Photochemical and photoexcitation effects on the gas-phase chemistry in disks

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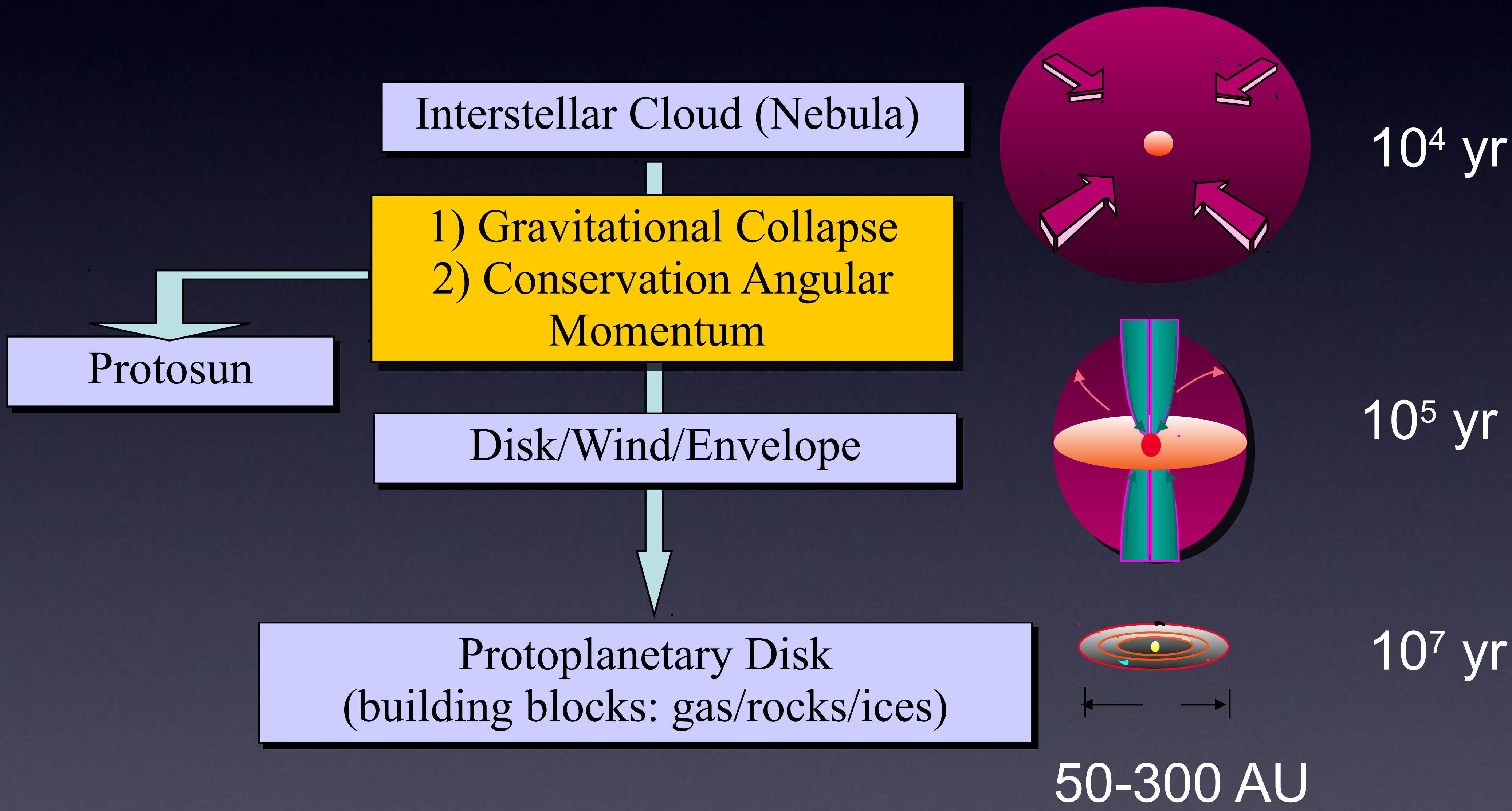
SEVENTH FRAMEWORK PROGRAMME

