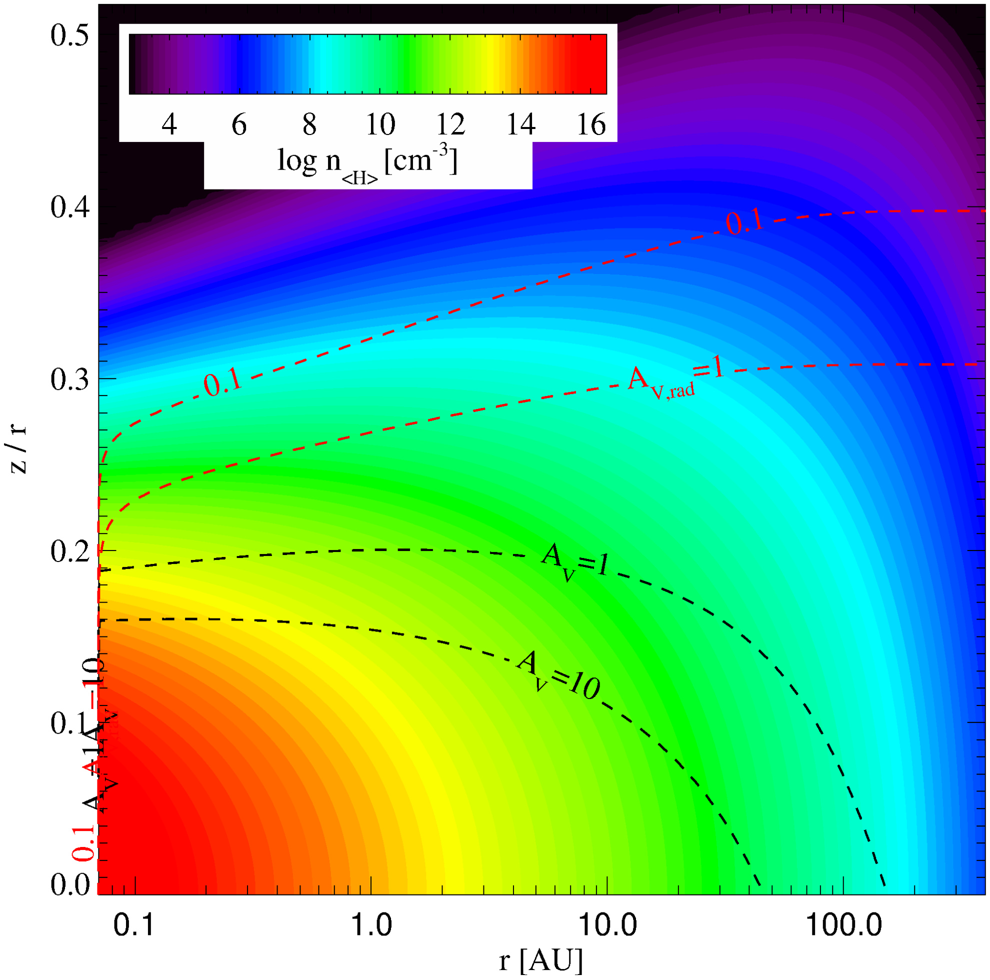


Gas Heating & Cooling

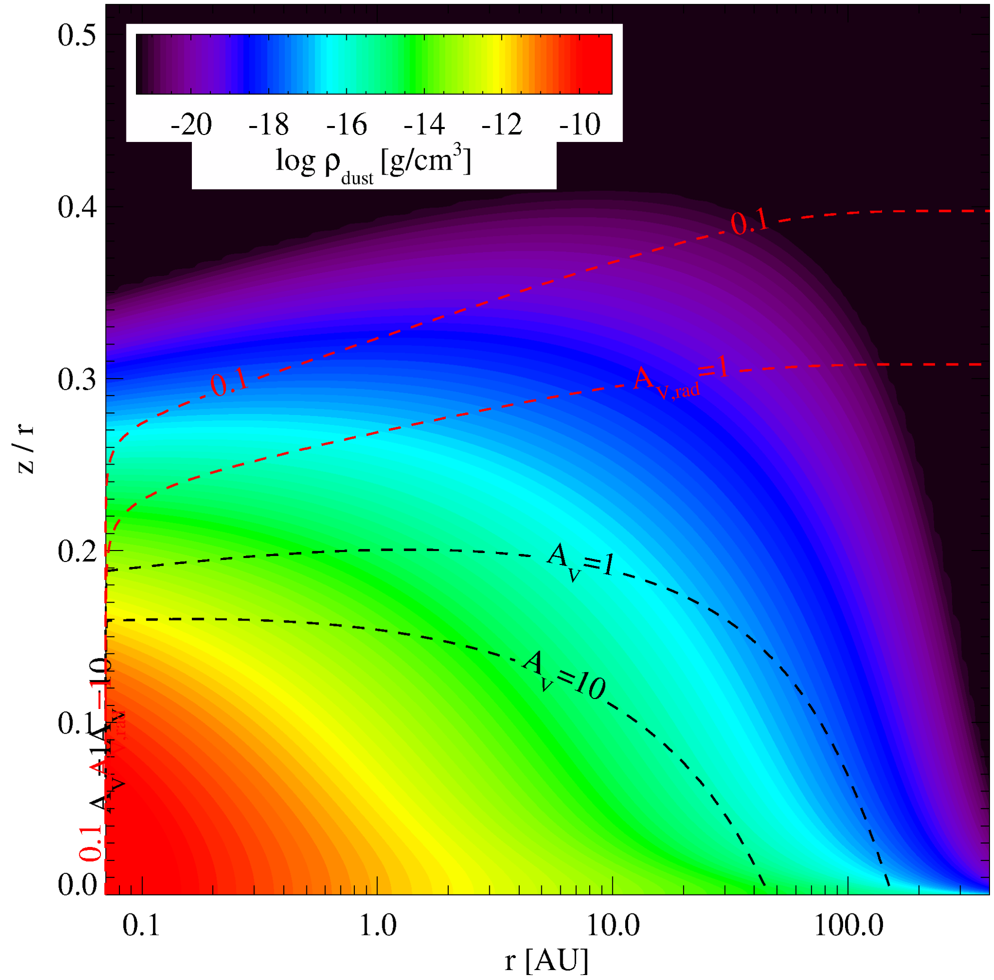


