HYACINTH: HYdrogen And Carbon chemistry in the INTerstellar medium in Hydro simulations

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Prachi Khatri & Cristiano Porciani

Khatri, PC, RDE, 2024, A&A, 688, A194

Khatri, RDE, CP, 2025, A&A, 697, A174

SFB 1601

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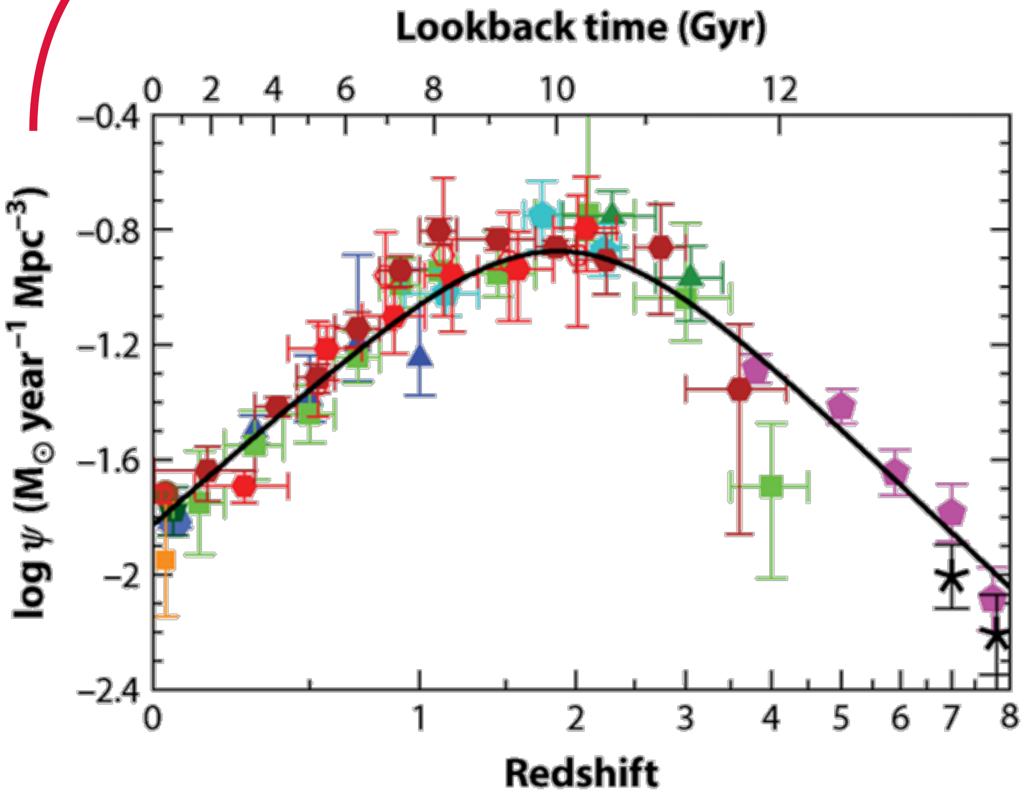
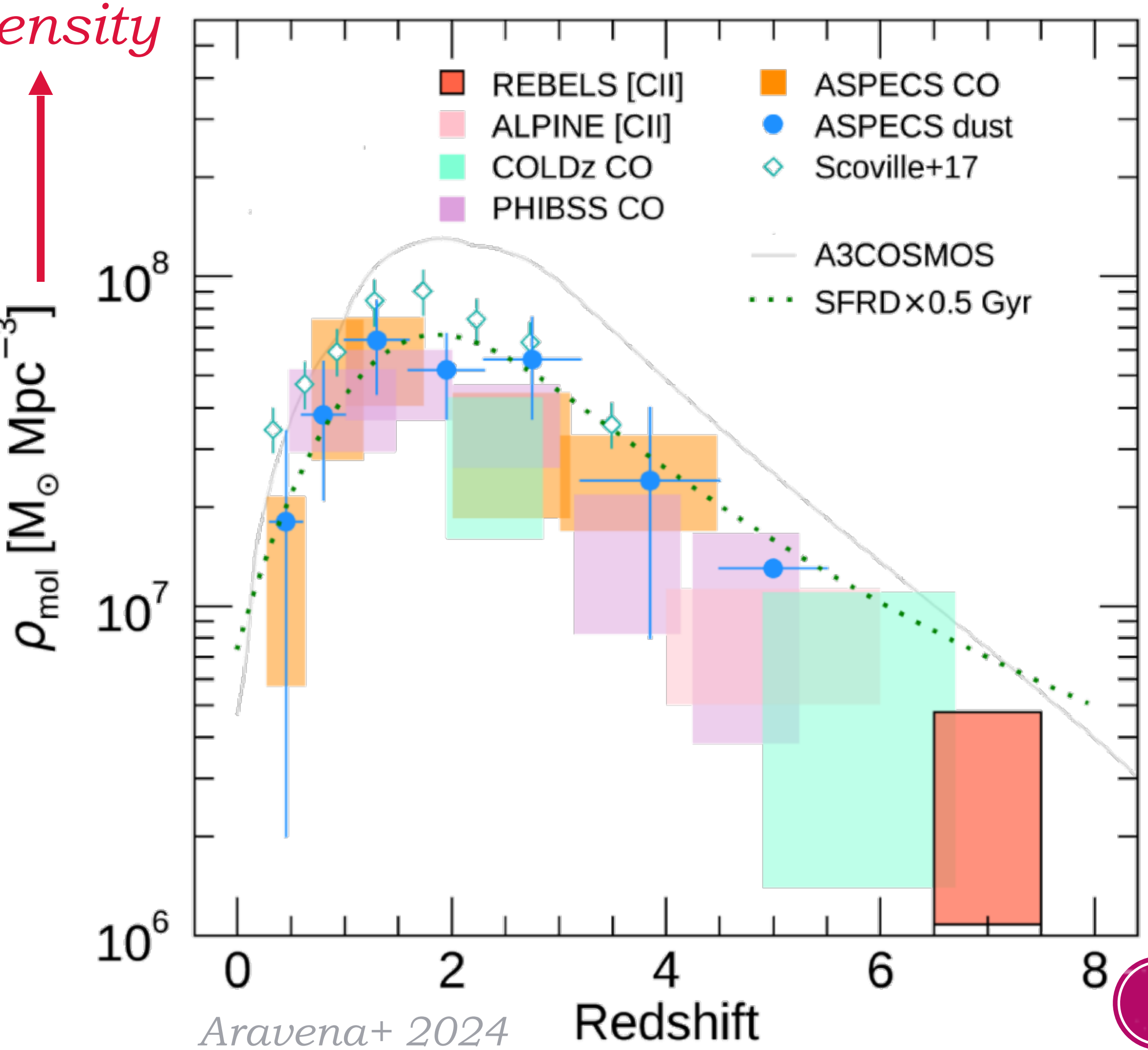
STAR FORMATION ACROSS COSMIC TIME

