Modelling

Planet-forming Circumstellar Discs

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The GASPS modelling team

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Grenoble: Wing-Fai Thi, Francois Ménard, Christophe Pinte, Gaspard Duchêne

Edinburgh: Ian Tilling

Thanks to: Uma Gorti, Simon Bruderer, Dmitry Semenov Edwin Bergin, Hideko Nomura, ...

University of St Andrews

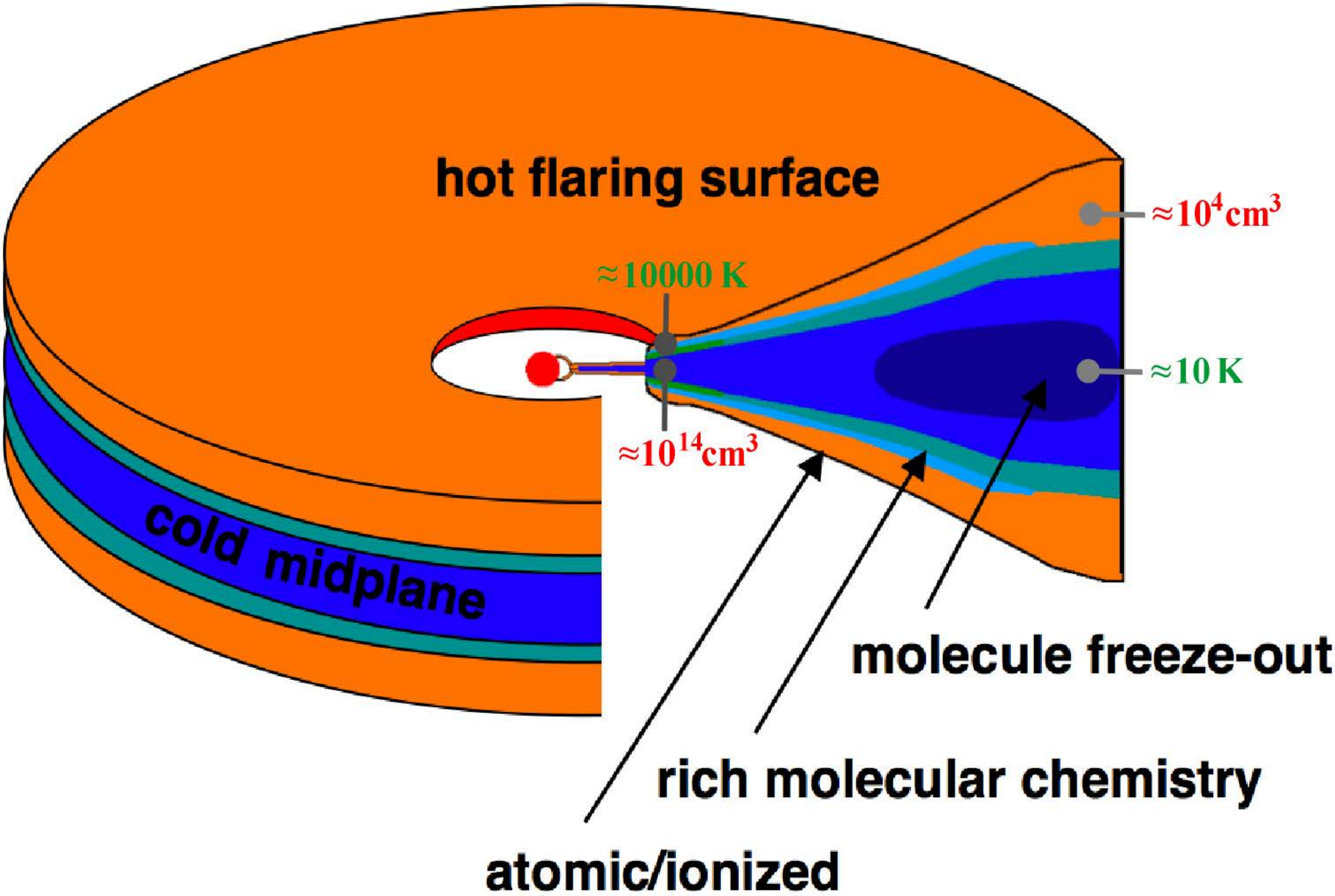
RuG

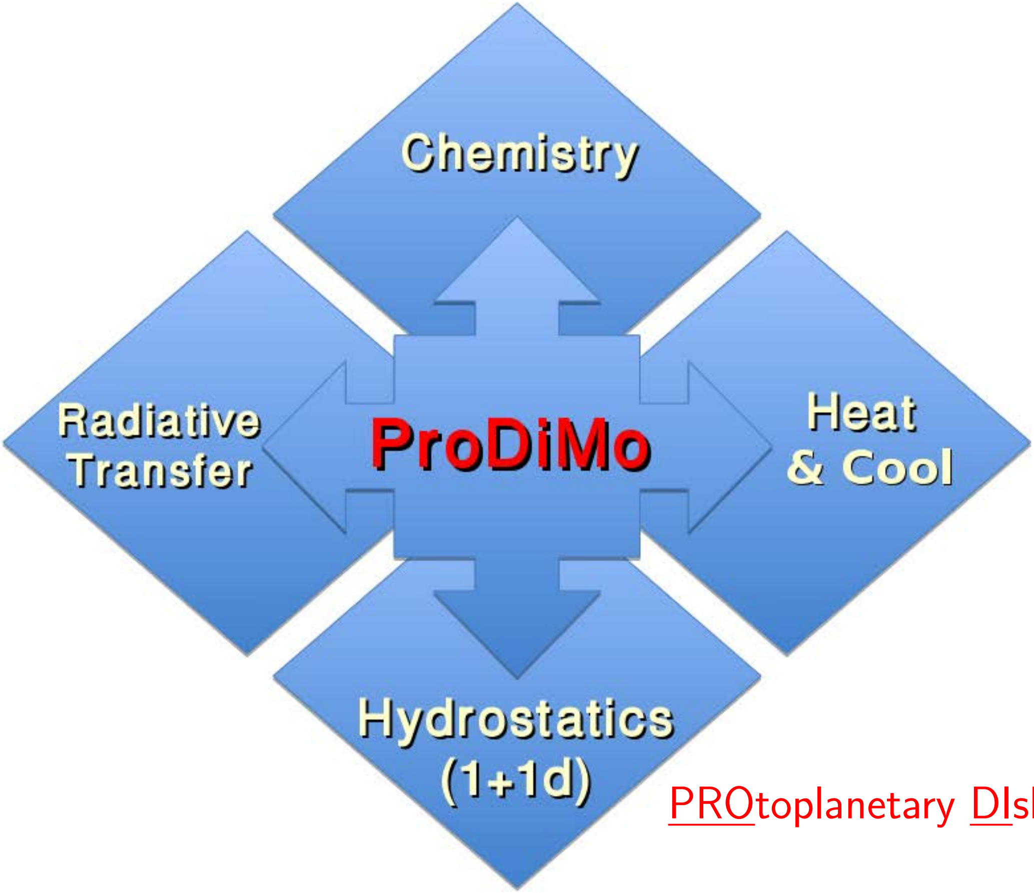
IPAG Institut de Planétologie et d'Astrophysique de Grenoble

THE UNIVERSITY OF EDINBURGH

What means (radiation) thermo-chemical disk modelling?

Gas in Protoplanetary Disks





PROtoplanetary DIsk MOdel

main paper	→ Woitke, Kamp & Thi (2009, A&A 501, 383)
improved RT coupling	→ Kamp et al. (2010, A&A 510, 18)
inner rim & SED calculation	→ Thi, Woitke & Kamp (2011, MNRAS 412, 711)
PAH charge & line transfer	→ Woitke et al. (2011, A&A 534, 44)
X-ray chemistry & heating	→ Aresu et al. (2011, A&A 526, 163)
application to individual targets	→ 7 papers so far (2010 – 2012)
this conference	→ used in 4 talks, 8 posters (!)

Chemistry

$$\frac{dn_i}{dt} = \sum_r n_k n_l R^r_{kl\to ij}(T_{\rm gas}) - n_i \sum_r n_j R^r_{ij\to kl}(T_{\rm gas}) \;\pm\; \ldots$$

elements:	~10	e.g. H, He, C, N, O, Ne, Na, Mg, Si, S, Ar, Fe, PAHs
species:	~100	atoms, ions, double ions, molecules, vib. exc. $H_2^\star$, ices, PAHs
reactions:	~1000	gas-phase, including 3-body (UMIST 2006), UV-photo-reactions with detailed $\sigma(\nu)$ (Leiden database), 2-directional self-shielding by H_2, CO, C (various papers), X-ray primary and secondary (Meijerink & Glassgold 2008) H_2 formation of grain surfaces (e.g. Cazaux & Tielens 2010) $H_2^\star$ chemistry (Tielens & Hollenbach 1985) ice formation ($H_2O^\#$, $CO^\#$, $CO_2^\#$, $CH_4^\#$, ...) (Aikawa 1996) (including thermal, UV-photo, and cosmic-ray desorption) PAH photo-ionisation, recomb. (Draine & Li 2007, ...)

$$\frac{dn_i}{dt} = 0 \quad \Rightarrow \quad \text{“kinetic chemical equilibrium”}$$

- dependent on **dust properties** (total surface area, $T_{\rm dust}$)
- coupled to **radiative transfer** results (UV, X-rays)
- **new:** more ices, simple surface chemistry (Kamp et al. 2012, in prep.)
- **open issues:** warm and dense chemistry?