DiscAnalysis DIANA

Low-mass star formation

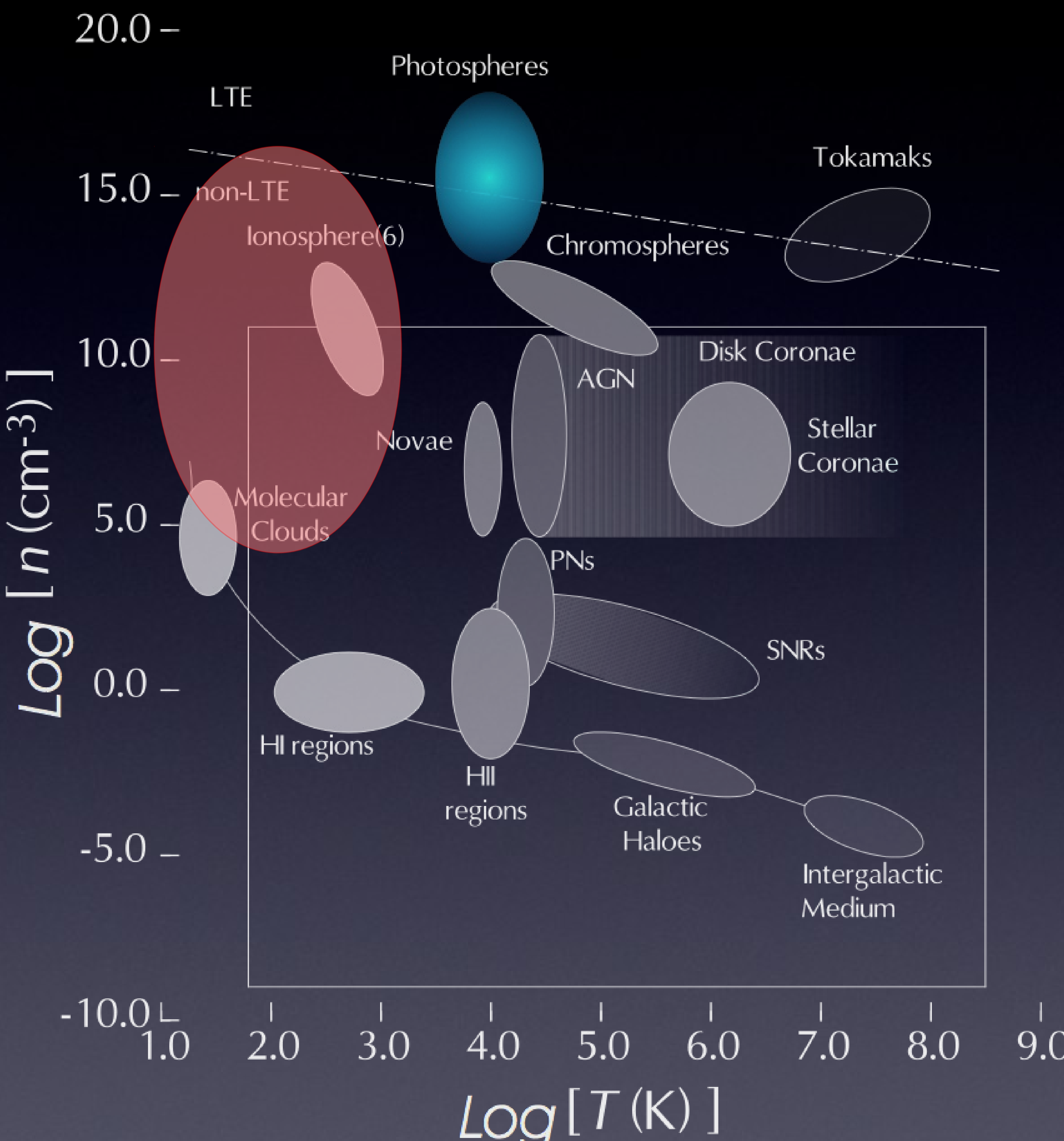
Low-mass stars



Protoplanetary discs: large range of temperatures and densities

T=10-5000K

$n=10^5$-10^{15} cm^{-3}



Disc modelling with (MFOST+) ProDiMo

Disks are exposed to stellar UV & X-rays, interstellar UV and cosmic radiation

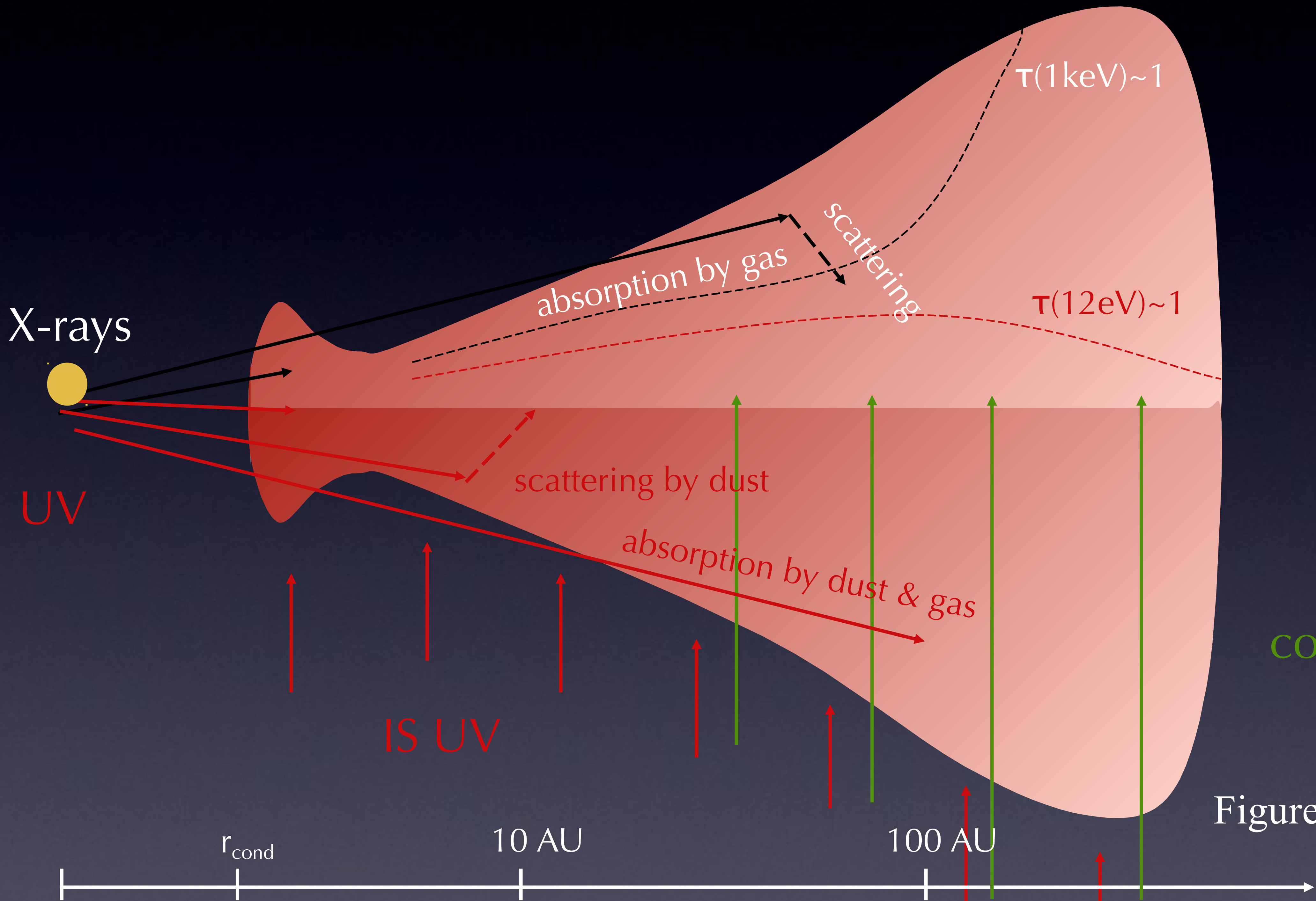
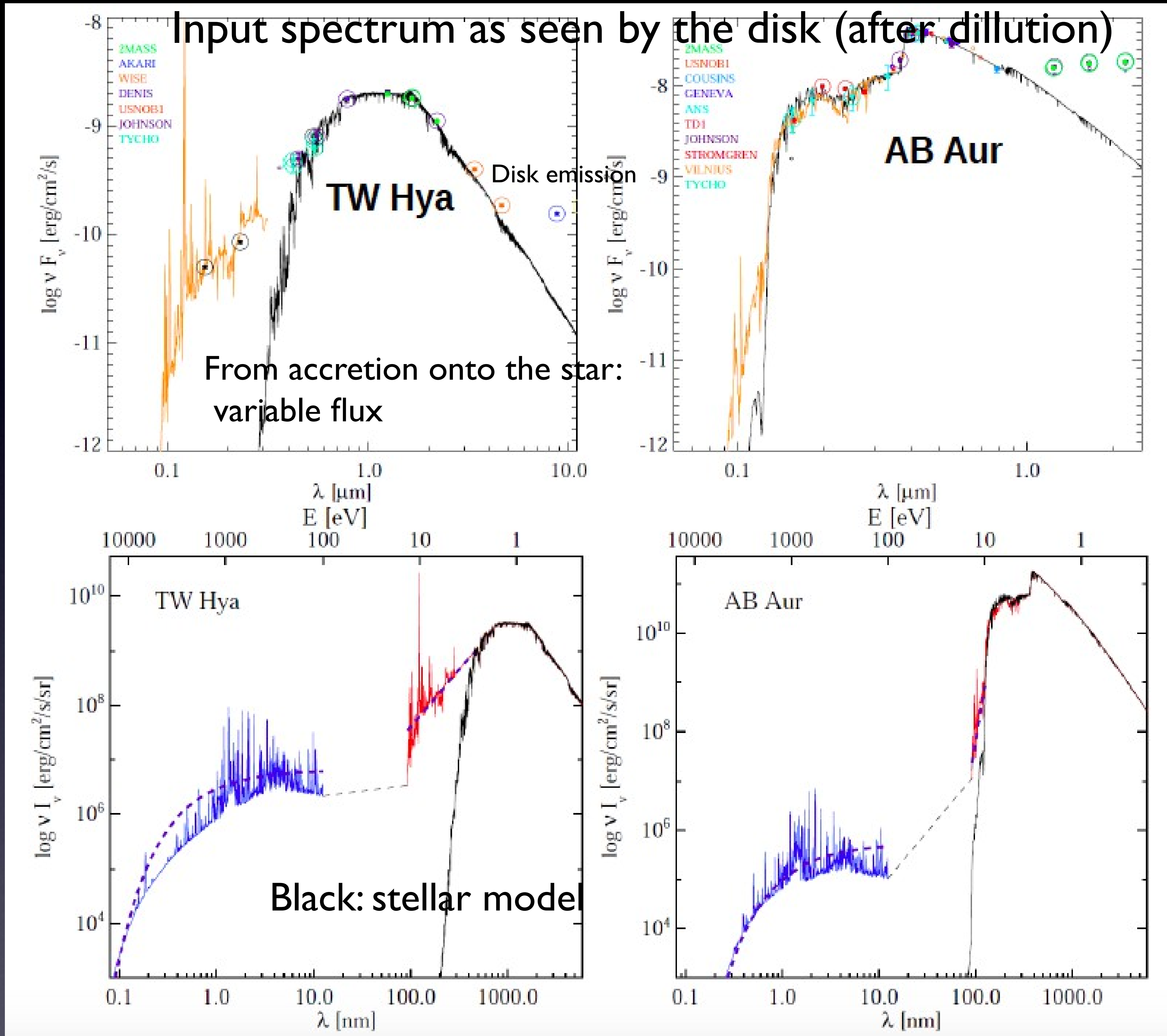