Star formation rate density (SFRD)



Madau & Dickinson 2014

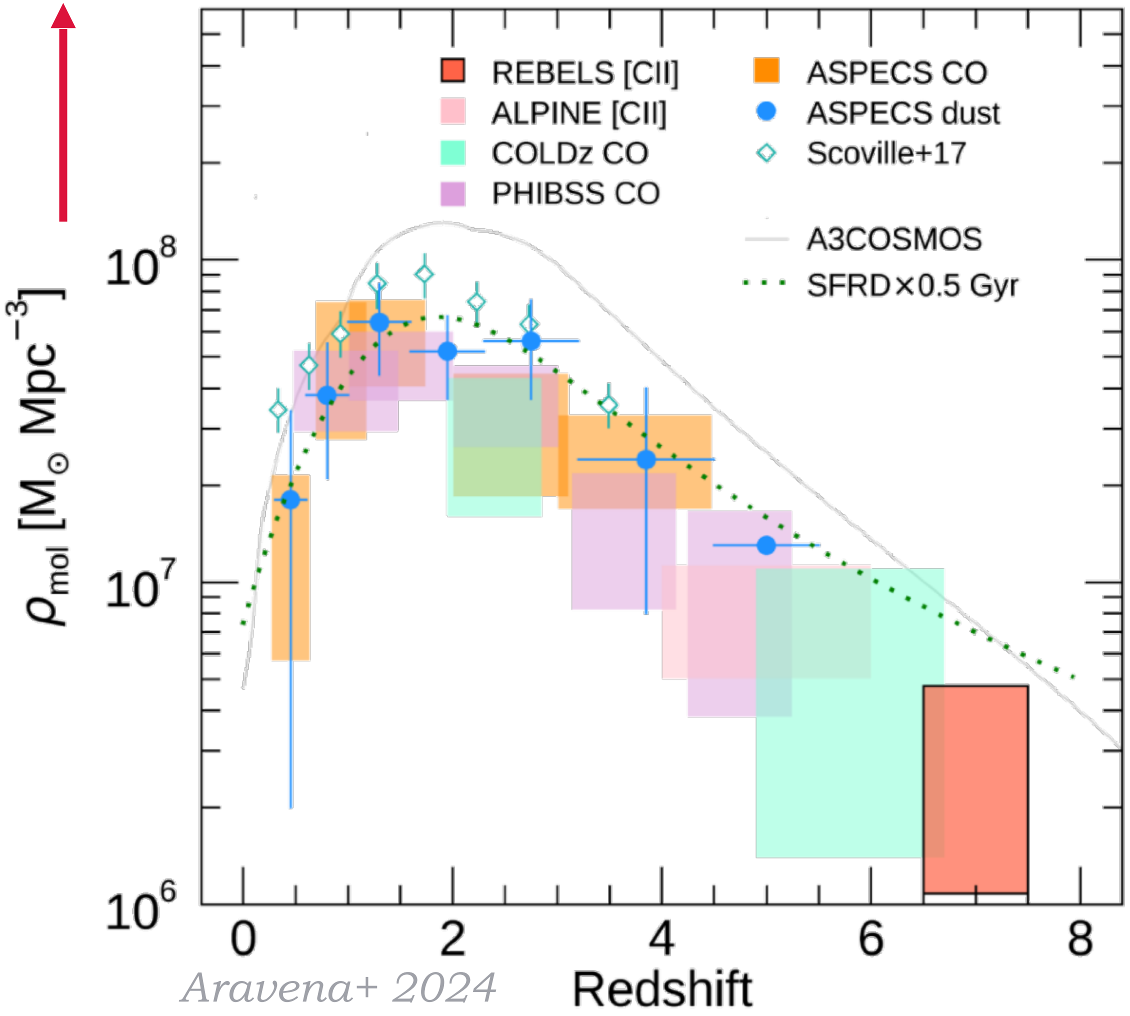
Molecular gas density



Aravena+ 2024

MOLECULAR GAS ACROSS COSMIC TIME

Molecular gas density



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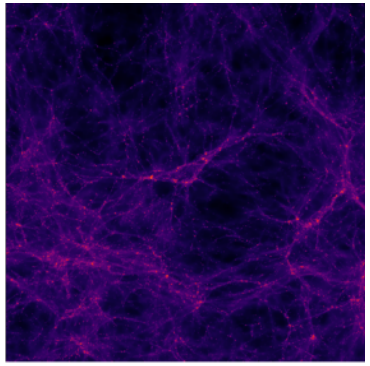
We need simulations to complement these observations.

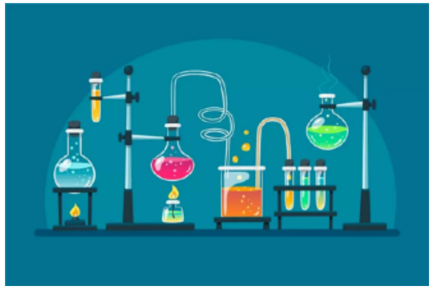
Simulations that model:



✓ The formation of galaxies in a cosmological context

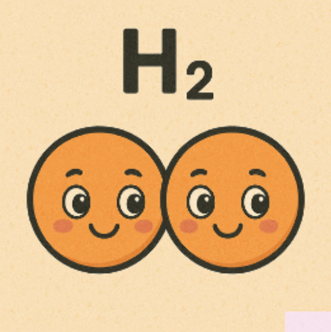
✓ Follow the evolution of molecular gas in galaxies.
||
H_2 and other molecules

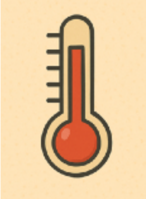
Model chemistry



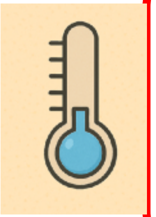
THE STORY OF H_2

Lacks a permanent dipole moment
⟹ no electric dipolar transitions





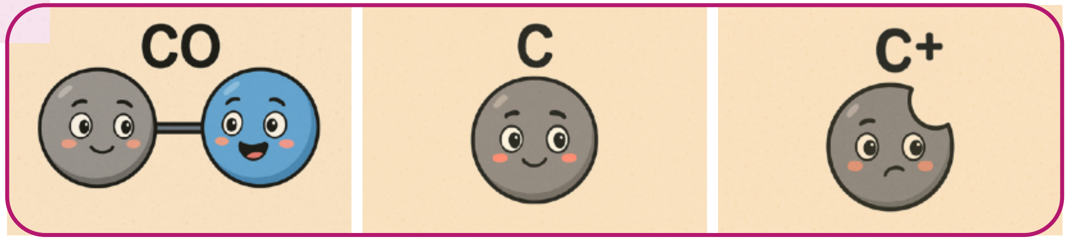
Lowest possible transition
(quadrupole rotation)
requires T ~ 510 K



Does not emit under typical conditions of molecular clouds (T~10-100 K)

