Science and Technology Facilities Council

UNIVERSITY OF LEEDS

ASTROCHEMISTRY

FROM THE BIG BANG TO LIFE

Global Astrochemistry Lecture Series (GALS) 2024

PHYSICAL AND CHEMICAL PROCESSES IN PROTOPLANETARY DISKS

Catherine Walsh. *University of Leeds, UK*

07.03.2024 | 15:00 - 17:00 CET

cost EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

NanoSpace

Funded by the European Union

Outline of lectures

- Lecture 1: observations of dust in protoplanetary disks
  - Dust physics and evolution
  - Spectral energy distributions
  - Observations at
    - optical to infra-red wavelengths
    - mid-infrared wavelengths
    - (sub)mm to cm wavelengths
  - Hunting for protoplanets

- Lecture 2 : observations of gas and chemistry in protoplanetary disks
  - The chemical anatomy of a protoplanetary disk
  - Astrochemistry
  - ALMA observations of molecular emission from disks
  - Observing chemistry at high spectral and spatial resolution
  - The chemistry of planet formation

Our origins

What are the initial conditions of planet formation?
How do planets form?
What are our origins?



the protostellar disk

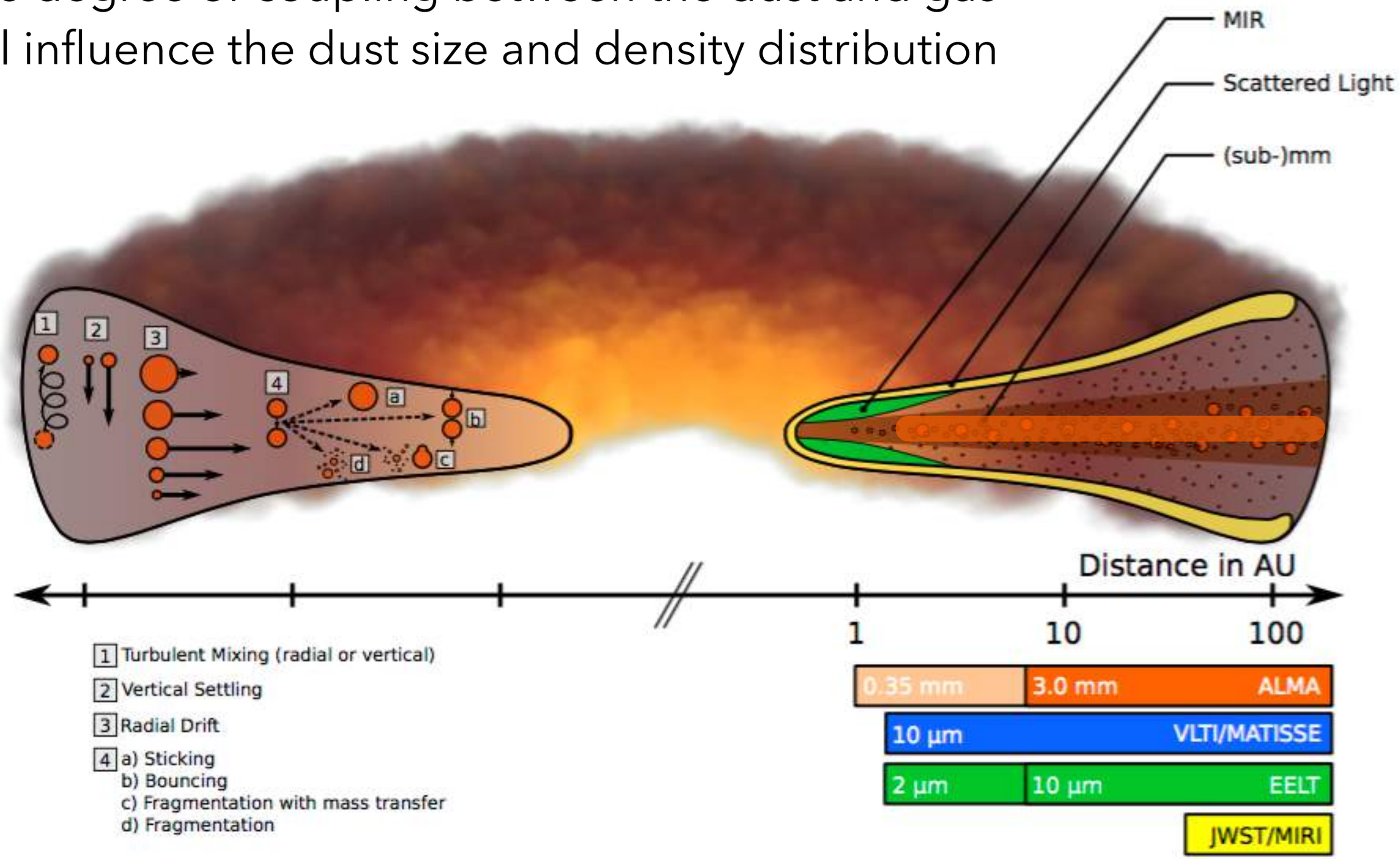


the protoplanetary disk

Credit: B. Saxton (NRAO/AUI/NSF)

Dust structure and physics in protoplanetary disks

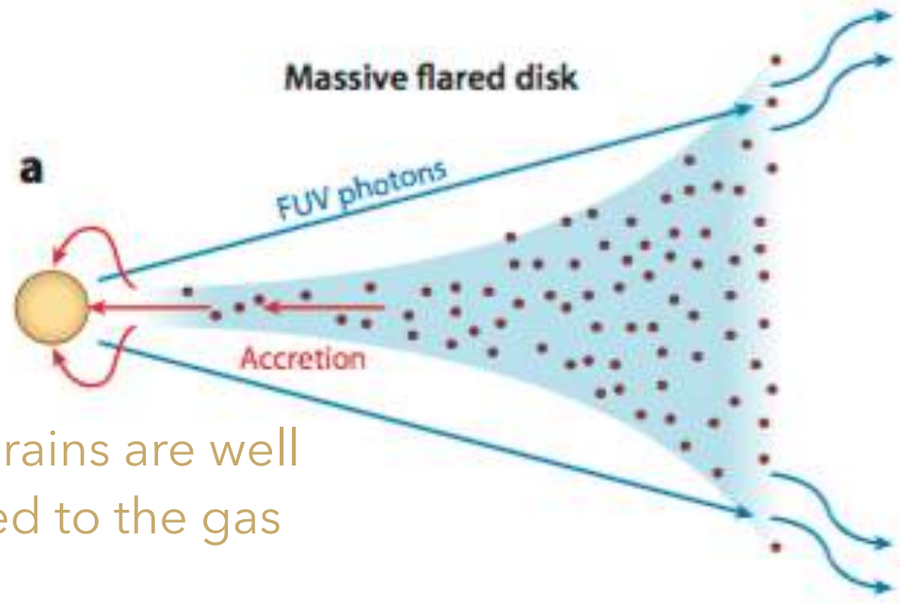
The degree of coupling between the dust and gas will influence the dust size and density distribution



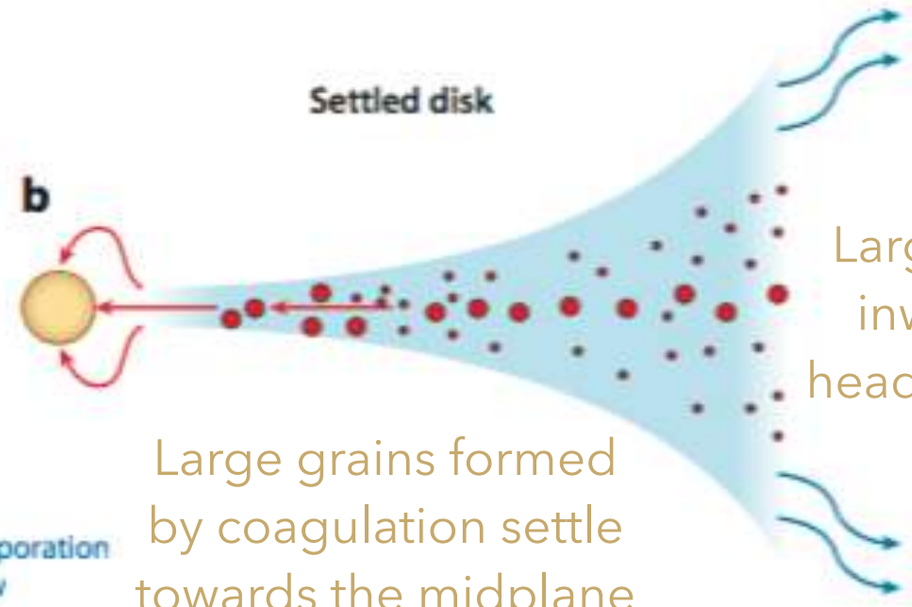
Testi, L., et al. 2014, PPVI, 339

Dust structure and physics in protoplanetary disks

Generalised picture of dust evolution in protoplanetary disks



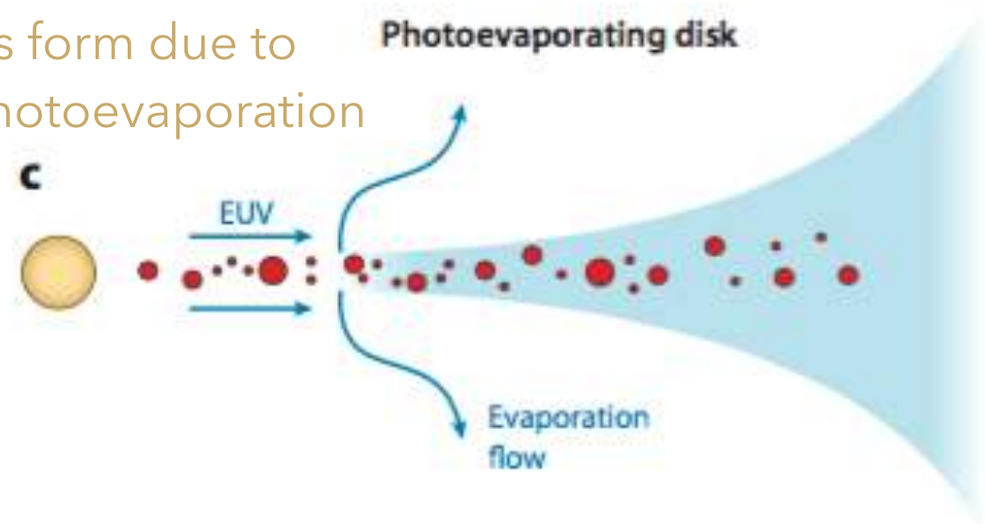
Small grains are well coupled to the gas



Large grains drift inwards due to headwind from gas

Large grains formed by coagulation settle towards the midplane

Cavities form due to planets/photoevaporation





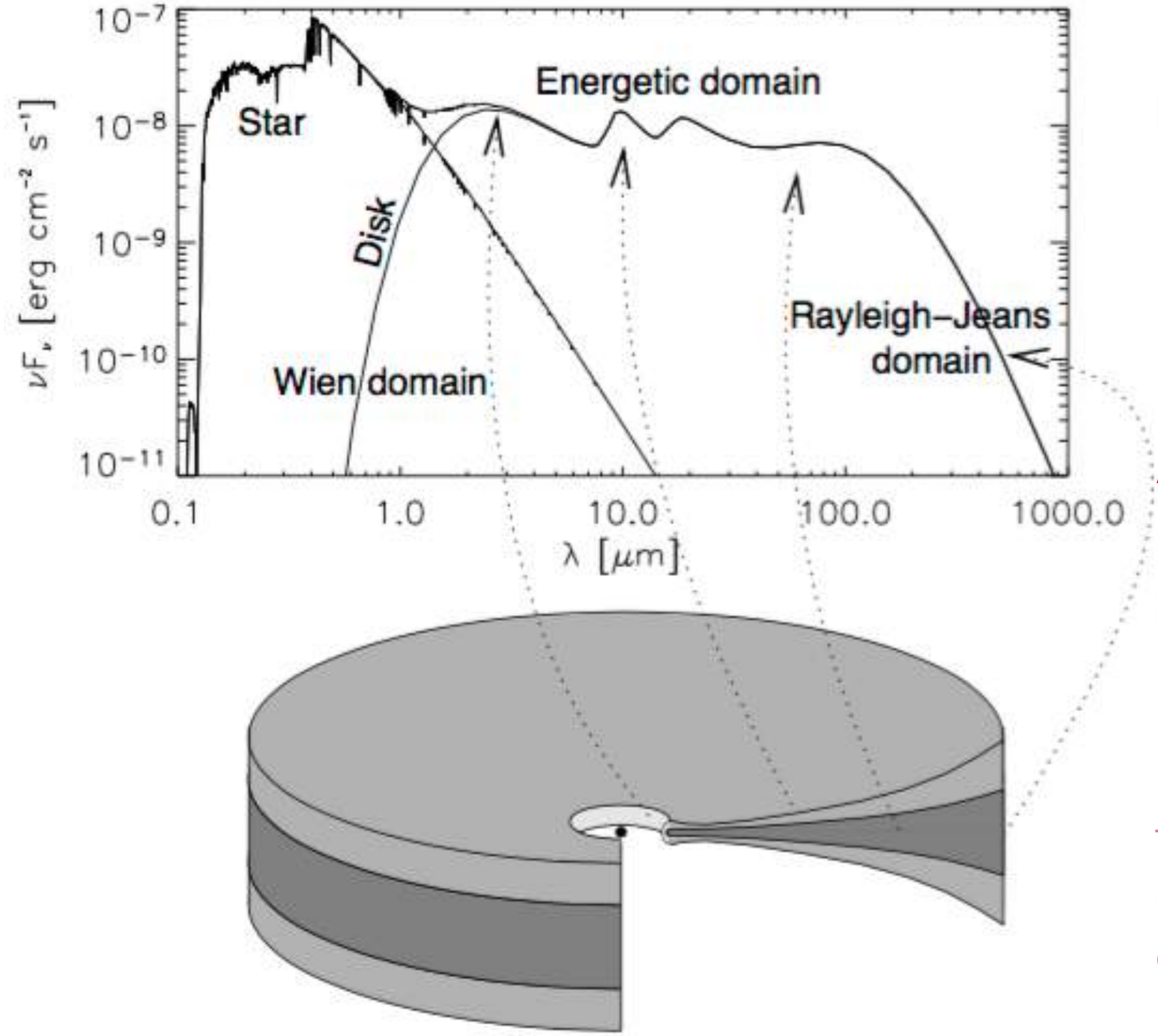
Eventually dust is incorporated into larger bodies or expelled in photoevaporative flow

Small (~ micron-sized) and large (mm-sized) grains follow different paths

Williams & Cieza 2011, ARA&A, 49, 67

Spectral energy distribution (SED)

Early detections of disks were made from SEDs



- Optical wavelengths: scattered light; hence no temperature/density information

- Near-infrared wavelengths: originates mainly from "hot" inner rim

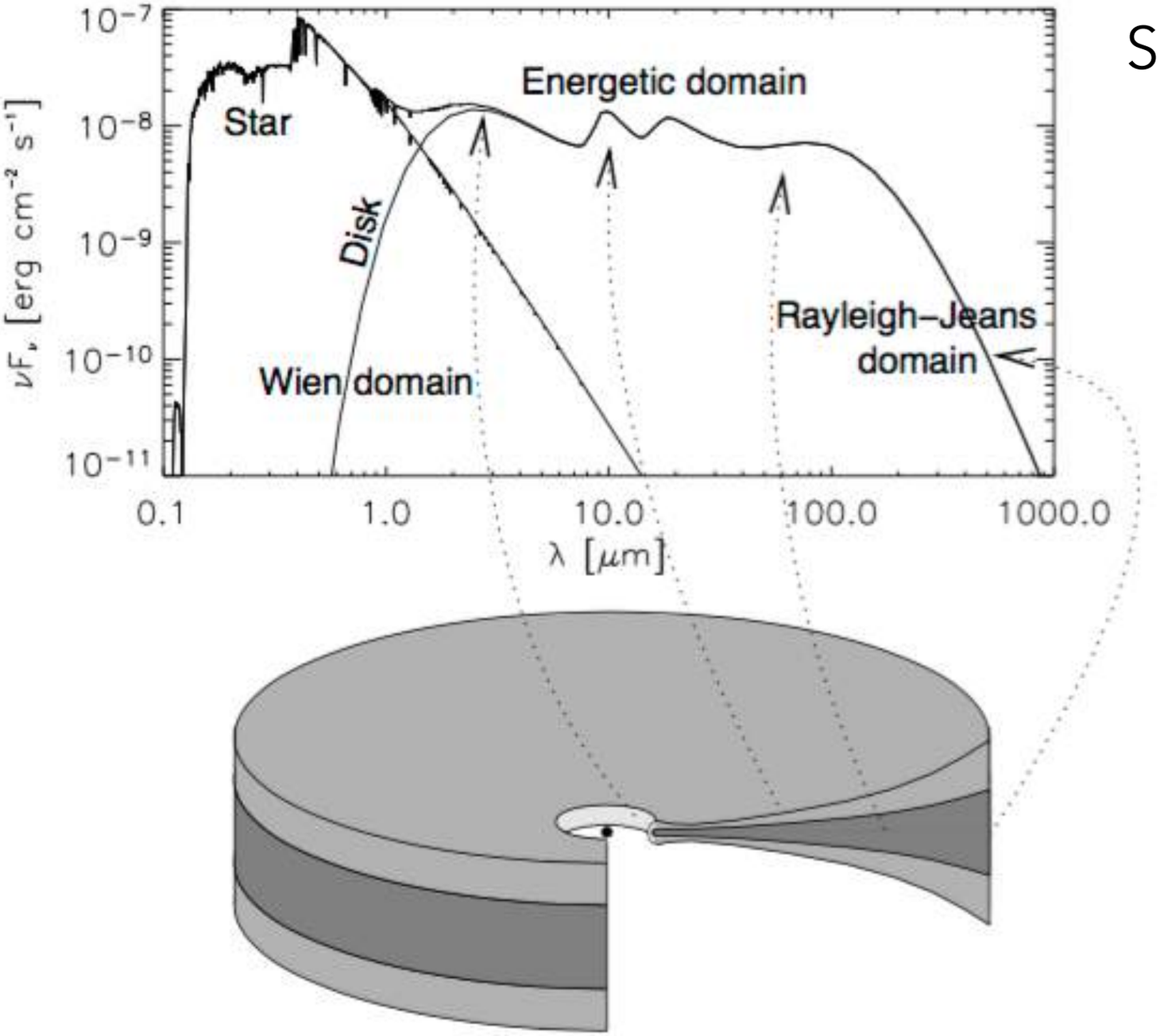
- Mid-infrared wavelengths: originates from "warm" dust close to the star (< 10 au) and is typically optically thick; hence, no density information but probes temperature of dust photosphere

- Sub-mm/mm wavelengths: originates from "cold" dust in outer disk (> 10 au) and is typically optically thin; hence, provides density information

Beckwith et al. 1990, AJ, 99, 924; Williams & Cieza 2011, ARA&A, 49, 67

Spectral energy distribution (SED)

Early detections of disks were made from SEDs



Simple assumptions can yield a dust mass from spatially unresolved observations

Optical depth

$$\tau_\nu = \int \rho \kappa_\nu \, ds = \kappa_\nu \Sigma$$

Mass opacity

$$\kappa_\nu \propto \nu^\beta$$

Dust mass

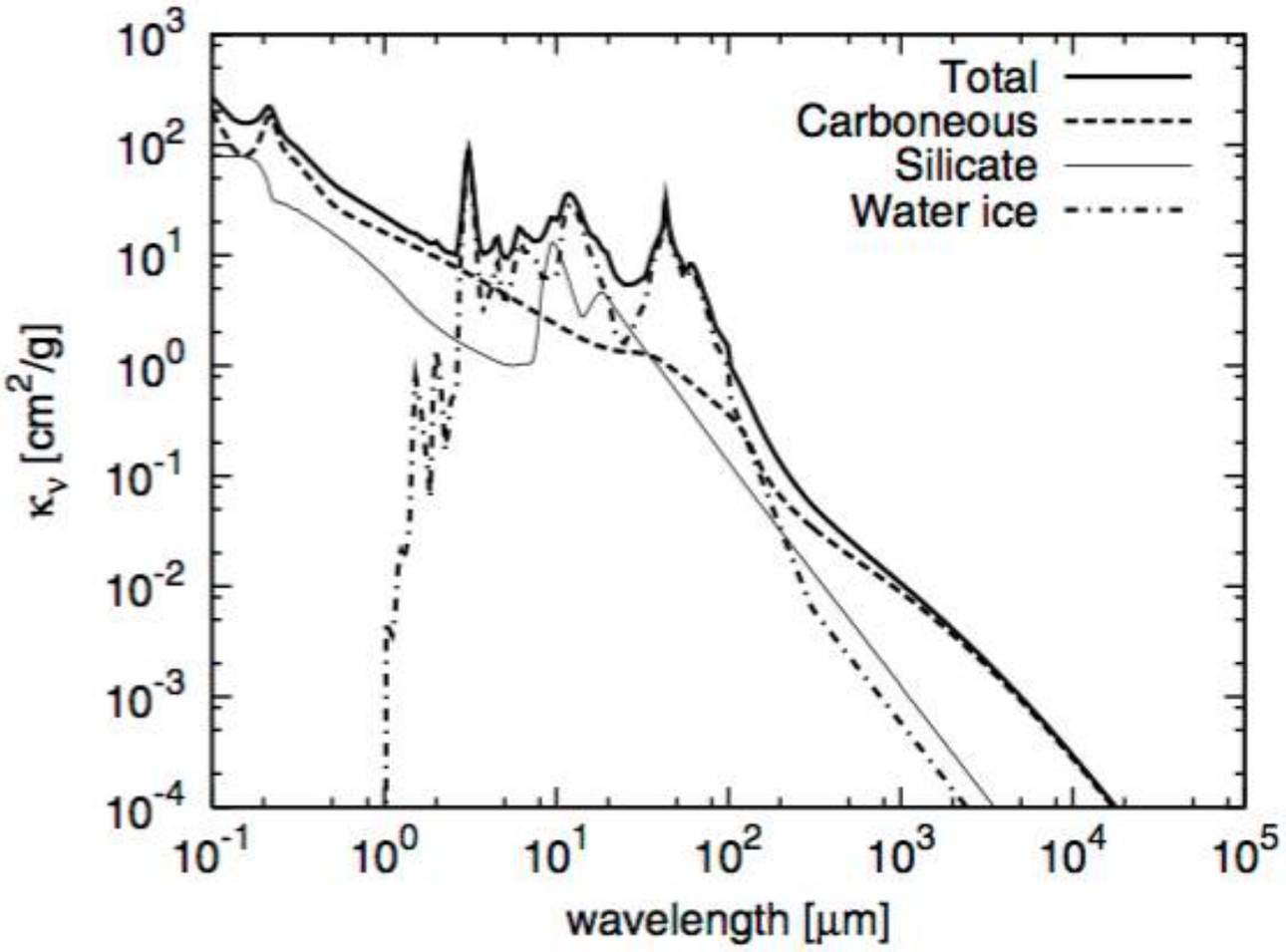
$$M_{\rm dust} \approx \frac{F_\nu d^2}{\kappa_\nu B_\nu(T)}$$

Beckwith et al. 1990, AJ, 99, 924; Andrews & Williams 2005, ApJ, 631, 1134; Williams & Cieza 2011, ARA&A, 49, 67

Observations of dusty protoplanetary disks at optical to infra-red wavelengths

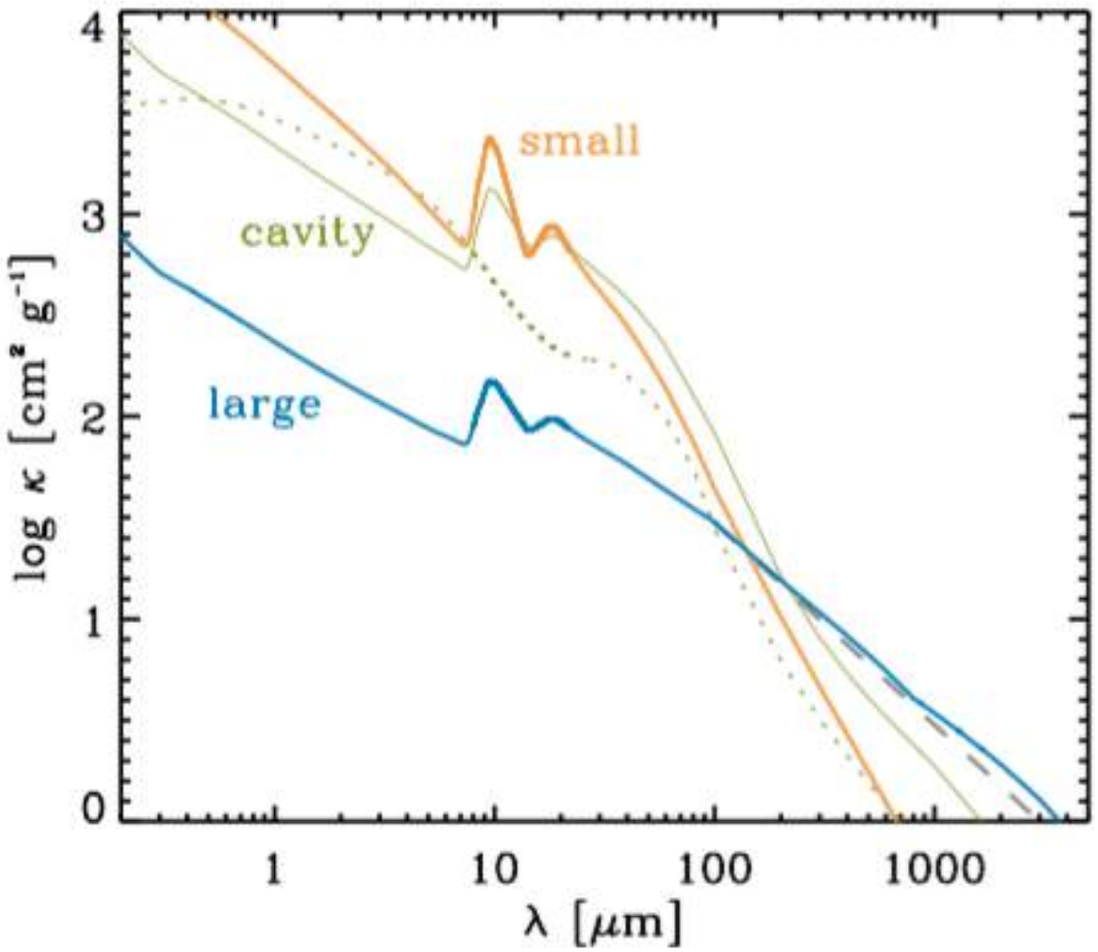
Dust opacity

The composition and size and density distribution of the dust grains controls how light propagates through and is scattered from the disk



Single MRN size distribution

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

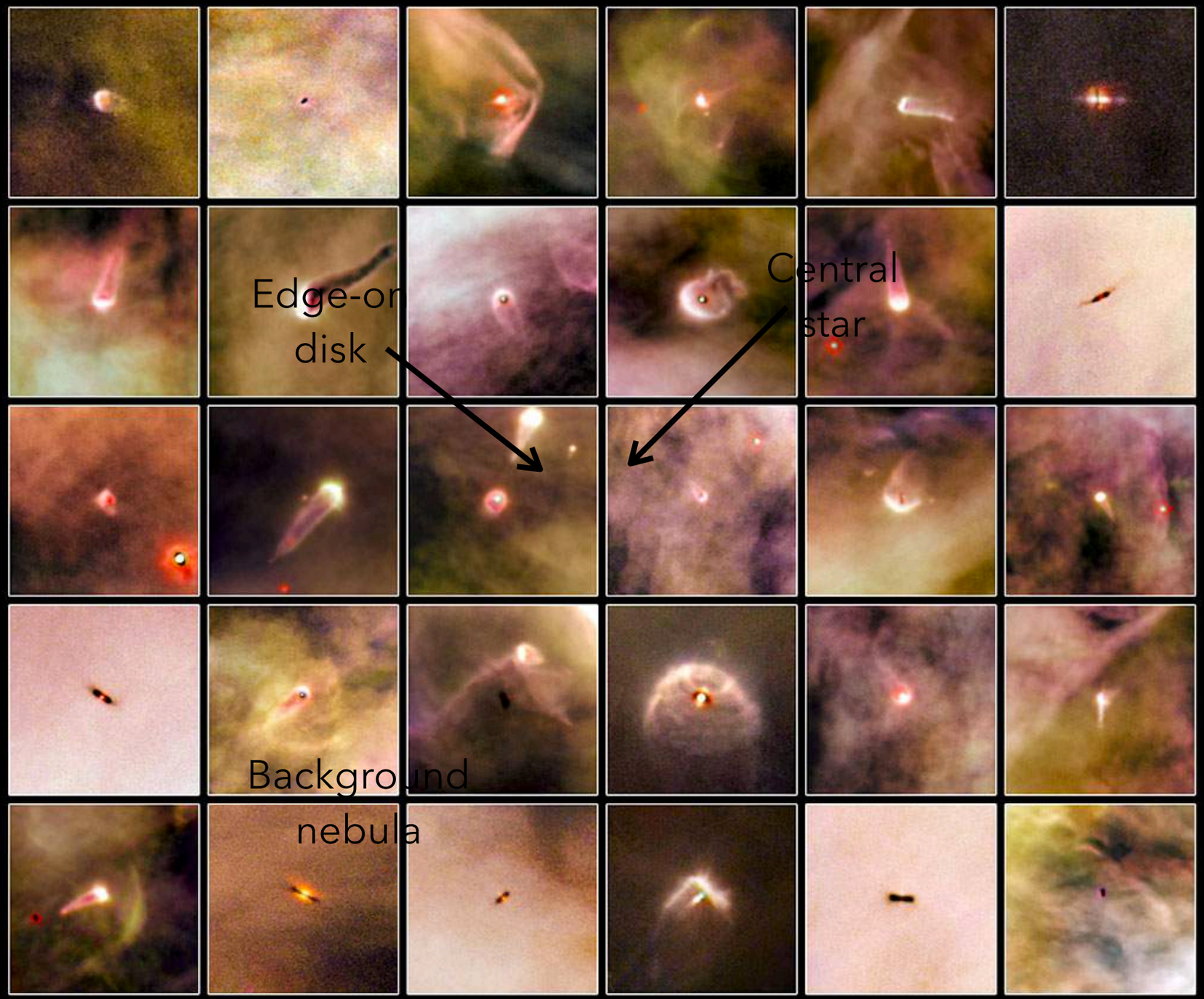


Two MRN-like populations

"Small" (micron) & "Large" (mm)

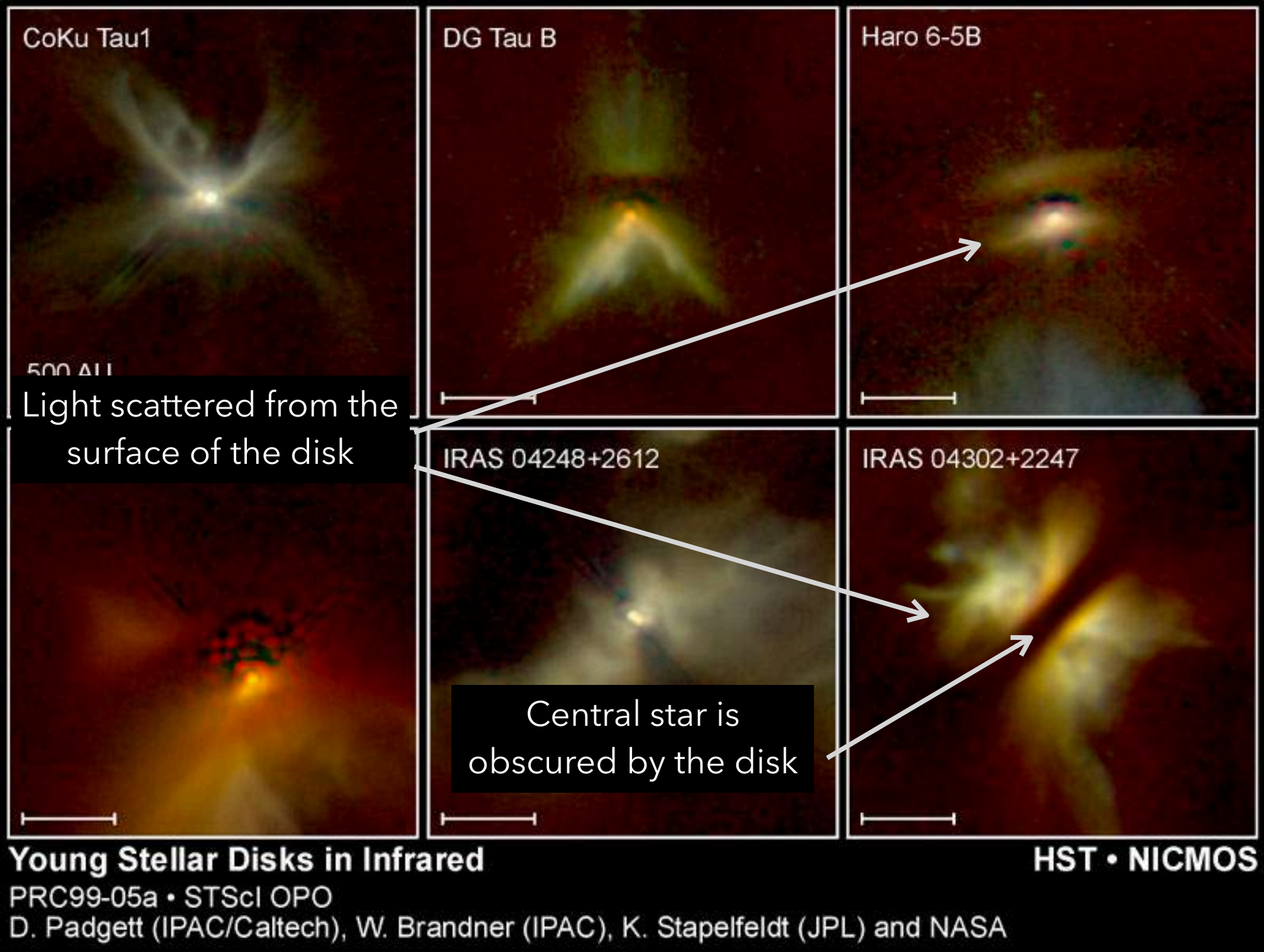
Nomura, H. & Millar, T. J., 2005, A&A, 438, 923; Andrews S. M., et al. 2011, ApJ, 732