Figure courtesy Inga Kamp

ProDiMo: Woitke, Kamp, Thi, Aresu, Meijeirnk, Spaans

MCFOST: Pinte, Ménard, Duchêne

Input spectrum as seen by the disk (after dillution)



Modelling the gas in discs with ProDiMo

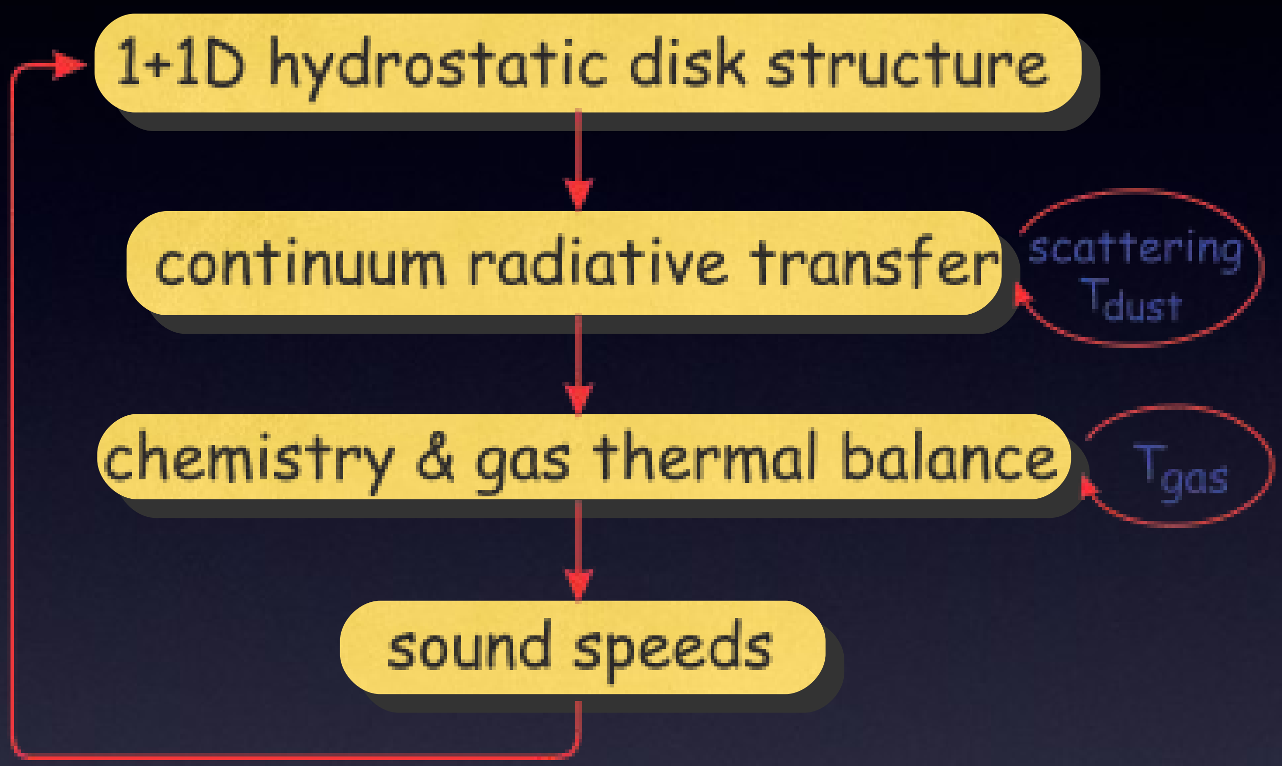
1. 2D dust radiative transfer: grain thermal balance

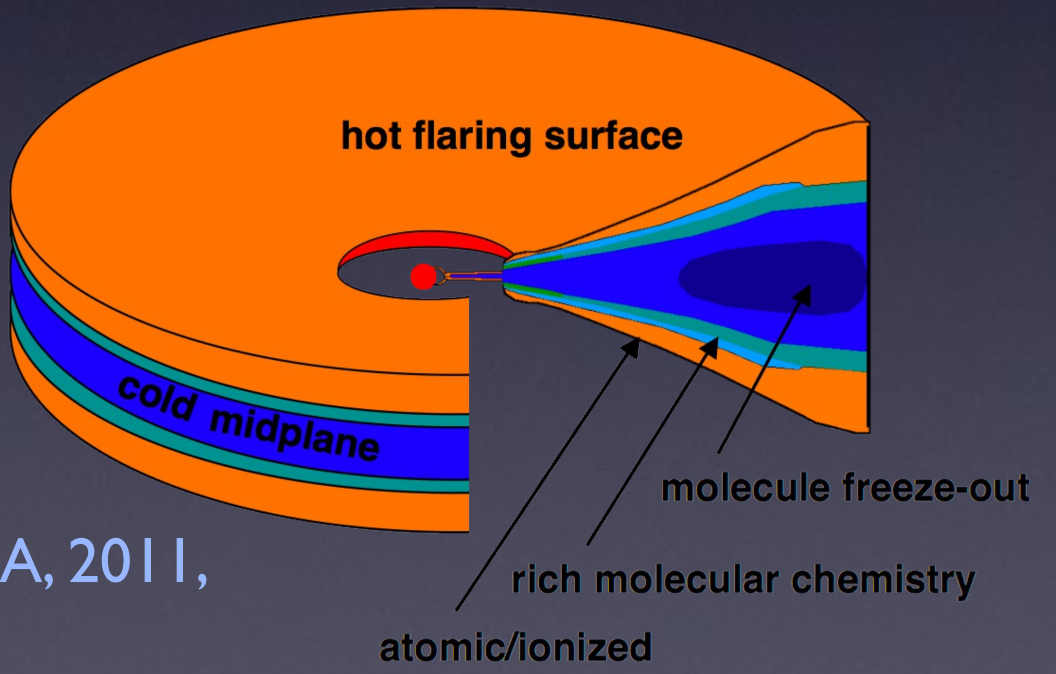
• 1+1D for the gas cooling using escape probability (checked against 3D Monte-Carlo): atomic and ro-vibrational cooling lines