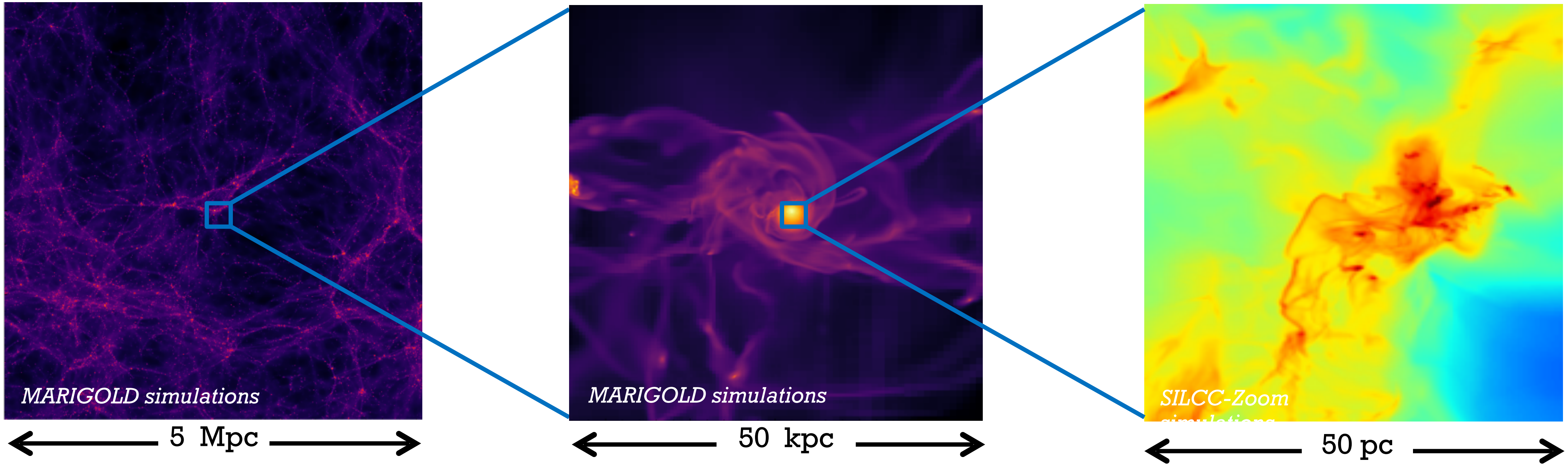
Caveat in Using Tracers

Mapping between emission and H_2 abundance sensitive to:
physical conditions like density, metallicity, UV radiation, etc.



CO, C, and C^+ emission lines serve as indirect tracers of H_2.

COSMOLOGICAL SIMULATIONS OF GALAXY FORMATION



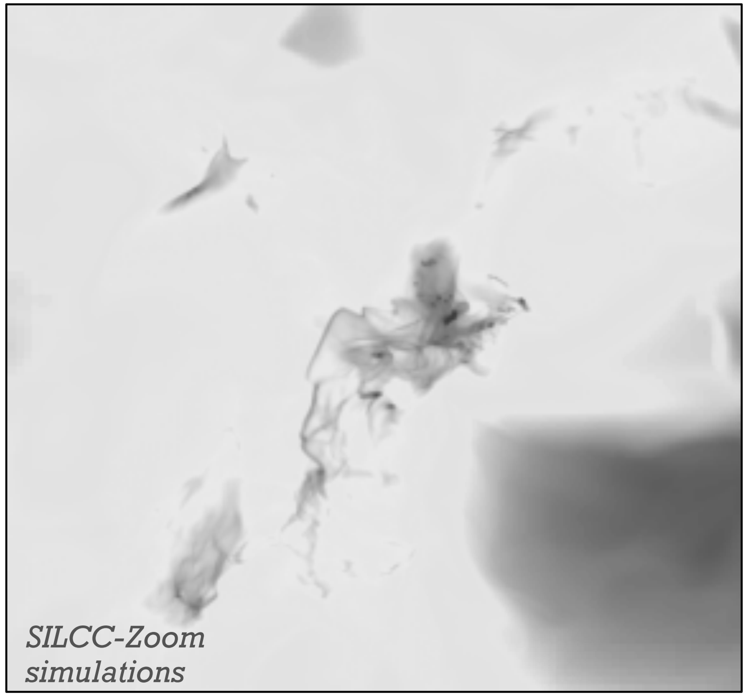
Modelling galaxy formation is a multiscale and multiphysics problem

DENSITY STRUCTURE OF THE ISM

Realistic ISM

Simulated ISM

100 pc



*The finite resolution of simulations misses the **intricate density structure (and other properties)** of the ISM, important for modelling chemical abundances and emission.*

DENSITY STRUCTURE OF THE ISM

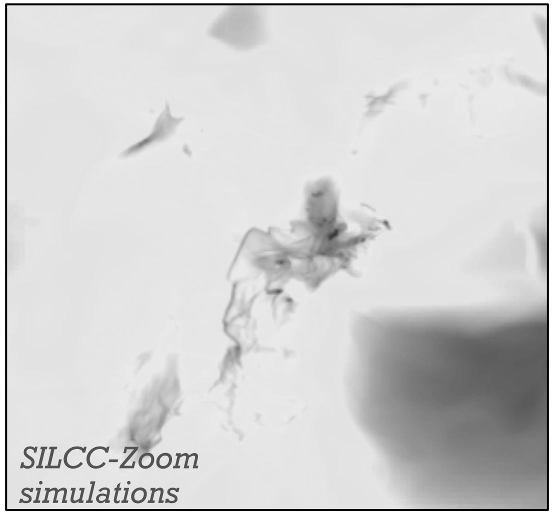
Turbulence-driven log-normal (LN)