Heating & Cooling

$$\sum_k \Gamma_k(T_{\rm gas}, n_i, {\rm dust}) \;=\; \sum_k \Lambda_k(T_{\rm gas}, n_i, {\rm dust})$$ $\Rightarrow$ $T_{\rm gas}$ *"thermal balance"*

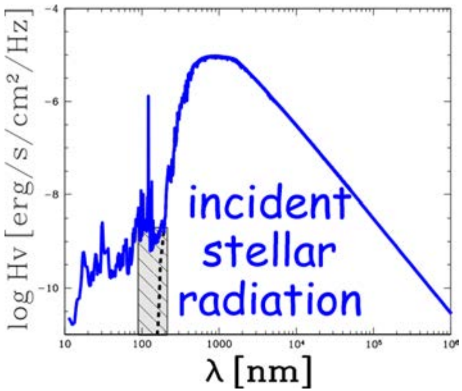
heating	~60	PAH photo-ionisation heating, photo-electric heating, X-ray Coulomb heating, cosmic ray heating, exothermal reactions, viscous ("α") heating, coll. de-excitation of $H_2^\star$, H_2-formation on grains, C photo-ionisation, H^- bound-free, line pumping (in particular Fe II, H_2O ro-vib, CO ro-vib, ...)
cooling	~50	thermal accomodation on grains, PAH recombination cooling, Ly α, OIII (6 levels / 11 lines), MgII (8 / 12), ArII, NeII, FeII semi-forbidden (120 levels / 956 lines), OI (91 / 647), CII (10 / 31), CI, SiII, SI, SII, NII, CO ro-vibrational (e.g. $v=0,1,2$, $J=0,...,35$), o/p-H_2 ro-vibronic (327/342 levels, 3984/4232 lines), o/p-H_2O ro-vibrational (411/413 levels, 4248/3942 lines), OH, SiO, NO, CS, HCN, HNC, CN, HCO^+, CH^+ rotational, ^{13}CO, HD, HDO, SO, SO_2, OCS, o/p-NH_3, p/o-H_2CO rot.

- escape probibility (vertically upwards, radially inwards/outwards)
- background radiation field from continuum RT
- **new:** CO ro-vibronic (Thi et al. 2012 in prep., also poster)
- **open issues:** more chem. pumping? more stellar-atmosphere-like?

Continuum & Line Radiative Transfer

$$\frac{dI_\nu}{d\tau} = S_\nu - I_\nu$$, dust in radiative equilibrium (+ non-rad. heating)

incident stellar:



incident interstellar:

- far UV (Draine)
- CMB (2.7 K)
- isotrop

EITHER use ProDiMo ...

– *isotropic scat. ray-based, long-char., accelerated Λ-iteration*

OR use MCFOST (Pinte et al. 2009; Ménard's previous talk) **...**

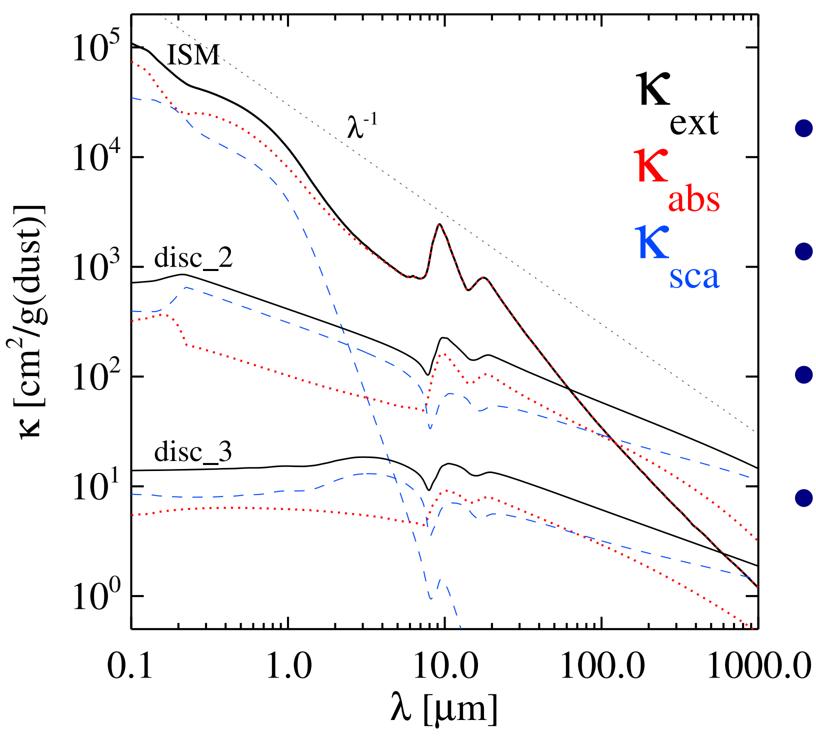
– *anisotropic scattering, Monte-Carlo, diffusion solver, ...*

- ray-tracing of continuum and non-LTE line transfer, for given inclination, to get simulated observations
- **open issues:** gas opacities? X-ray RT with Compton scattering?

Disc dust is special ...

(from Mie and effective medium theory, $f(a) \propto a^{-3.5}$ size distribution, gas/dust$\,=100$)

	a_{min}	a_{max}	carbon	surface/H [cm^2]	A_V/N_H [cm^2]	albedo$_V$
ISM	0.005 μm	0.25 μm	25%	5.3×10^{-21}	6.9×10^{-22}	0.36
disc_1	0.05 μm	1 mm	25%	2.6×10^{-23}	$1.6 \times \mathbf{10^{-23}}$	0.48
disc_2	0.05 μm	1 mm	0%	2.6×10^{-23}	1.3×10^{-23}	**0.76**
disc_3	1 μm	10 cm	0%	5.9×10^{-25}	$3.5 \times \mathbf{10^{-25}}$	0.56



- more difficult to form H_2 (even more so if dust is settled!)
- UV penetrates much deeper than used from ISM
- unusual combinations of high densities & high UV fluxes
- be careful with any formula from ISM research!

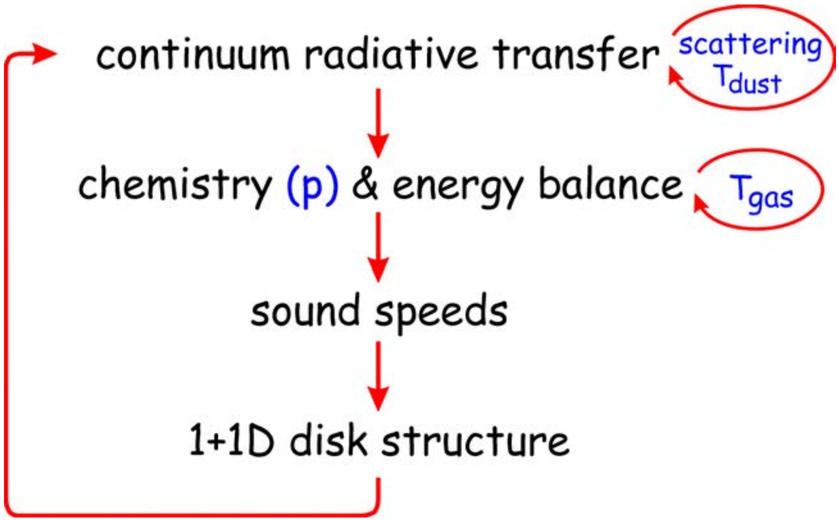
Vertical Structure and Global Iteration

vertical: $$\frac{1}{\rho}\frac{\partial p}{\partial z} = -\frac{z\,GM_\star}{(r^2+z^2)^{3/2}}$$ with $p = c_T^2\,\rho$ and $c_T^2 = c_T^2(r,z)$

radial: $$\Sigma(r) = \int \rho(r,z)\,dz \;\propto\; r^{-\epsilon}$$ with $M_{\rm disk} = \int 2\pi r\,\Sigma(r)\,dr$

+ inner soft edge
or any other law (holes, gaps, ...)

iterative solution:



Radiation thermo-chemical disc models usually have ...

- *no* magnetic fields
- *no* hydrodynamics, except ...

  photoevaporation wind models
  → Alexander, Clarke, Pringle et al. (2006 –2012);
  → Owen, Ercolano, Clarke et al. (2009 – 2012)

  some models run on stream-lines of disc evolution (quasi-1D), see e.g.
  → Visser, van Dishoeck et al. (2009 – 2012),
  also poster by Harsono et al.