2. Over 71 gas and solid species (including deuteratred species) steady-state+time-dependent. Xray and UV chemistry

• Hydrostatic equilibirum

3. Entire disc is modellized



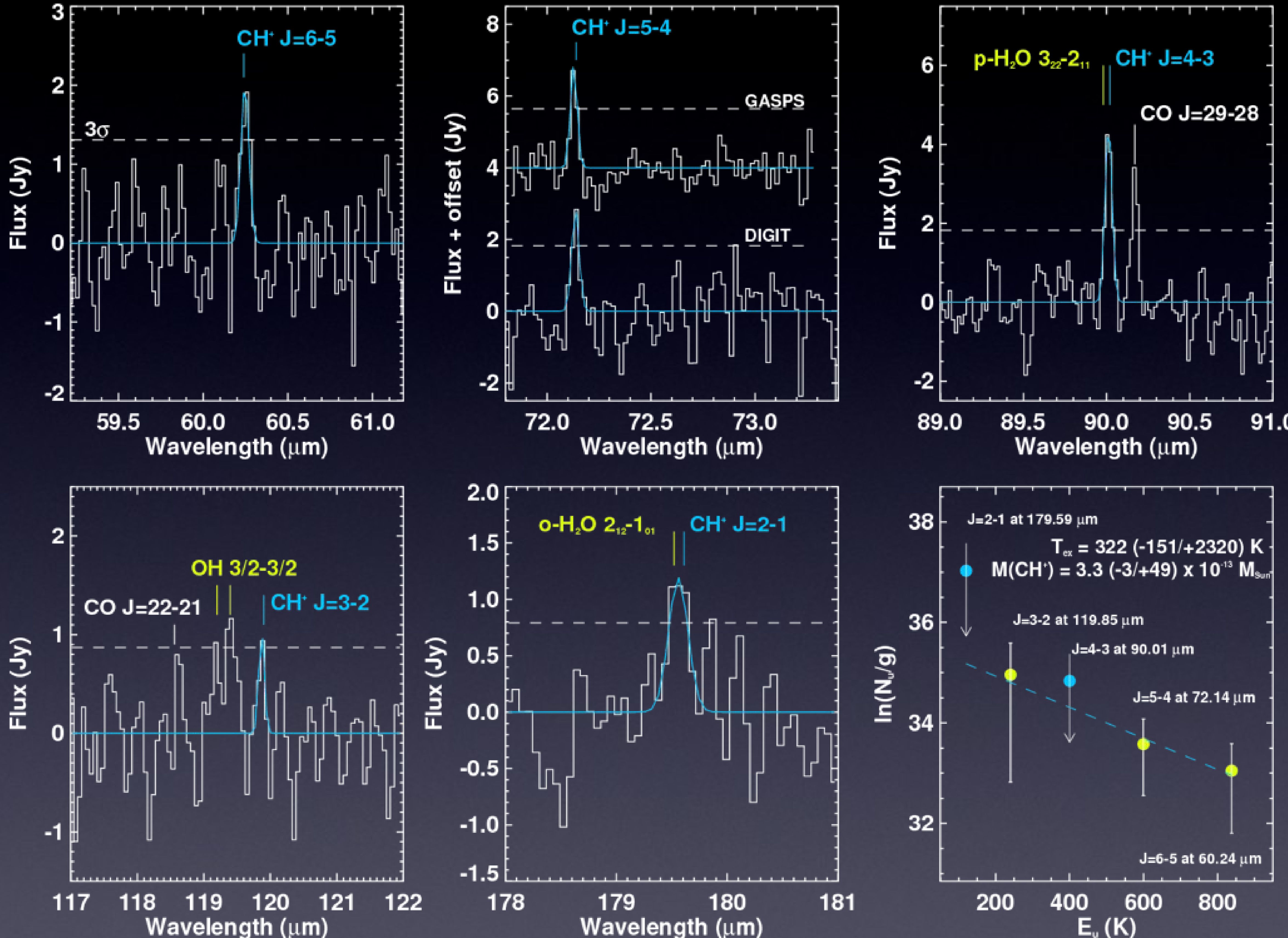


Woitke et al. 2009a, 2009b; Kamp et al. 2009; Thi et al. 2010A, 2011, Aresuetla. 2011, 2014, , Meijeink et al. 2012, 2013

Photochemical and photoexcitation effects on the gas-phase chemistry in disks

- Inner disk gas-phase chemistry: hot gas?, state-to-state reactions? Reactions with UV-excited H_2? Chemical effects of differencial photodissociation?
  - Detection of warm HCN, C_2H_2 with Spitzer (Najita+; Pascucci+; ...)
  - Detection and modelling of CH^+ in a protoplanetary disks: the role of excited H_2
  - Differential H_2/HD photodissociation as a cause of enhanced HDO/H_2O in hot gas
  - Pumping [OI] optical lines through photodissociation of OH (and H_2O?)
  - CO rovibrational levels pumping of UV (see Inga Kamp's talk)

CH^+ in HD100546: Herschel-PACS



Thi et al. 201, Fedele et al. 2013 continuum subtracted archival data (Sturm et al. 2010 A&A 518 L129)

CH^+ chemistry

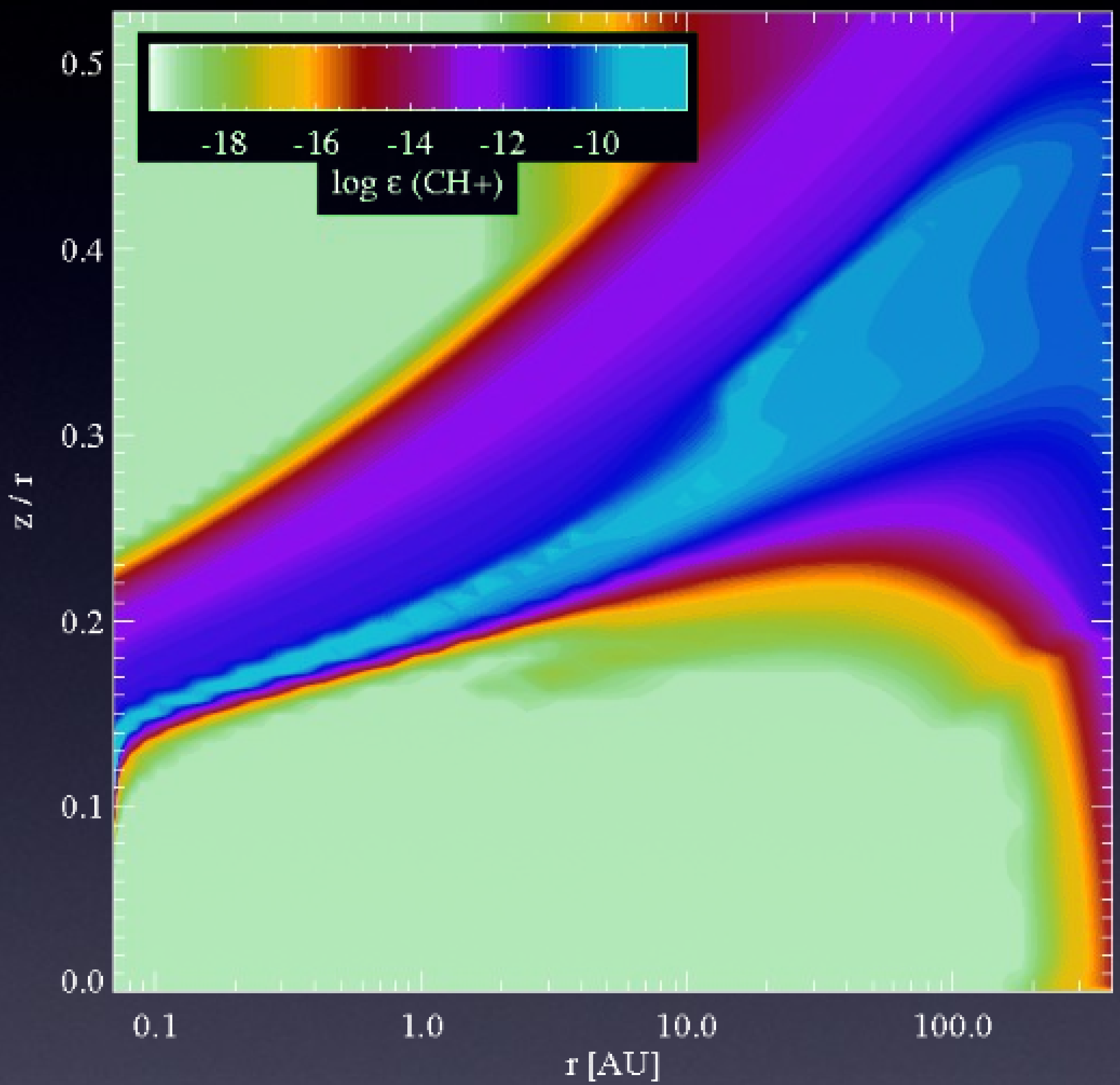
- $C^+ + H_2$ (v=0) → $CH^+ + H$ (activation barrier 0.4eV or 4600K), Hierl et al. 1997 J. Chem Phys 106, 10145
- $C^+ + H_2$(v>0) → $CH^+ + H$ (no barrier) Hierl et al. 1997; see also Agundez et al. 2010 ApJ 713, 662 (H_2^* = H_2(v>0))
- $C^+ + H_2$ radiative association rate is vey small (Barinovs & van Hemert 2006 ApJ 636, 923)
- $CH^+ + H_2$ → $CH_2^+ + H$ (CH^+ is very reactive)
- CH^+ + e- → C + H (electron recombination)
- CH^+ + UV → C^+ + H (rate calculated using cross-section and stellar+accretion UV)
- + other rates from UDFA: www.udfa.net