Tomassetti+15

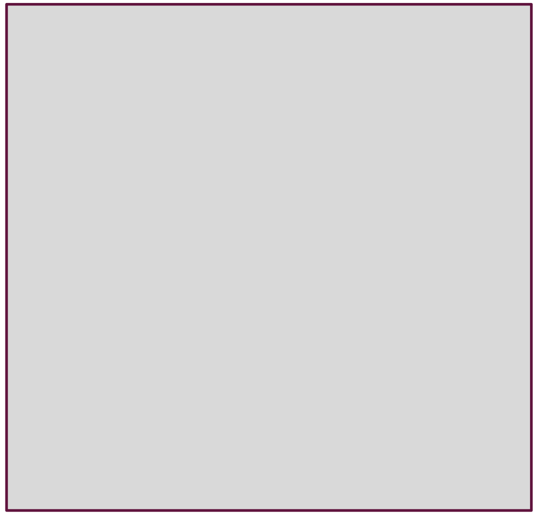
A PDF to mimic the distribution of unresolved (sub-grid) densities

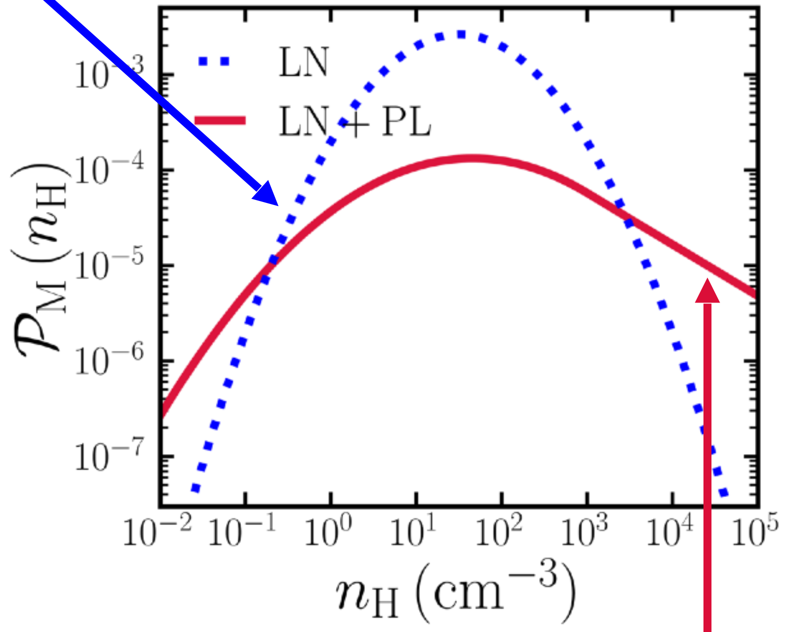
100 pc

Realistic ISM



Simulated ISM





*The finite resolution of simulations misses the **intricate density structure** of the ISM, important for modelling chemical abundances and emission.*