Dust settling

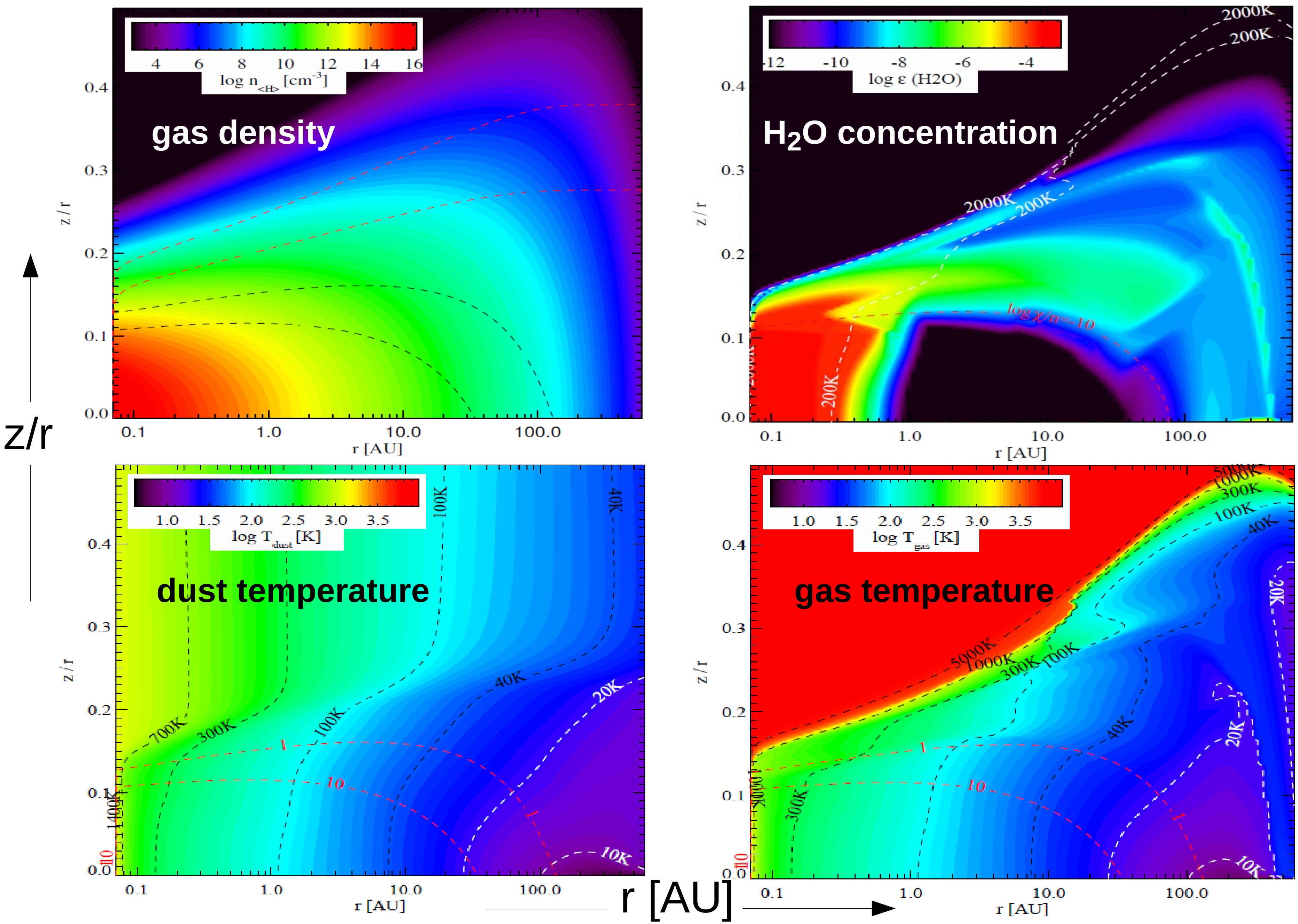
gas (assumed): exponential tapering-off