Protoplanetary disks in silhouette in Orion with HST/WFC



O'dell, et al. 1993, ApJ, 410. 696; O'dell & Wen 1994, ApJ, 436, 194; https://www.spacetelescope.org/images/heic0917bb/; Credit: NASA, ESA , L. Ricci (ESO)

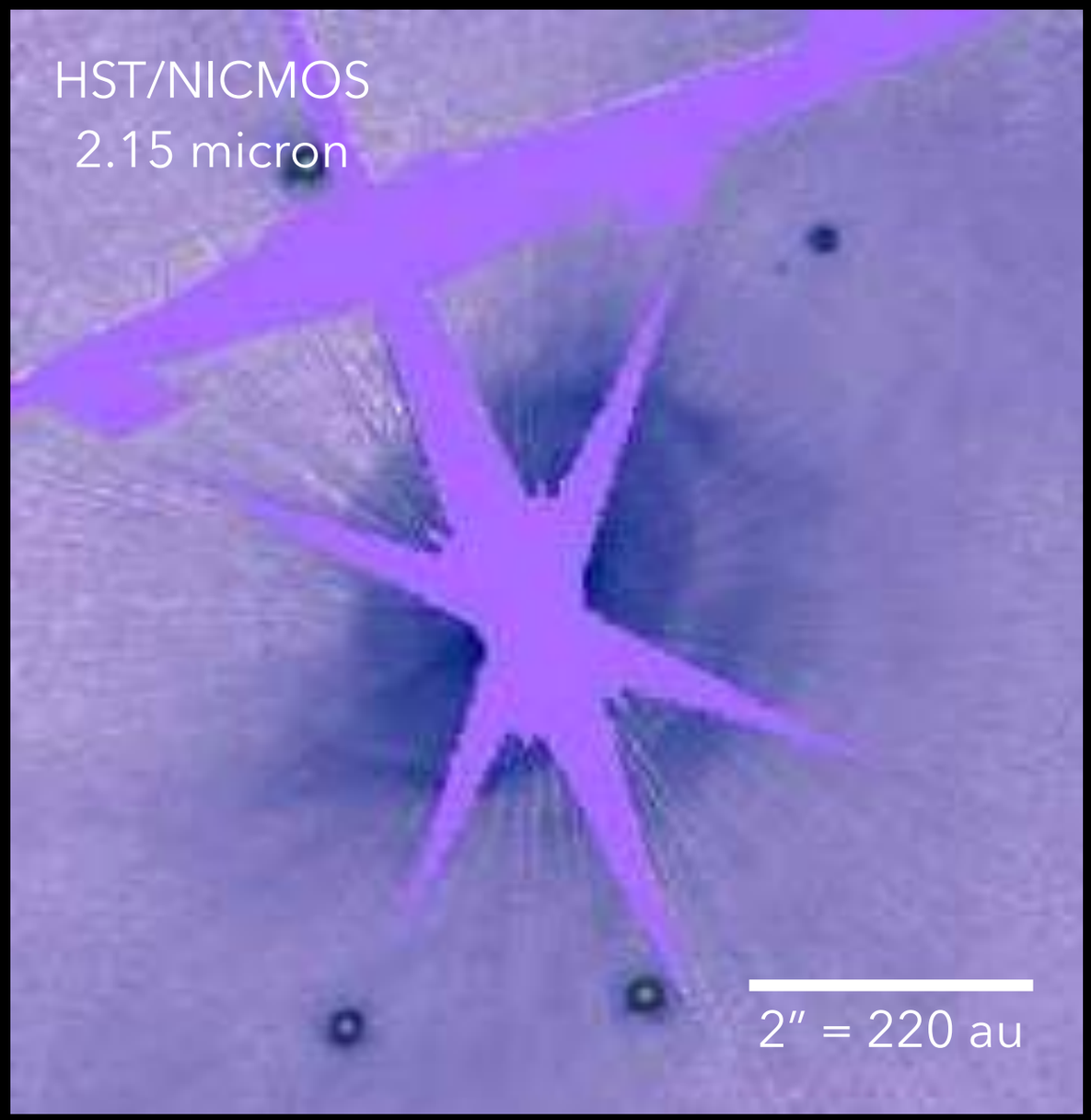
Protoplanetary disks in scattered light in Taurus with HST/NICMOS



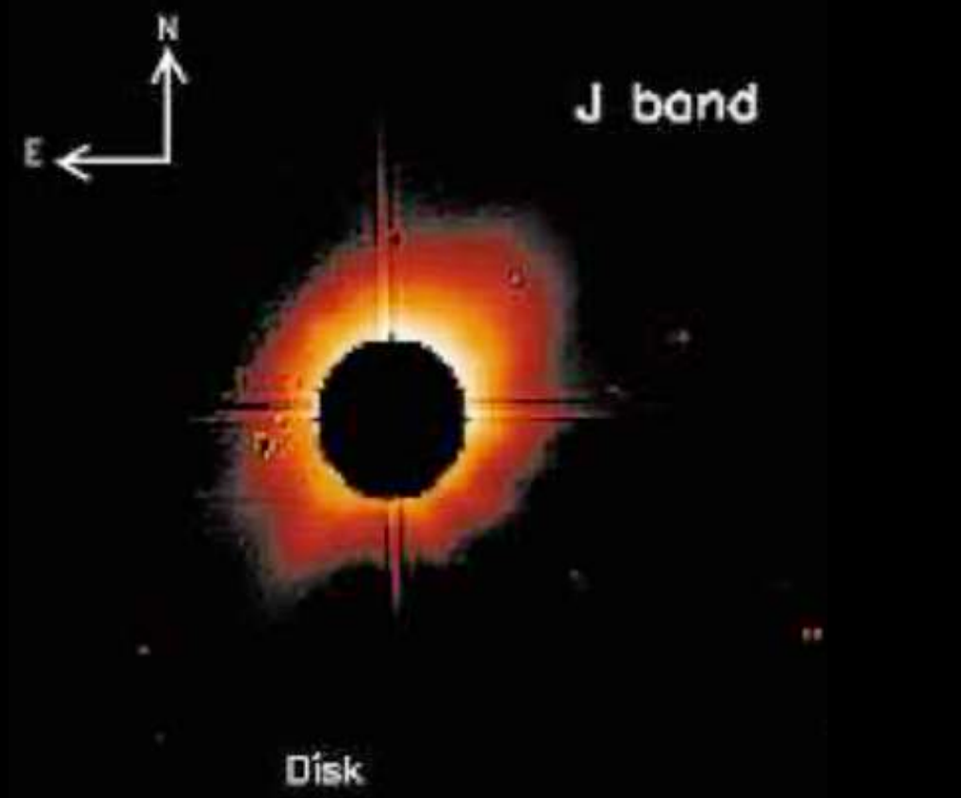
Padgett et al. 1999, AJ, 117, 1490

Coronography reveals extended disks in scattered light

Observations of the disk around HD 100546

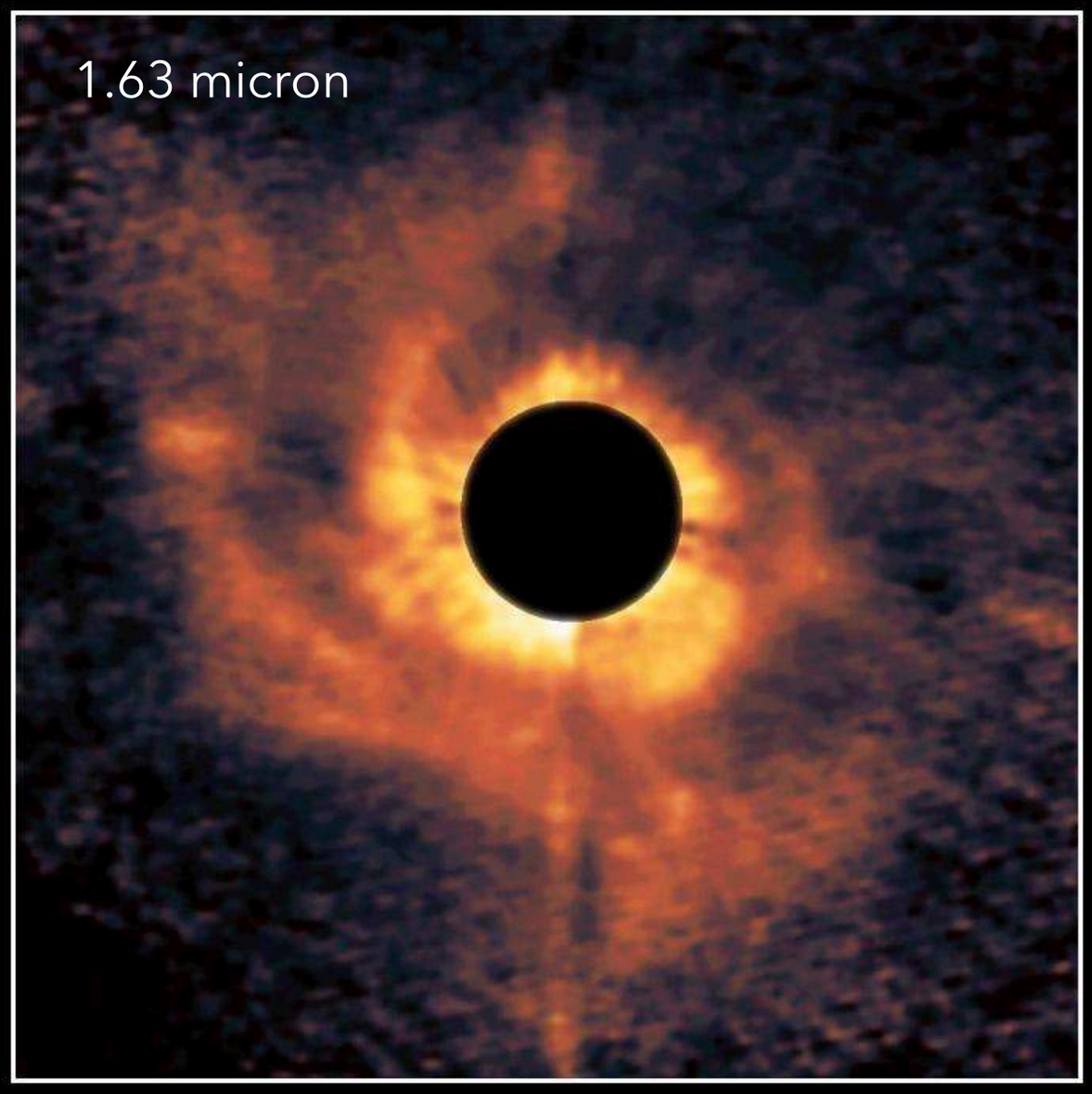


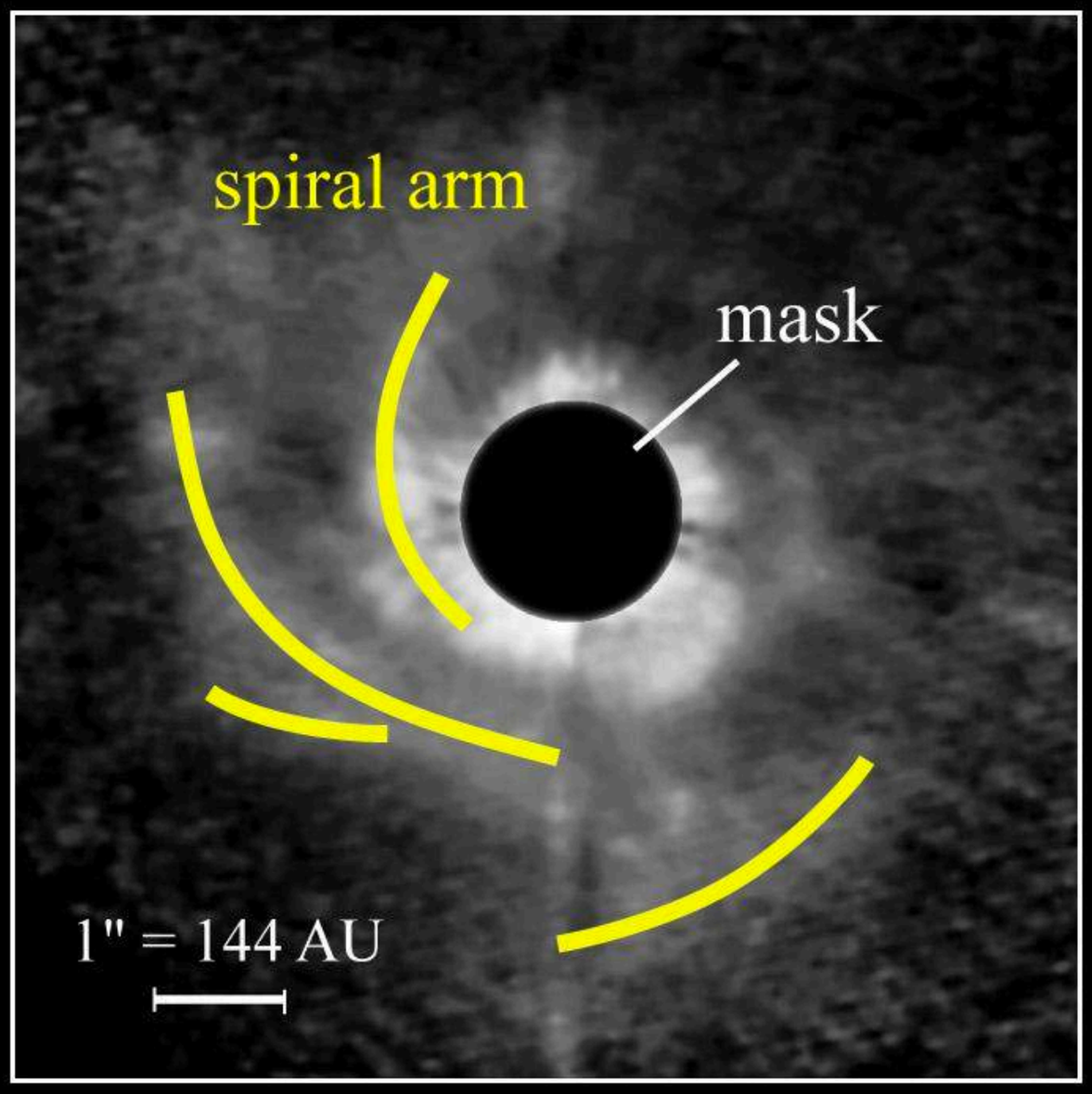
3.6m/ADONIS
1.25 micron



Grady et al. 2001, ApJ, 122, 3396; Pantin et al. 2000, A&A, 361, L9; NOAO, NASA/GSFC CTIO, ESO, NSF

Coronography reveals complex structures in scattered light





Protoplanetary Disk Surrounding the Star AB Aurigae CIAO+AO (H)

April 18, 2004

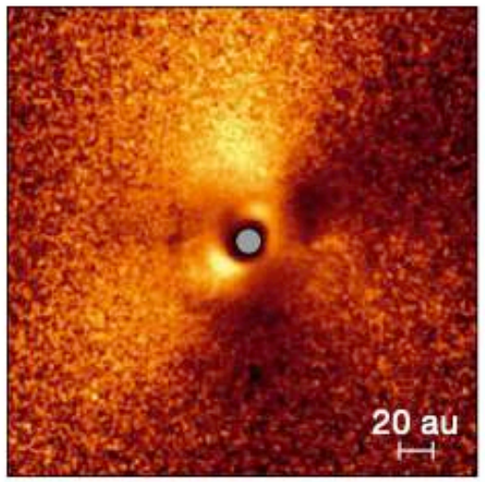
Subaru Telescope, National Astronomical Observatory of Japan

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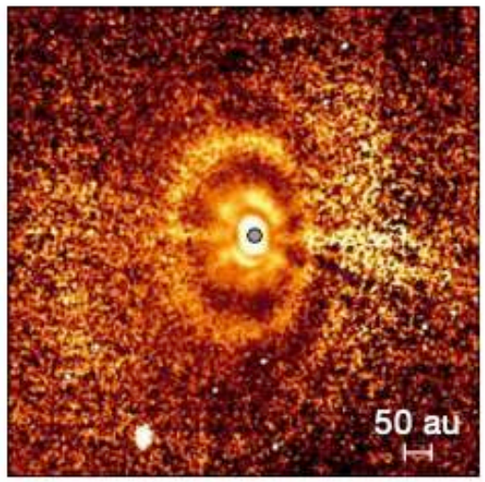
Fukagawa et al. 2004, ApJ, 605, L53

High-contrast imaging of protoplanetary disks

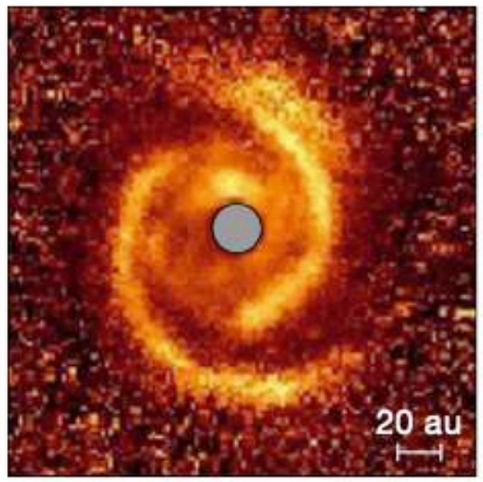
A compendium of disk morphologies revealed by VLT/SPHERE



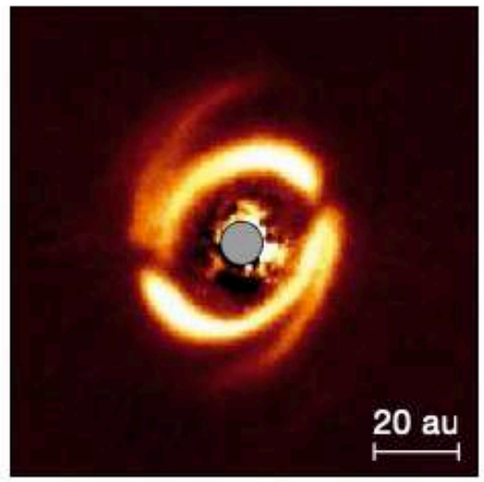
HD 100546



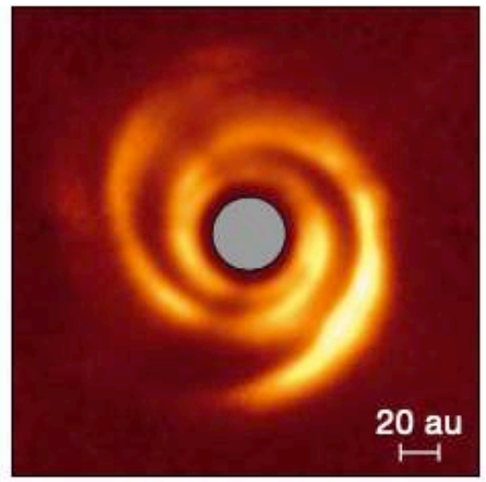
HD 97048



MWC 758

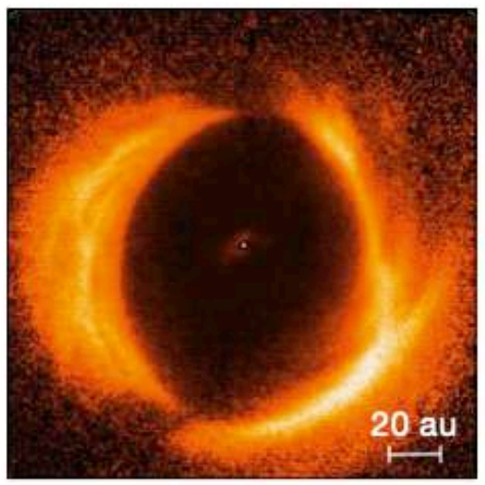


HD 100453

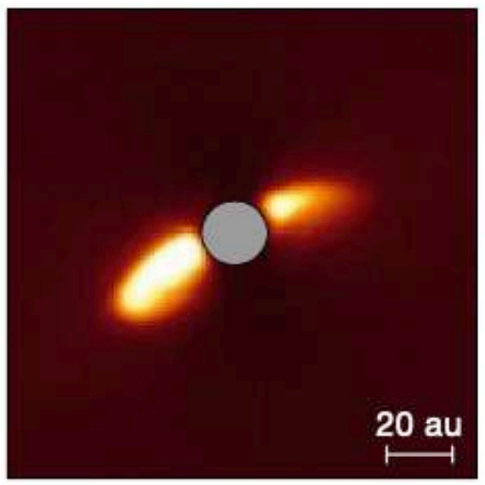


HD 135344B

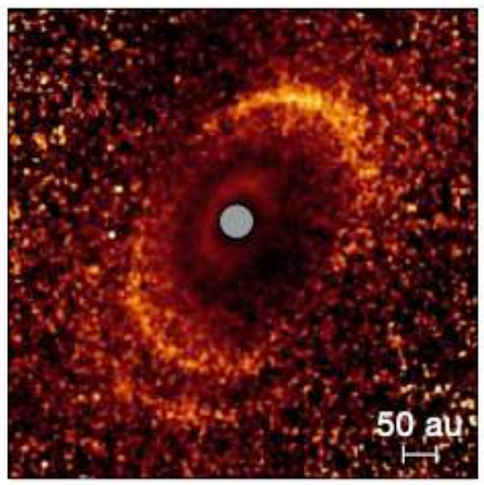
Early stellar type ⟵ Herbig Ae/Be stars ⟶ ⟵ F stars ⟶



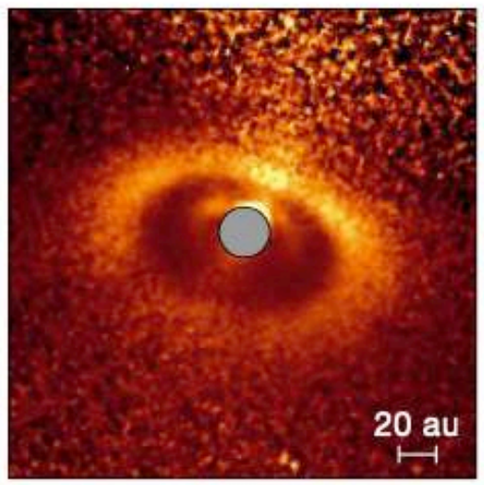
HD 142527



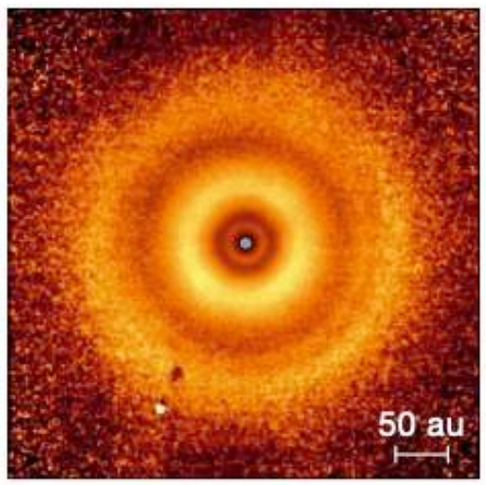
T Cha



RX J1615-3255



LkCa15



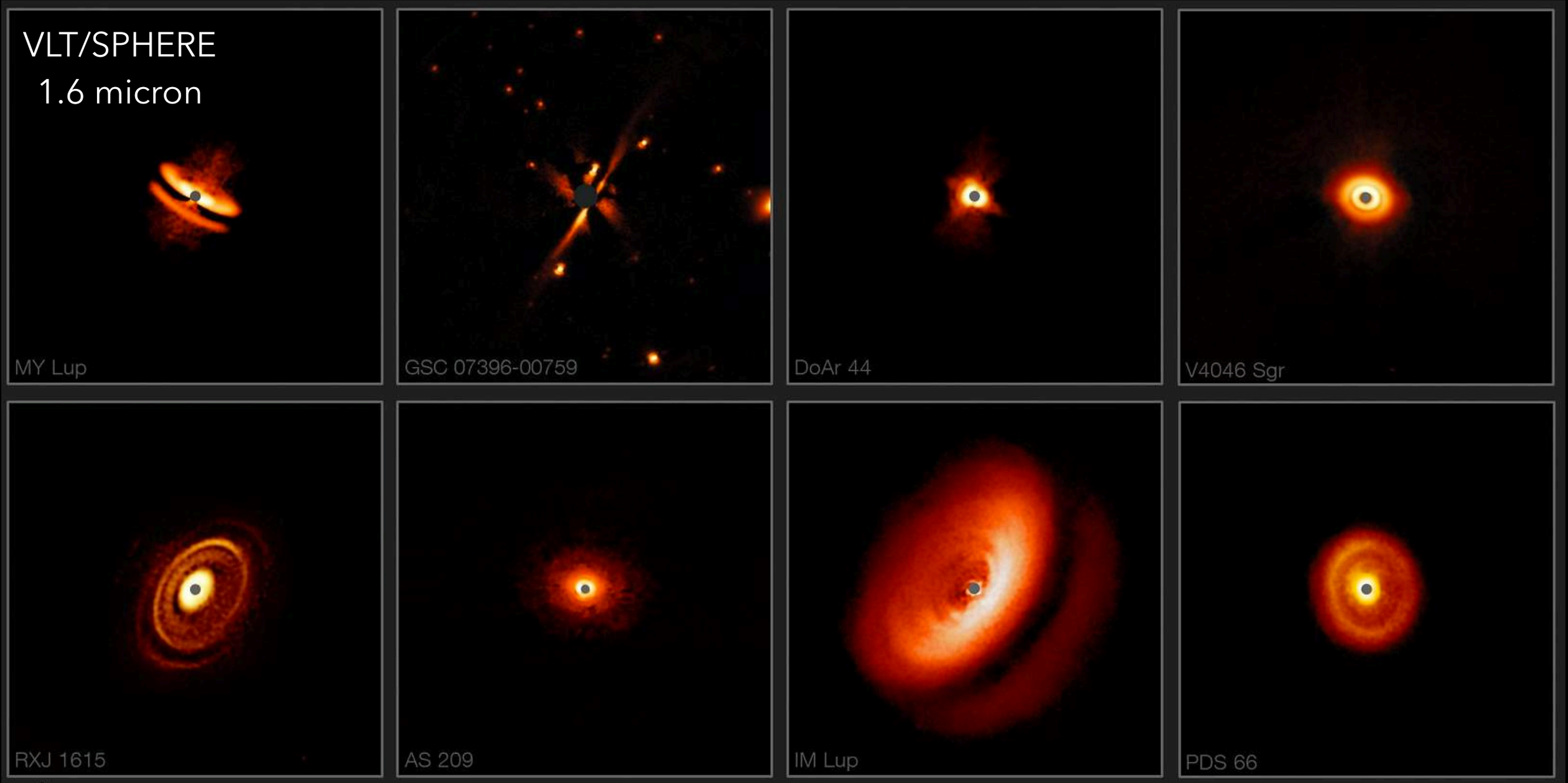
TW Hya

T Tau stars ⟶ Late stellar type

Marois et al. 2006, ApJ, 641, 556; Garufi et al. 2017, Messenger, 169, 32

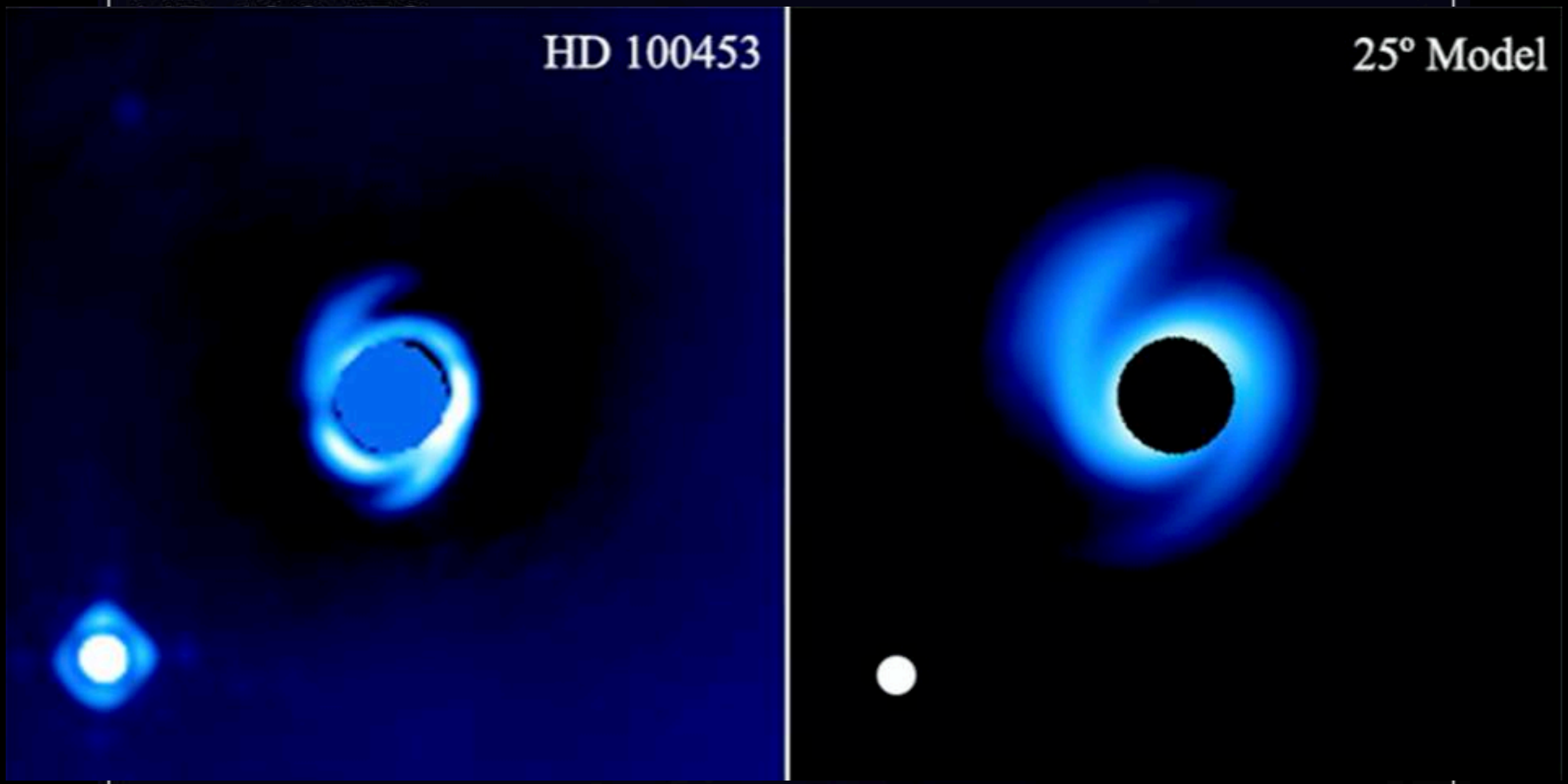
High-contrast imaging of protoplanetary disks

A compendium of disk morphologies revealed by VLT/SPHERE



Avenhaus et al. 2018, ApJ, 863, 44; ESO/H. Avenhaus et al./E. Sissa et al./DARTT-S and SHINE collaborations

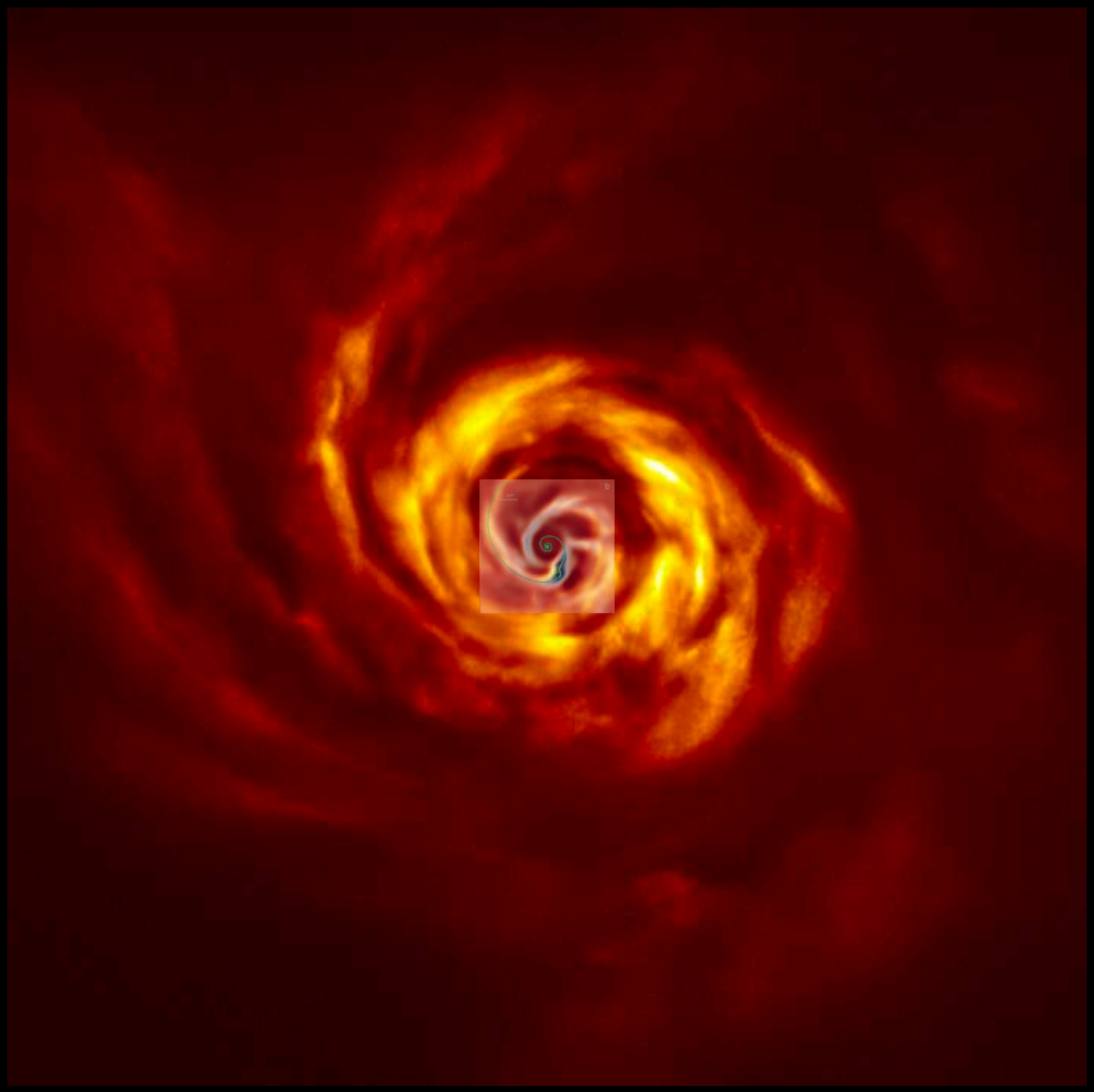
Drivers of spiral arms seen in scattered light