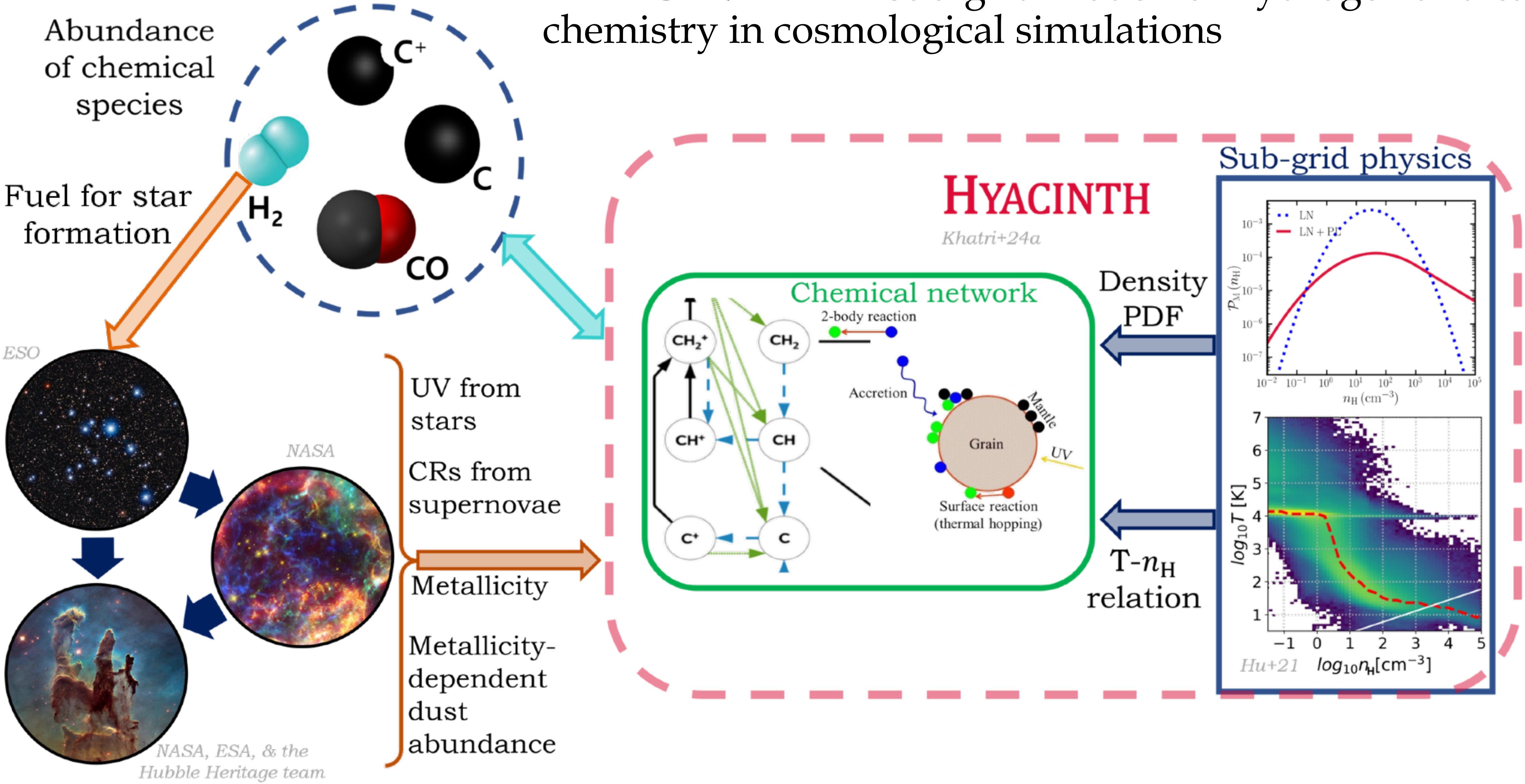
Self-gravity induces a power-law tail

log-normal + power-law (LN+PL)

Functional forms of density PDF:
Kainulainen+09,
Kritsuk+11, Federrath+13, Girichidis+14

Sub-grid model HYACINTH