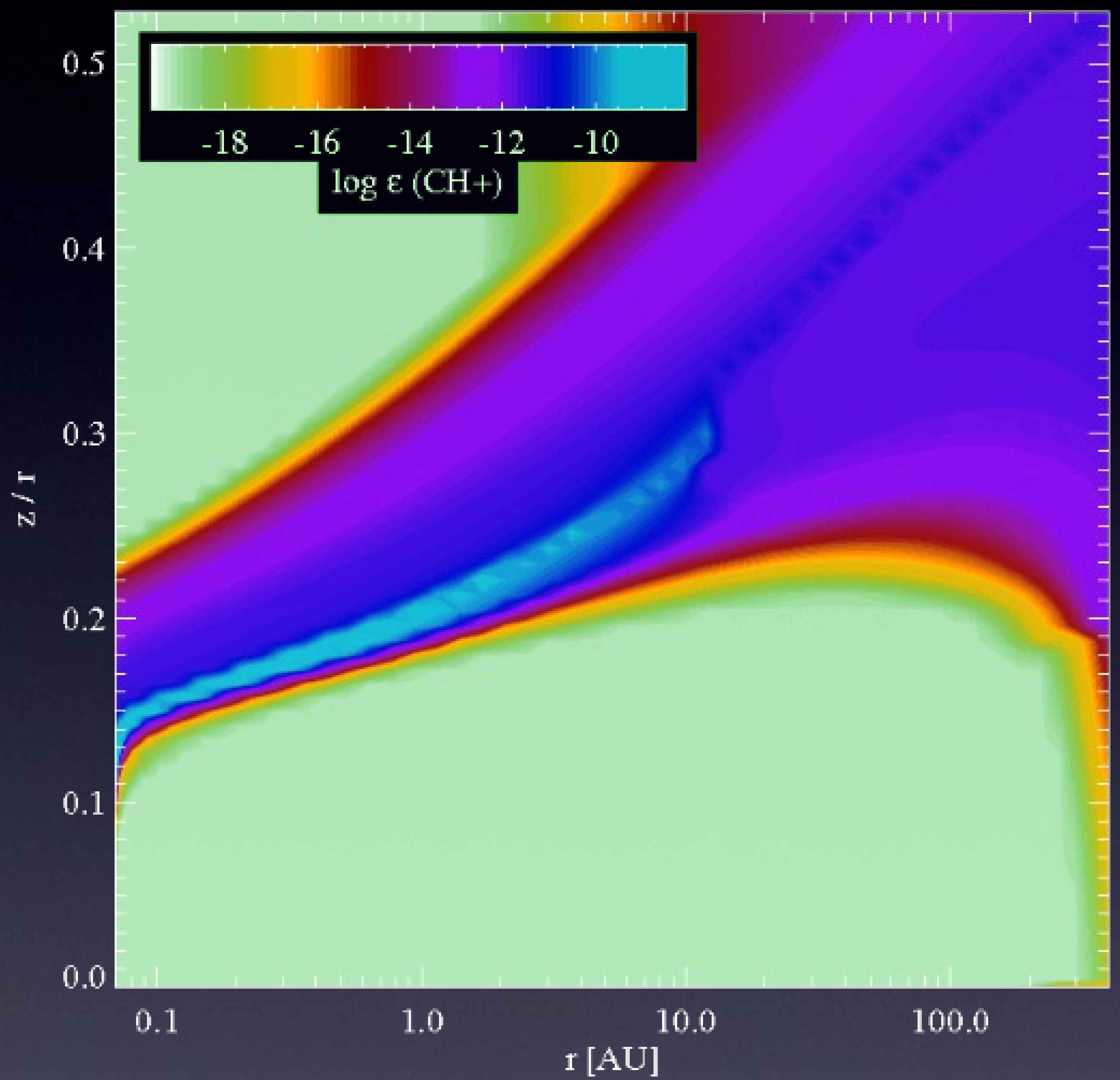
How to overcome the activation barrier?

- UV-pumped excited H_2 (e.g., Agundez et al. 2010)
- Shock heated gas (Draine & Katz 1986) but no velocity shifts detected between species as expected (Gredel 1997). However recent WISE images show shocked gas structures
- Turbulence heated gas (e.g., Godard et al. 2009) for the ISM gas or acccretion heating for the inner disk midplane.
- Photoelectric heated hot gas: possible for protoplanetary discs and enveloppe around massive young stellar objects (Benz et al. 2010, Bruderer et al. 2010a,b)
- (hot)-electrons excitation to electronic levels followed by decays to high-v levels (Cosmic-Rays, stellar wind, X-ray interaction with the gas)