Wagner et al. 2018, ApJ, 854, 130

Drivers of spiral arms seen in scattered light

AB Aur
VLT/SPHERE

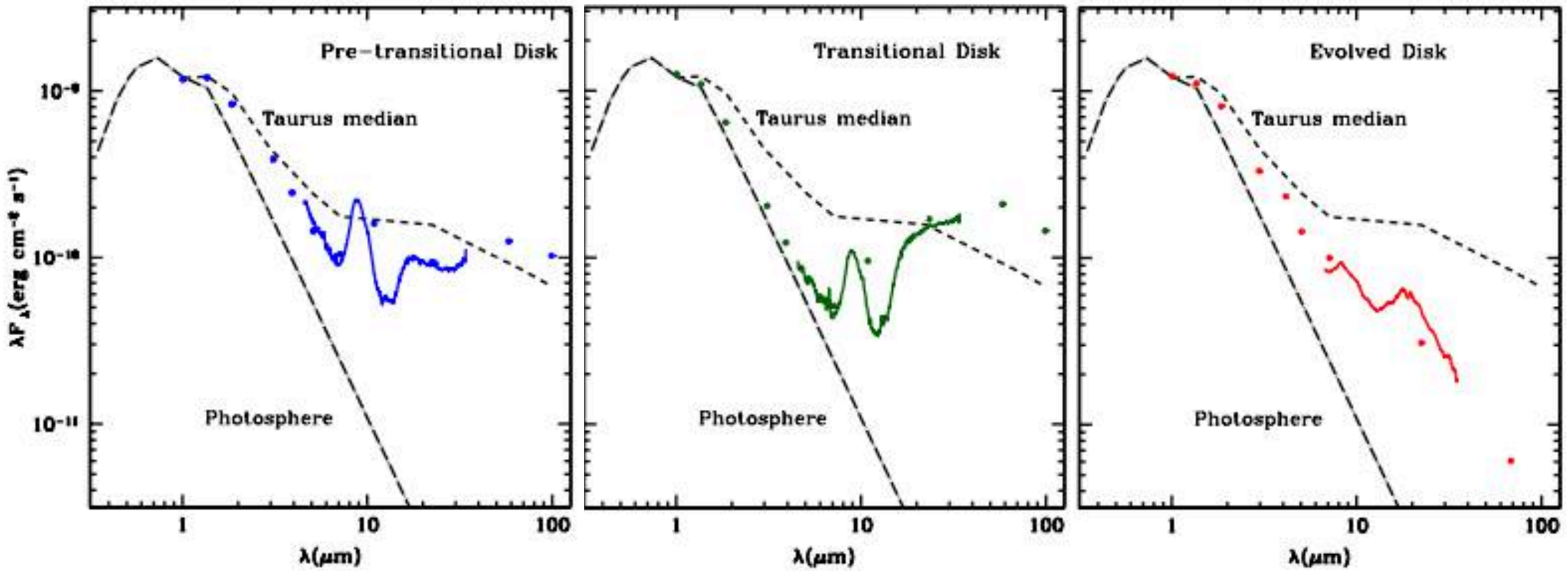


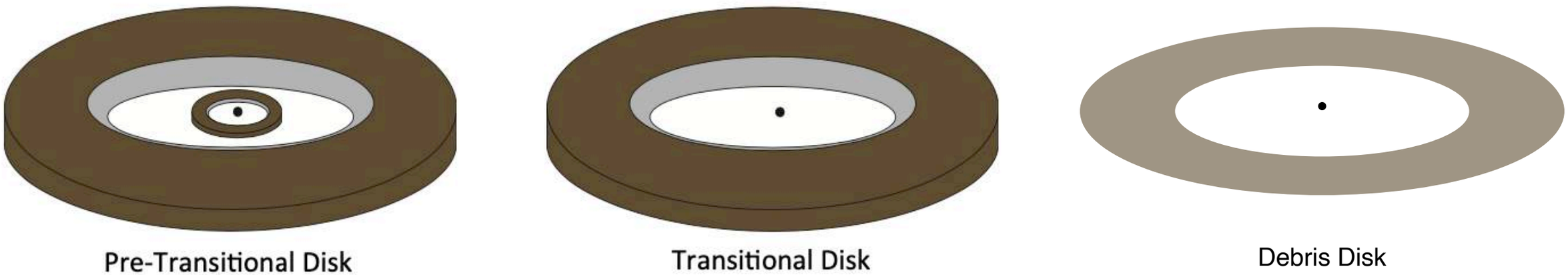
ESO/Boccaletti et al. 2020, A&A, 637, L5

Observations of dusty protoplanetary disks at (mid)infra-red wavelengths

Spectral energy distribution (SED)

Transitional disks: disks “in transition”?

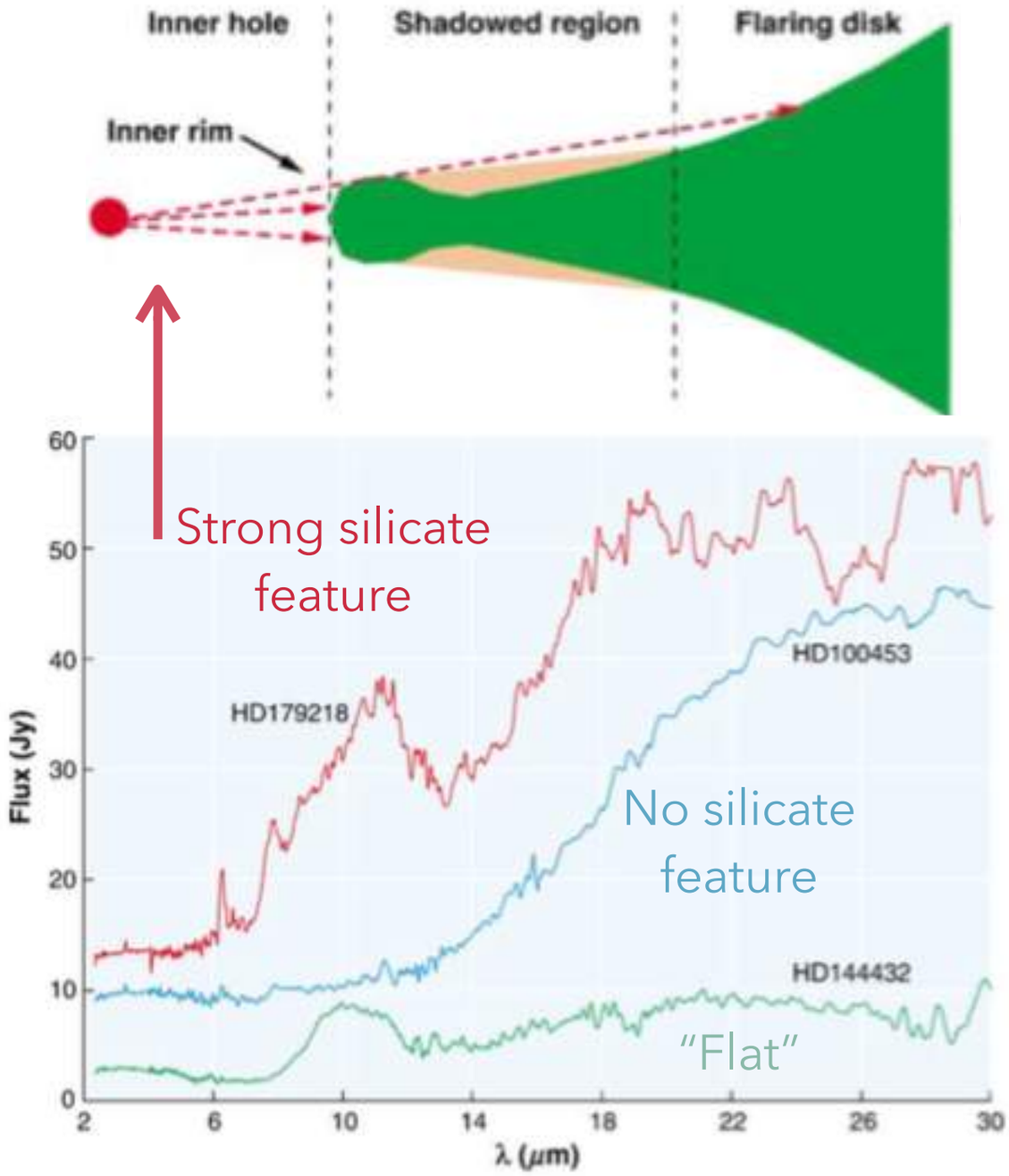


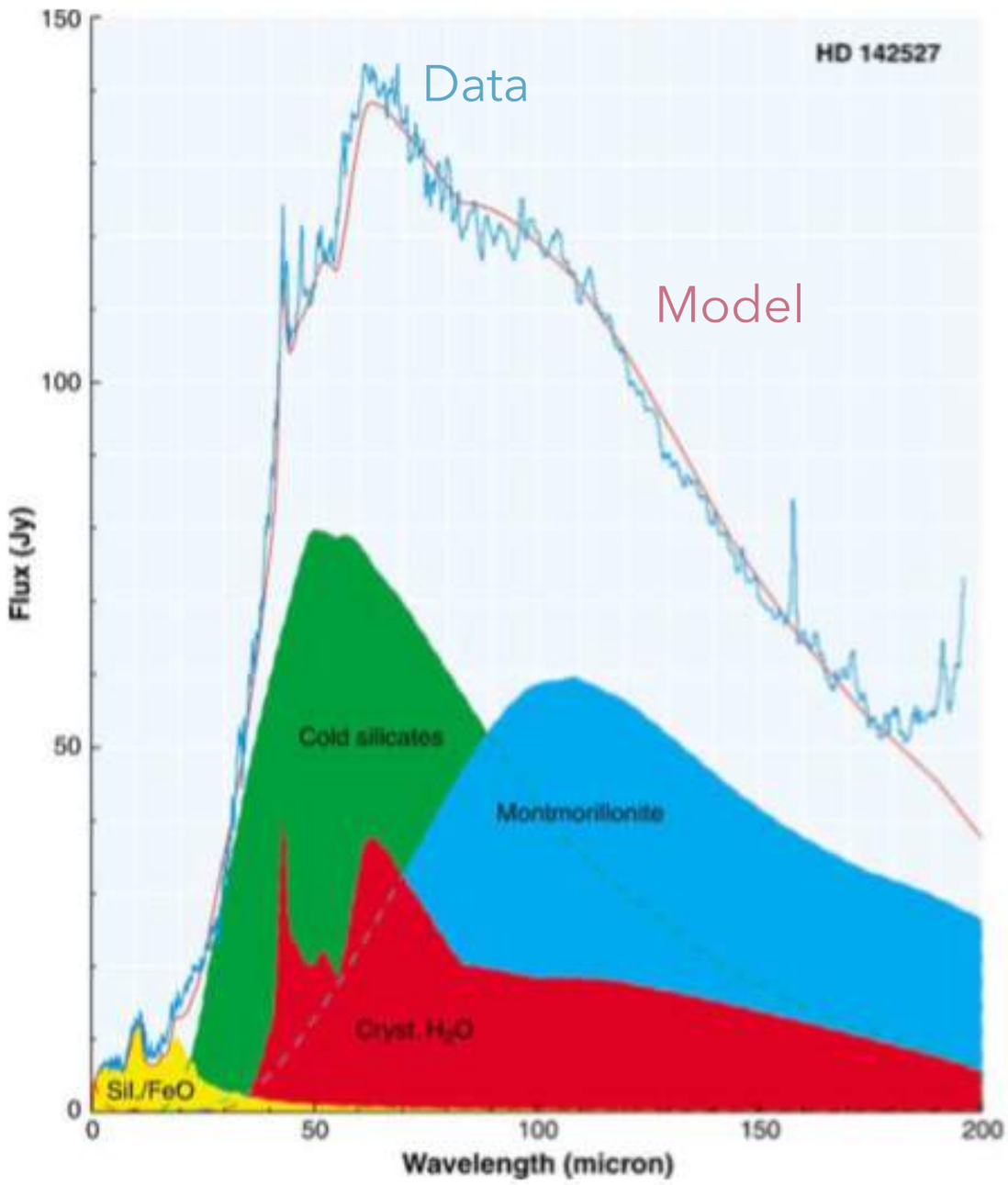


Espaillat et al. 2014, PPVI,497

Spectrally-resolved (mid) infrared emission

Revealing the inner disk structure and dust composition



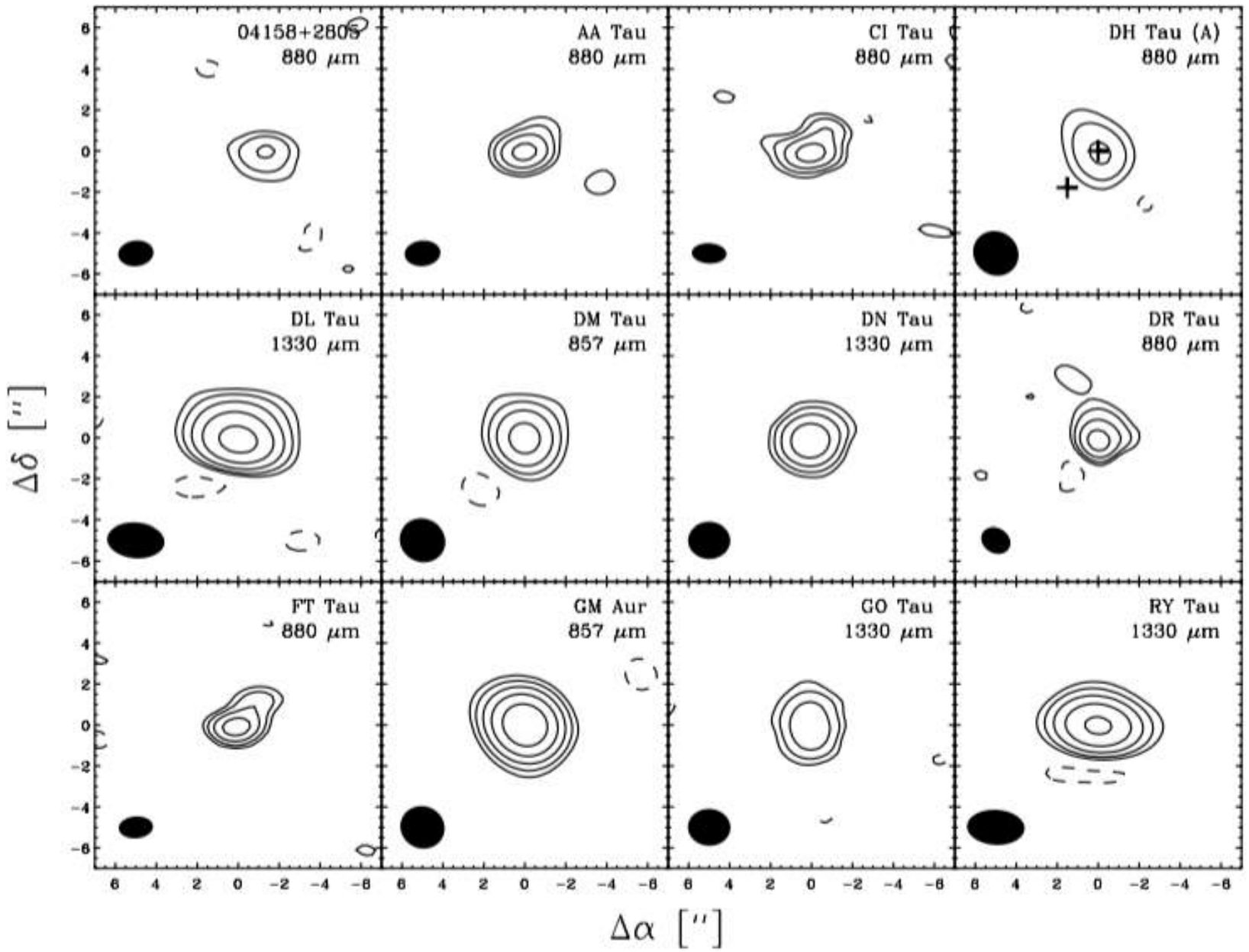


van Dishoeck, E. F. 2004, ARA&A, 42, 119; Meeus et al. 2001, A&A, 365, 476; Malfait et al. 1999, A&A, 345, 181

Observations of dusty protoplanetary disks at mm to cm wavelengths

The advent of (sub) mm interferometry

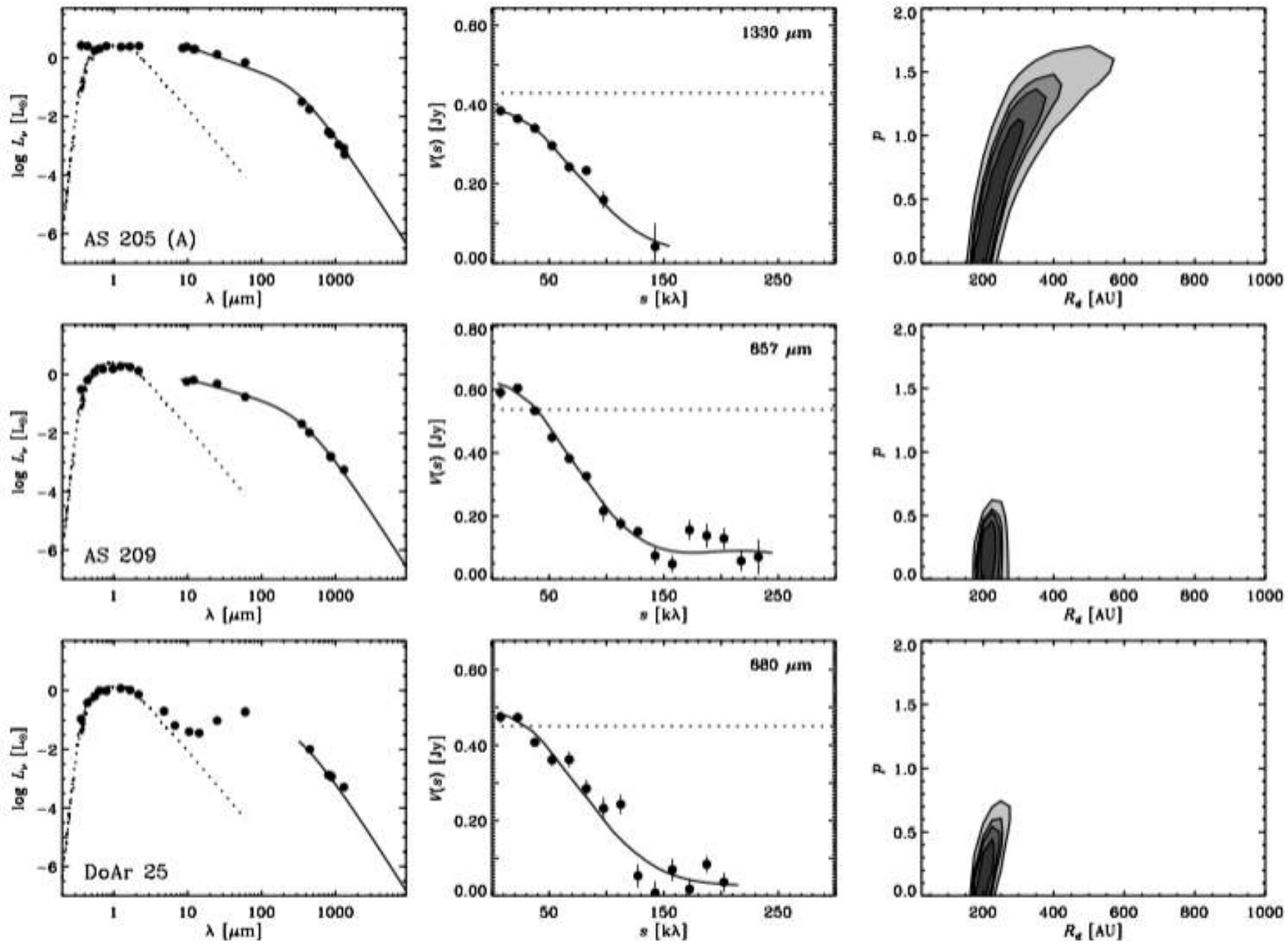
Submillimeter Array (SMA) survey of disks in Taurus-Auriga/ Ophiuchus-Scorpius at 1″ - 2″ resolution



Andrews & Williams 2007, ApJ, 659, 705; Williams & Cieza 2011, ARA&A, 49, 67

The advent of (sub) mm interferometry

Fitting done direct to the visibilities (raw interferometric data) can constrain the radial disk structure



Data are fit using power laws for the midplane temperature and dust surface density

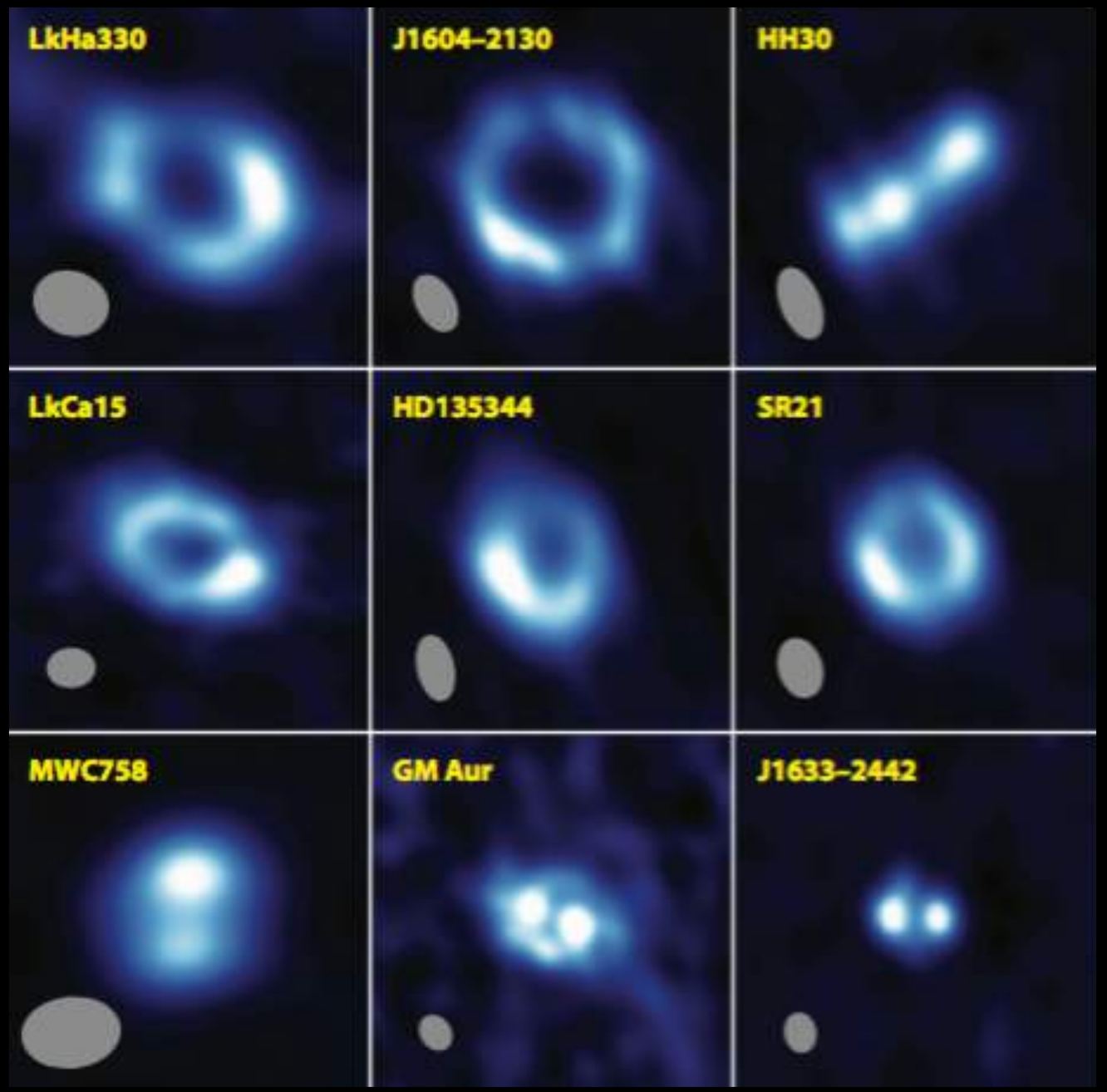
$$T_r = T_1 \left(\frac{r}{1\ \mathrm{AU}} \right)^{-q},$$

$$\Sigma_r = \Sigma_5 \left(\frac{r}{5\ \mathrm{AU}} \right)^{-p},$$

Andrews & Williams 2007, ApJ, 659, 705; Williams & Cieza 2011, ARA&A, 49, 67

The advent of (sub) mm interferometry

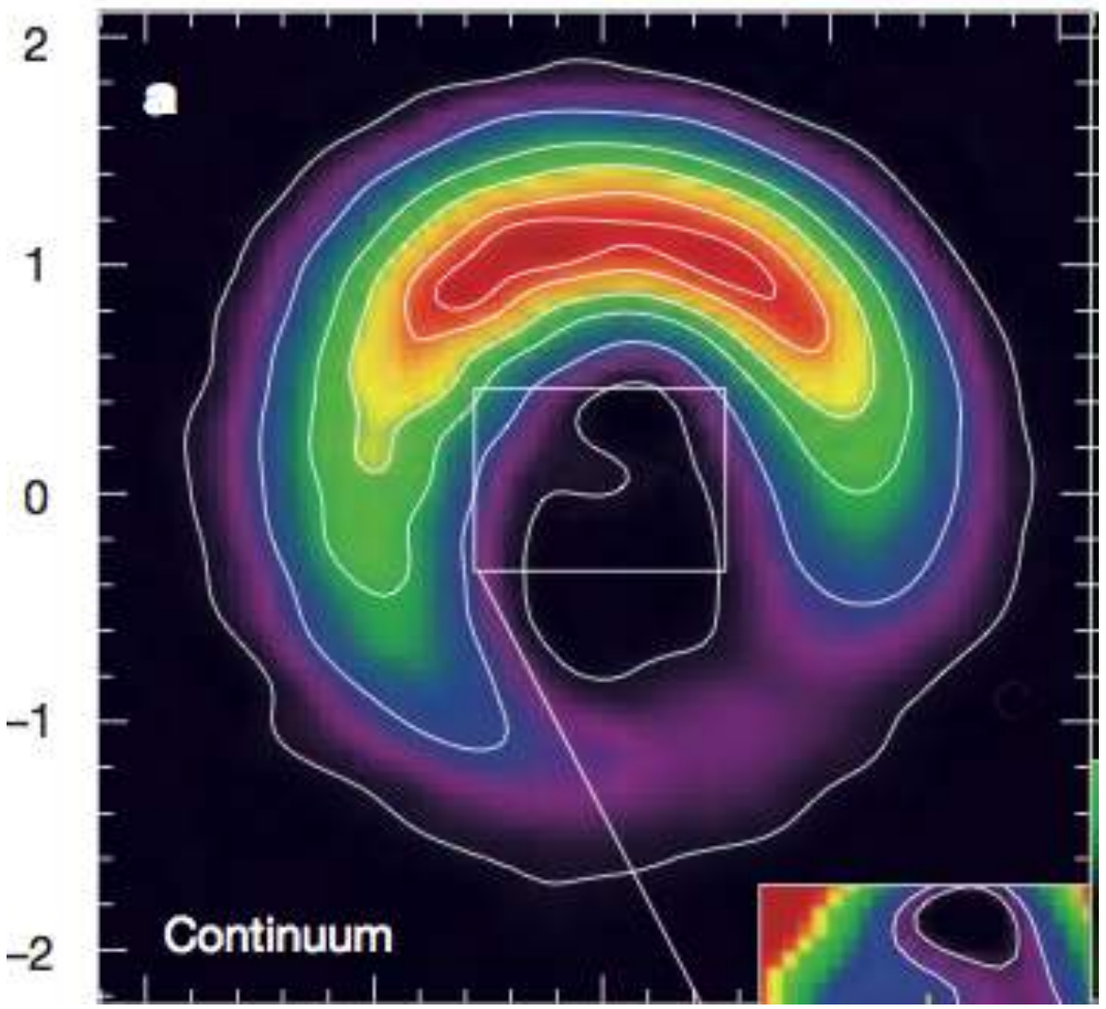
Sub-arcsecond resolution revealed rings, gaps, and asymmetries



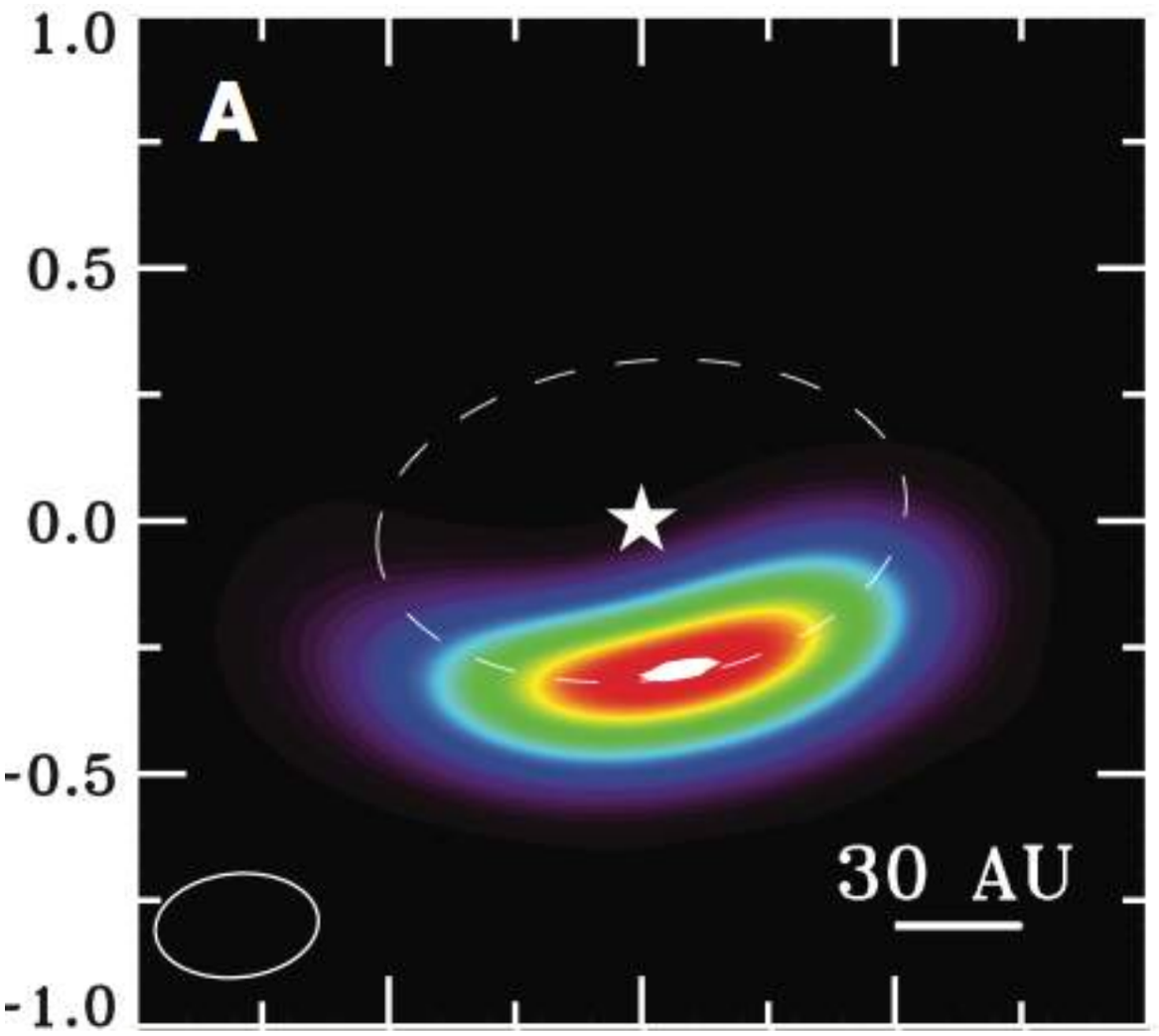
Williams & Cieza 2011, ARA&A, 49, 67

Dusty disks in the era of ALMA

ALMA Early Science revealed highly asymmetric (sub)mm emission attributed to dust trapping by vortices induced by planets/companions