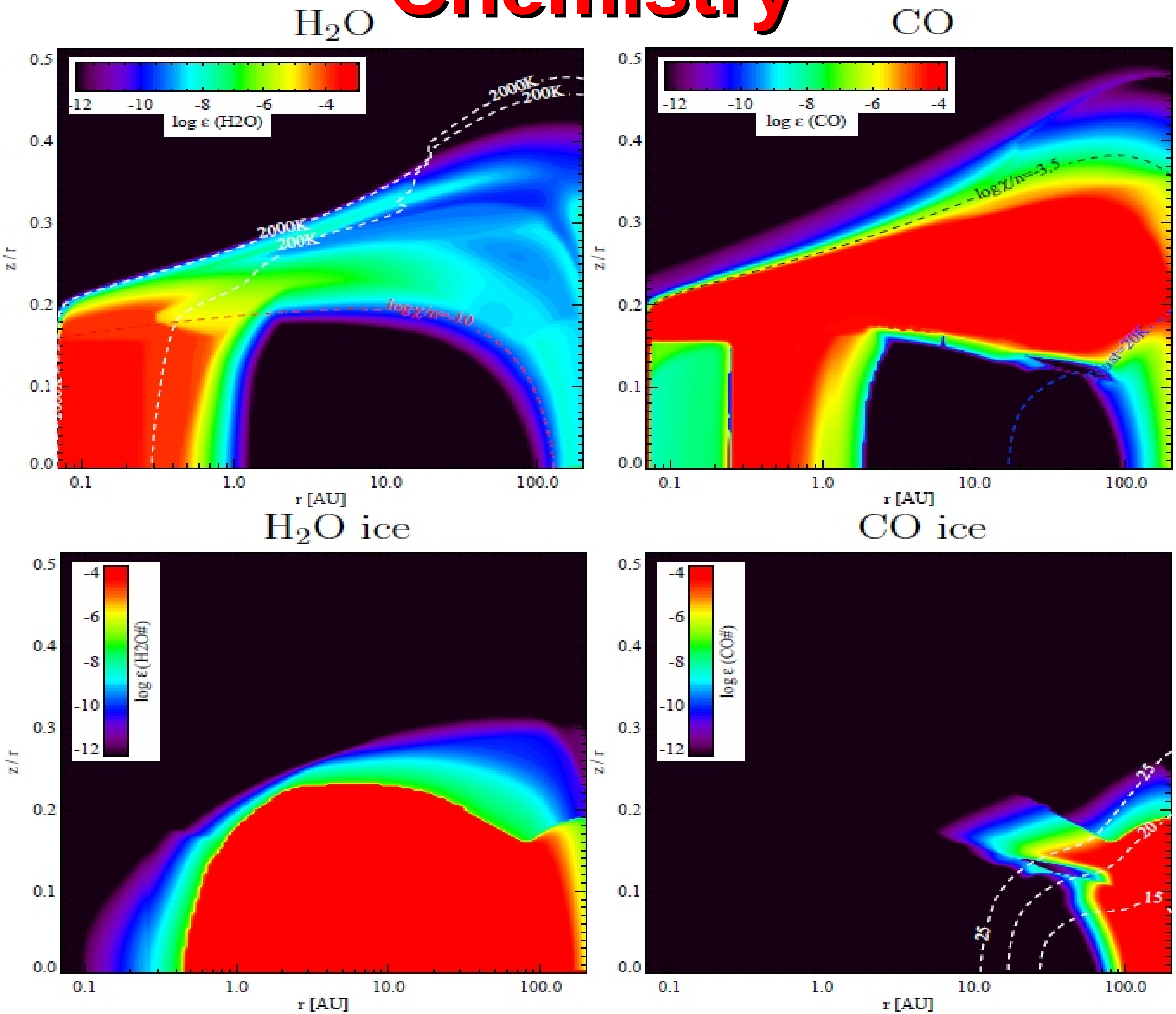
dust (calculated): Dubrulle-settling $\alpha = 10^{-3}$