- *no* non-LTE beyond escape probability method, except ...

  on given structure, temperatures, concentrations, etc.
  → e.g. Hogerheijde et al. (2000 – 2012)

Overview of Disc Models

	RT	chemistry	X-rays	heat & cool	vert. struc.	transport & mixing
Gorti, Hollenbach et al.	*	**	✓	**	***	-
Heinzeller, Normura et al.	*	***	✓	**	***	*
Bruderer et al.	***	**	✓	**	(fixed)	-
Semenov, Bergin et al.	*	****	✓	$(T_{\rm g}=T_{\rm d})$	(fixed)	***
ProDiMo	**	**	✓	***	***	-
ProDiMo & MCFOST	***	**	✓	***	(fixed)	-

Gorti, Hollenbach, Najita, Pascucci (2011, ApJ 735, 90)

Heinzeller, Nomura, Walsh, Millar (2011, ApJ 731, 115)

Bruderer, van Dishoeck, Doty, Herczeg (2012, A&A in press)

Fogel, Bethell, Bergin, Calvet, Semenov (2011, ApJ 726, 29)

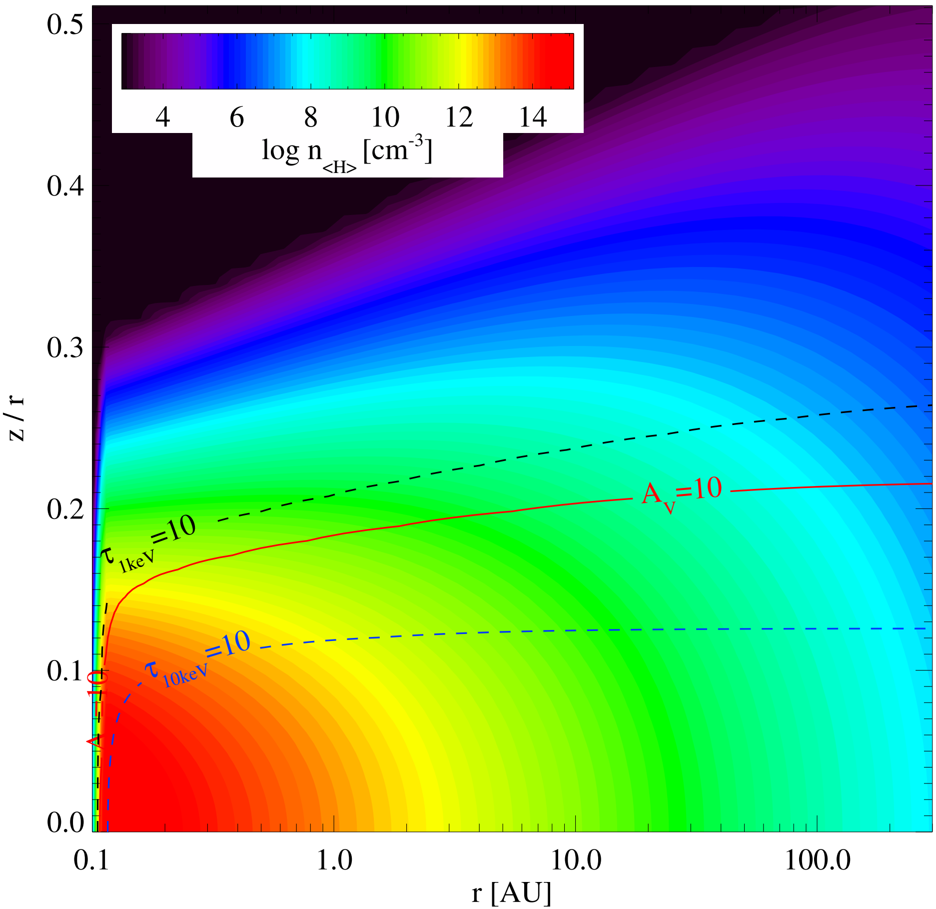
Woitke, Thi, Kamp, Aresu, Meijerink, Spaans (various papers 2009–2012)

Pinte, Ménard, Duchêne (2006, A&A 459, 797)

Apologies, if I misread something, or missed your model!

Some remarkable results and latest tendencies ...

X-rays penetrate much deeper than UV - really?



Aresu et al. (2011, A&A 526, 163)

→ poster by Aresu et al., this conference

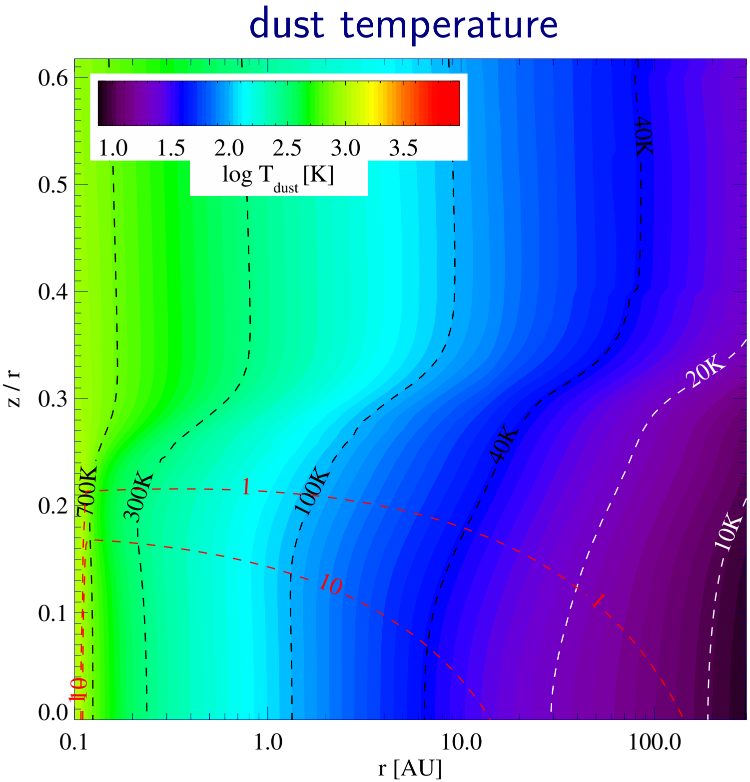
→ poster by Liebhart, Güdel, Meeus, Woitke, Kamp

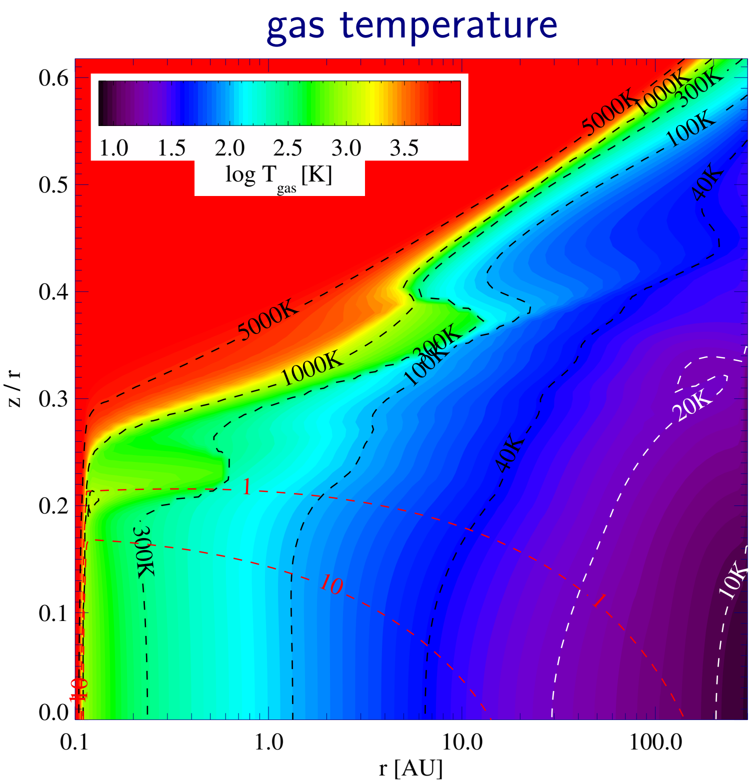
Dust and Gas Temperature

T Tauri type: $L_\star = 0.7\,L_\odot$, $T_{\rm eff} = 4400\,$K, $L_{\rm UV} = 1.4 \times 10^{31}\,$erg/s, $L_X = 10^{30}\,$erg/s

$r = (0.1 - 300)\,$AU, rad. exponent $\epsilon = -1$, scale height $H_0 = 1\,$AU @ 10 AU, flaring $\beta = 1.1$