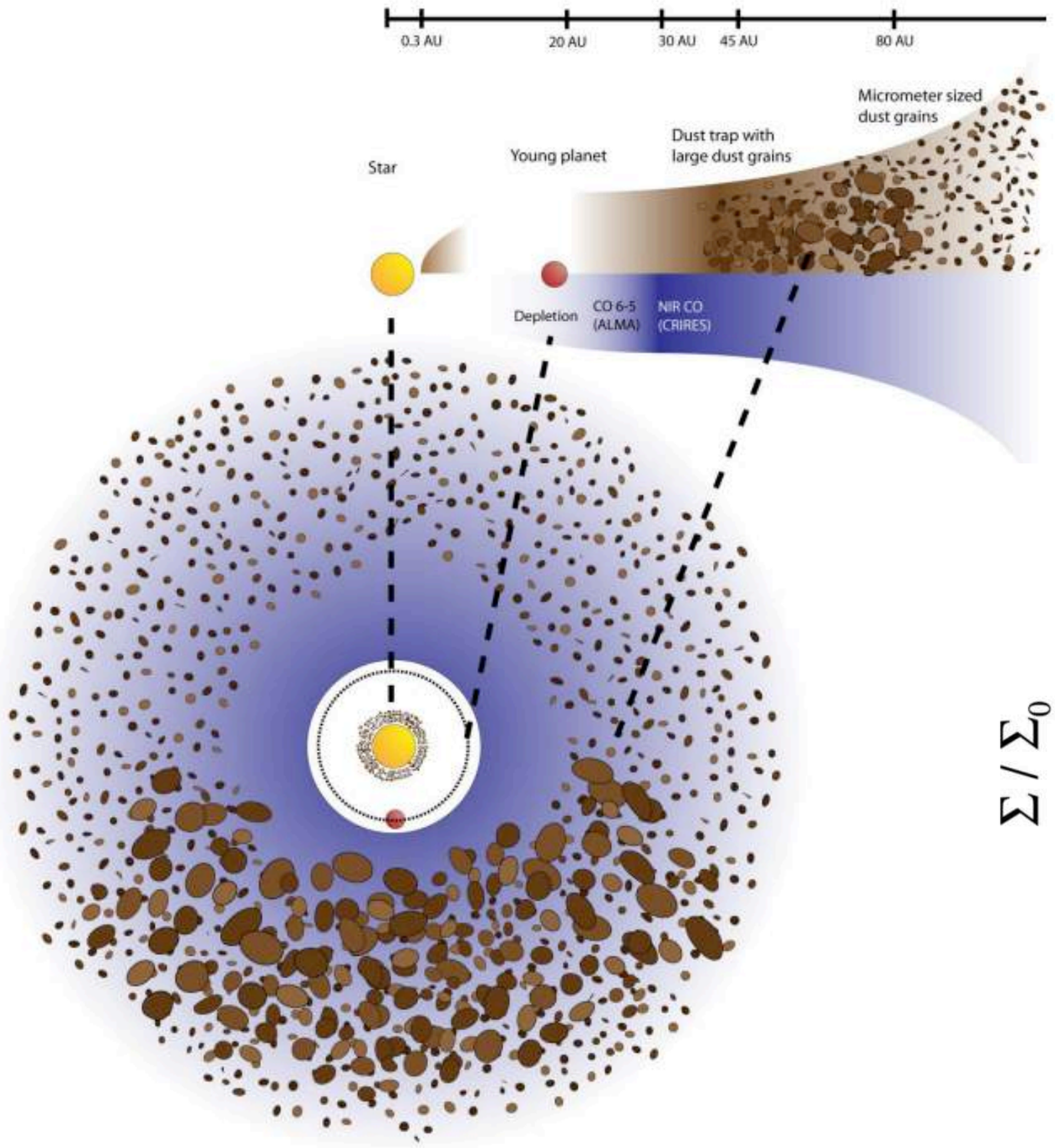
HD 142527



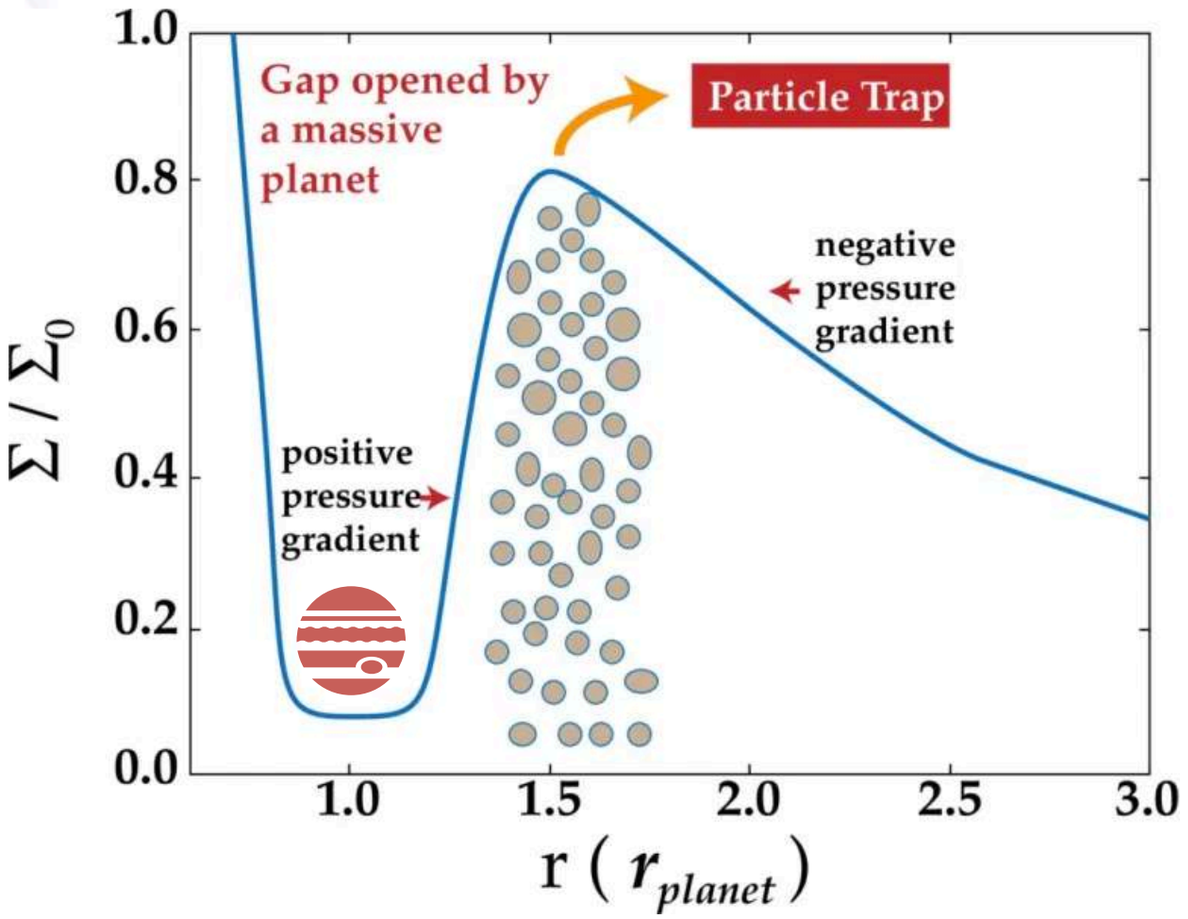
IRS 48

Casassus, S., et al. 2013, Nature, 493, 191; van der Marel, N., et al. 2013, Science, 340, 1199

Dusty disks in the era of ALMA



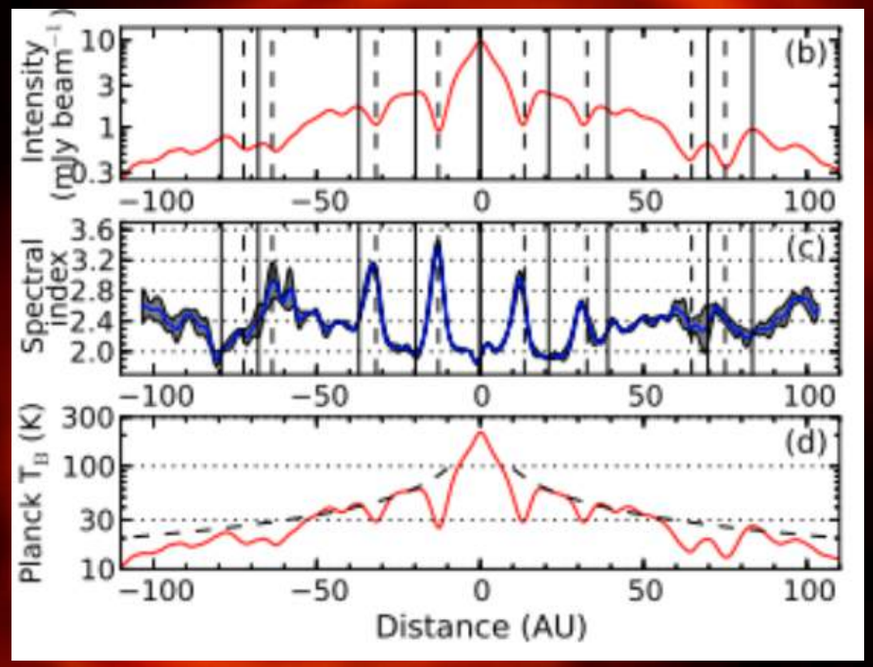
Models with dust growth/ fragmentation and radial drift show trapping at pressure maxima

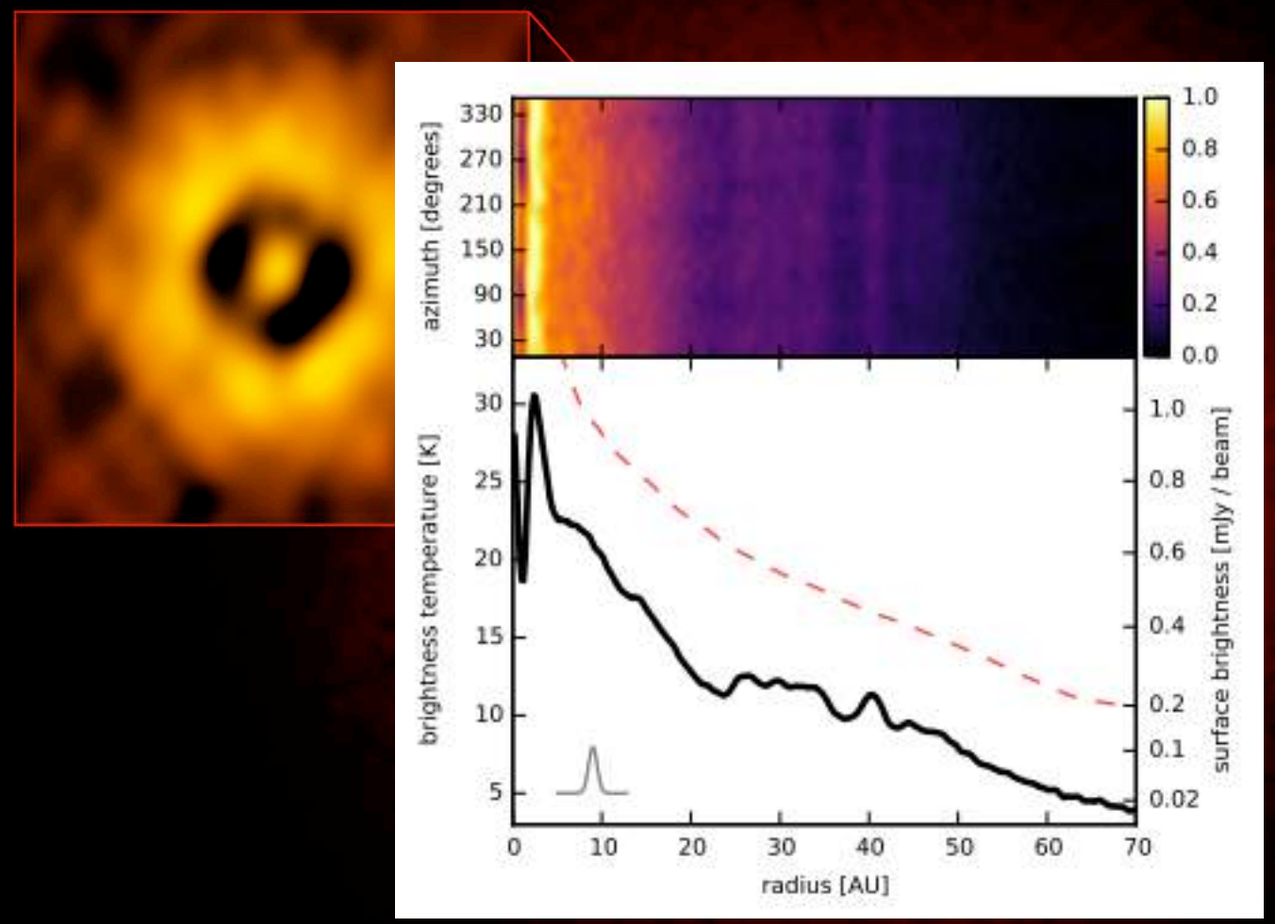


van der Marel, N., et al. 2013, Science, 340, 1199; P. Pinilla

Dusty disks in the era of ALMA

Long baseline observations: towards ~ au resolution



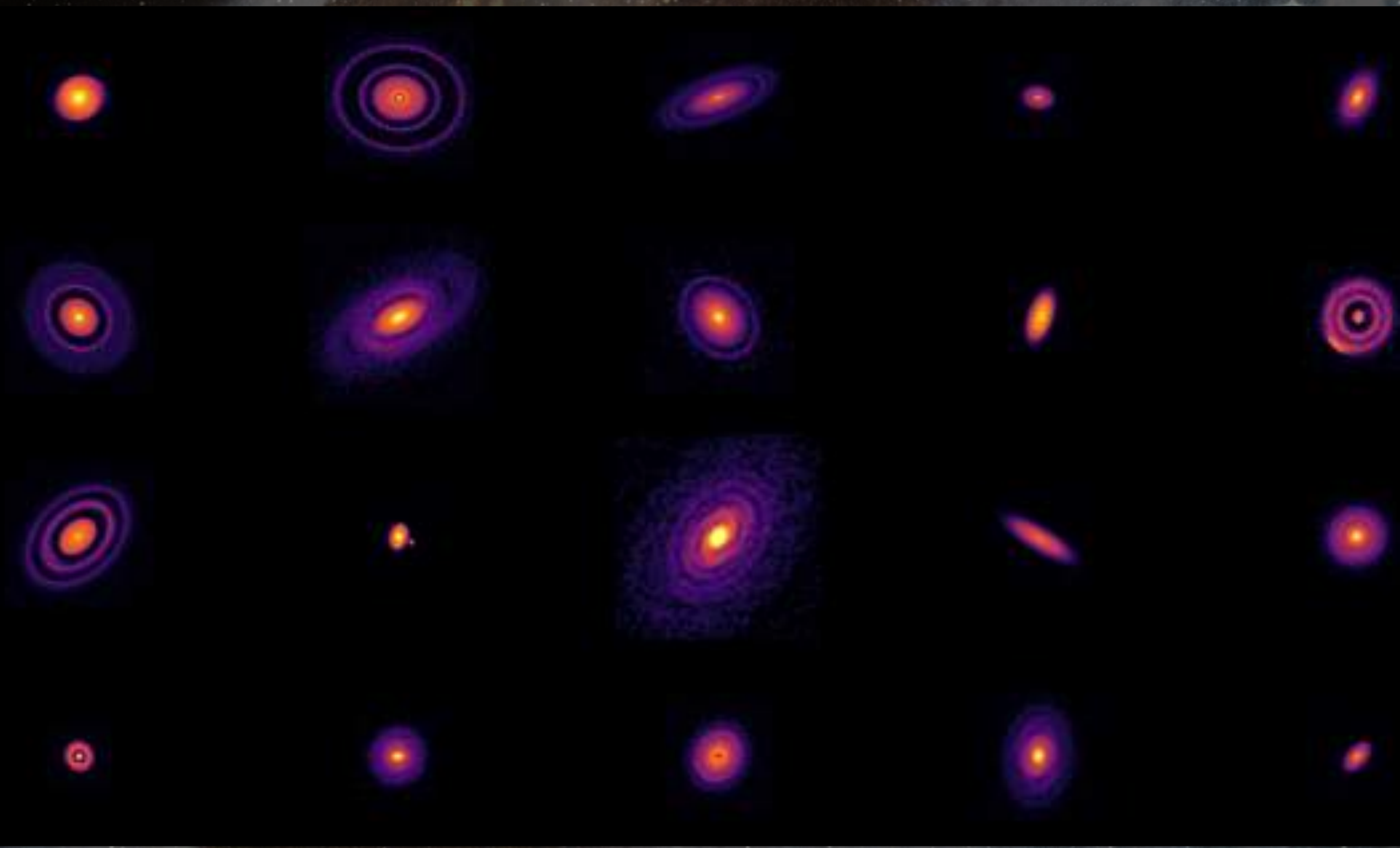


HL Tau

TW Hya

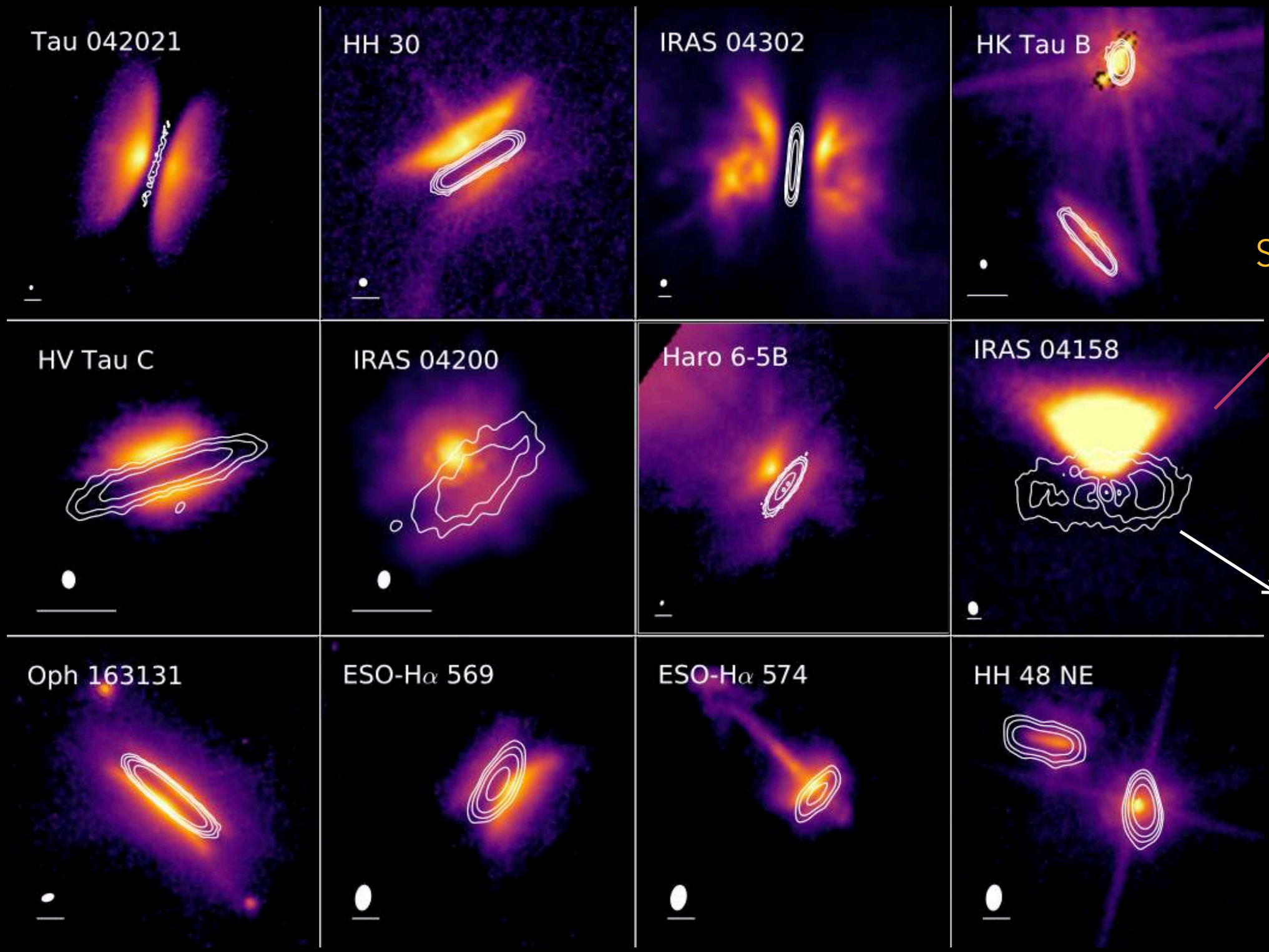
ALMA Partnership 2015, ApJL, 808, L3; Andrews, S. M., et al, 2016, ApJ, 820, L40

Dusty disks in the era of ALMA: DSHARP



Andrews, S. M., et al. 2018, ApJ, 869, L41; Credit: ALMA (ESO/NAOJ/NRAO), S. Andrews et al.; NRAO/AUI/NSF, S. Dagnello

Dusty disks in the era of ALMA: edge-on systems

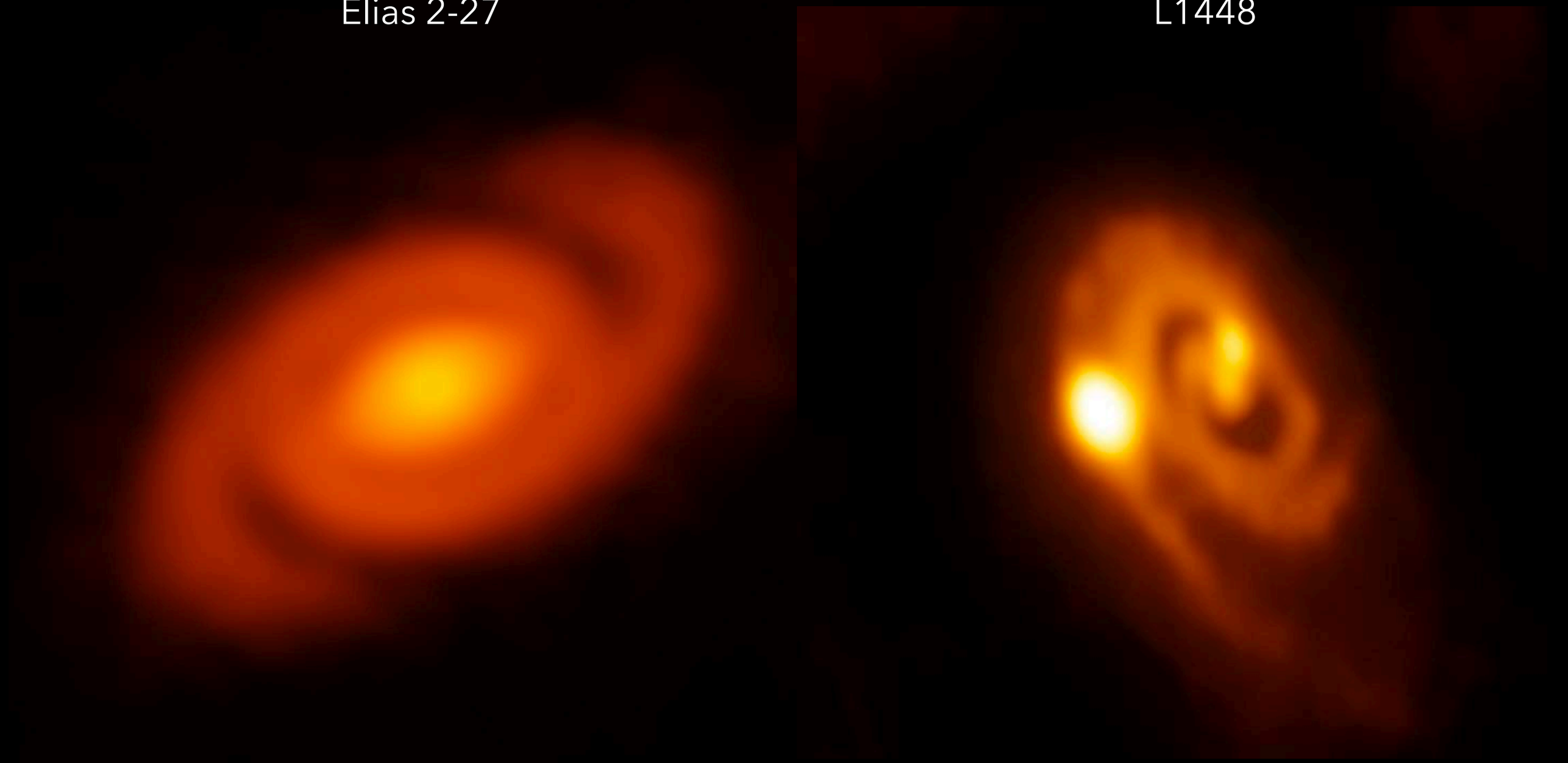


Villenave et al. 2020, A&A, 642, A164

Dusty disks in the era of ALMA: spirals

Elias 2-27

L1448

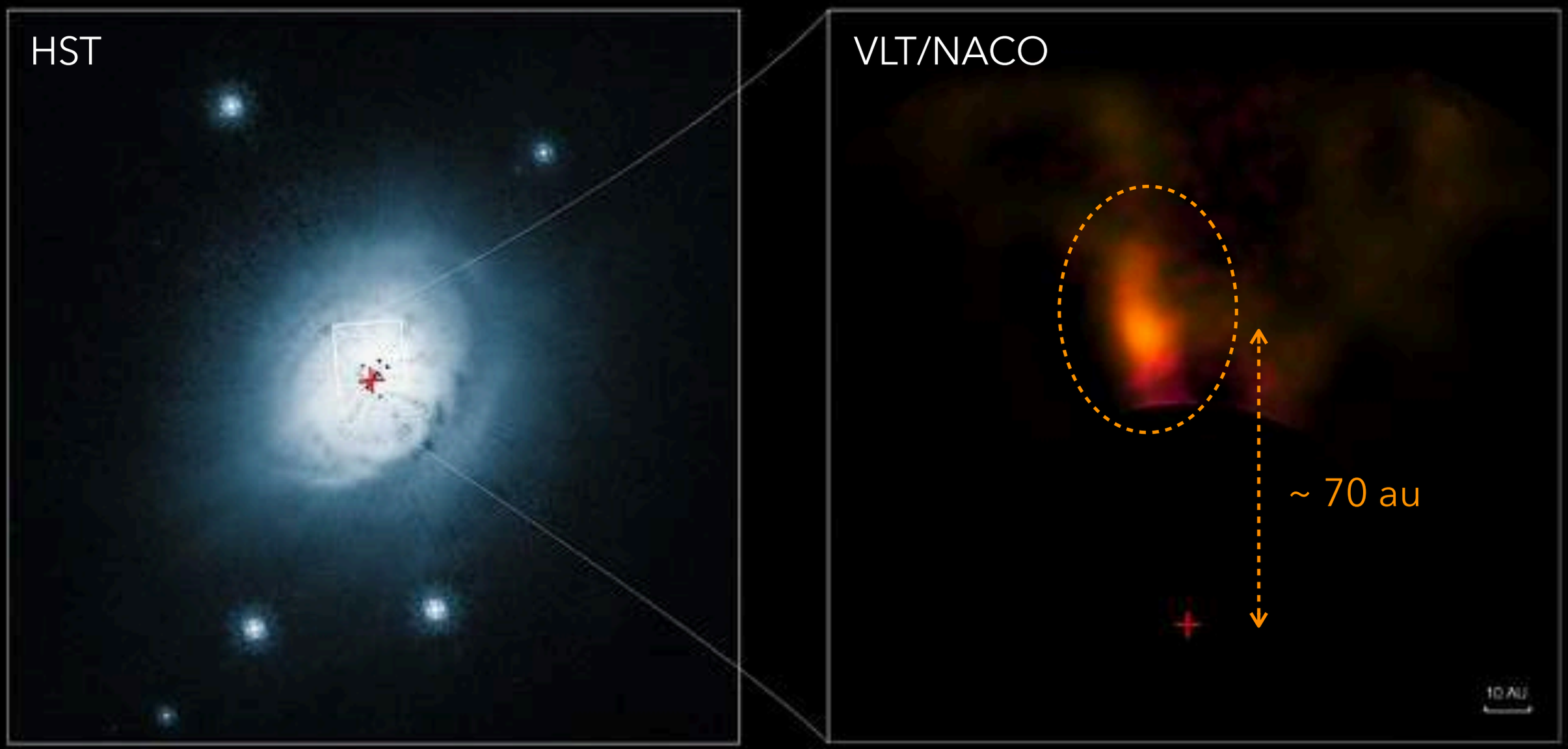


Perez et al. 2016, Science, 353, 1519; Tobin, et al. Nature, 538, 438; ALMA (ESO/NAOJ/NRAO)

Hunting for forming planets in the dust

Hunting for forming planets

A candidate protoplanet in the disk around HD 100546?



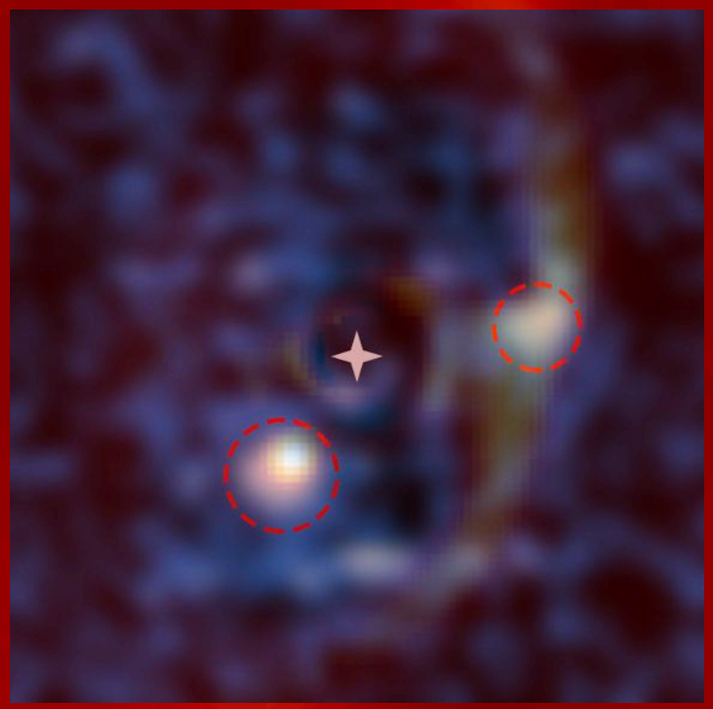
Also detected with Gemini/GPI

Quanz et al., 2013, ApJL, 766, L1; Currie et al. 2017, RNAAS, 1, 1

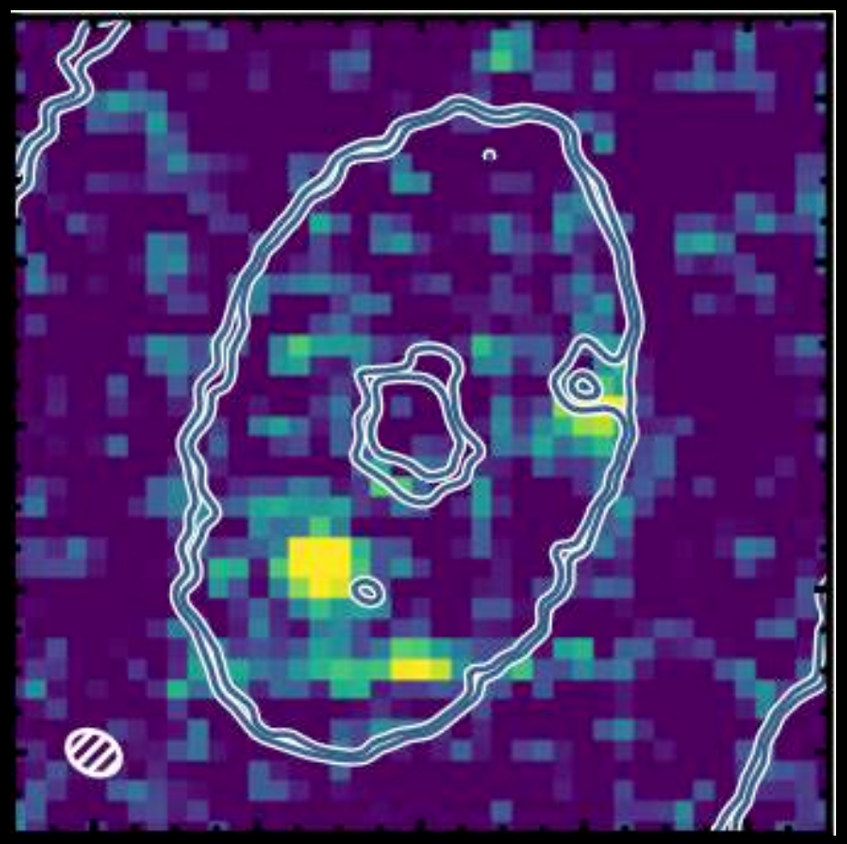
Hunting for forming planets

Two accreting protoplanets in the PDS 70 disk

VLT/SPHERE + VLT/MUSE



ALMA + VLT/MUSE



ESO/MPIA; Keppler et al. 2018, A&A, 617, A44; Haffert et al. 2019, Nature Astronomy, 3, 749; Isella et al. 2019, ApJL, 879, L25

Resolved observations of dust in protoplanetary disks

- Optical to IR wavelengths
  - Scattered light: morphology (gaps, spirals, rings, flaring)
  - Disk “surface”
  - Spectrally resolved: inner disk shape, dust composition
  - Signatures of accretion: H-alpha

- Sub-mm to cm wavelengths
  - Thermal emission: morphology (gaps, rings, traps, spirals)
  - Disk “midplane”
  - Radial dust mass distribution, dust scale height

Observations of gas and chemistry in protoplanetary disks

Our origins

A unique astrochemical laboratory
What is the origin (or heritage) of planet- and comet-building material?
What are our origins?