HYACINTH – A sub-grid model for hydrogen and carbon chemistry in cosmological simulations



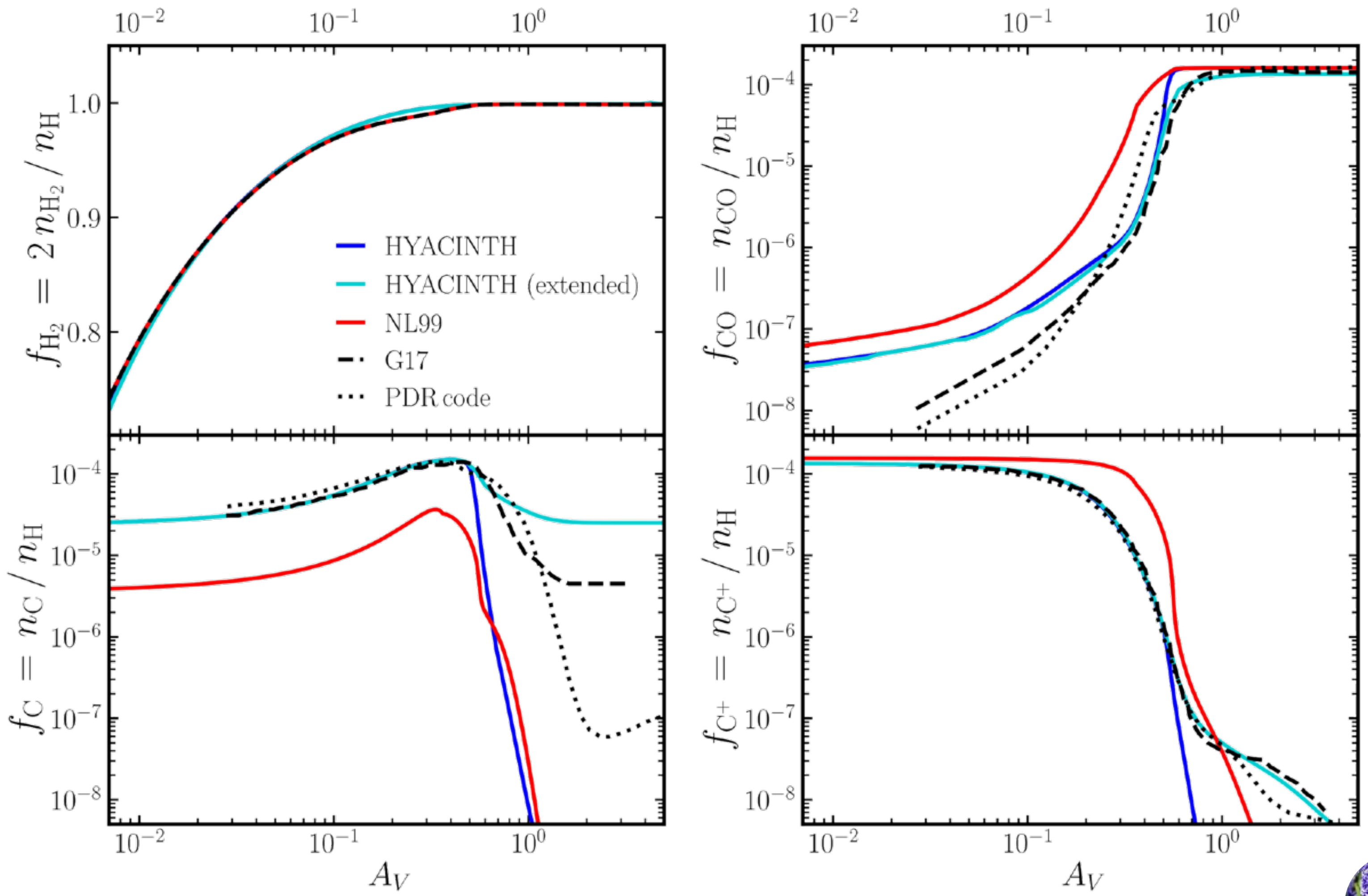
TEST OF CHEMICAL ABUNDANCES –
Comparison of equilibrium abundances using the slab test