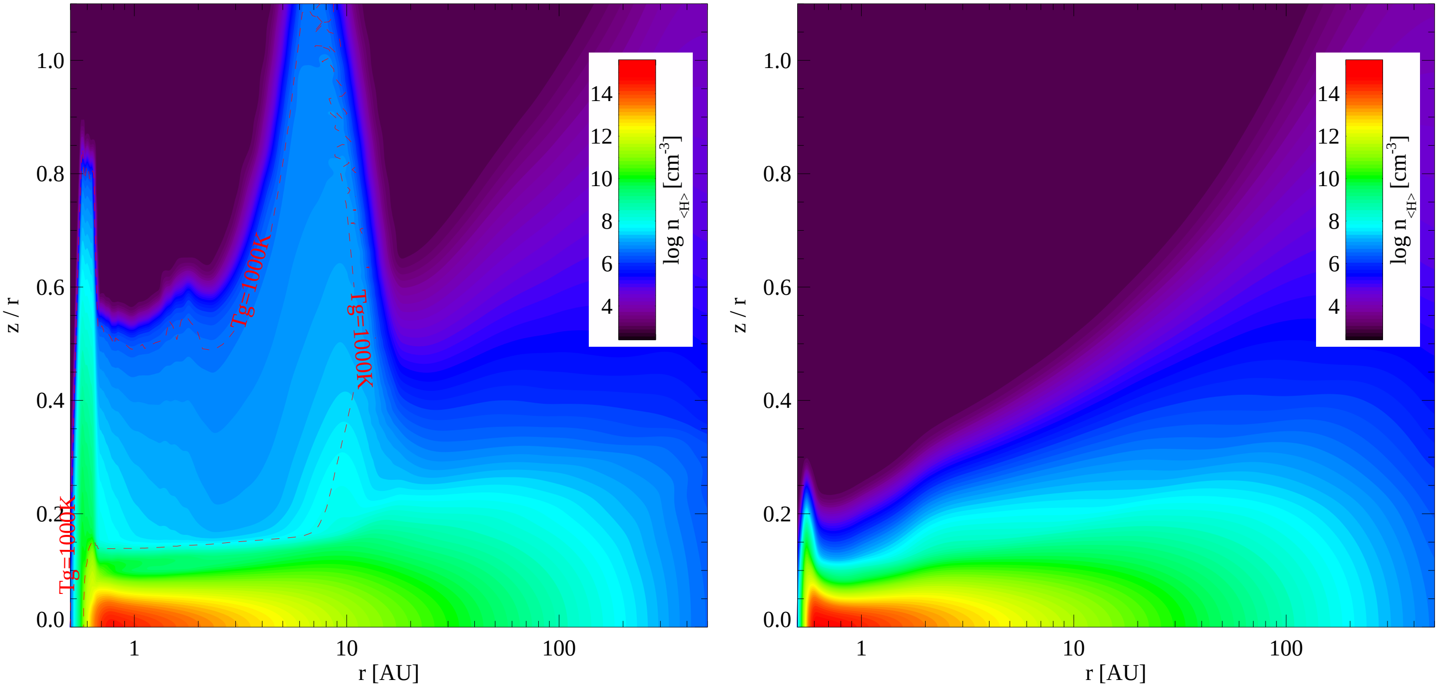
$M_{\rm gas} = 10^{-2}\,M_\odot$, dust/gas $= 0.01$, astro. sil. ($a = 0.05\,\mu$m $- 1\,$mm, $p = -3.5$), $f_{\rm PAH} = 0.01$





Density Structure

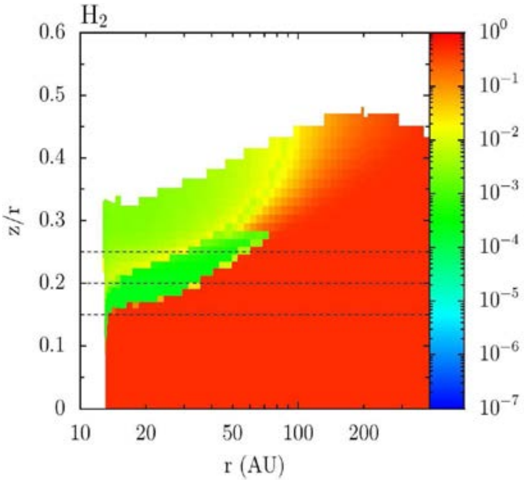
gas in thermal balance | $T_{\rm g} = T_{\rm d}$ assumed



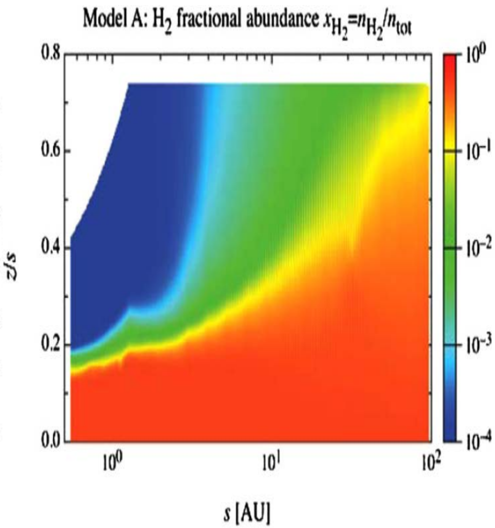
Woitke, Kamp & Thi (2009, A&A 501, 383);
Thi, Woitke, Kamp (2011, MNRAS 412, 711)

Do the models agree?

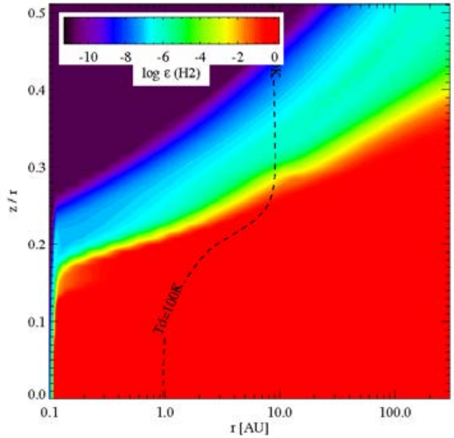
Bruderer et al.



Heinzeller at al.



ProDiMo

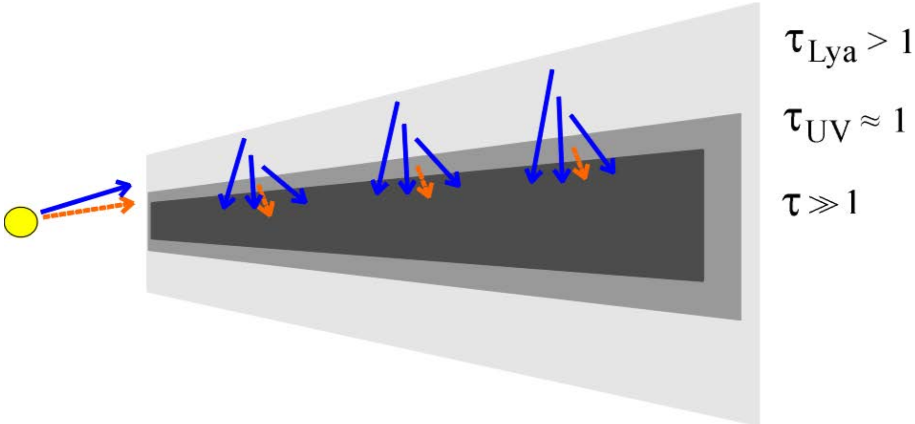


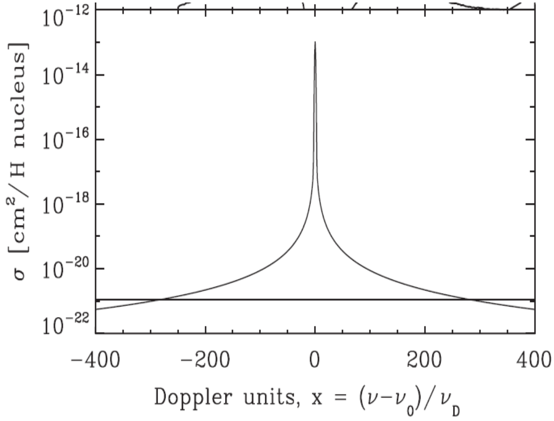
- well, of course **they don't** – what did you expect?
- but **qualitatively**, they often do!
- different disc **parameters**, different **understanding** of parameters, different **approximations**, different **numerics**, ...

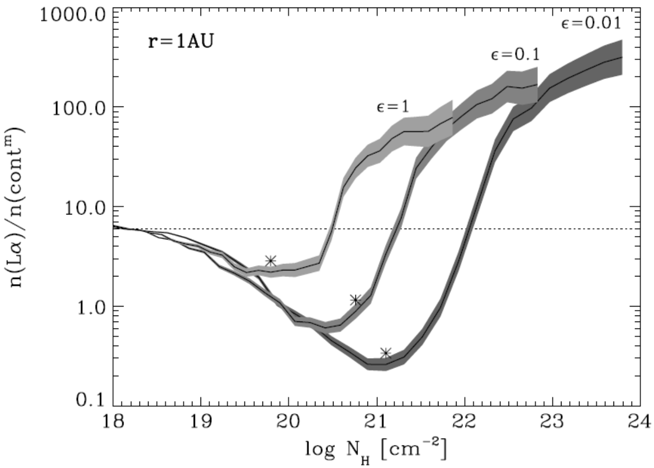
  → need for a disc modelling **benchmark**?