the protostellar disk



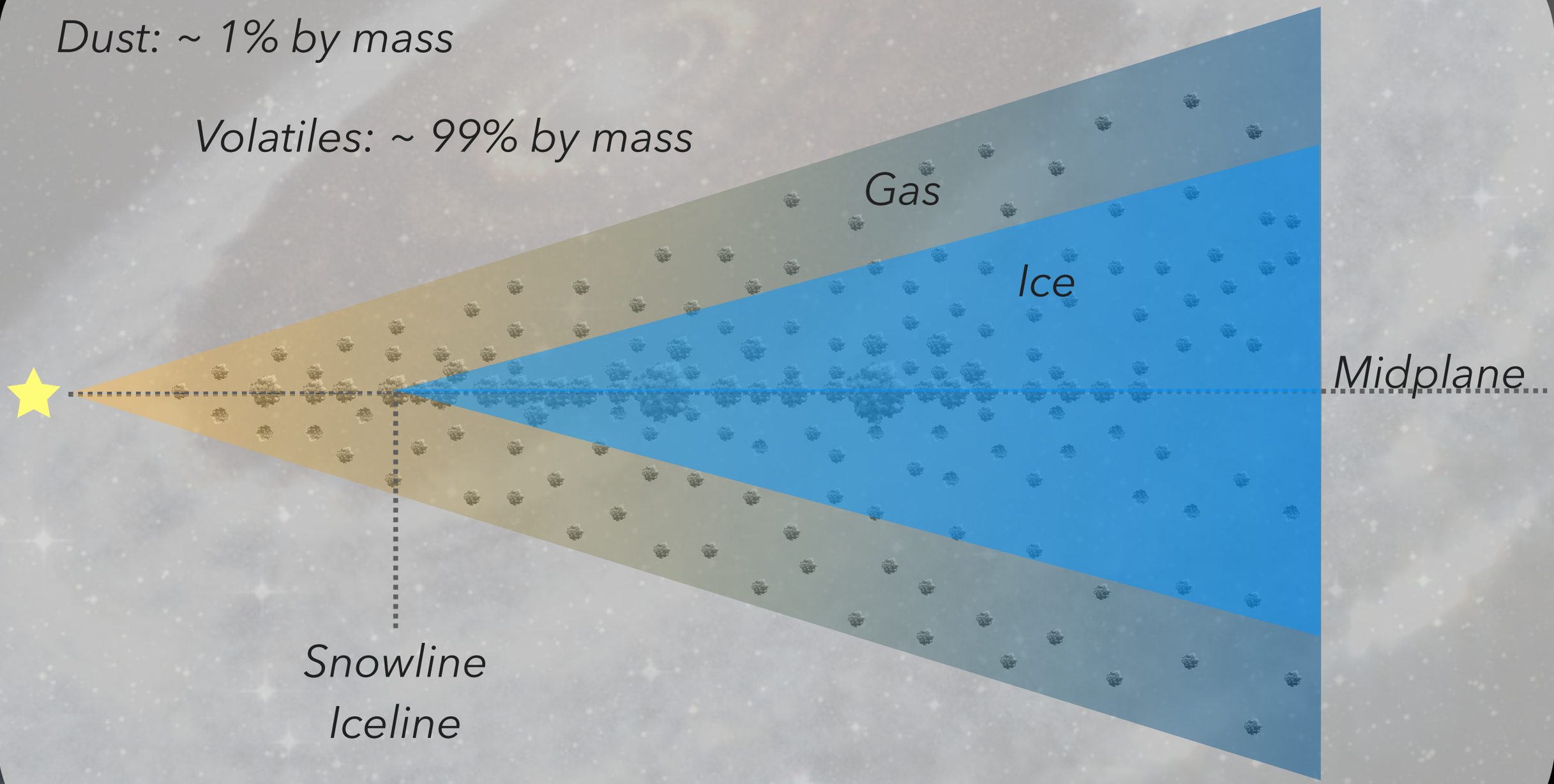
the protoplanetary disk

Credit: B. Saxton (NRAO/AUI/NSF)

The anatomy of a protoplanetary disk

Dust: ~ 1% by mass

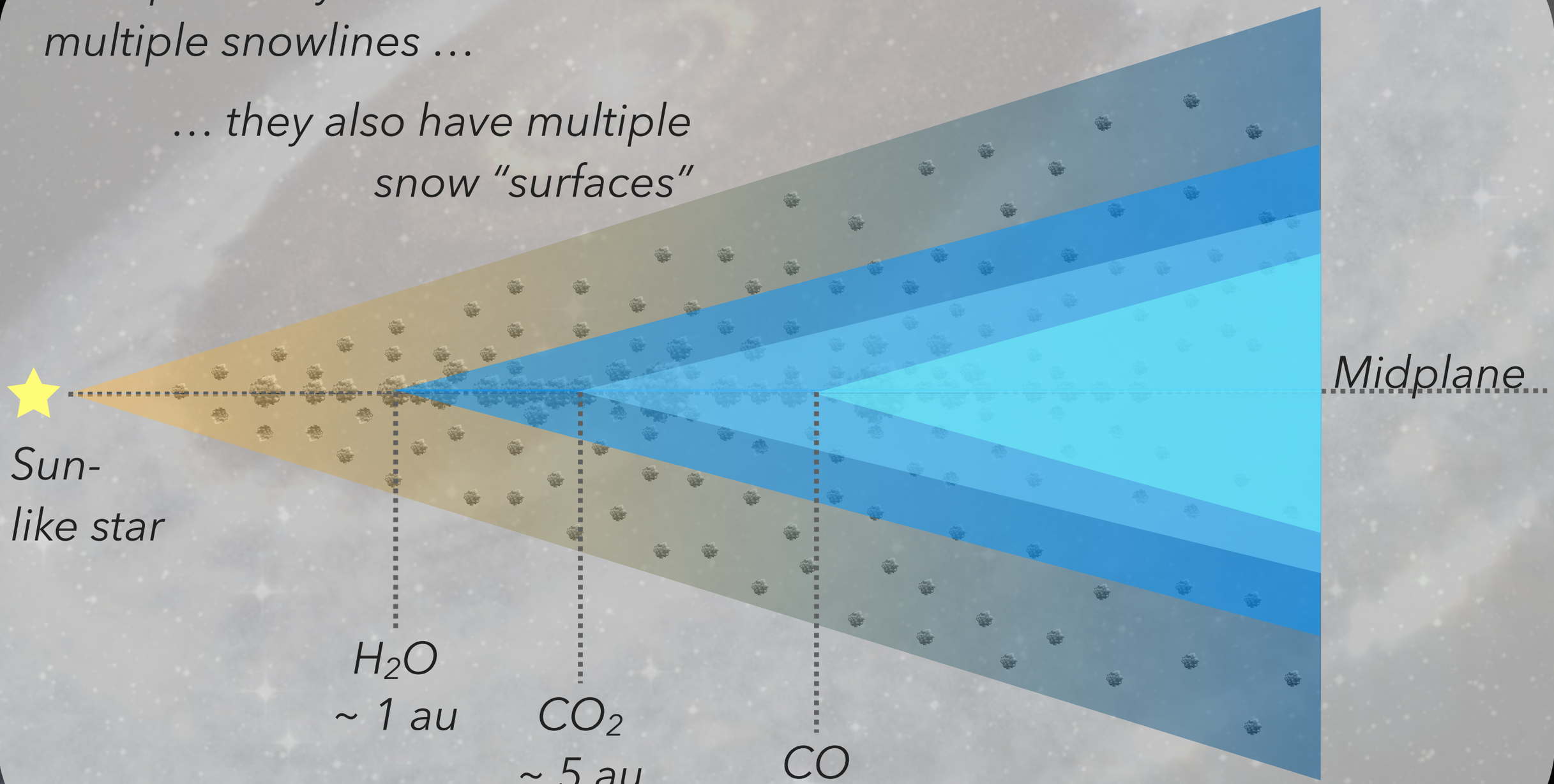
Volatiles: ~ 99% by mass



The anatomy of a protoplanetary disk

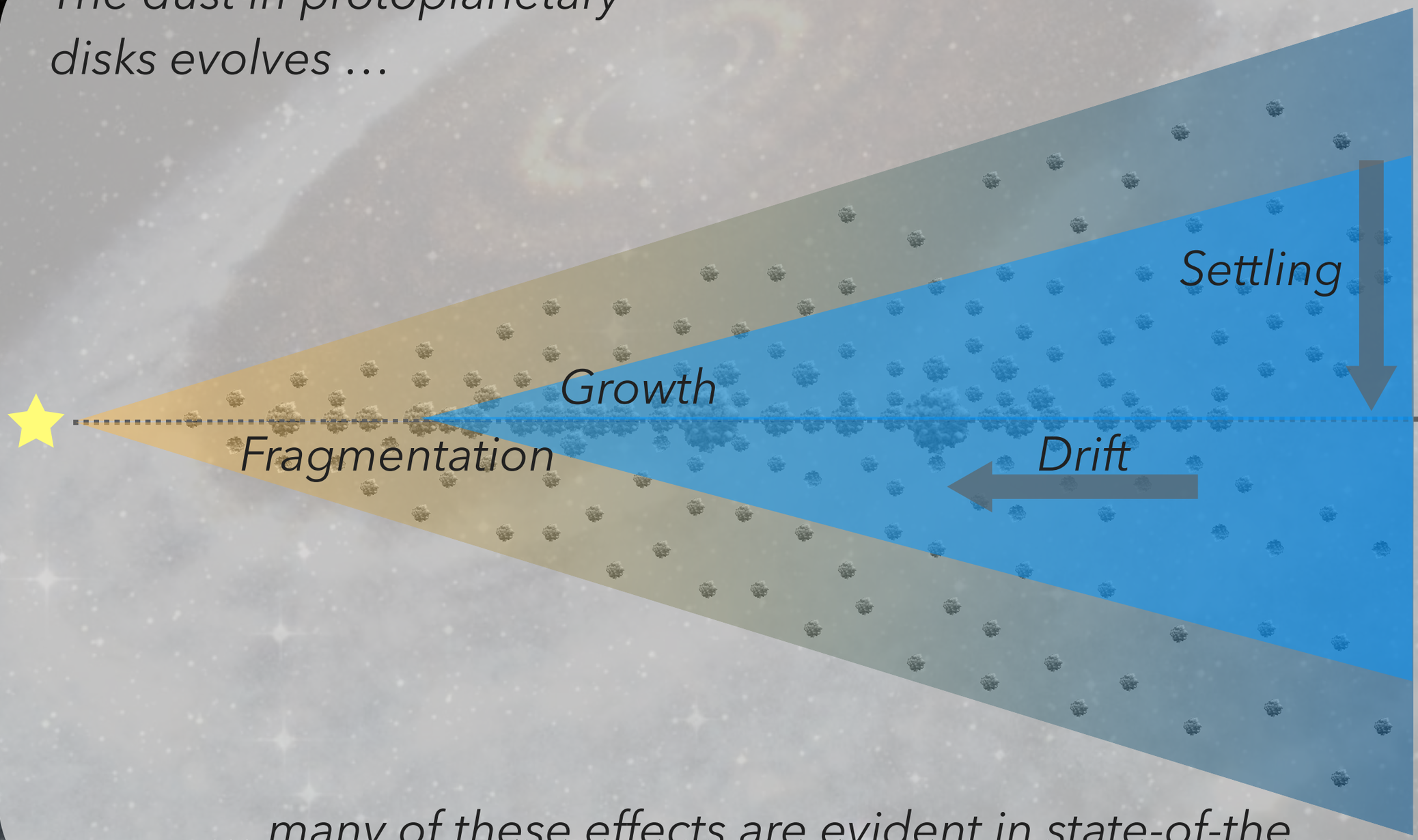
Protoplanetary disks have multiple snowlines …

… they also have multiple snow "surfaces"



The anatomy of a protoplanetary disk

The dust in protoplanetary disks evolves …

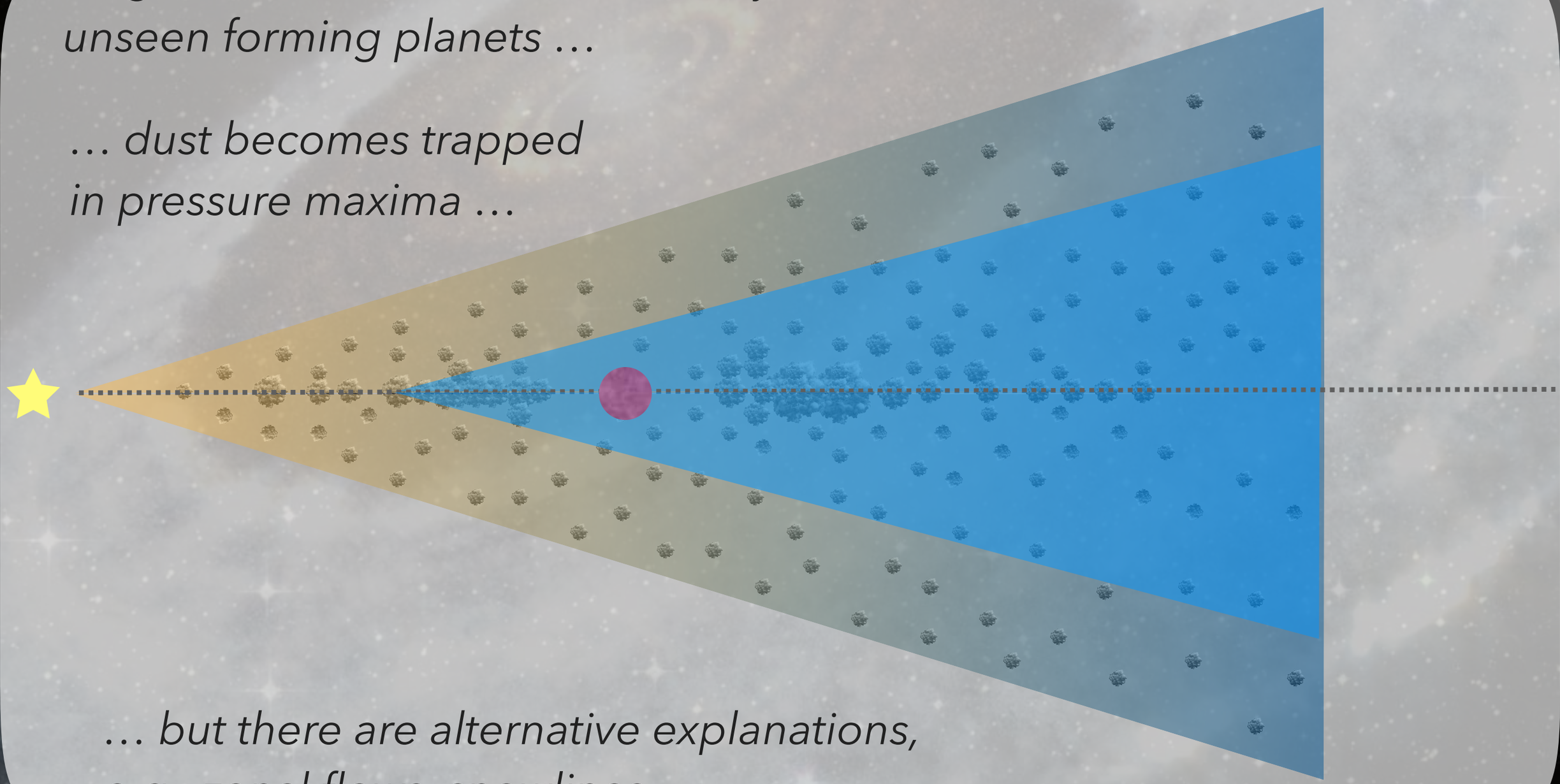


… many of these effects are evident in state-of-the art observations of dust scattering/emission

The anatomy of a protoplanetary disk

Rings in the sub(mm) emission may be due to unseen forming planets …

… dust becomes trapped in pressure maxima …



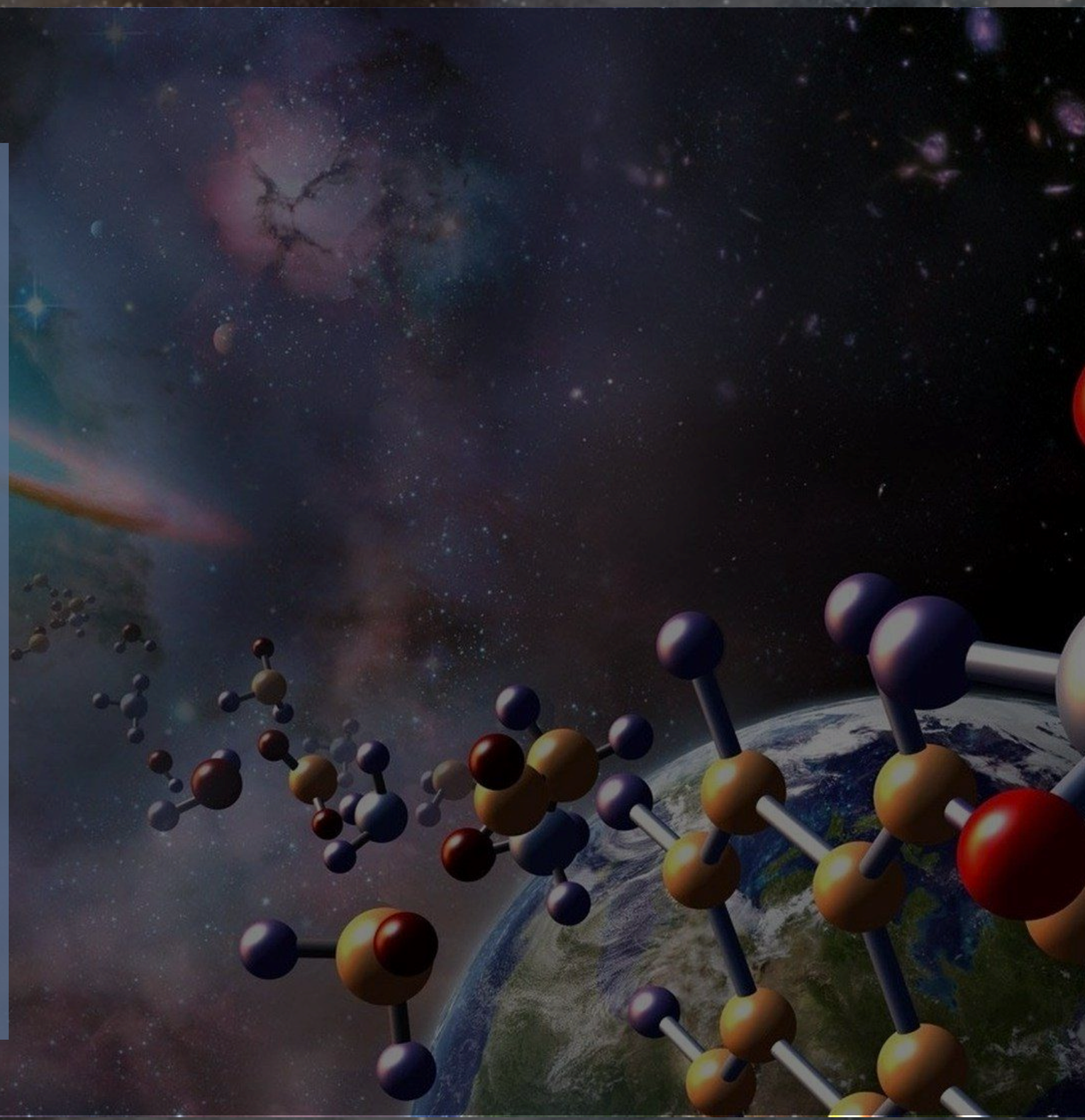
… but there are alternative explanations, e.g., zonal flows, snowlines.

Astrochemistry

Protoplanetary disks are molecular in nature

Molecular spectroscopy offers insight into:

- *Gas mass and distribution*
- *Gas temperature*
- *Gas density*
- *Gas composition*
- *Ice composition*
- *Gas kinematics*
- *Turbulence*
- *Ionisation fraction*



Credit: NASA/Jenny Mottar

Molecular diagnostics at mm wavelengths

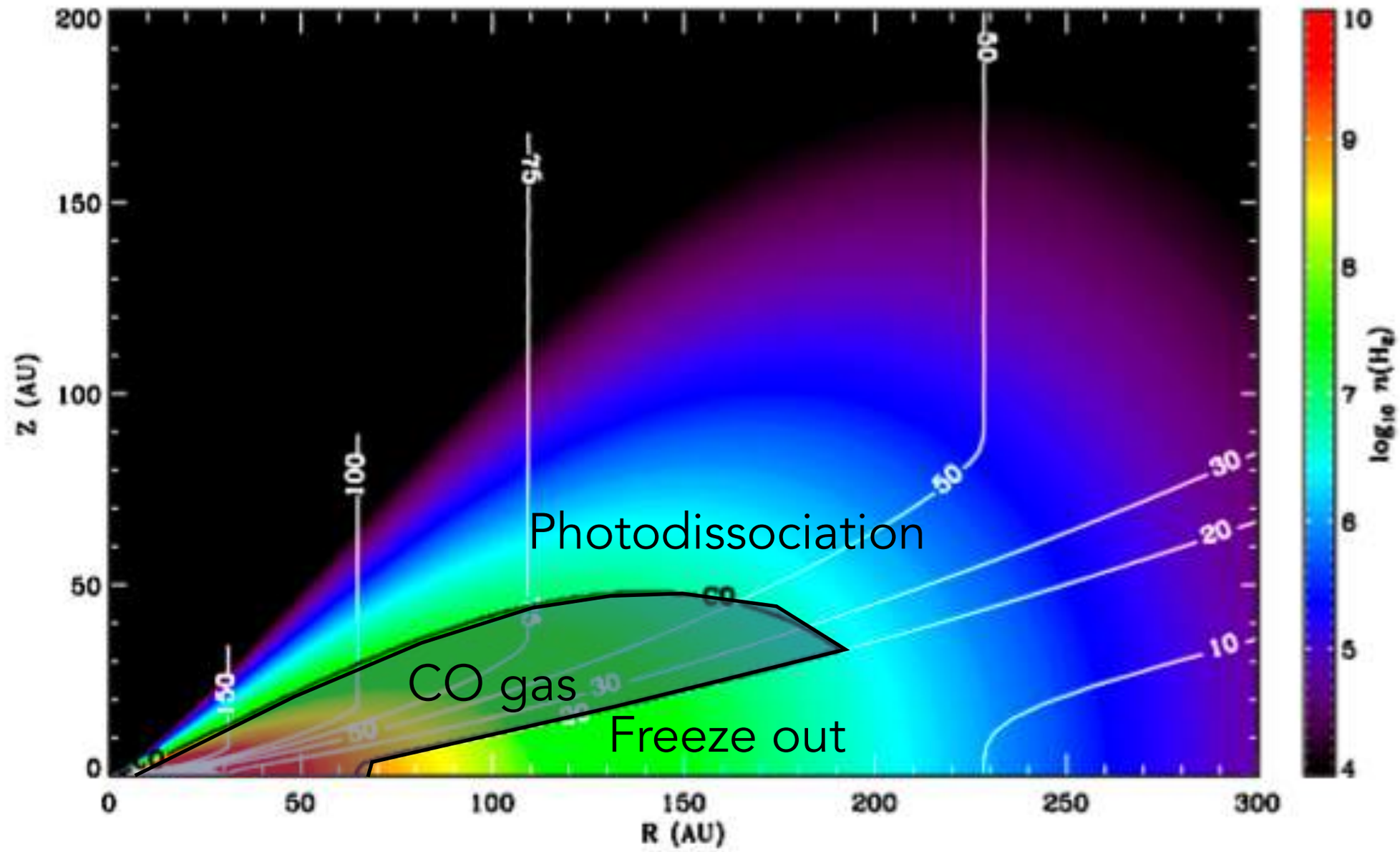
Quantity	Example Tracers
Mass	$^{x}C^{y}O$, HD
Temperature	$^{x}C^{y}O$
Density	CS, H_2CO, HC_3N
Kinematics	$^{x}C^{y}O$, HCO^+
Photodissociation	CN, HCN, C_2H
Ionisation	HCO^+, N_2H^+, CH^+
Deuteration	DCO^+, N_2D^+, DCN
Turbulence	$^{x}C^{y}O$, CS, HC_3N
C/N/O fractionation	$^{x}C^{y}O$, $^{x}C^{z}N$, $H^{x}C^{z}N$
Shocks	SO, SiO, H_2O, CH_3OH
Snow lines	$^{x}C^{y}O$, N_2H^+, DCO^+, HCO^+
Grain-surface processes	Complex molecules

x = 12,13; y = 16,17,18; z = 14,15

Adapted from Henning, & Semenov 2013 Chem Rev., 113, 9016

Disk gas mass measurements

Gas is mainly H_2 (90%) and He (10%) which are difficult to observe: CO (~0.01%) is used as a proxy as the second-most abundant molecule

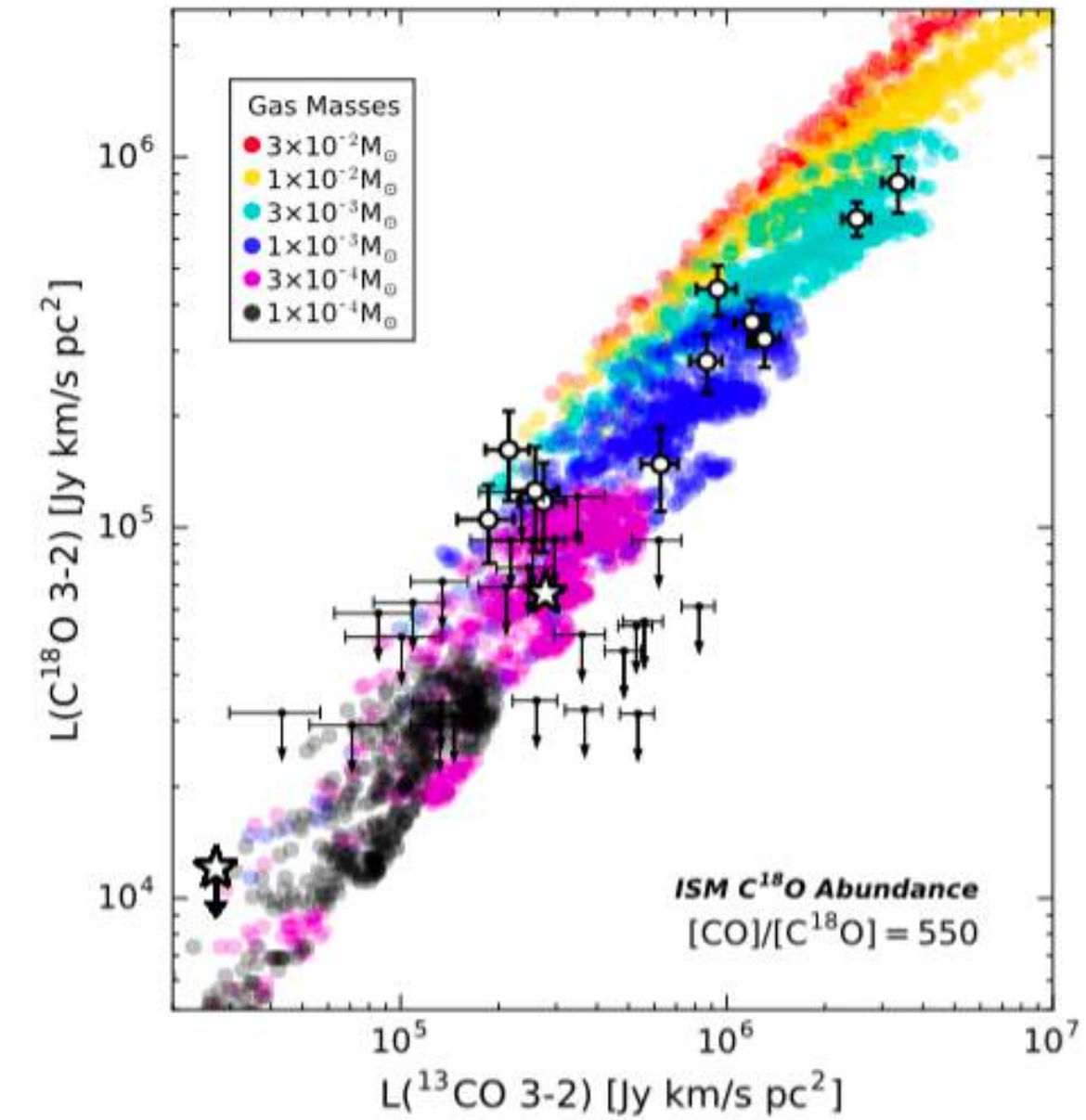


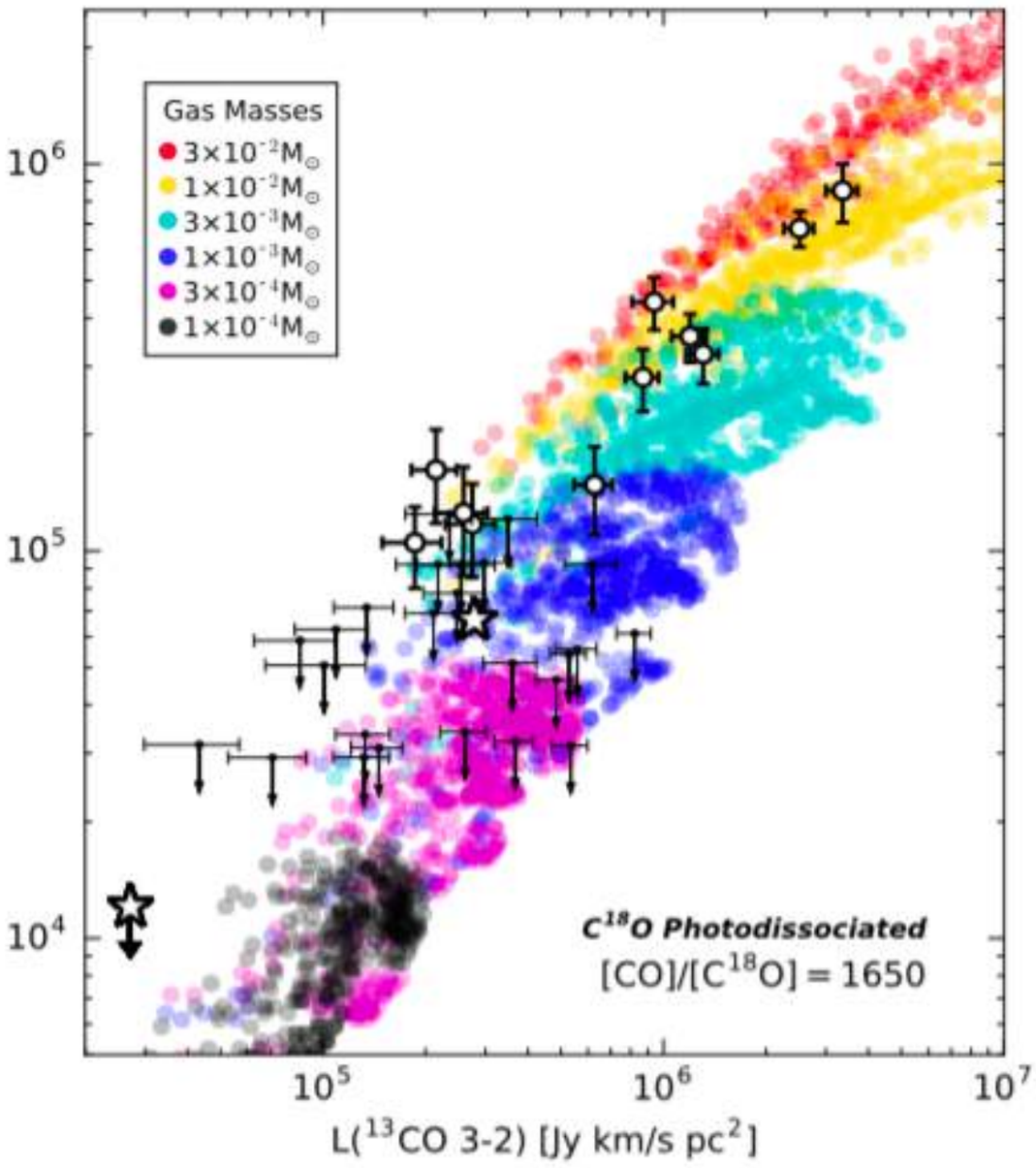
Warning! CO can have a complex distribution due to the disk structure

Williams, J. P & Best, W. M. J. 2014, ApJ, 788, 59

Disk gas mass measurements

Emission from the main CO isotopologues (^{12}CO and ^{13}CO) are optically thick, hence less abundant isotopologues are used (C^{18}O and C^{17}O)



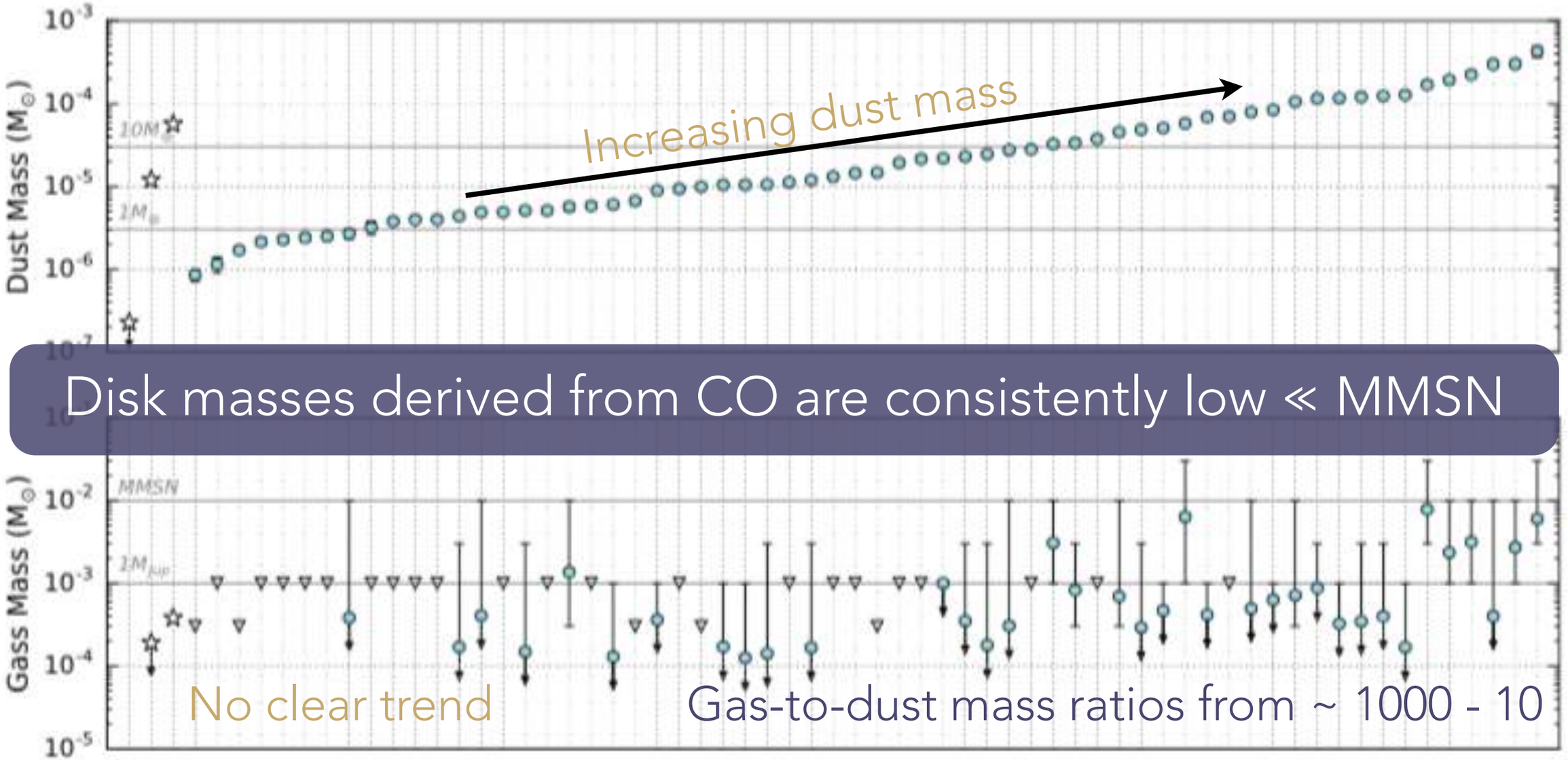


Models are used to provide line fluxes/ratios as a function of gas mass

Ansdell, M., et al. 2016, ApJ, 828, 46; Miotello, A., et al. 2017, A&A, 599, A113