- 19 chemical reactions

- Additional chemical species – He^+ and HCO^+ -- important for CO chemistry

- 29 chemical reactions in total

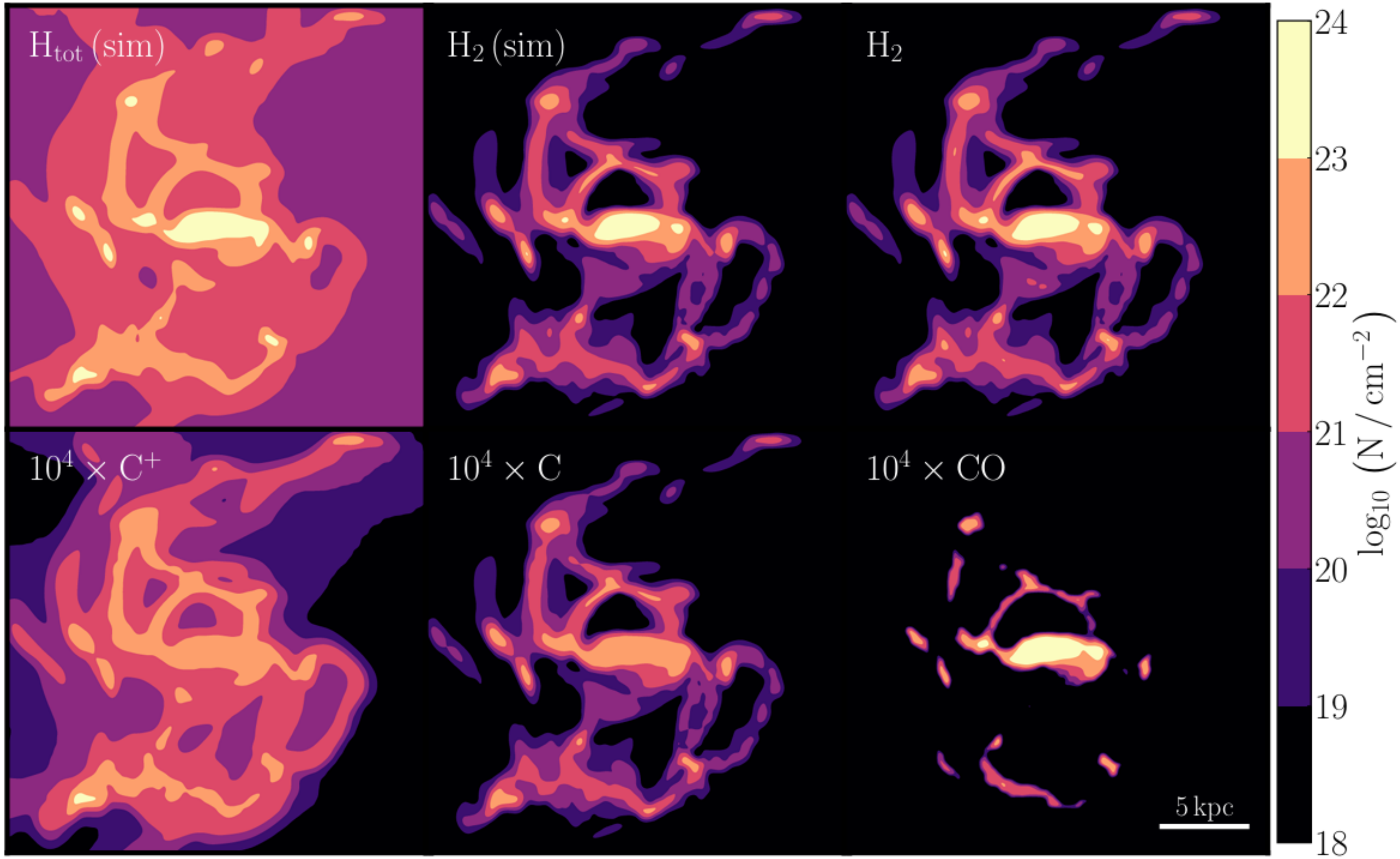
- ≈3.3x computational time



NL99= Nelson & Langer 1999
G17 = Gong et al. 2017
PDR code from Tielens & Hollenbach 1985