  → poster (Thi, Bruderer et al.) on HD 141569A

Enhancement of Lyα in disc geometry



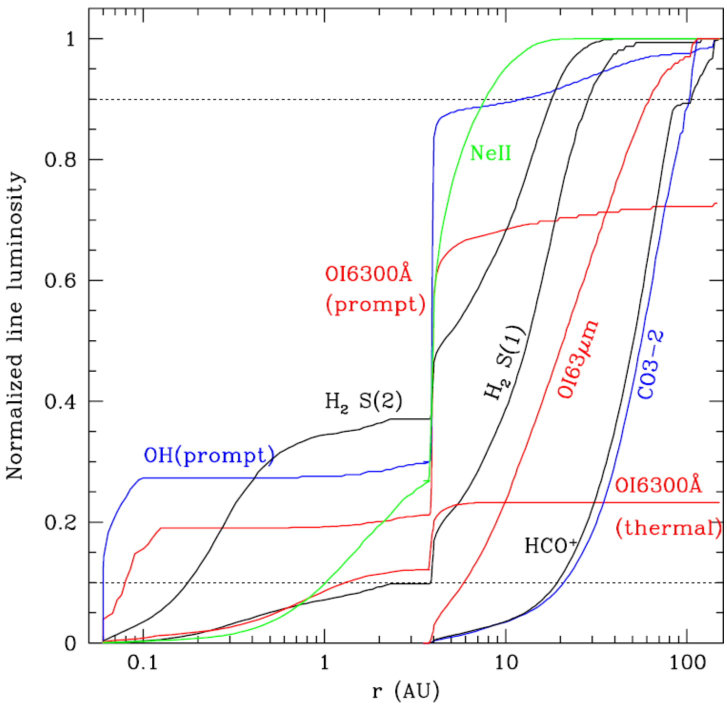




- resonance scattering of Lyα in teneous disc surface leads to amplification of photo-dissociation in discs
- selective destruction of HCN, NH_3, and CH_4, which have 1216Å photo-coss-sections > 0
- enhancement of CO, CN, and SO

Bethell & Bergin (2011, ApJ 739, 11)
Fogel, Bethell, Bergin, Calvet, Semenov (2011, ApJ 726, 29)

Using optical−sub-mm lines to constrain the distribution of gas



TW Hya

- [OI] 6300 Å and 5577 Å forbidden lines, pumped by OH photo-dissociation
- OH mid-IR lines, pumped by H_2O photo-dissociation
- mid-IR S(1) and S(2) H_2-lines
- [NeII] 12.8μm
- [OI] 63μm
- CO and HCO^+ sub-mm lines

Gorti, Hollenbach, Najita, Pascucci (2011, ApJ 735, 90)

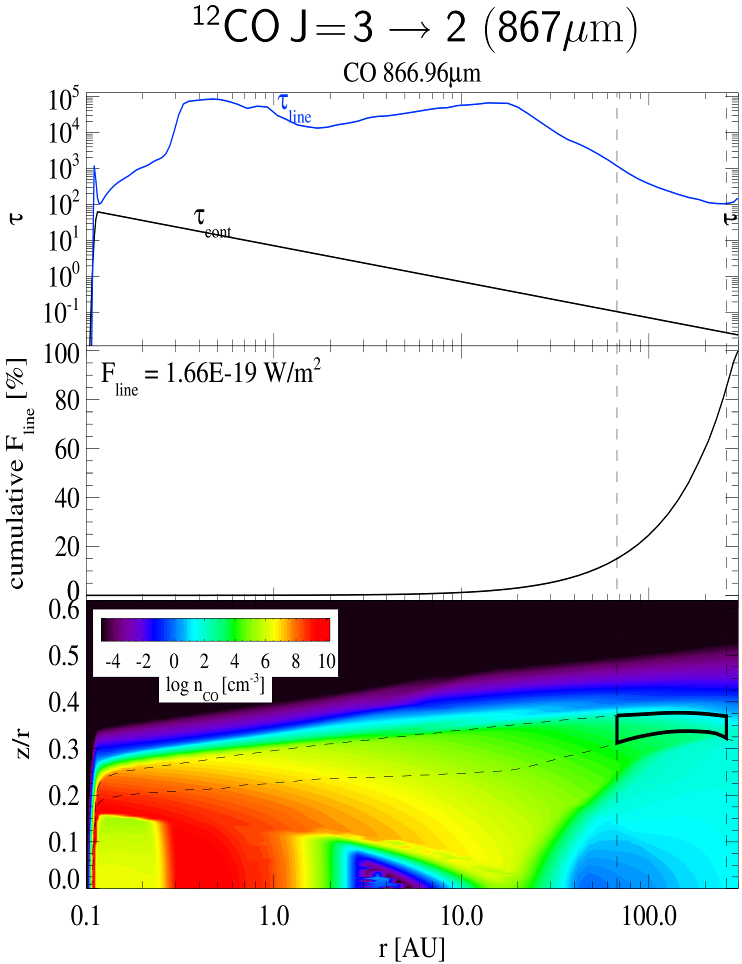
→ related posters about H_2 near/mid IR, [NeII] 12.8 μm, ro-vib CO and OH (Carmona et al., Thi et al., Liskowsy et al.)

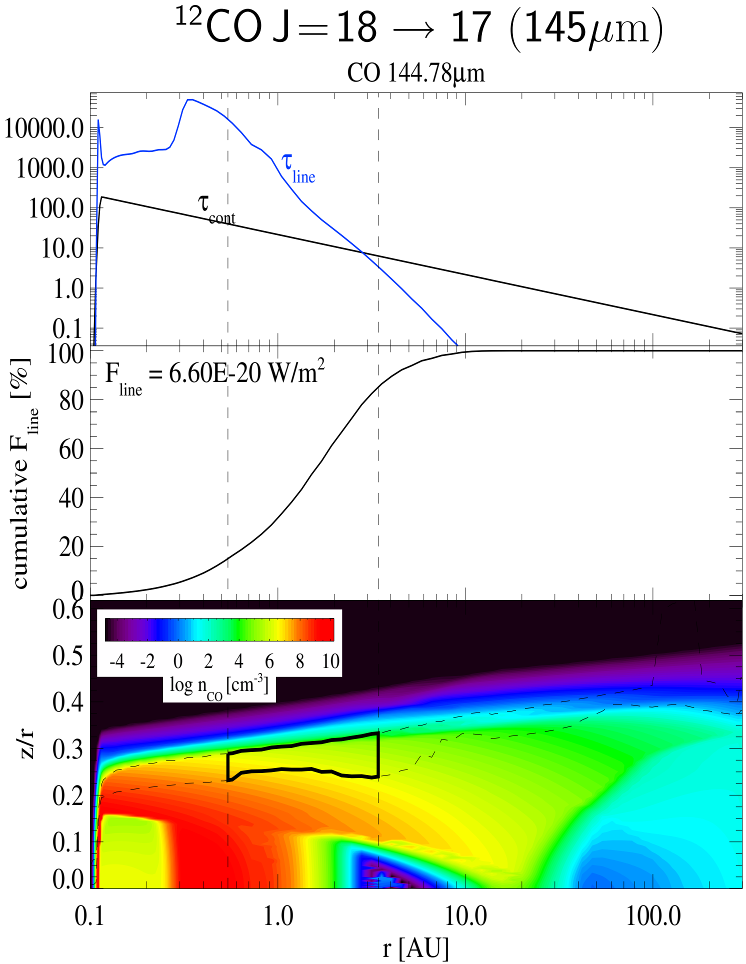
Recent modelling "trends"

- merging radiative transfer ↔ chemistry
  (Bruderer et al., Woitke et al.)
- believe in results from gas energy balance —
  $T_{\rm gas} = T_{\rm dust}$-models can't explain the Herschel results
  (Gorti et al., Bruderer et al., Nomura et al., Woitke et al.)
- include X-rays, merge PDR and XDR physics and chemistry (all)
- investigate more complicated disc shapes, such as inner holes, gaps, zones with different scale heights, puffed-up inner rim, etc.
  (Gorti et al., Woitke et al., Pinte et al.)
- use multi-wavelength line data, from optical to mm
  (Gorti et al., Woitke et al.)
- try to fit dust and gas observations at the same time
  (Woitke et al., see also poster by Pinte et al.)
- use dust properties & settling from dust evolution models
  (e.g. Pinte et al.)

Important results from Herschel

Where do the emission lines come from?