Disk gas mass measurements

Emission from the main CO isotopologues (^{12}CO and ^{13}CO) are optically thick, hence less abundant isotopologues are used (C^{18}O and C^{17}O)



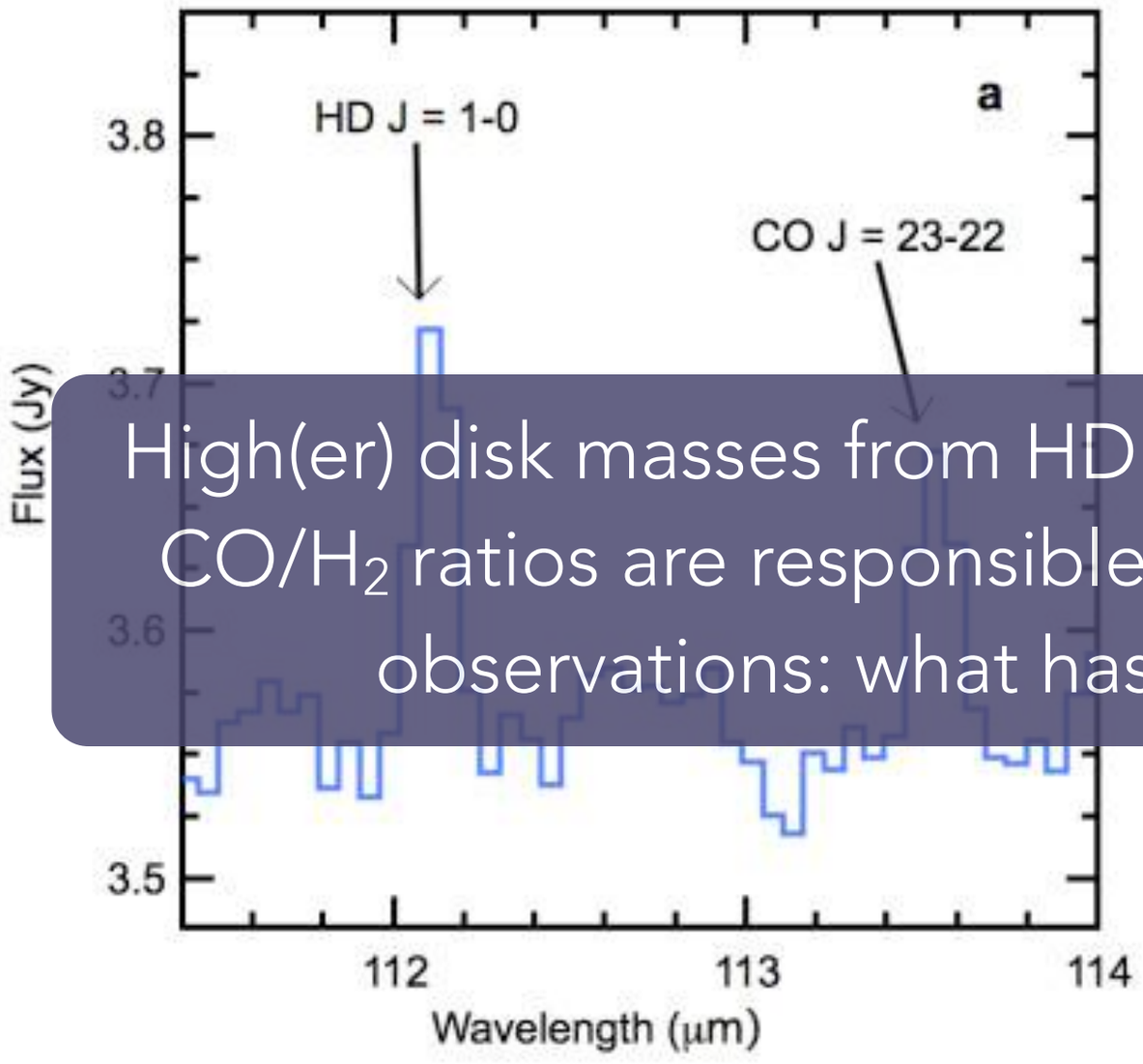
Disk masses derived from CO are consistently low ≪ MMSN

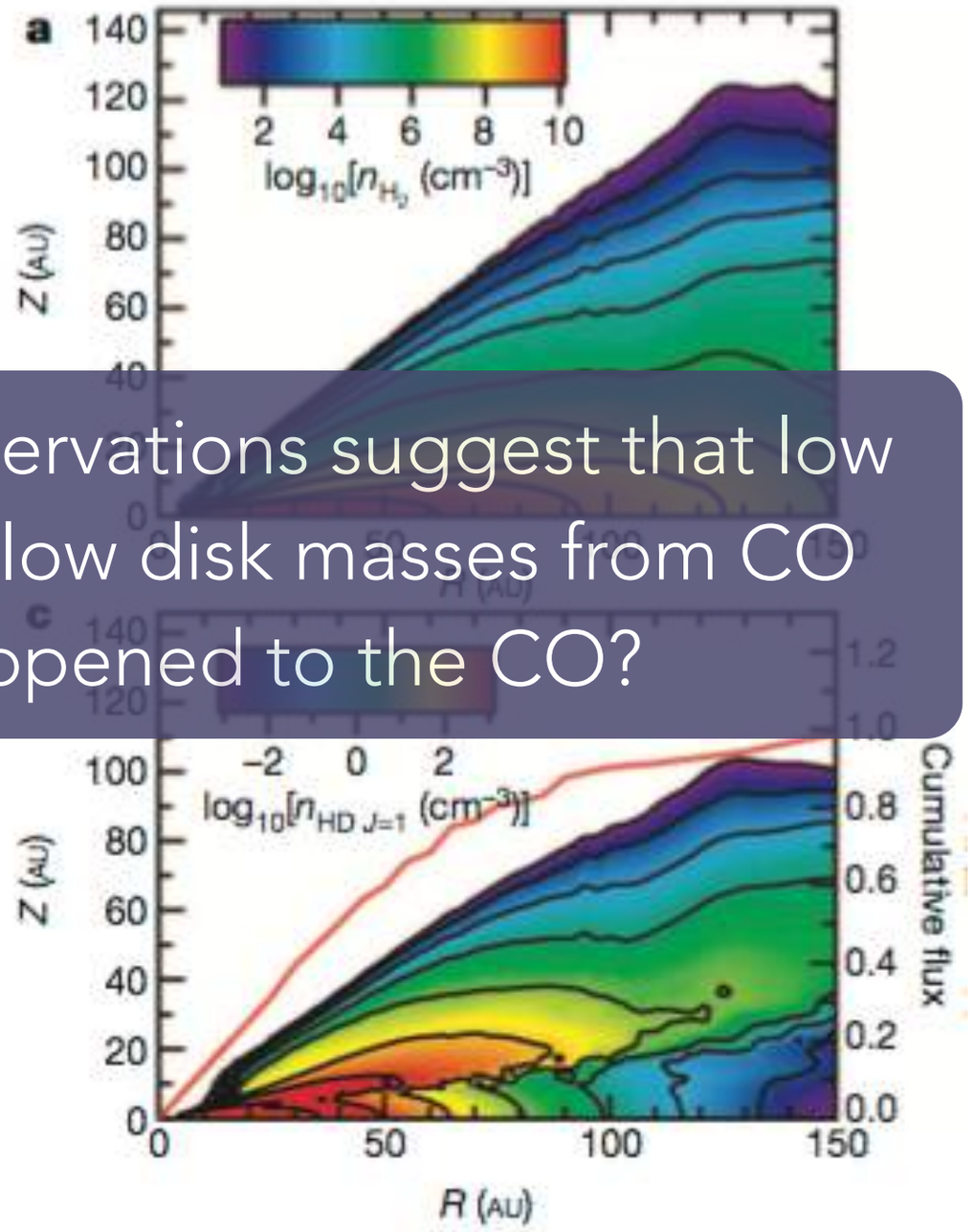
Dust and gas masses from the ALMA Survey of Lupus

Ansdell, M., et al. 2016, ApJ, 828, 46; Miotello, A., et al. 2017, A&A, 599, A113

Disk gas mass measurements

HD is insensitive to chemistry, has a homogeneous distribution ($HD/H_2 \sim 10^{-5}$) and was observable in disks with Herschel



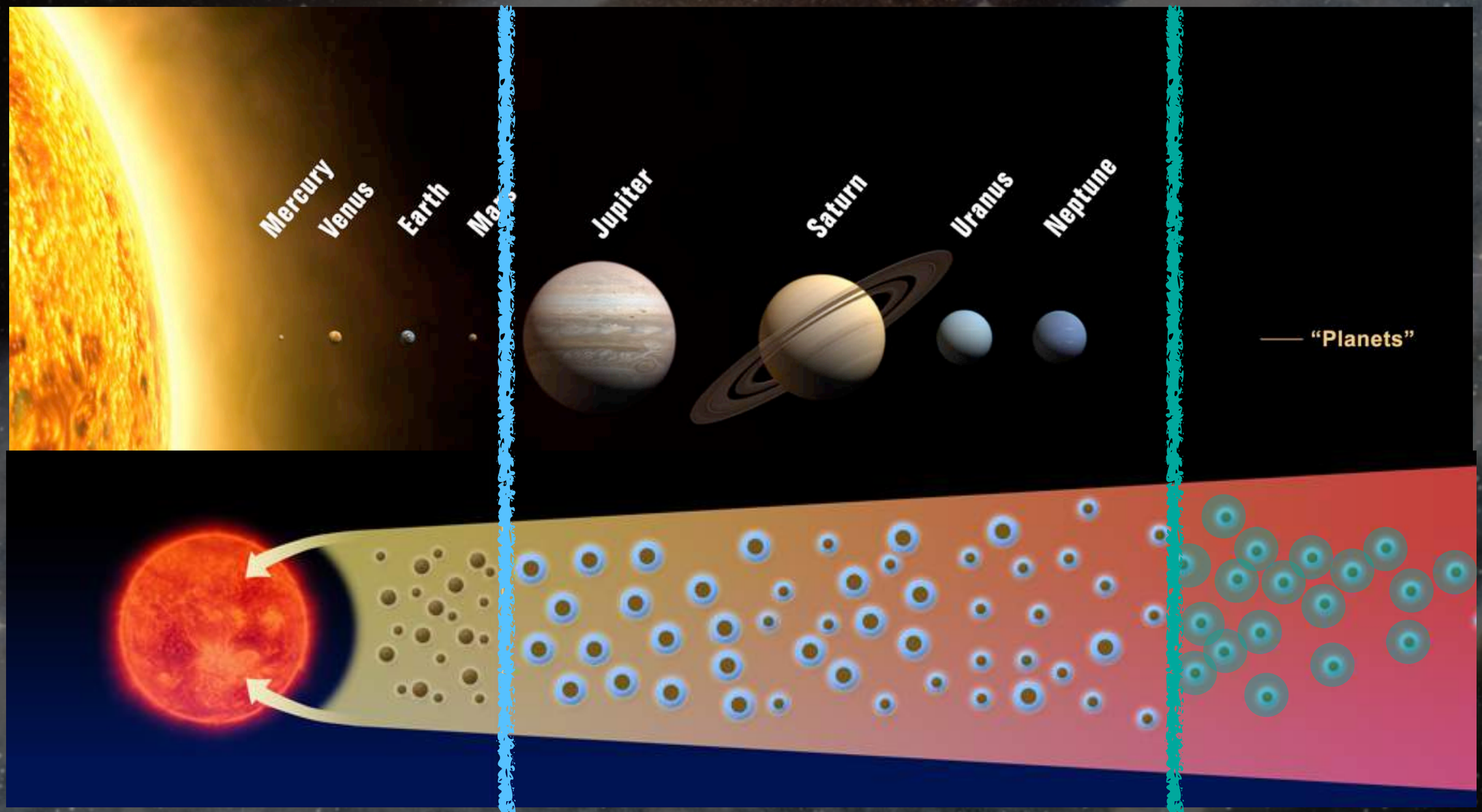


High(er) disk masses from HD observations suggest that low CO/H_2 ratios are responsible for low disk masses from CO observations: what has happened to the CO?

Disk mass (TW Hya) > 0.05 $M_\odot$

Bergin, E. A., et al. 2013, Nature, 493, 644; McClure M. et al. 2016, ApJ, 831, 167; Trapman, L., et al. 2017, A&A, 605, A69

Snowlines



H_2O snow line
~ 1 au

CO snow line
> 10s au

Credit: ALMA (ESO/NAOJ/NRAO)/L. Cieza; IAU

Chemical tracers of snowlines

TW Hya

N_2H^+



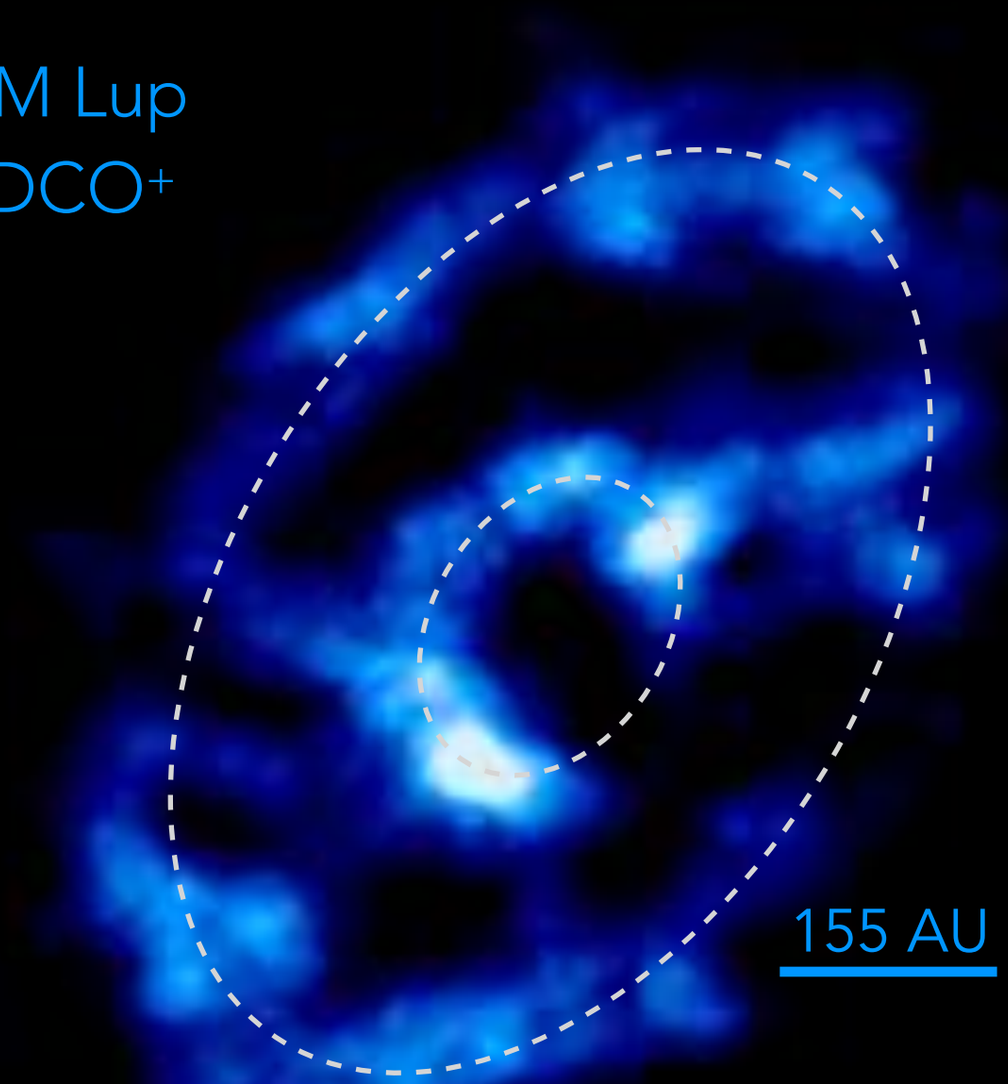
50 AU

$N_2 + H_3^+ \rightarrow N_2H^+ + H_2$

$CO + N_2H^+ \rightarrow HCO^+ + N_2$

IM Lup

DCO^+



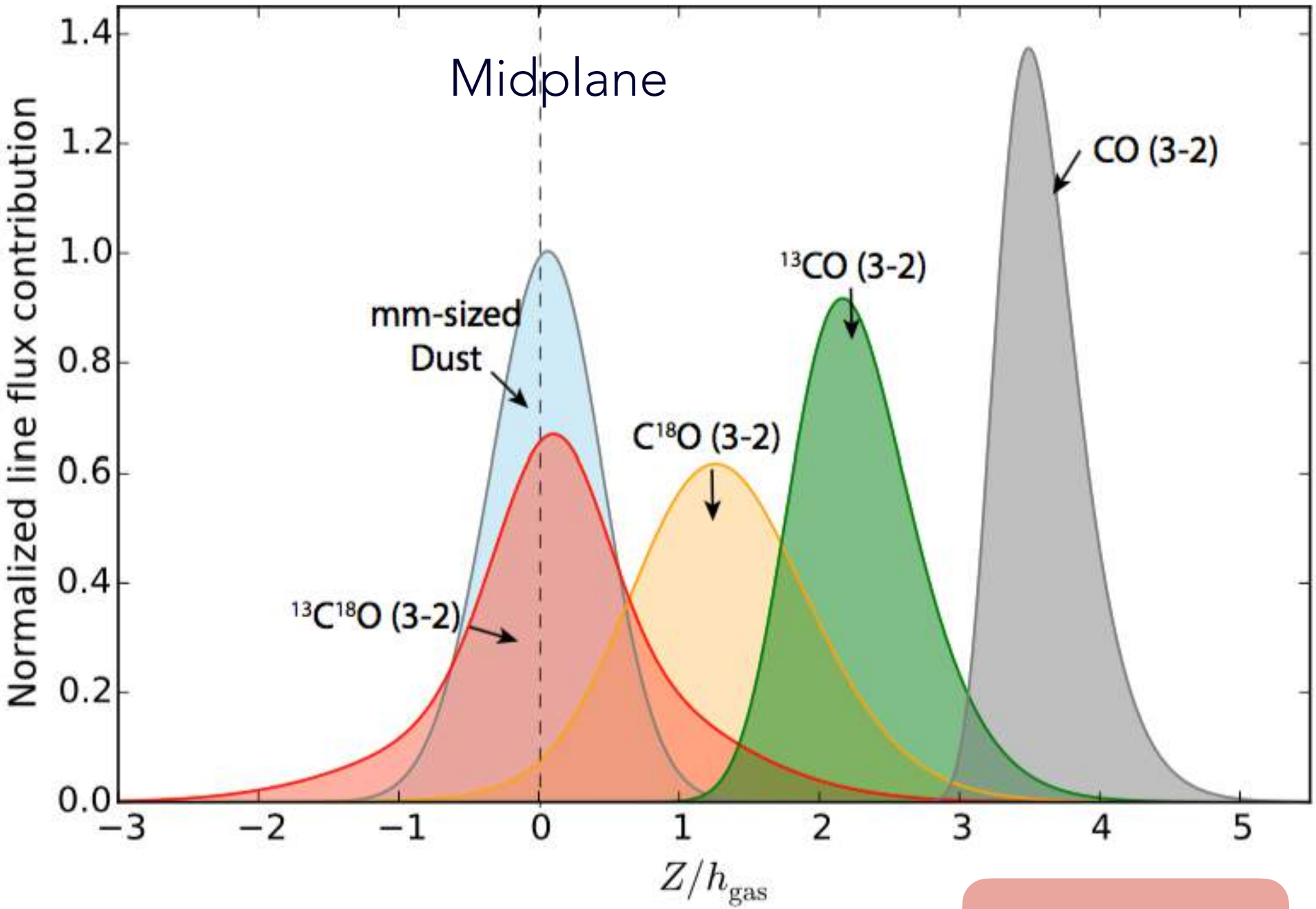
155 AU

$HD + H_3^+ \rightarrow H_2D^+ + H_2$

$CO + H_2D^+ \rightarrow DCO^+ + H_2$

Qi, C., et al. 2013; Öberg, K. I., et al. 2015

Direct detection of CO snowline in TW Hya

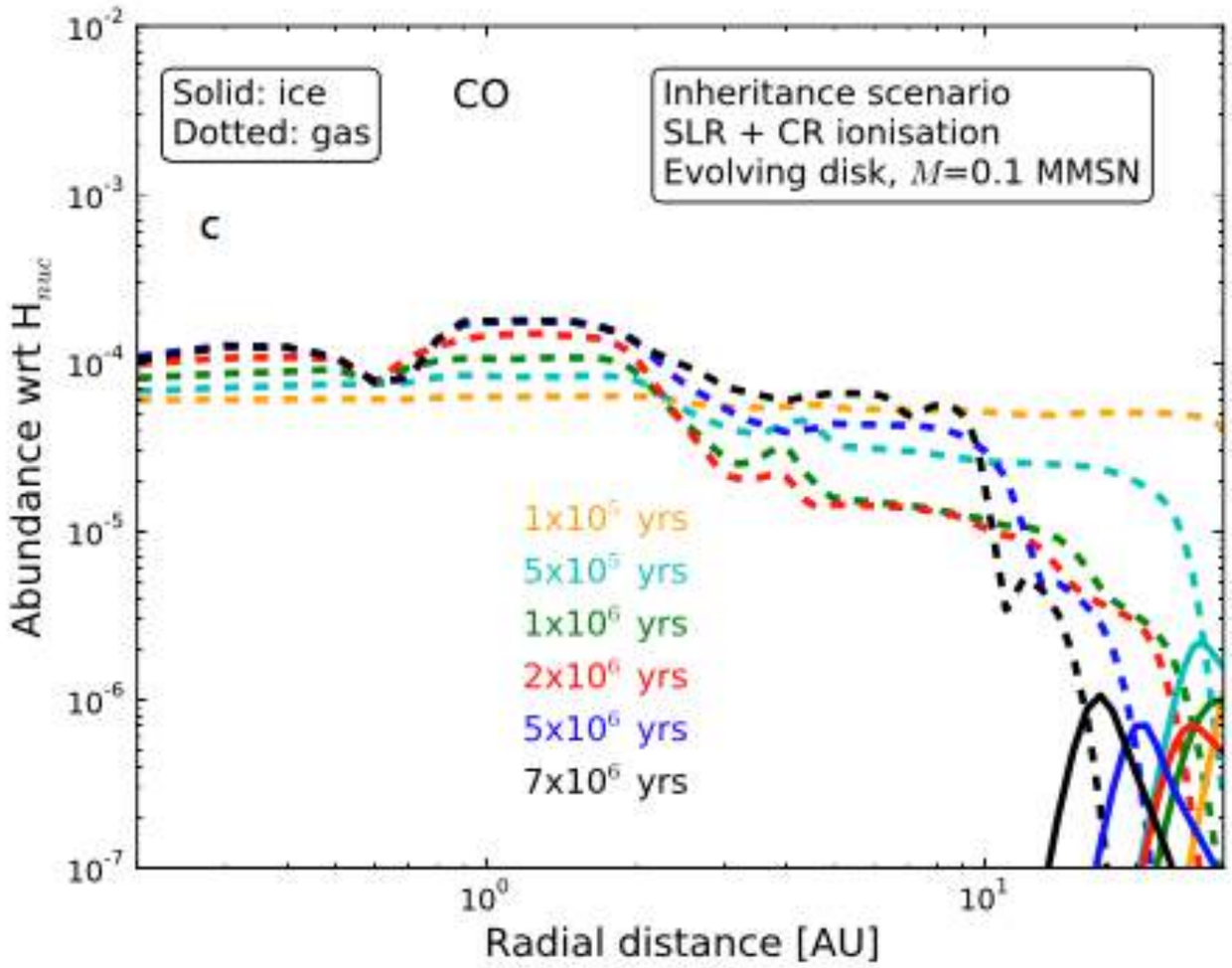


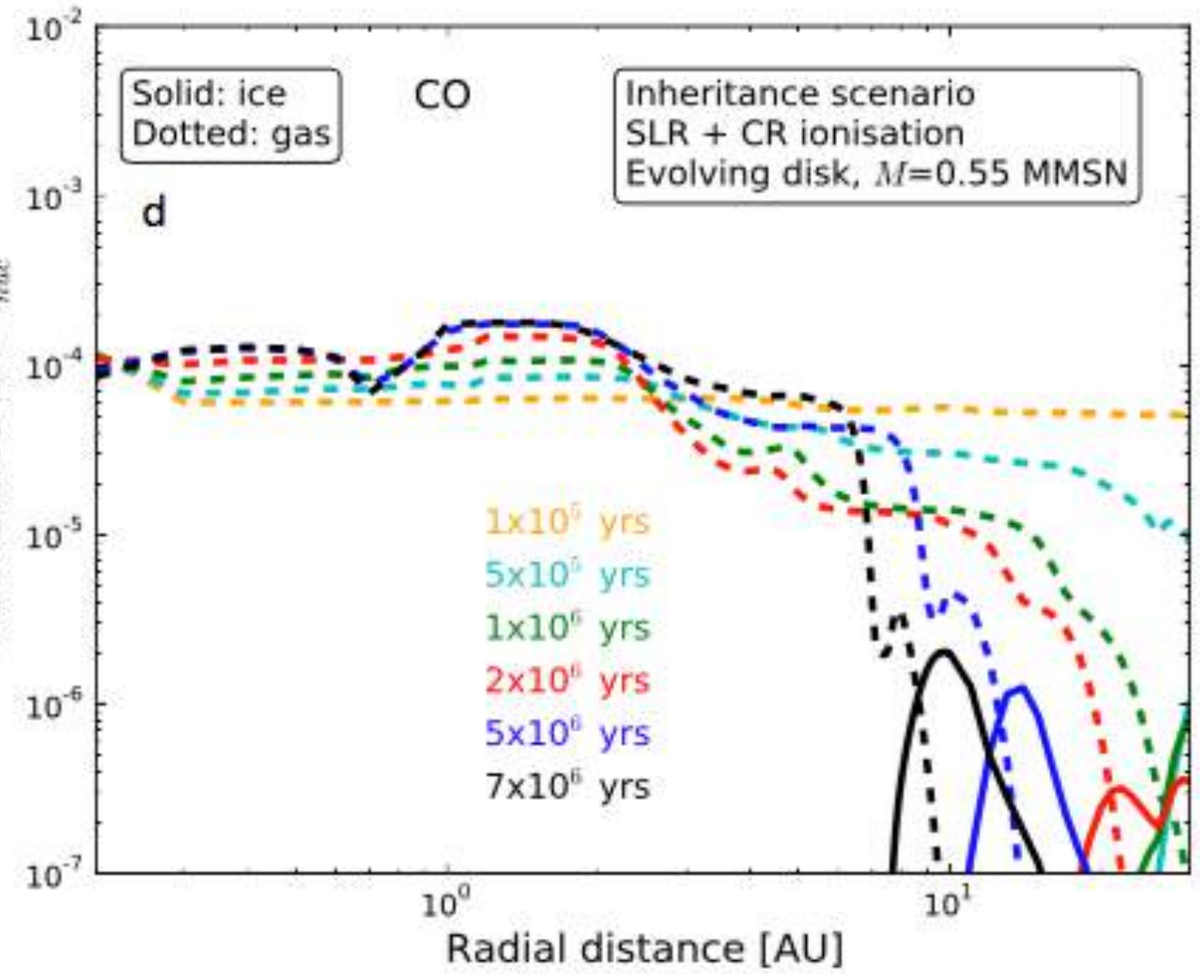
R_{snow} = 20.5 ± 1.3 au; T_{snow} = 27 ± 3 K; $CO/H_2 \sim 10^{-6}$

Schwarz, K., et al. 2016,ApJ, 823, 91; Zhang, Ke, et al. 2017, Nature Astronomy, 1, 130

What is happening to the CO?

Chemical models with gas and ice chemistry predict a chemical conversion of CO into a less volatile form: CO_2, C_xH_y, COMs





Results in a "fake" CO snowline which evolves in time

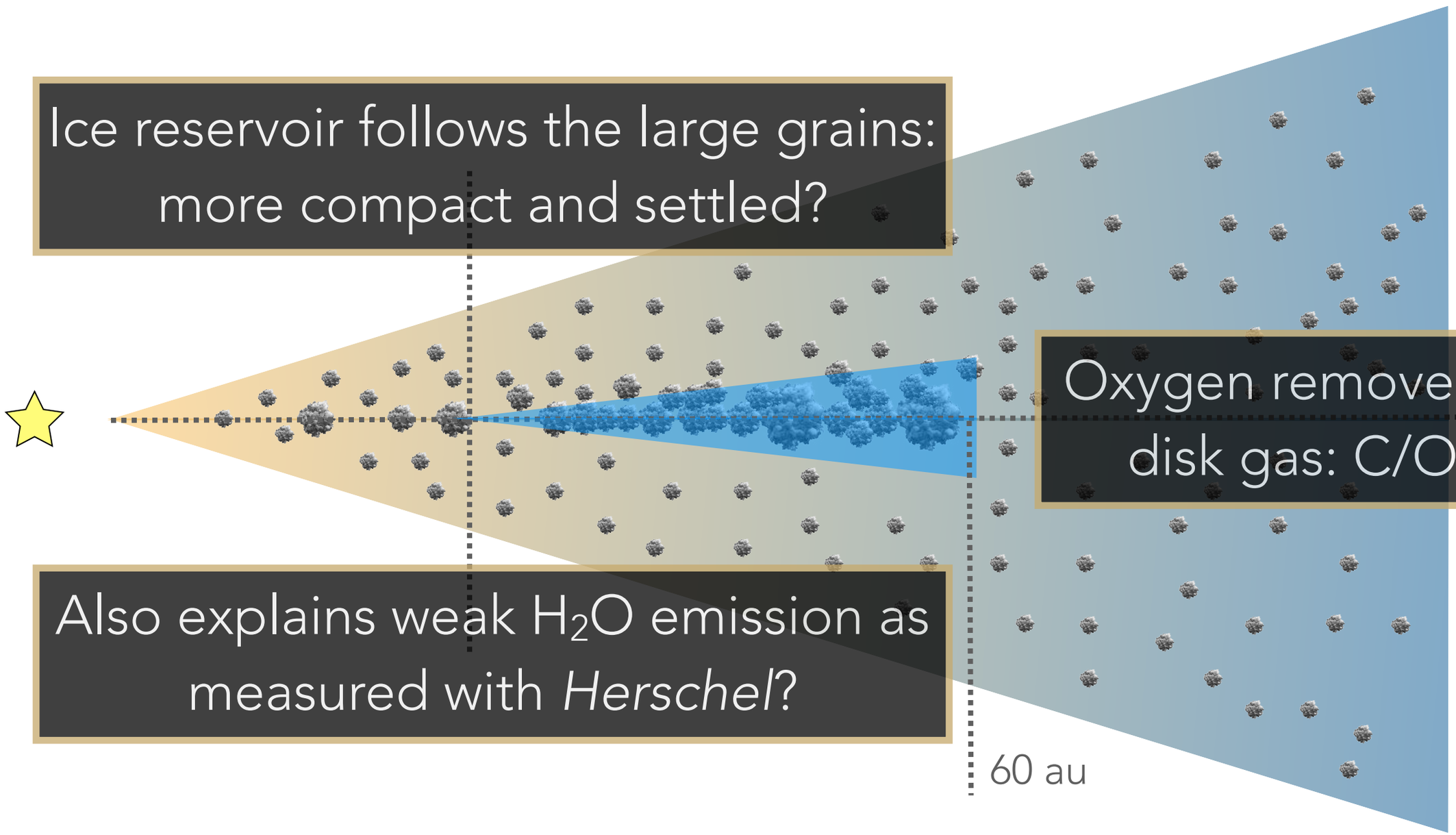
The gas-phase CO in the outer disk is also depleted over time

Aikawa, Y., et al. 1997; Helling, C., et al. 2014; Reboussin, L., et al. 2015; Eistrup, C., et al. 2016, 2017; Yu, M., et al. 2016, 2017

What is happening to the CO?

Large grains in the outer disk will also be coated with oxygen-rich ices: growth, settling, and drift can remove oxygen (and CO) from the gas

Ice reservoir follows the large grains: more compact and settled?