WISE image towards Zeta Oph

Standard TTauri disk model



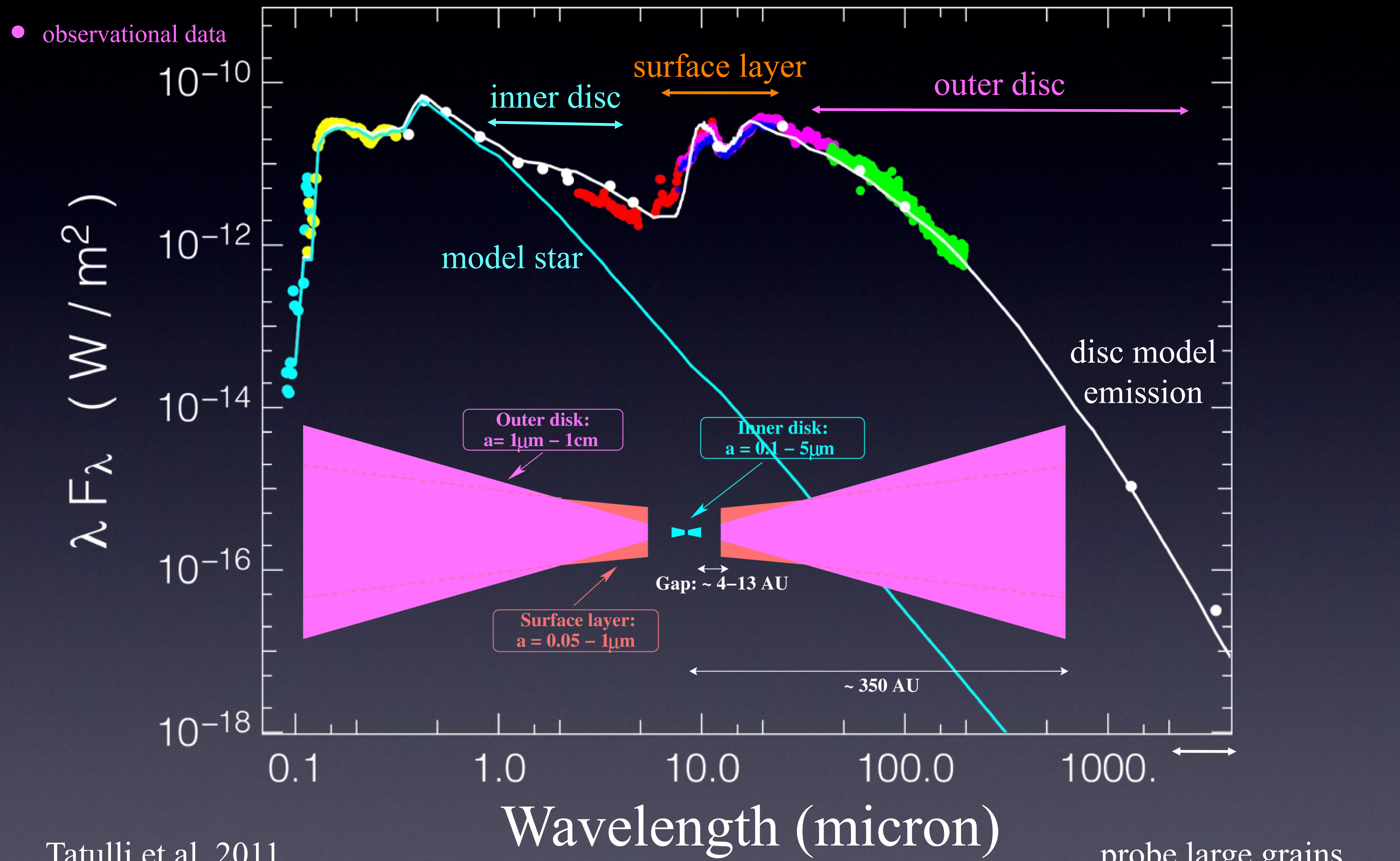


With excited H2

Without

Bouma & Kamp

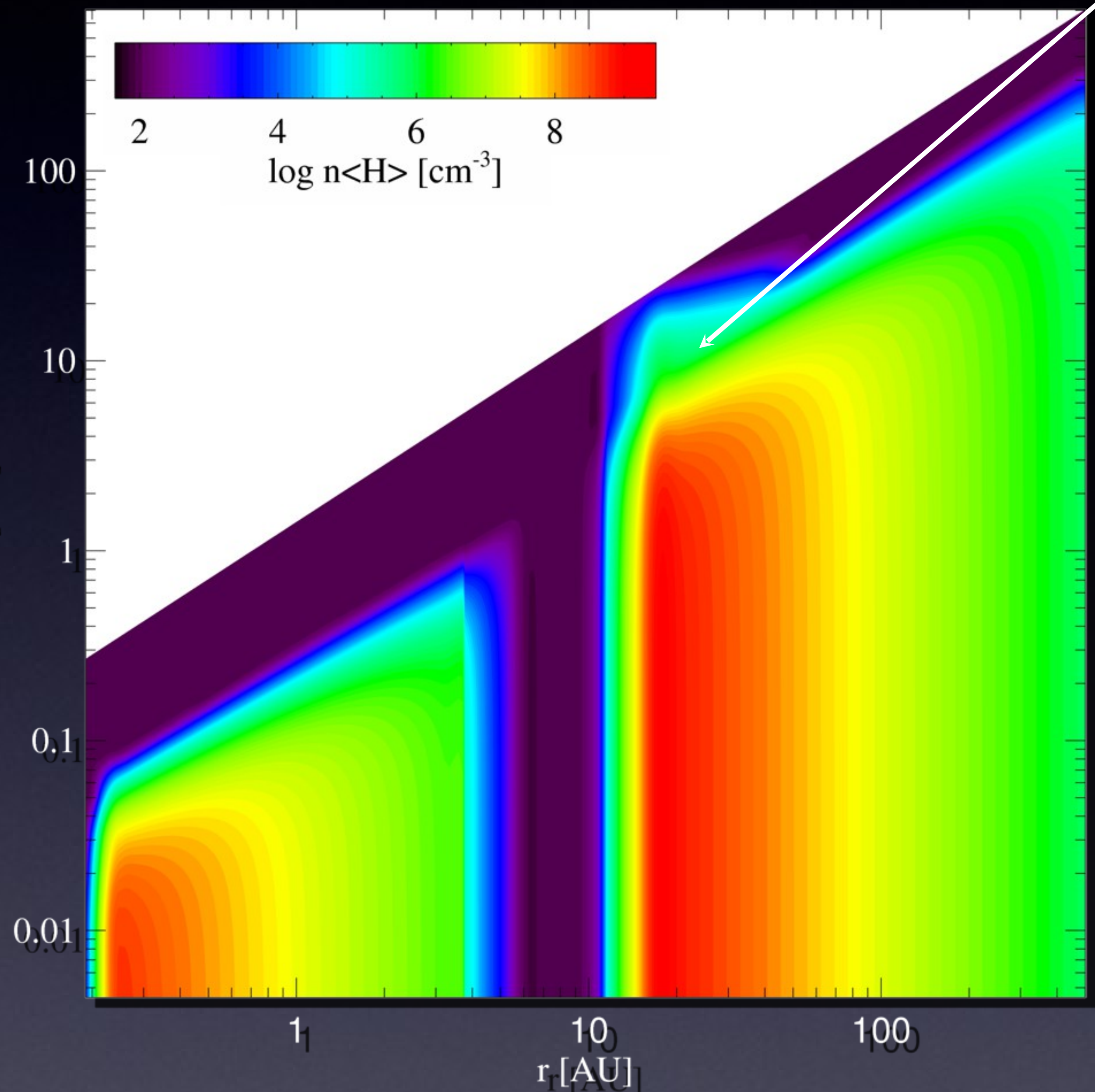
HD100546 SED fitting with 3D Monte-Carlo code MCFOST



Tatulli et al. 2011

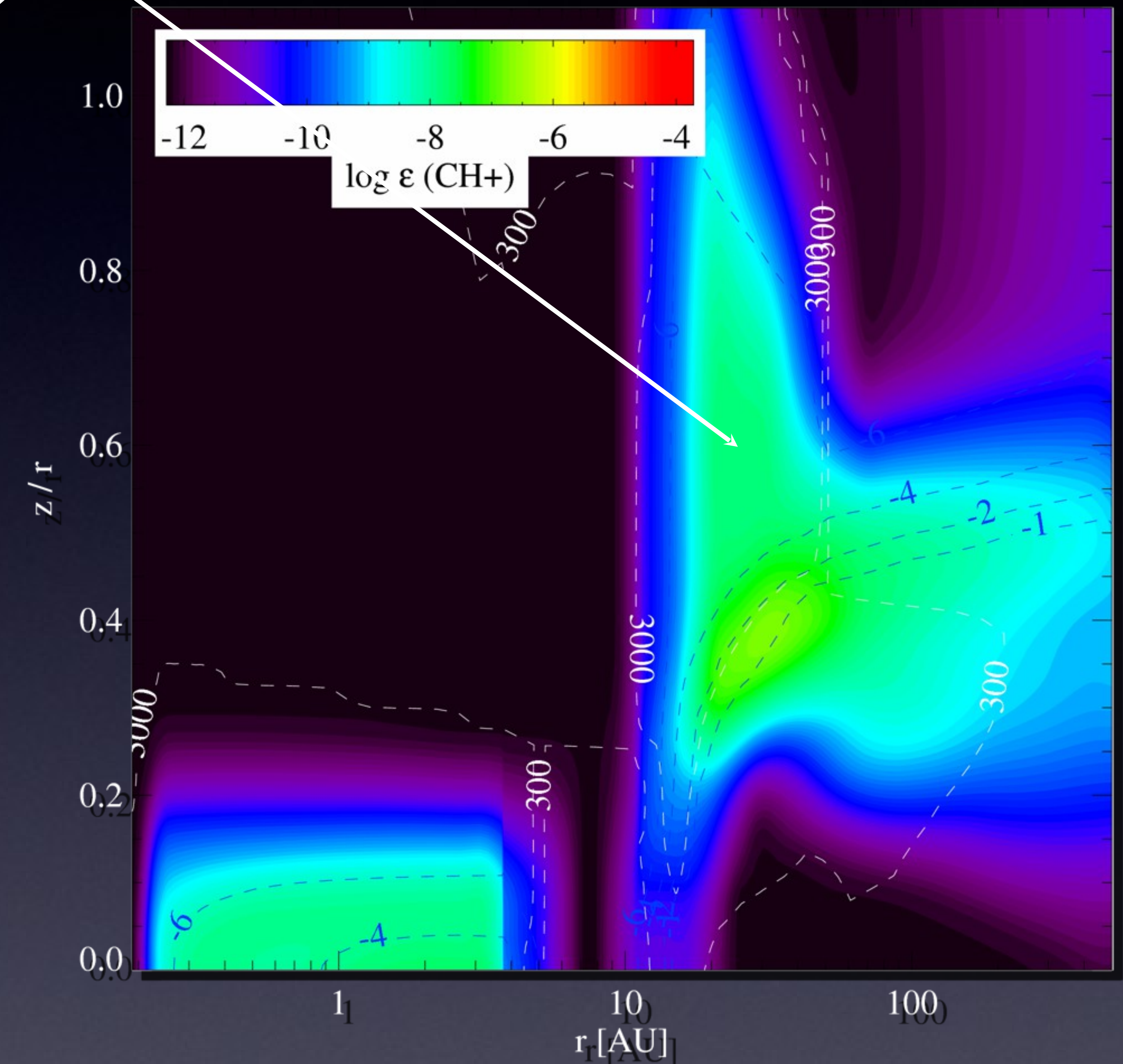
CH^+ is located at the rim HD100546
model with excited H2