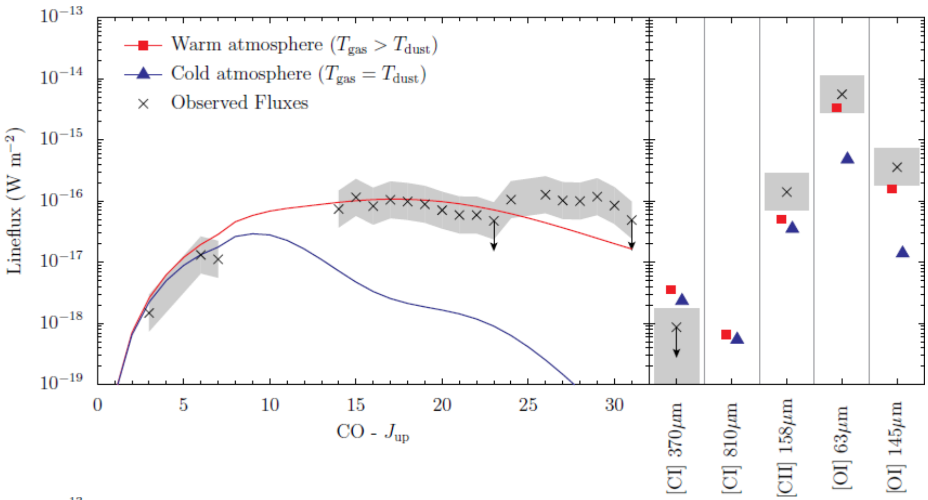




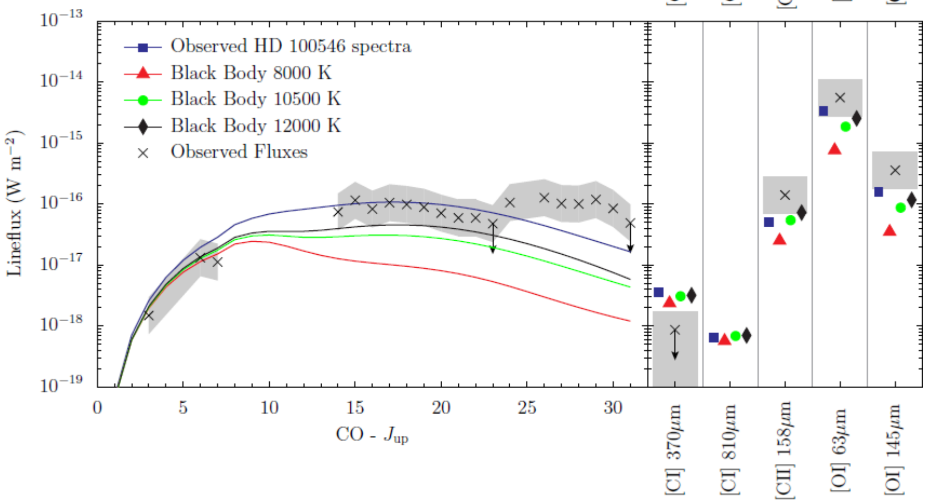
- optically **thick**
- continuum is optically thin

- still optically **thick**
- in front of optically thick dust

HD 100546: analysis of PACS/DIGIT data



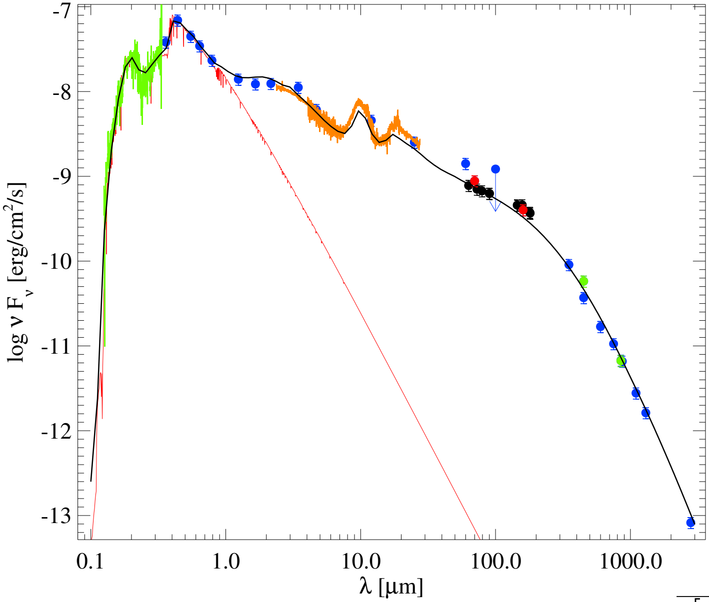
- warm surface $T_{gas} \gg T_{dust}$ excites high-J Herschel lines
- $T_{gas} = T_{dust}$ models are fine for the sub-mm CO lines, but fail for the high-J Herschel lines



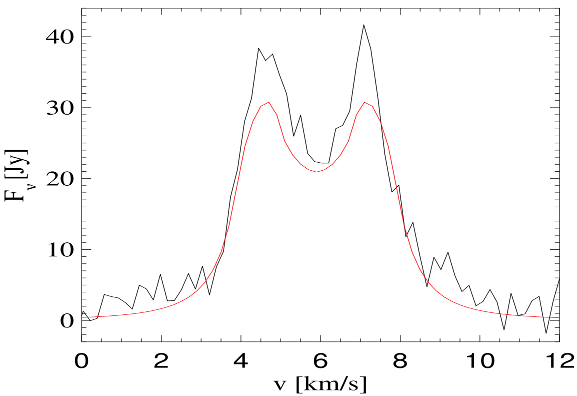
- hard FUV is what counts
- better use the observed UV input spectrum

Bruderer, van Dishoeck, Doty, Herczeg (2012, A&A in press), → Simon's talk soon

HD 163296: analysis of PACS/GASPS data



$M_\star = 2.5\,M_\odot$, type AIVe,
$T_{\rm eff} = 9250\,$K, $L_\star = 37.7\,L_\odot$,
disk: $0.45 - 850\,$AU,
exponential outer edge
dust: $0.01\,\mu$m $- 2\,$mm (p $= 3.7$),
$M_{\rm dust} = (0.0007 \ldots 0.001)\,M_\odot$,
$M_{\rm gas} = (0.02 \ldots 0.07)\,M_\odot$,
gas/dust $= 20 - 100$

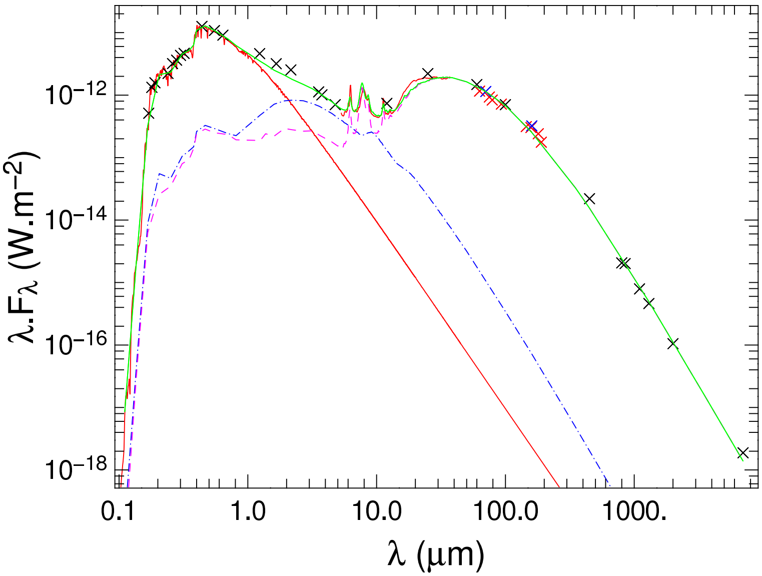


	observed	model
[OI] 63.18 μm	**193** $\pm$ 6	**191**
[OI] 145.52 μm	$<$ 8.5	5.4
p-H_2O 89.99 μm	$<$ 9.4	1.2
o-H_2 17.03 μm	$<$ 28	1.1
CO 144.78	$<$ 13.1	1.5
CO 3 $\rightarrow$ 2	**1.65** $\pm$ 0.4	**1.2**
CO 2 $\rightarrow$ 1	**0.38** $\pm$ 0.12	**0.40**
^{13}CO 1 $\rightarrow$ 0	**0.0124** $\pm$ 0.007	**0.012**

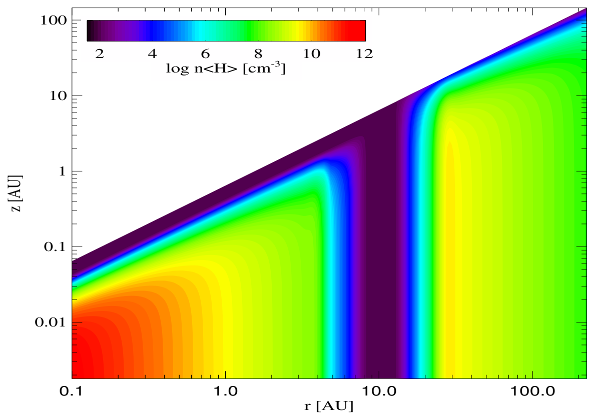
line fluxes in $[10^{-18}\,{\rm W/m^2}]$

Tilling, Woitke, et al. (2012, A&A 538, 20)

HD 169142: analysis of PACS/GASPS data



$M_\star = 2.0\,M_\odot$, age $= (6-8)$ Myr,
$T_{\rm eff} = 3400$ K, $L_\star = 8.5\,L_\odot$,
inner disk: 0.1 − 5 AU,
outer disk: 20 − 235 AU,
dust: 0.03 μm − 1 cm,
$M_{\rm dust} = 1.5\,(0.5)\,10^{-4}\,M_\odot$,
$M_{\rm gas} = (5 \pm 2)\,10^{-3}\,M_\odot$,
gas/dust $= 33^{+17}_{-11}$