Oxygen removed from disk gas: C/O ~ 1

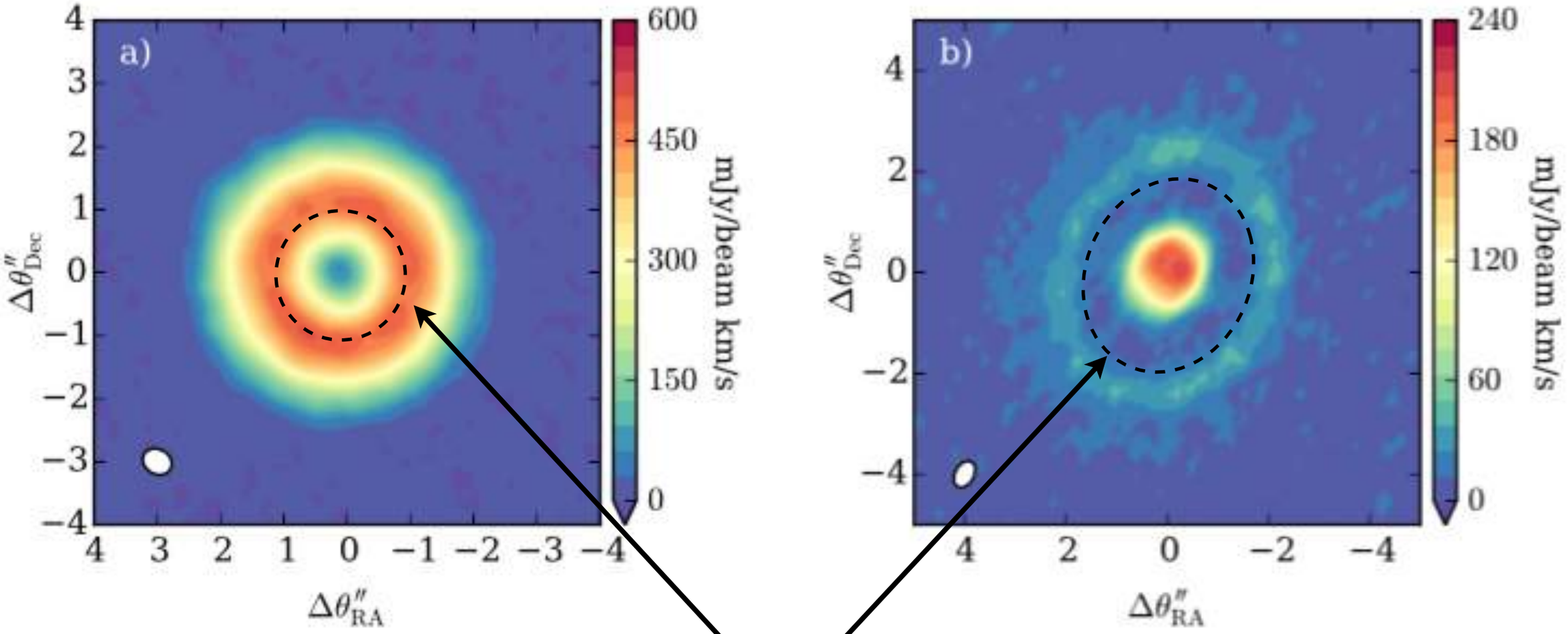
Also explains weak H_2O emission as measured with *Herschel*?

Hogerheijde, M. R., et al. 2011, 2016; Andrews, S., et al. 2016; Bergin, E. A., et al. 2016; Kama, M., et al. 2016; Walsh, C. et al. 2016; Du, F., et al. 2017

Further chemical evidence of dust evolution

TW Hya
C_2H

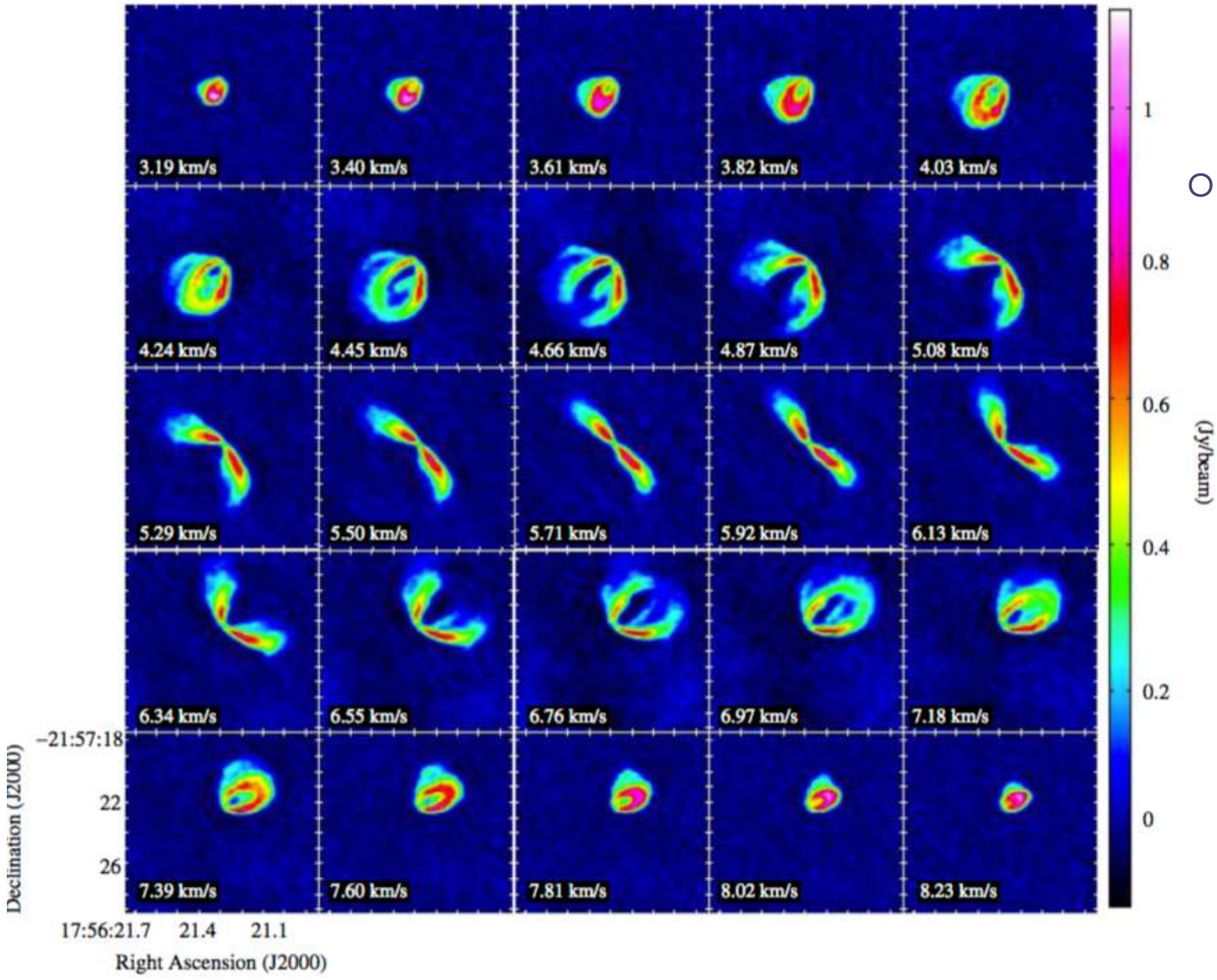
DM Tau
C_2H



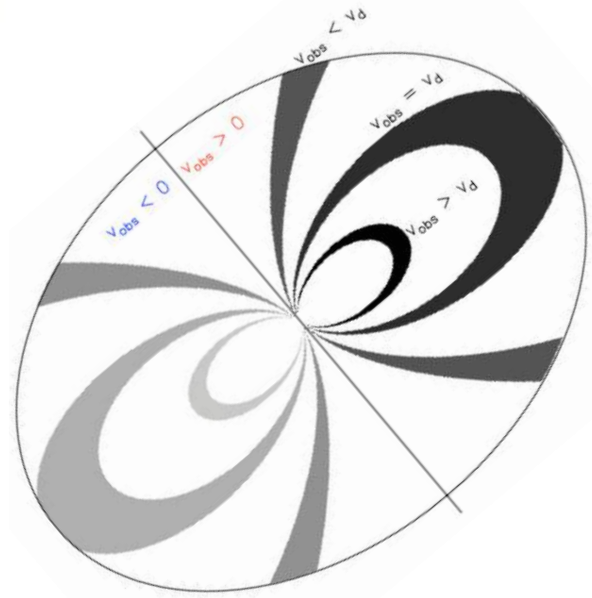
C_2H emission traces the outer edge of the “large” (mm-sized) dust grains: tracing enhanced gas-phase C/O (~ 1) ratio?

Bergin, E. A., et al. 2016, ApJ, 831, 101

CO remains an excellent tracer of gas kinematics



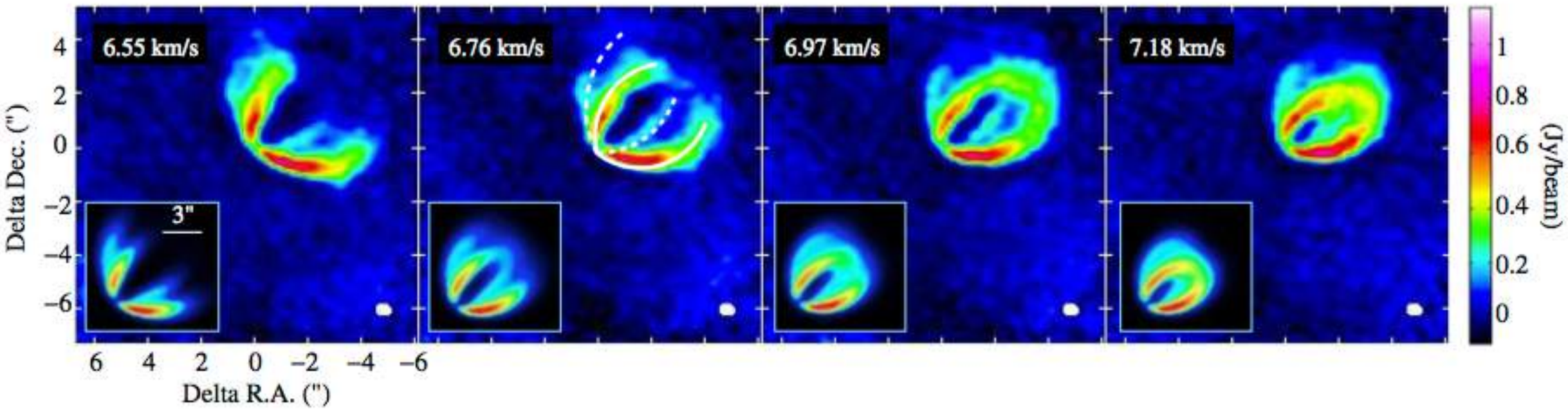
ALMA Cycle 0 observations of CO J=3-2 emission from HD 163296



de Gregorio-Monsalvo, et al. 2013, A&A, 557, 133

CO remains an excellent tracer of gas kinematics

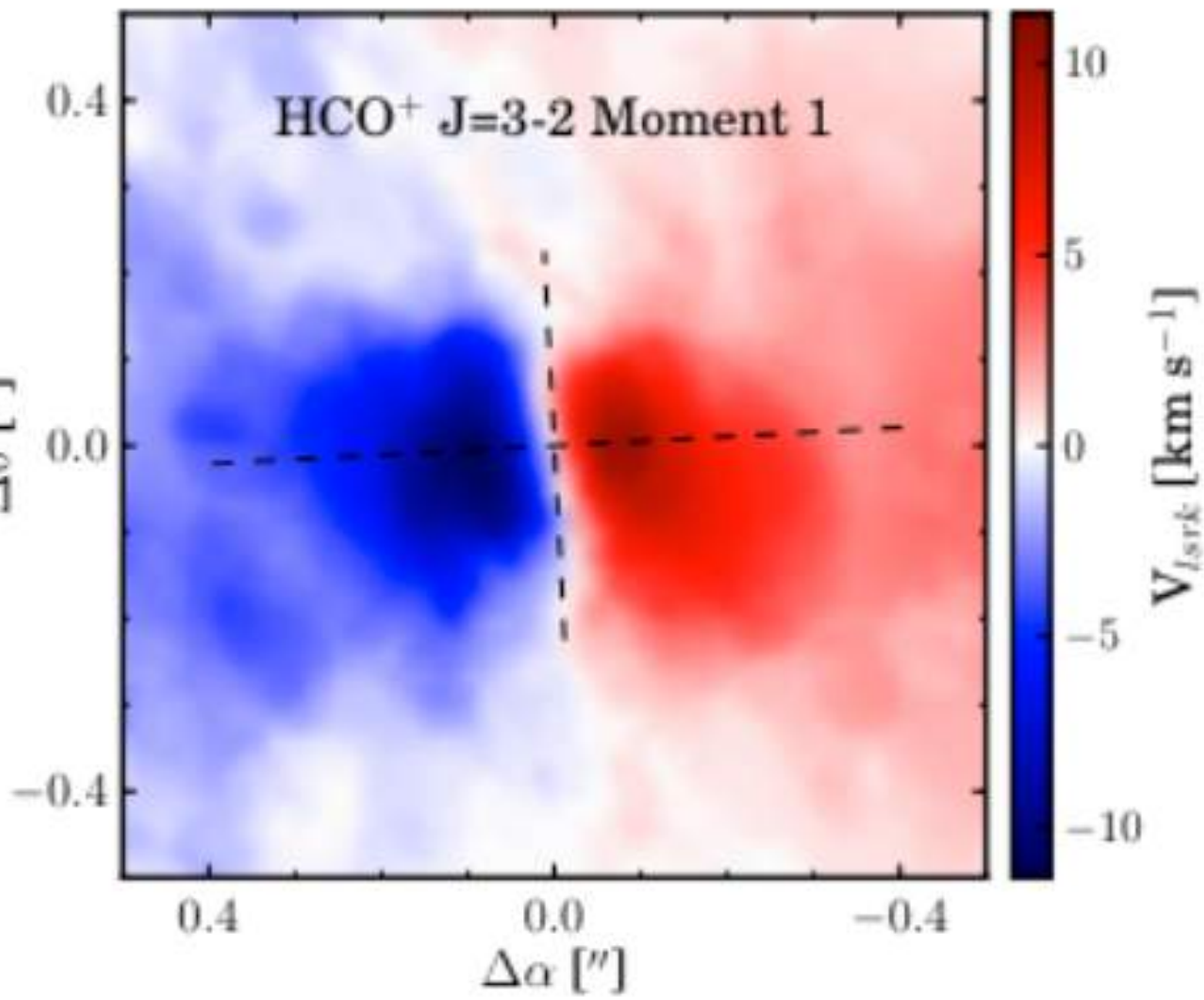
CO J=3-2 shows emission from a moderately flared disk (z/r ~ 0.1) and reveals direct evidence of CO freezeout in the disk midplane



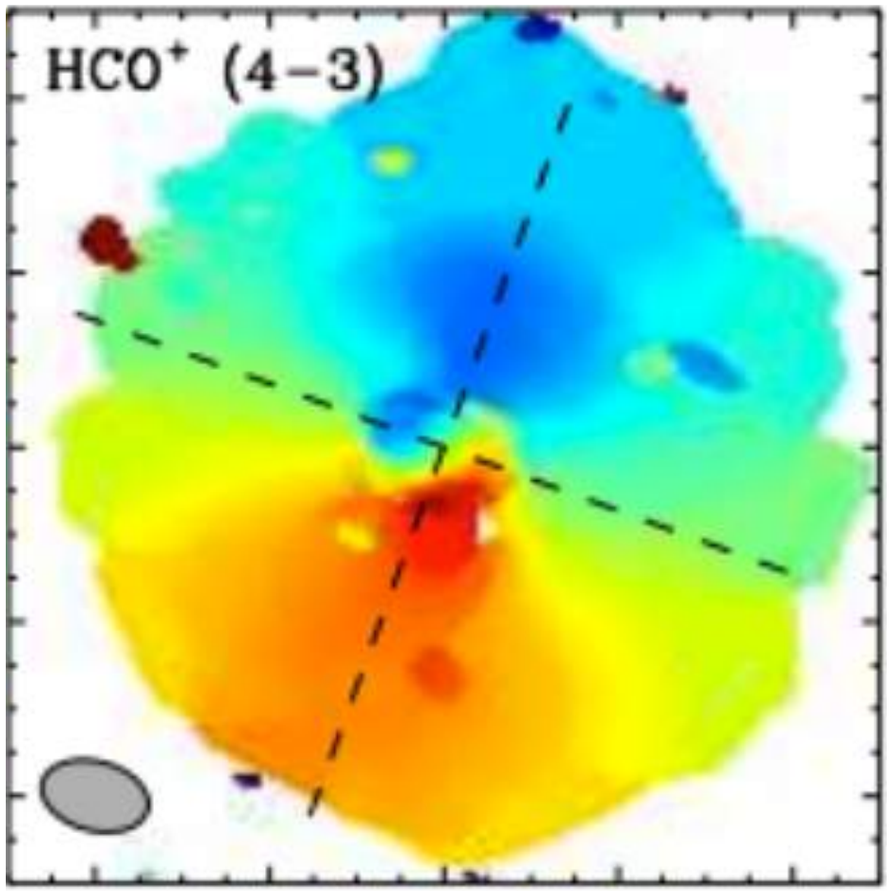
de Gregorio-Monsalvo, et al. 2013, A&A, 557, 133

HCO^+ tracing inner disk kinematics

AA Tau



HD 142527

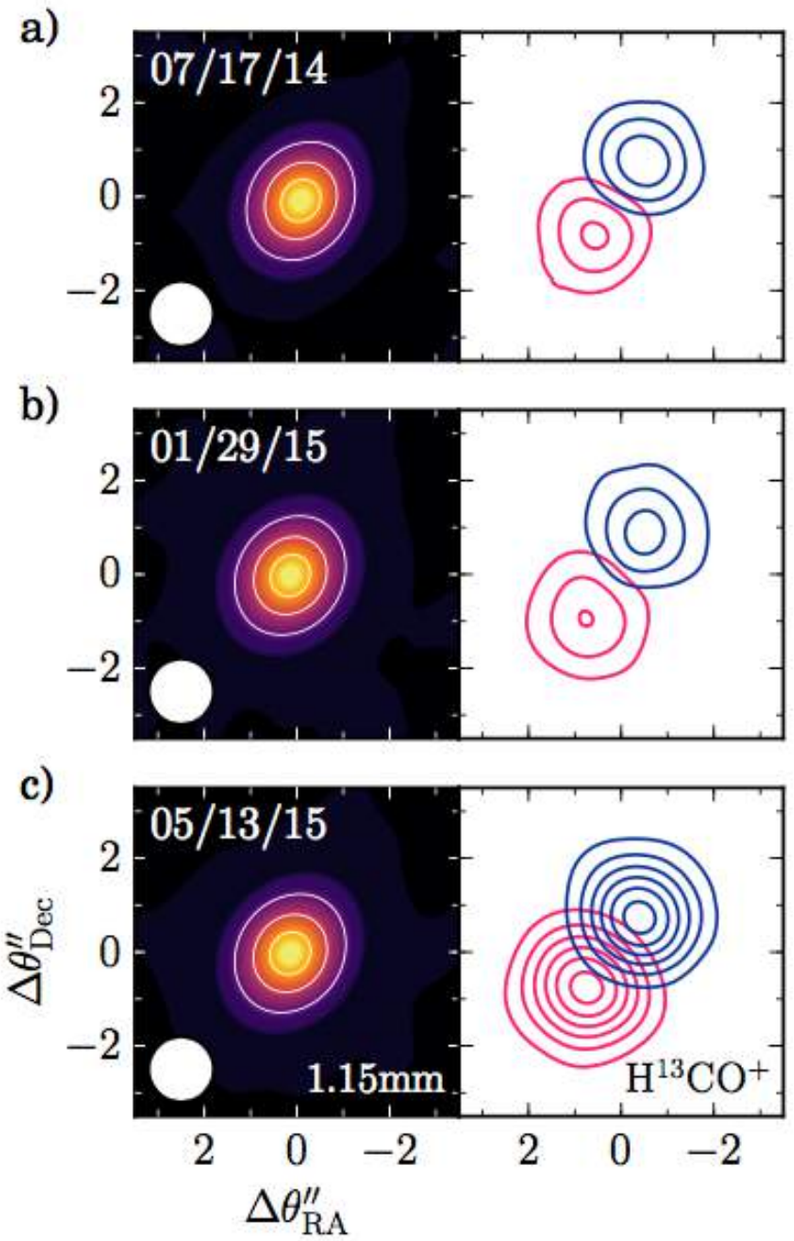


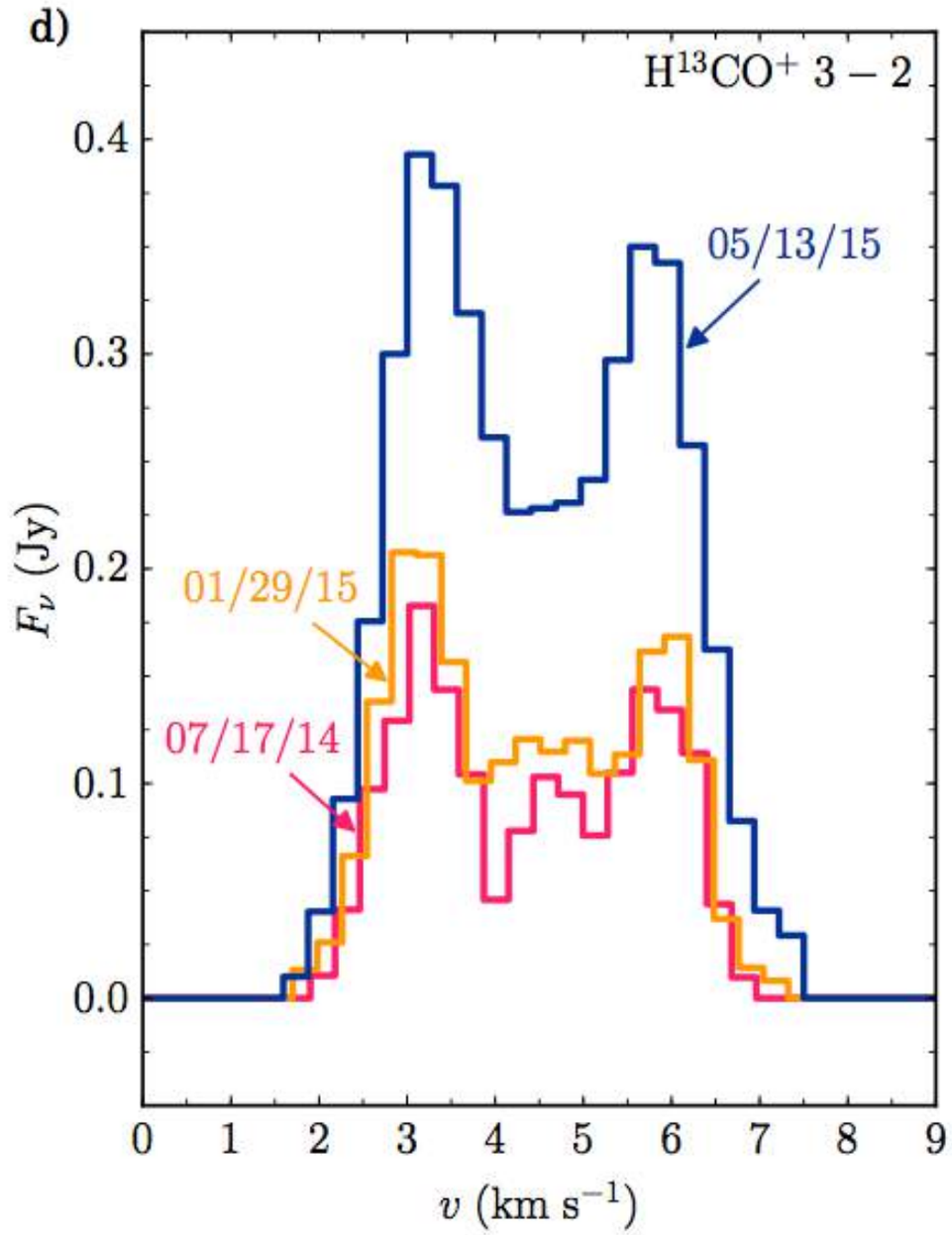
Twist in the first moment map caused by fast (close to free fall) radial flows across dust cavities or warps?

Casassus, S., et al., 2015; Rosenfeld, K. A., et al. 2014; Loomis, R. A., et al. 2017

Stellar variability traced in cation emission

Multi-epoch observations of $H^{13}CO^+$ in IM Lup



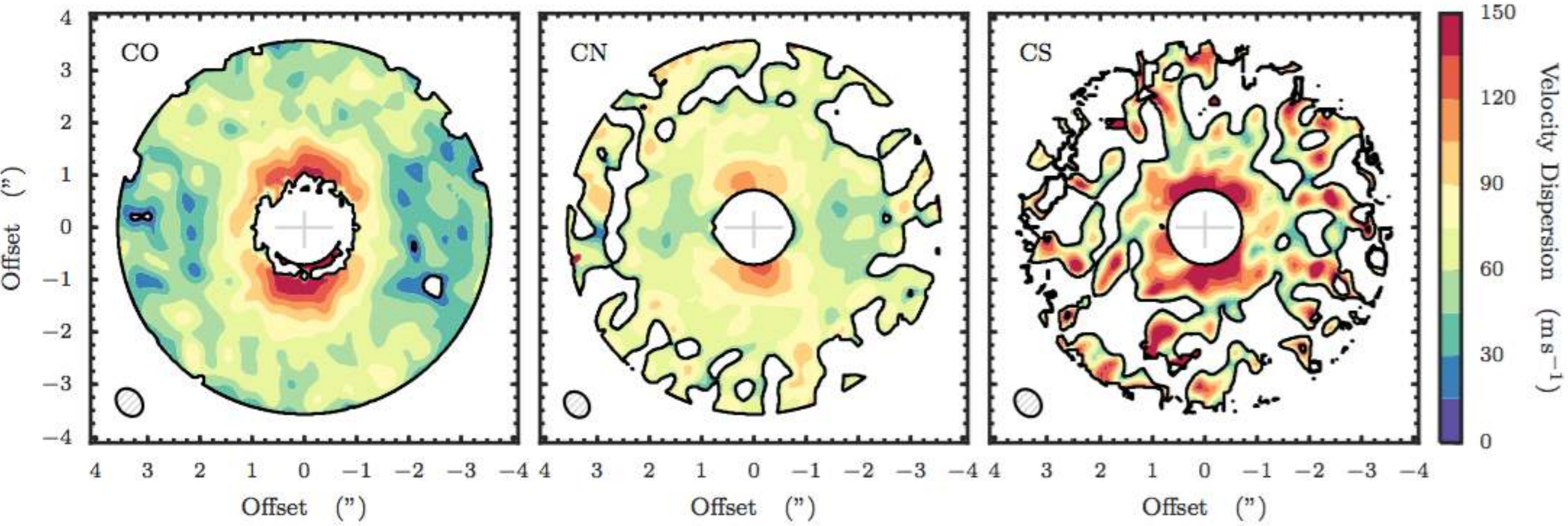


Confirmation of real-time variability in ionisation in the disk atmosphere

Cleeves, L. I., et al. 2017, ApJL, 843, L3

Constraining turbulence in disks

Contribution to line broadening by turbulence constrained in TW Hya through subtraction of thermal and rotational components



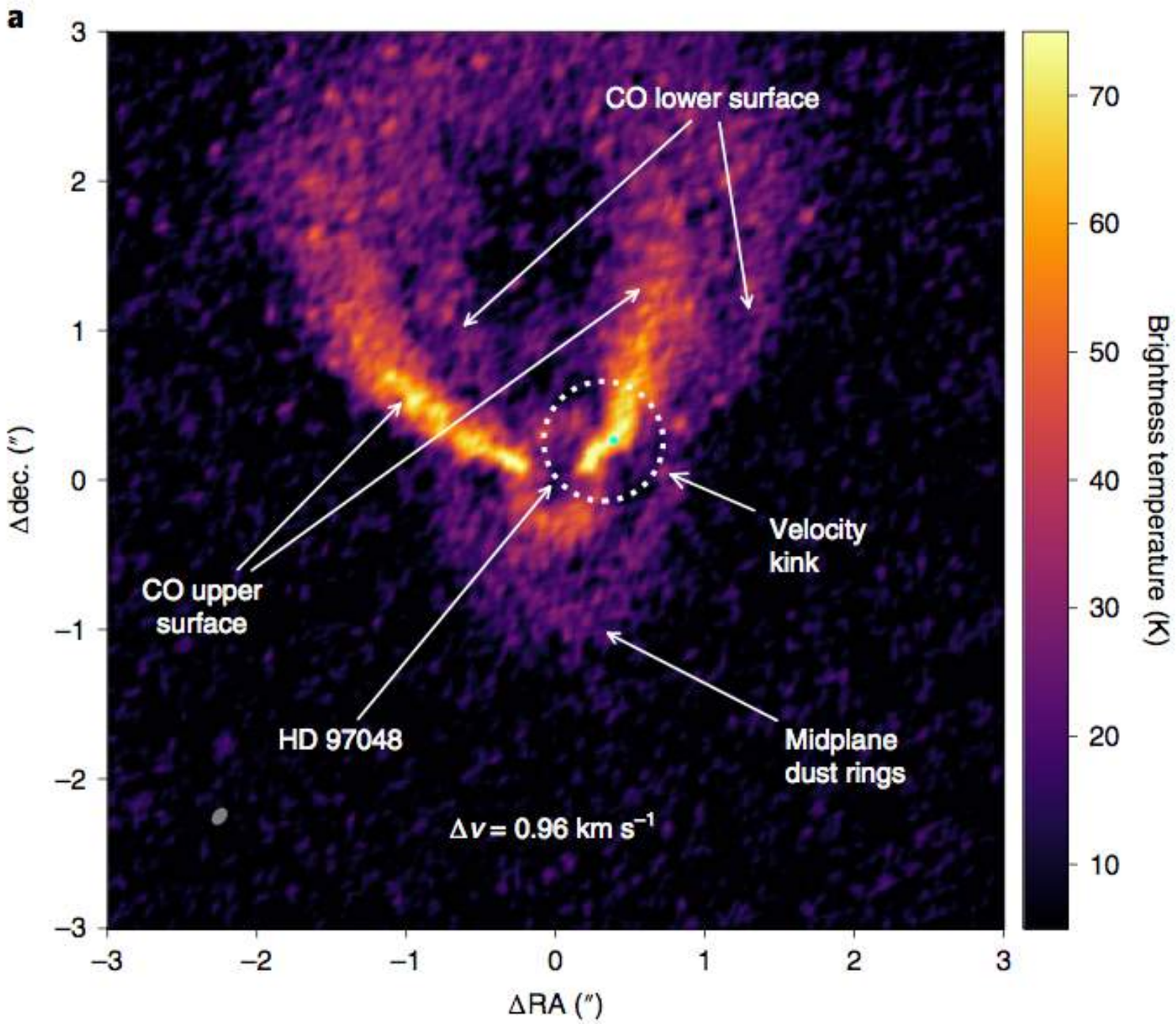
δv_{turb} = 130 m/s @ 40 au to 50 m/s in outer disk

Corresponds to 0.2 - 0.4 times the local sound speed

Hughes, M., et al. 2011; Guilloteau, S., et al. 2011; Flaherty, K., et al. 2015, 2017; Teague, R., et al. 2016

Molecular emission at high spatial resolution

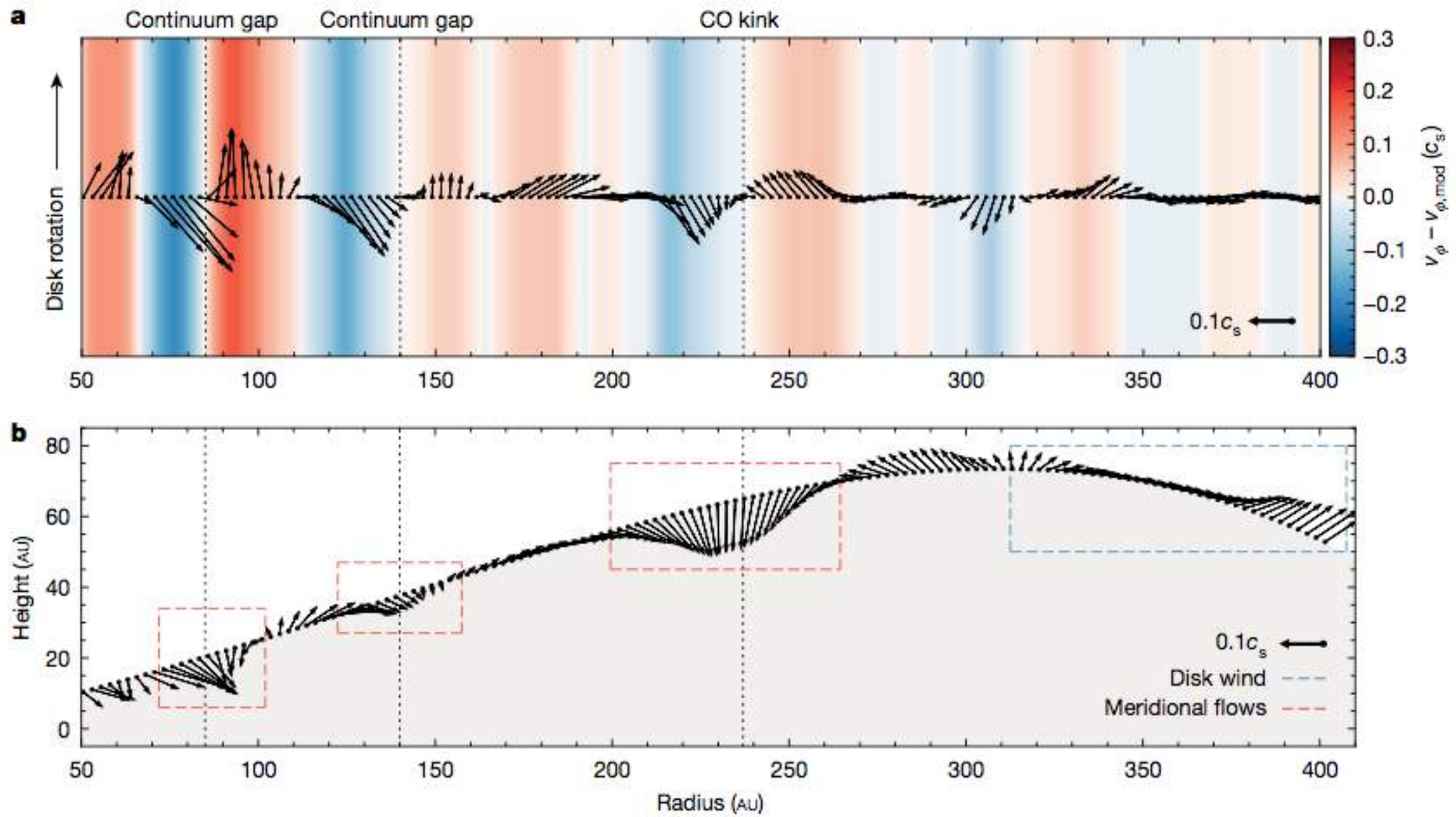
Velocity wiggle/kink coinciding with a dust gap in HD 97048



Pinte et al. 2019, Nature, Astronomy, 3, 1109; 2020, ApJ, 890, L9

Molecular emission at high spatial resolution

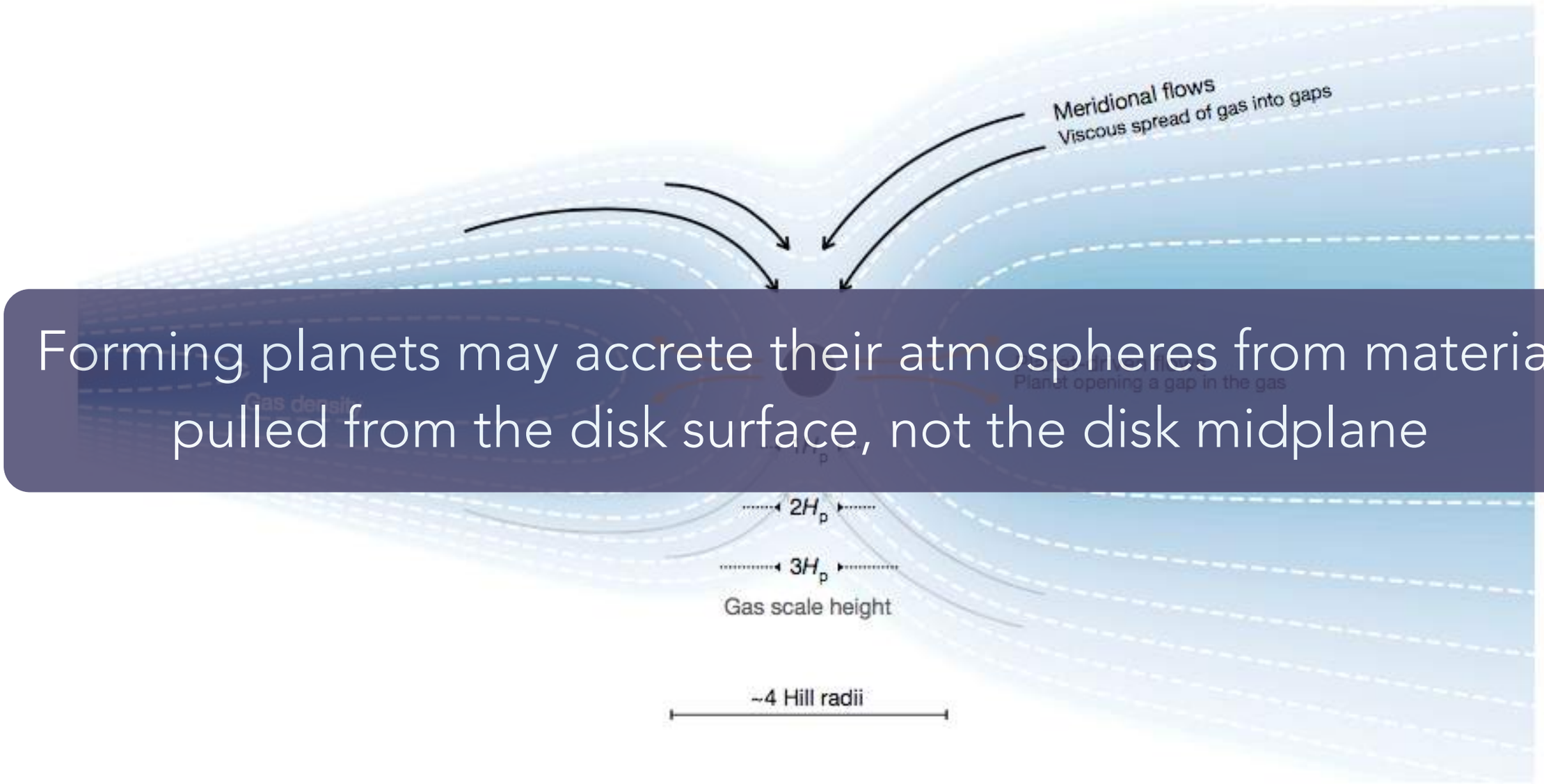
Velocity mapping of HD 163296 revealing meridional flows in CO



Teague et al. 2019, Nature, 574, 378

Evidence for still-accreting (forming) planets?