outer disc rim



inner disc

outer disc

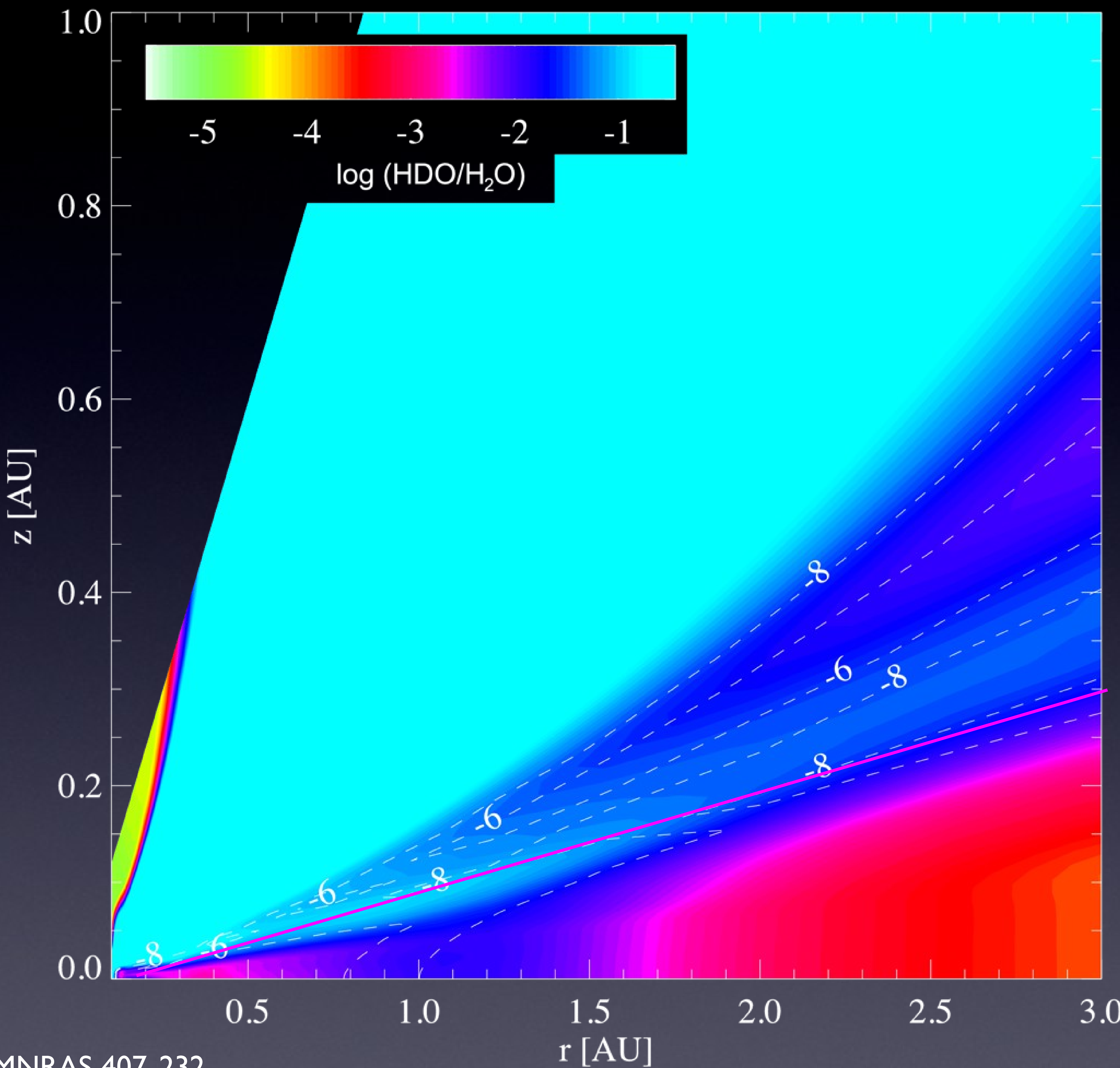


Water deuterium enrichment at high gas temperature in photodissociation regions

- H2 self-shielding implies that [D]/[H]>>[HD]/[H_2] in photodominated regions
- UV-excited H_2 promotes the (neutral-neutral) reactions $H_2^* + O \rightarrow OH + H$
- The exchange $D + OH \rightarrow OD + H$ is favored
- $H_2^* + OH \rightarrow H_2O$ and $H_2^* + OD \rightarrow HDO$: in photodominated regions [HDO]/[H_2O] is enhanced even at T=100-500 K

How to deal with all the neutral – H_2^* reactions with activation barriers? (Kamp+ 2015)