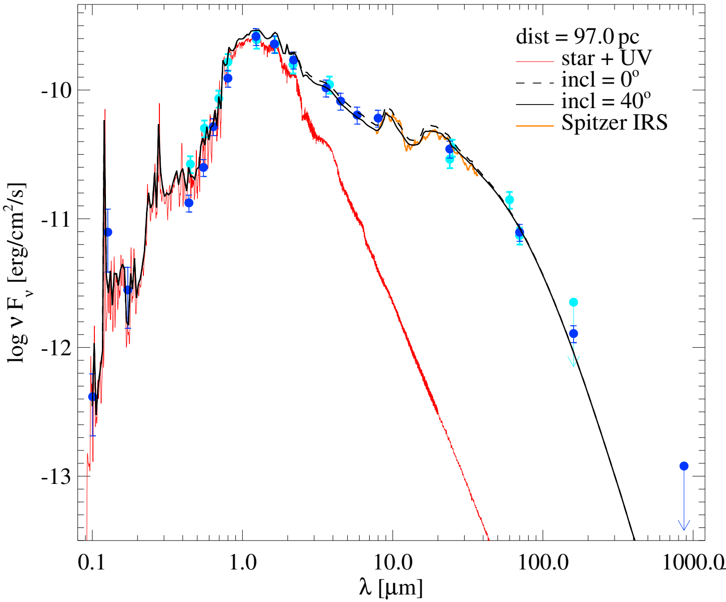


	observed	**model**
[OI] 63 μm	**71.7** ± 3.8	**71.6**
CO 2 → 1	**0.093** ± 0.004	**0.092**
^{13}CO 2 → 1	**0.048** ± 0.004	**0.048**

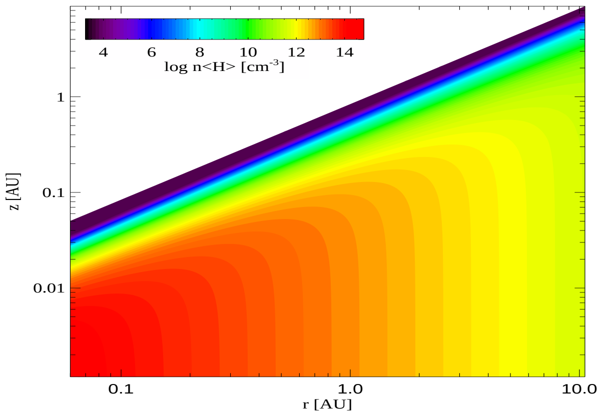
line fluxes in $[10^{-18}\,{\rm W/m^2}]$

Meeus, Pinte, Woitke, et al. (2010)
see also Maaskant et al. (poster)

ET Cha: analysis of multi-λ data



$M_\star = 0.2\,M_\odot$, age $= (6-8)$ Myr,
$T_{\rm eff} = 3400\,$K, $L_\star = 0.085\,L_\odot$,
$\dot{M}_{\rm acc} \approx 10^{-9} M_\odot/{\rm yr}$,
$\dot{M}_{\rm outflow} \approx 10^{-9} M_\odot/{\rm yr}$,
disk: $0.022 - 8.2\,$AU
dust: $0.05\,\mu$m $- 1\,$mm $(p = 4.1)$
$M_{\rm dust} = (2-5) \times 10^{-8}\,M_\odot$,
$M_{\rm gas} = (5\times10^{-5} - 3\times10^{-3})\,M_\odot$
gas/dust $= 2500 - 60000$



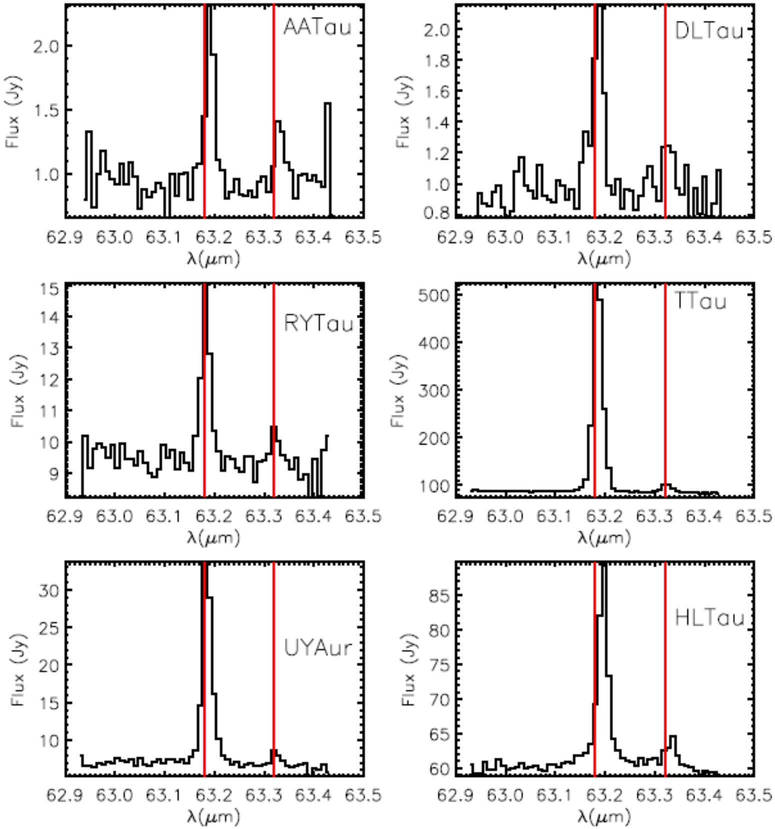
	observed	model
[OI] 63.18μm	**30.5** $\pm$ 3.2	**34.5**
[OI] 145.52μm	$<$ 6.0	2.6
[OI] 6300Å (LVC)	**65** $\pm$ 25	**69.6**
CO $J = 3 \rightarrow 2$	$<$ 0.05	0.014
CO $J = 29 \rightarrow 28$	$<$ 9.6	4.9
o-H_2 2.122μm	**2.5** $\pm$ 0.1	**2.4**

line fluxes in $[10^{-18}\,{\rm W/m^2}]$

Woitke et al. (2012, A&A 534, A44)

NEW: FT Tau (Garufi et al.), HD 135344B (Carmona et al.)

Herschel Water Lines I

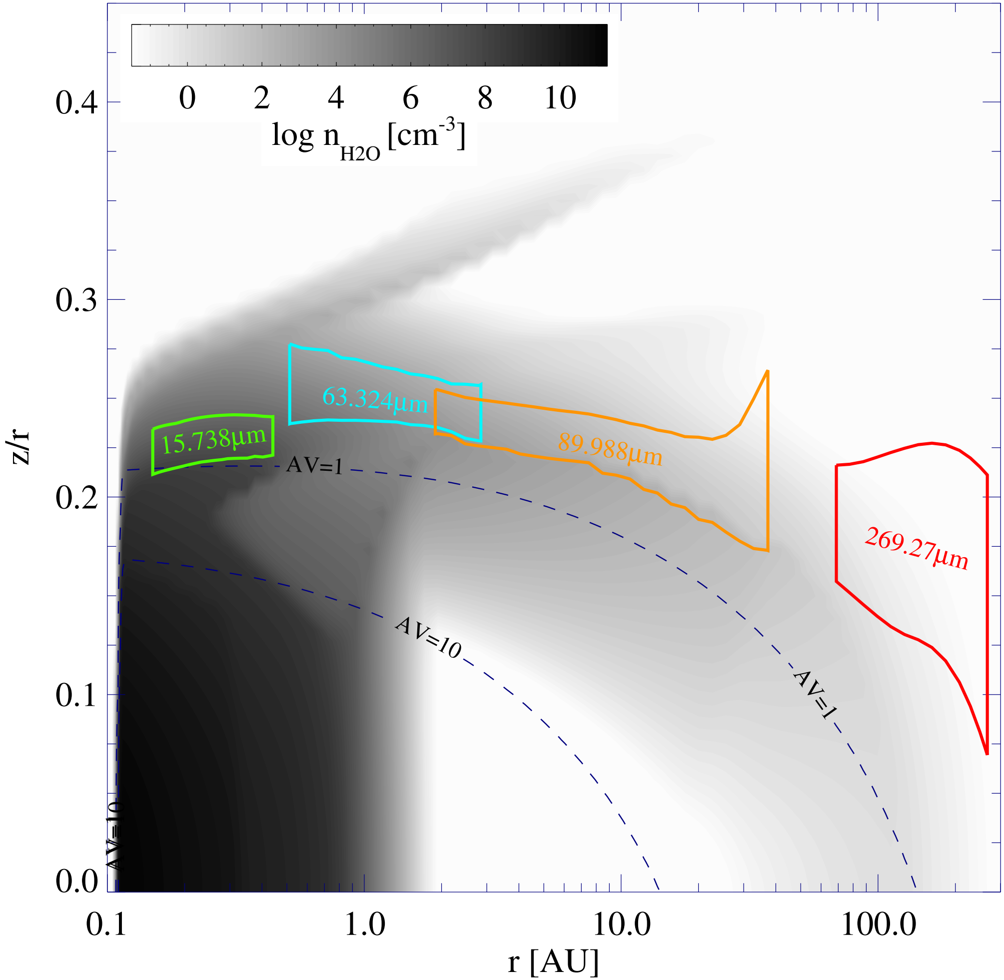


Herschel/PACS (GASPS:)
o-H_2O 63.32 μm $8_{18} \longrightarrow 7_{07}$
besides [OI] 63.18 μm
in 8/33 Taurus sample

Riviere-Marichalar et al. (2012, A&A 538, also poster)

BUT: Herschel/HIFI (WISH) found no water in discs, except in TW Hya
(tiny fluxes for fundamental lines at 269.27μm and 538.29μm)
E. van Dishoeck's talk; Hogerheijde et al. (2011, Science 334, 338)

Herschel Water Lines II



Too much water in outer regions?