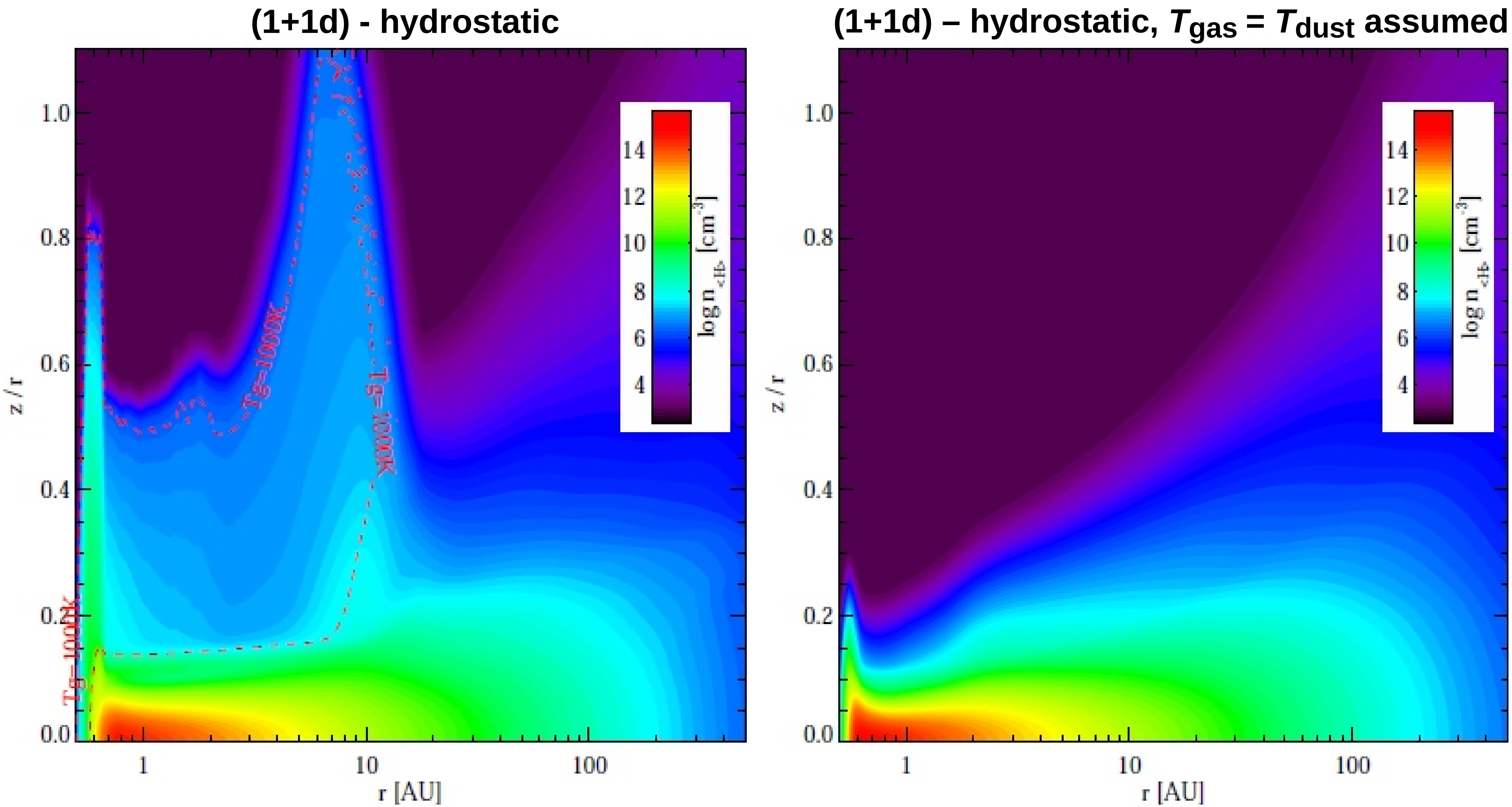
some modelling results



Chemistry


H2O
CO
H2O ice
CO ice
log ε (H2O)
log ε (CO)
log ε (H2O#)
log ε (CO#)
2000K
200K
logχ/n=-10
logχ/n=-3.5
Tdust=20K
z / r
r [AU]
0.1
1.0
10.0
100.0
25
20
15

Density Structure



Woitke, Kamp & Thi (2009, A&A 501, 383);
Thi, Woitke, Kamp (2011, MNRAS 412, 711)