Thi et al. 2010 MNRAS 407, 232

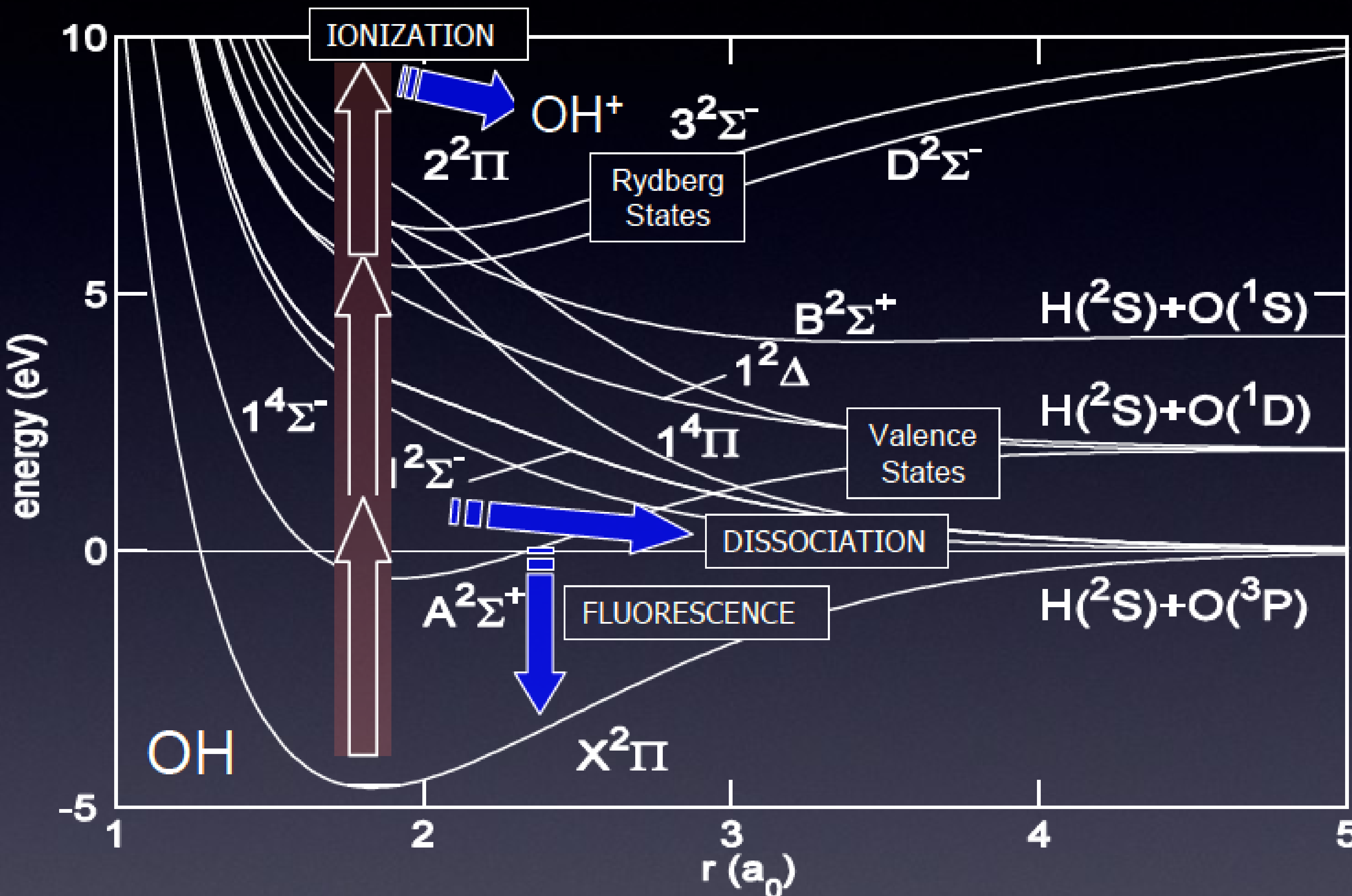


Thi et al. 2010 MNRAS 407, 232

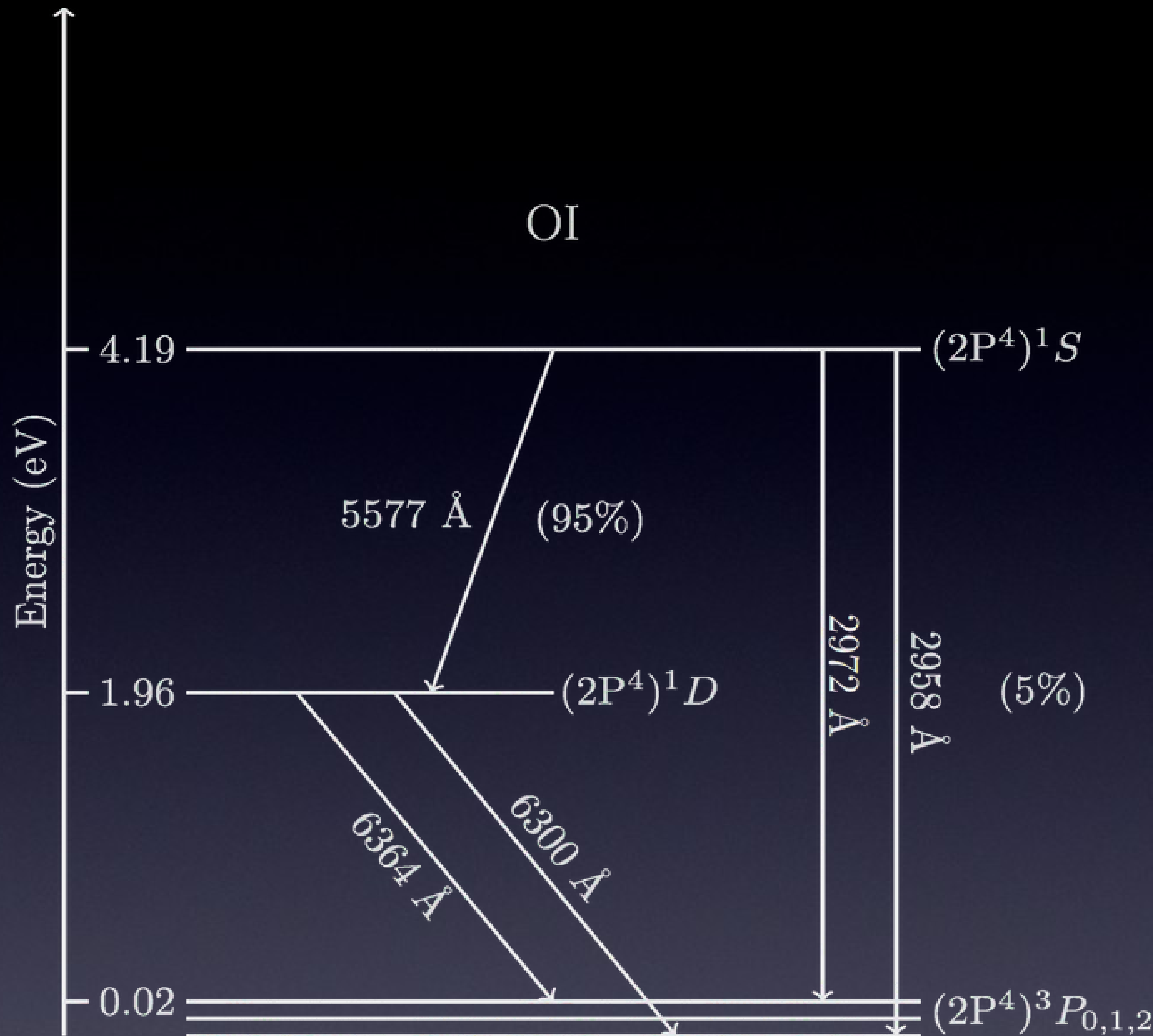
Modelling [OI]6300A line in disks

- [OI] optical line flux is too strong to be reproduced by thermally-excited atoms (B. Acke+; van der Plas+; Fedele+)
- O(^{1}D) can be fomed as the photodissocation product of OH (van Dishoeck+ 1983, 1984). Disk models by Gorti+2011; Rigliaco+ 2013
- Another possibilities are UV fluorescence or photodissociation of H_2O onto O(^{1}D) : branching ratio 10% at 1216A
- The excitation model of OI has to incorporate all the electronic levels (maximum UV energy of 13.6 eV) and electron collision rates
- The branching ratio between O(^{1}D) and O(^{1}P) has been computed (vD 1983, 1984; Storzer 2000; Zhou 2003)
- Chemical-pumping has to be included in the population model
- Detailed continuum and line UV-transfer has to be performed

Vincente+, in prep.



After Van der Loo & Groenenboom



Bhardwaj and Raghuram 2012 ApJ 748, 13 (Cometary [OI] emission model)

Conclusions

Photodissociation plays an important role in the disk surface chemistry (HDO. CH+, excitation of OI optical lines, $^{16}O/^{17}O/^{18}O$).

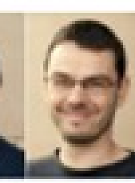
Photodissociaton cross-sections are needed in combination with

- Detailed treatment of the continuum and line (UV) radiative transfer
- Collision rates (to electronic levels) with electrons are required
- State-to-state chemistry
- UV levels to account for UV pumping

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 JCMT, eMERLIN astrobiology	obs./mod. XMM, Herschel high energy	mod./obs. VLT, JWST dust mod.	obs./mod. HST, Herschel interferometry	mod./obs. Herschel, JWST 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