Meridional flows triggered by an accreting embedded planet

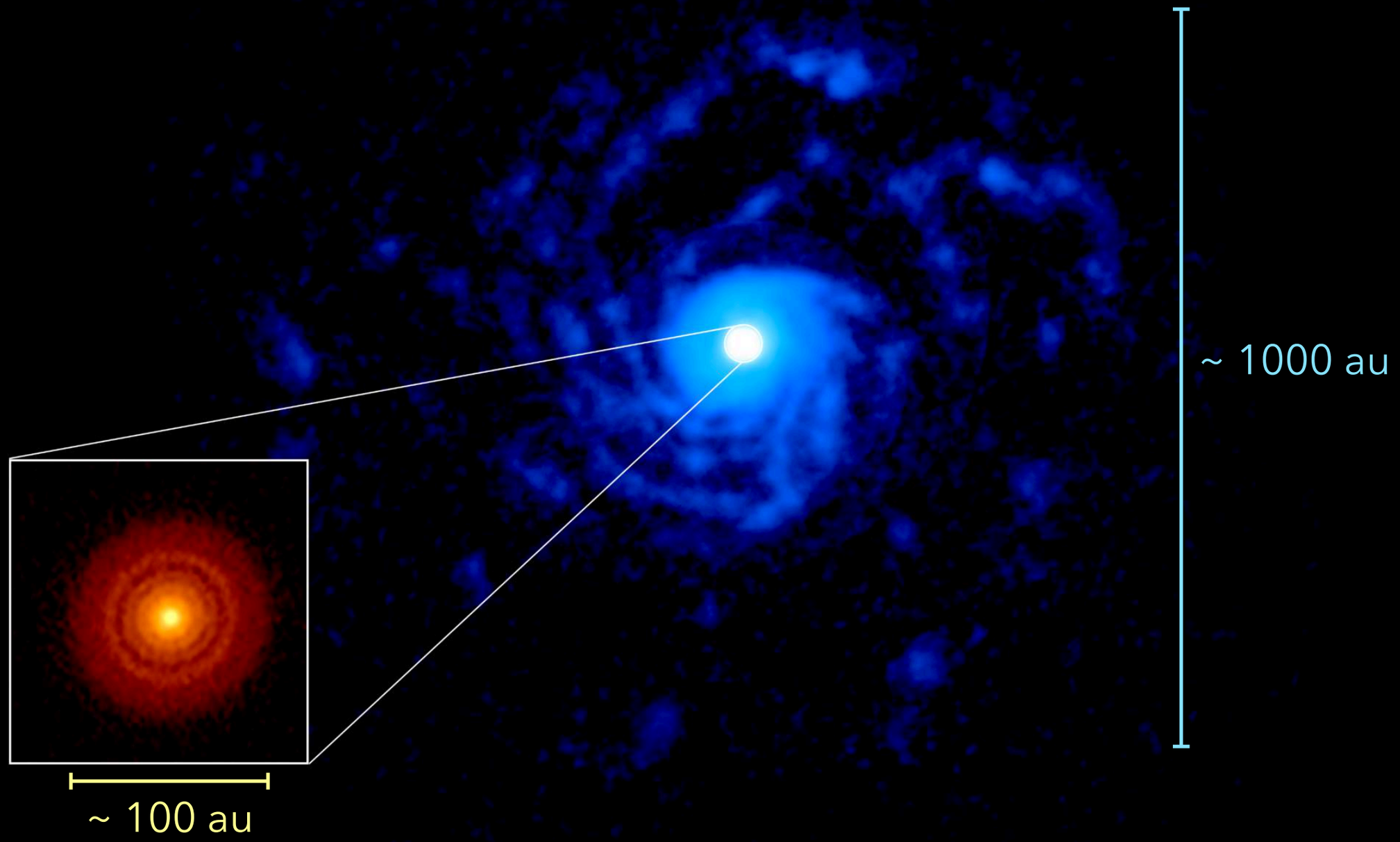


Forming planets may accrete their atmospheres from material pulled from the disk surface, not the disk midplane

Teague et al. 2019, Nature, 574, 378; Cridland et al. 2020, A&A, 635, A68

Evidence for ongoing large-scale accretion

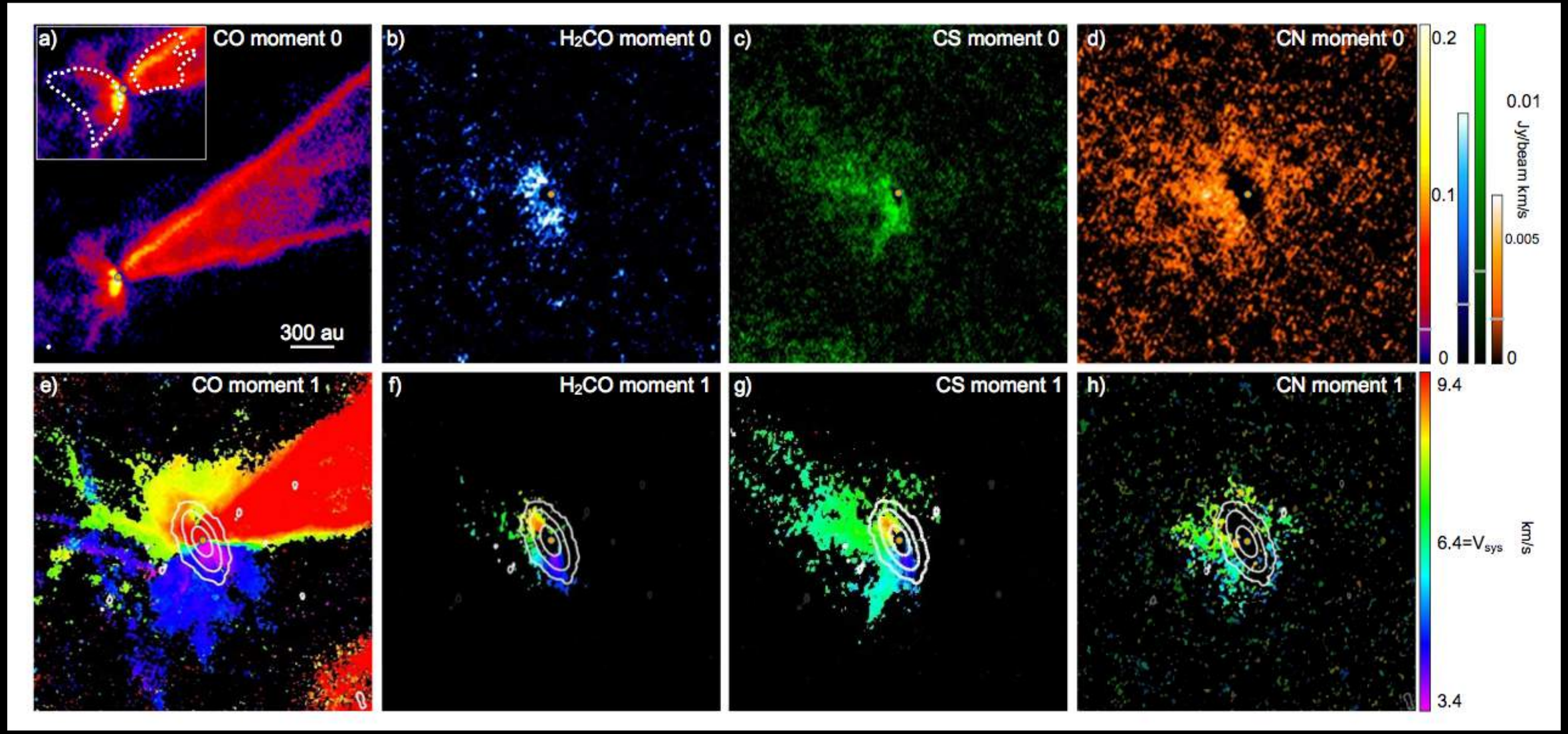
CO spirals detected well beyond the compact dust disk in RU Lup



ALMA (ESO/NAOJ/NRAO), J. Huang and S. Andrews; NRAO/AUI/NSF, S. Dagnello; Huang et al. 2020, ApJ, 898, 140

Chemistry at high spatial and spectral resolution

Molecular emission at ~ 0.1″ resolution towards DG Tau B



DG Tau B is a Class I source: molecular emission evident from disk, envelope, infall, and outflow

Garufi et al. 2020, A&A, 636, A65

The Chemistry of Planet Formation

Öberg, Aikawa, Bergin, Guzman, Walsh
MAPS ALMA Large Programme

To resolve the chemistry occurring in the planet-forming region, we require molecular line observations at high spectral (~ 0.1 km/s) and spatial resolution (~0.1"), and with high sensitivity (< 1 mJy/beam) at (sub)mm wavelengths



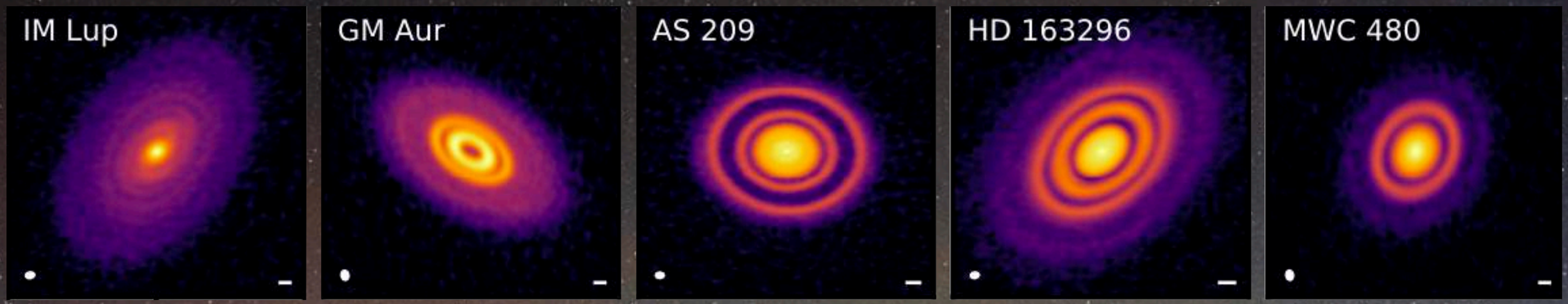
Credit: ESO/C. Malin

The Chemistry of Planet Formation

Öberg, Aikawa, Bergin, Guzman, Walsh
MAPS ALMA Large Programme

Younger
Lower-mass

Older
Higher-mass



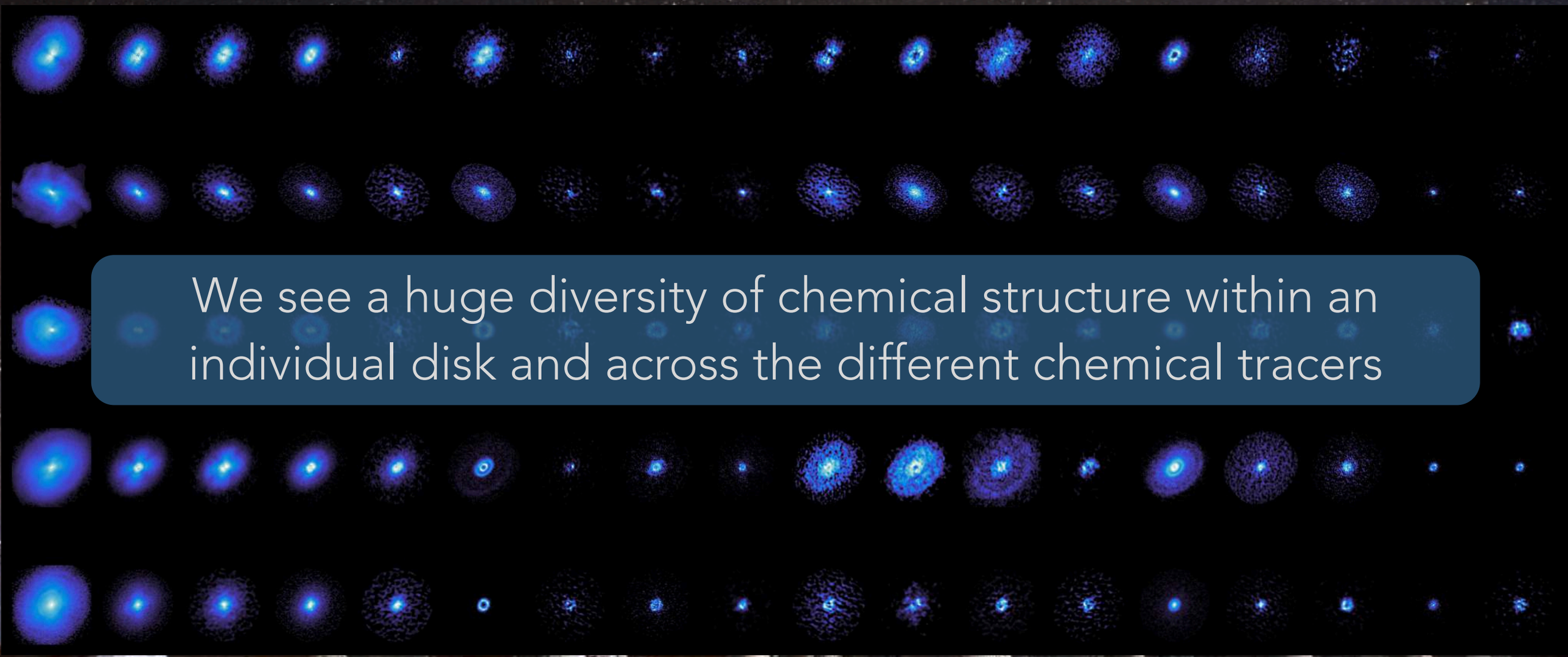
Continuum @ 220 GHz

Scale-bar = 20 au

Image credit: ESO/C. Malin: https://www.eso.org/public/images/ann12092a/; Öberg & MAPS Team 2021, ApJS, 257, 1

The Chemistry of Planet Formation

Öberg, Aikawa, Bergin, Guzman, Walsh
MAPS ALMA Large Programme

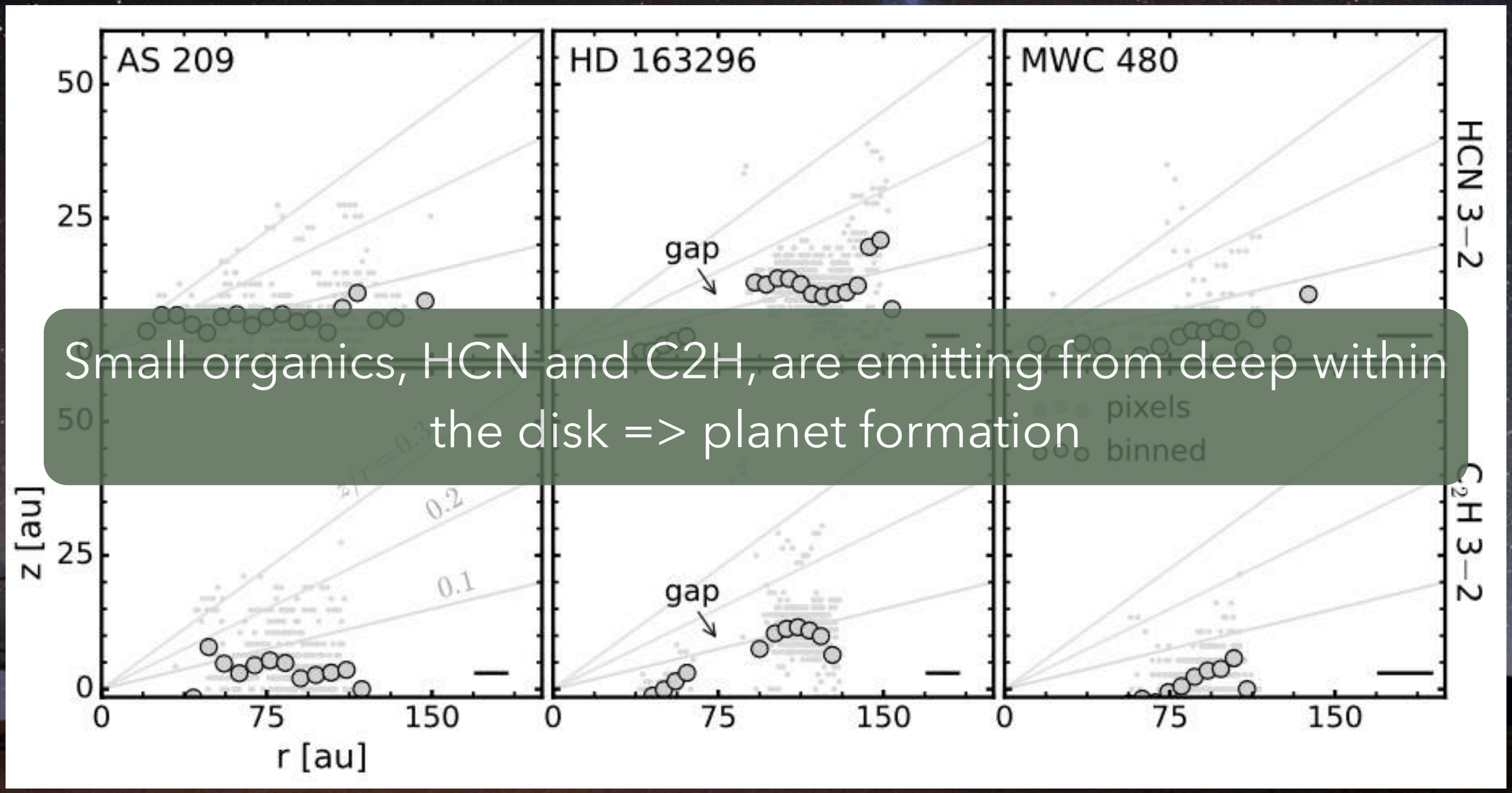


We see a huge diversity of chemical structure within an individual disk and across the different chemical tracers

Law & MAPS Team 2021, ApJS, 257, 3

The Chemistry of Planet Formation

Öberg, Aikawa, Bergin, Guzman, Walsh
MAPS ALMA Large Programme

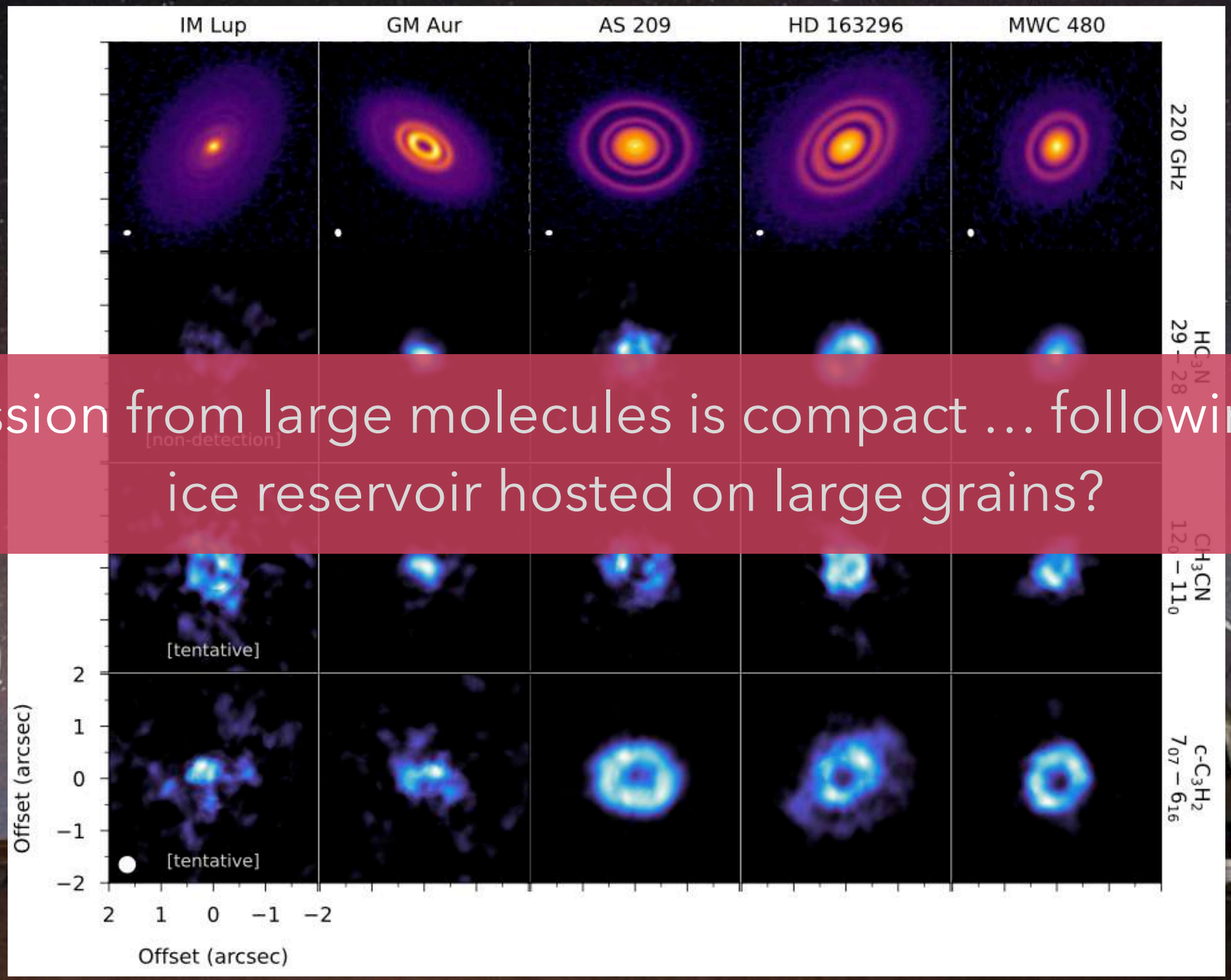


Small organics, HCN and C2H, are emitting from deep within the disk => planet formation

Law & MAPS Team 2021, ApJS, 257, 4

The Chemistry of Planet Formation

Öberg, Aikawa, Bergin, Guzman, Walsh
MAPS ALMA Large Programme

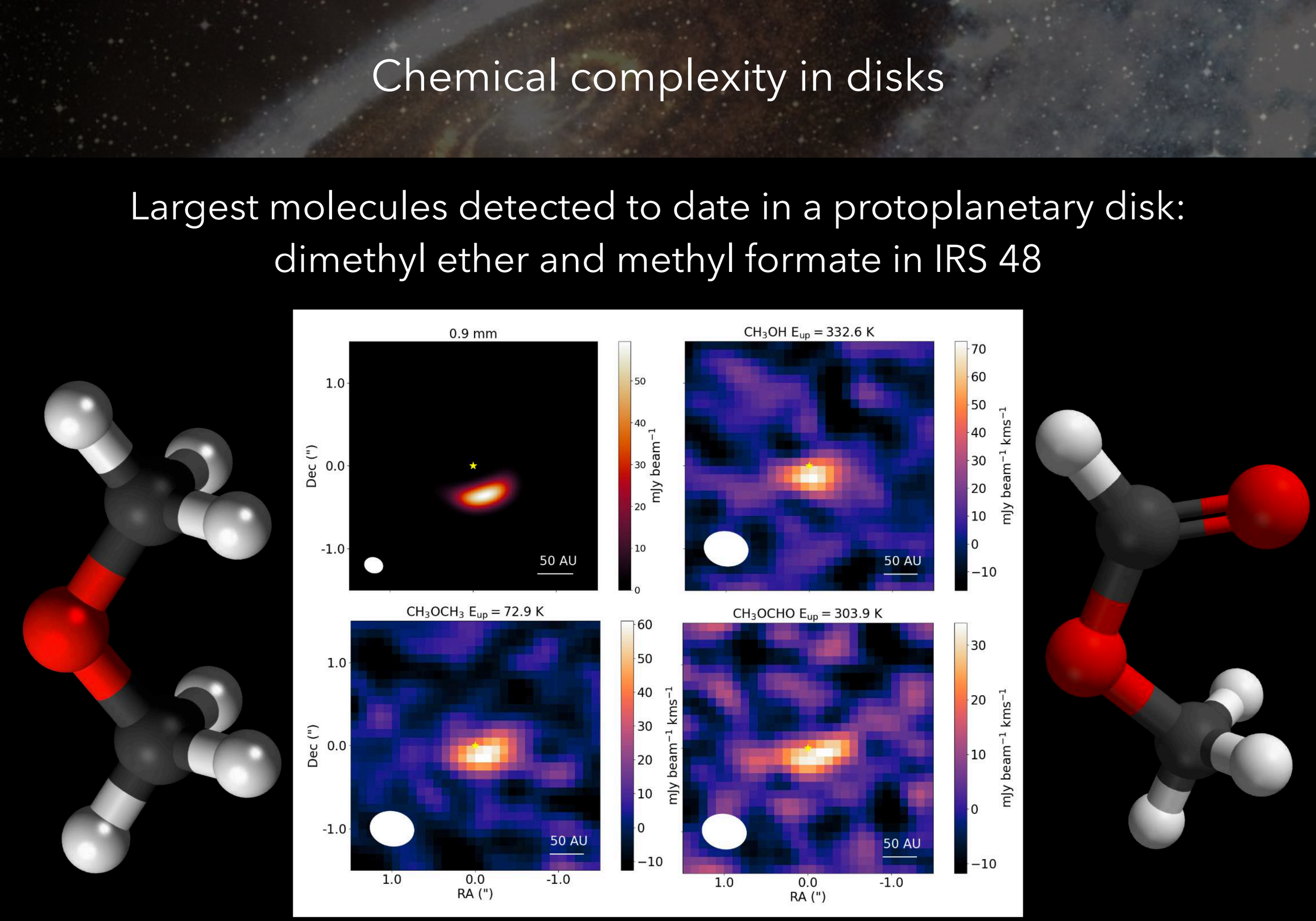


Emission from large molecules is compact … following the ice reservoir hosted on large grains?

Ilee & MAPS Team 2021, ApJS, 257, 9

Chemical complexity in disks

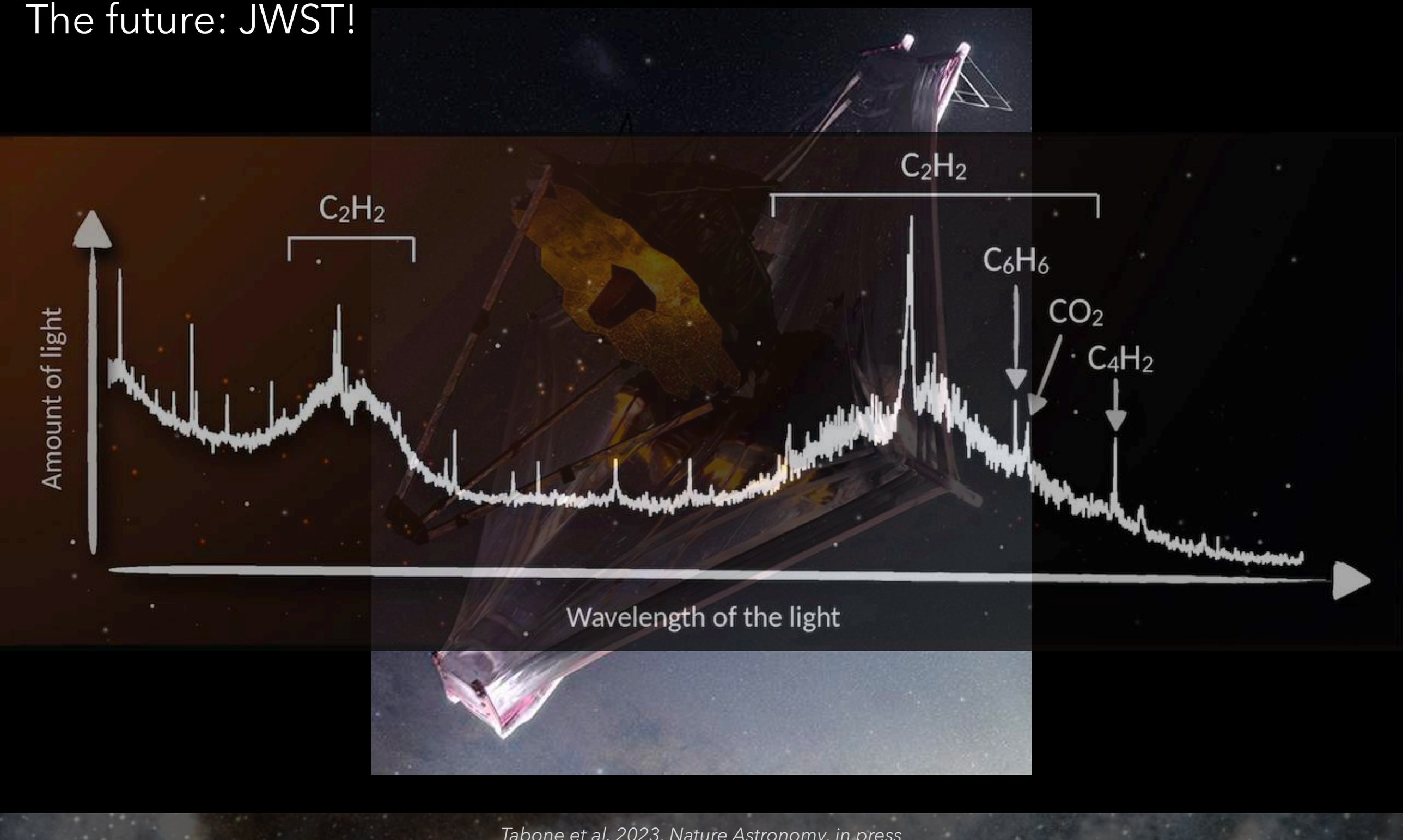
Largest molecules detected to date in a protoplanetary disk:
dimethyl ether and methyl formate in IRS 48



Brunken et al. 2022, A&A, 659, A29

Revealing the composition of the inner disk

The future: JWST!



Tabone et al. 2023, Nature Astronomy, in press

Resolved observations of gas and chemistry in protoplanetary disks can …

reveal snowline locations

reveal kinematic evidence of warps, planets, …

uncover coupled chemistry between dust, gas, and ice

resolve the composition of the planet-forming region