- settling of large icy grains below small ice-free grains ?

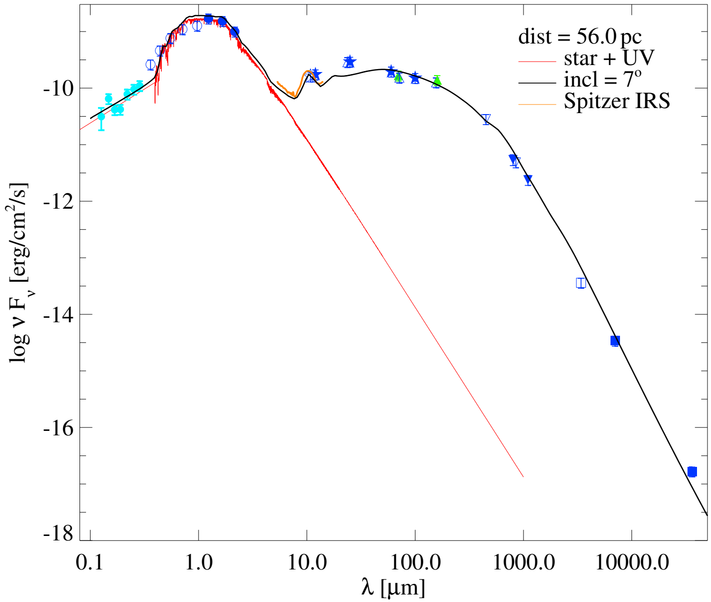
(Hogerheijde, previous talk)

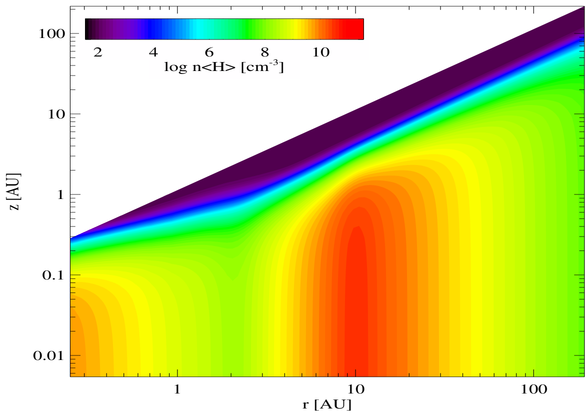
- gas/dust ratio ?
- surface chemistry ?
- UV photo-desorption yield ?
- metal abundances (Na, Mg, Si, S, Fe) ?

Rivière-Marichalar et al. (2012, A&A 538, L3), also poster

→ poster by Kamp et al., this conference

TW Hya: analysis of Herschel data





$M_\star = 0.6\,M_\odot$, age $= 10$ Myr,
$T_{\rm eff} = 4000$ K, $L_\star = 0.23\,L_\odot$,
inner disk: $0.25 - 4$ AU,
outer disk: $4 - 200$ AU,
dust: $0.03\,\mu$m $- 10$ cm(!),
$M_{\rm dust} \approx 0.0002\,M_\odot$,
$M_{\rm gas} = (0.005 - 0.05)\,M_\odot$, ($0.003^b$)
gas/dust $= 3 - 26$

	observed	**model**
[OI] 63 μm	**36.5** $\pm$ 4	$\approx 85^b$
CO 18 $\rightarrow$ 17	**3.5** $\pm$ 1.2	$\approx 0.33^b$
CO 3 $\rightarrow$ 2	**0.43** $\pm$ 0.13	$\approx 0.41^b$
^{13}CO 3 $\rightarrow$ 2	**0.044** $\pm$ 0.013	$\approx 0.084^b$
H_2O 538 μm	$\approx$ **0.22**^{a}	$\approx 0.32^b$
H_2O 269 μm	$\approx$ **0.29**^{a}	$\approx 0.79^b$
H_2O 89.9 μm	**5.6** $\pm$ 0.9^b	$\approx 0.53^b$

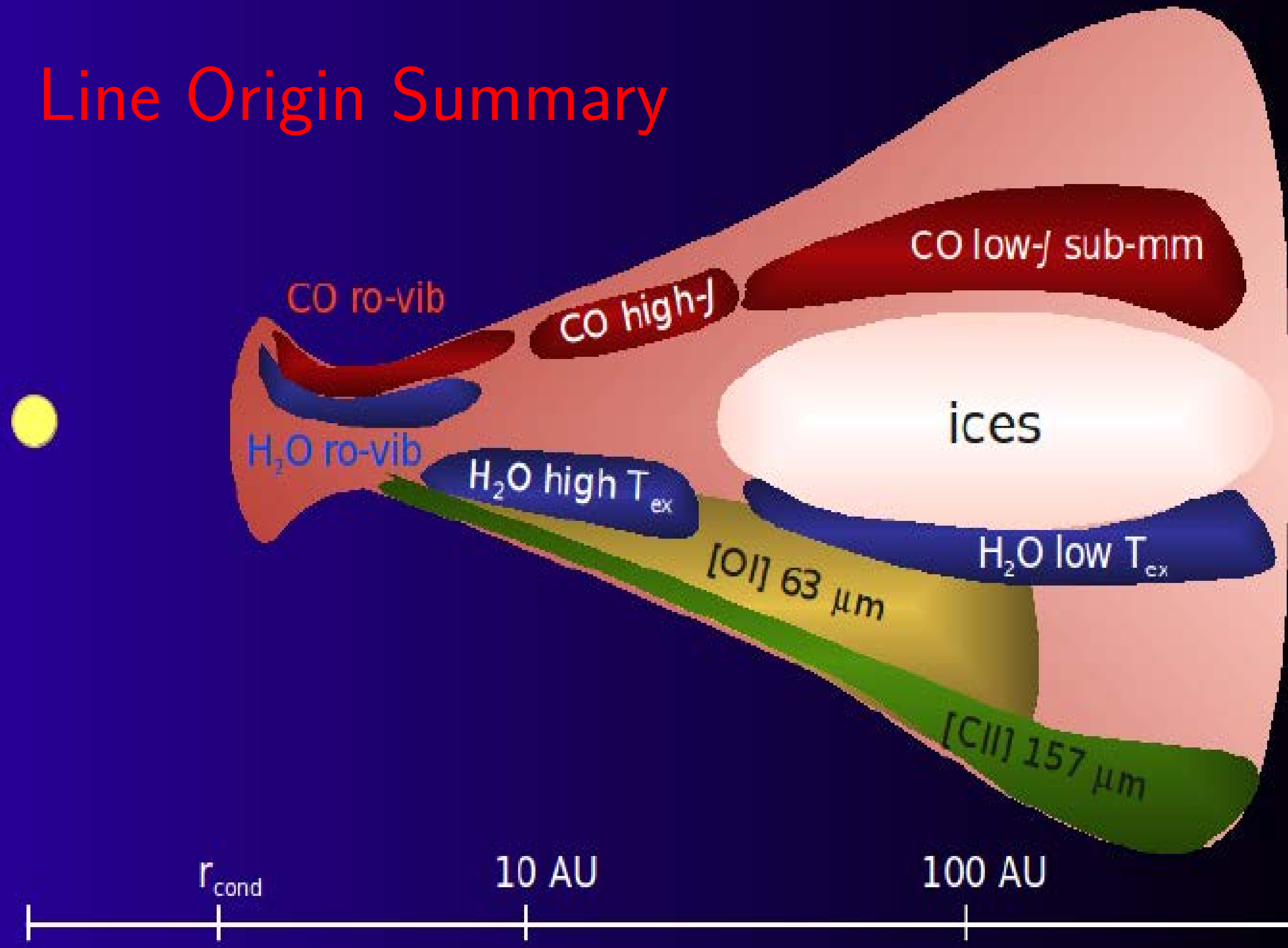
line fluxes in $[10^{-18}\,{\rm W/m^2}]$

Thi, Mathews, Ménard, Woitke et al. (2010)

[a]: Hogerheijde et al. (2011, Science 334, 338)

[b]: Kamp et al. (2012, A&A in prep. $\rightarrow$ see poster)

Line Origin Summary



Bad things (major uncertainties)

- dust properties uncertain, and probably varying throughout disc
- PAH size and abundance uncertain, and probably varying throughout disc
- H_2-formation rate on dust uncertain
- turbulence and degree of dust settling uncertain
  $\longrightarrow$ poster by Mulders & Dominik, this conference
- PDR and XDR physics uncertain for high densities $\gtrsim 10^{10}\,\mathrm{cm}^{-3}$
  $\longrightarrow$ planetary atmosphere physics & chemistry

Good things

- X-ray and UV irradiation directly measurable
- disk shape characterizable through SED & image modelling
- non-LTE often not so crucial

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

FP7-SPACE-2011 project DiscAnalysis ("DIANA")

Coordinator: Dr. Peter Woitke

- ★ EU-funded with 2 Mio Euro altogether
- ★ 1 academic, 3 PhD-students, 3 post-doc positions
- ★ in 5 places in Europe: St Andrews (UK), Vienna (AT), Groningen (NL), Amsterdam (NL) and Grenoble (FR)
- ★ for 51 months: 1.1.2012 – 31.3.2016