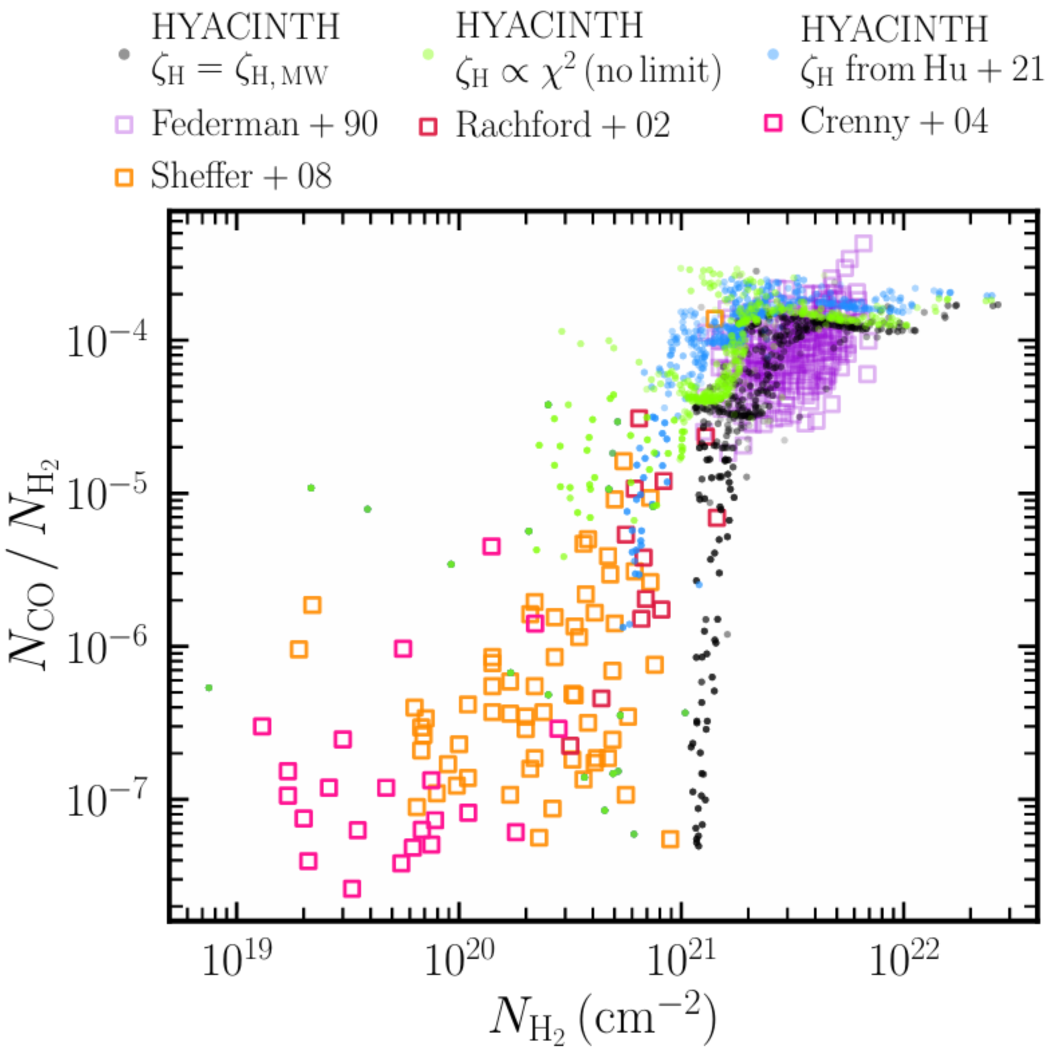
APPLICATION: POST-PROCESSING

- A RAMSES simulated galaxy at z=2.5 from Tomassetti+15 including H_2 chemistry and Lyman-Werner RT.



- Compute Eq. abundances: H_2, CO, C, and C^+ using HYACINTH.
  - Metallicity – from simulation
  - UV flux χ – from simulation
  - Different options for the cosmic-ray ionization rate ζ_H
    - constant
    - linear scaling with χ
    - quadratic scaling with χ

COMPARISON WITH OBSERVATIONS



THE MARIGOLD SUITE:
COSMOLOGICAL SIMULATIONS USING THE SUB-GRID MODEL HYACINTH

- Follow galaxy formation & evolution in a cosmological context (DM, gas & stars til z=3)

- Embed HYACINTH into RAMSES to track the abundances of H_2, CO, C, and C^+ in addition to the total gas.

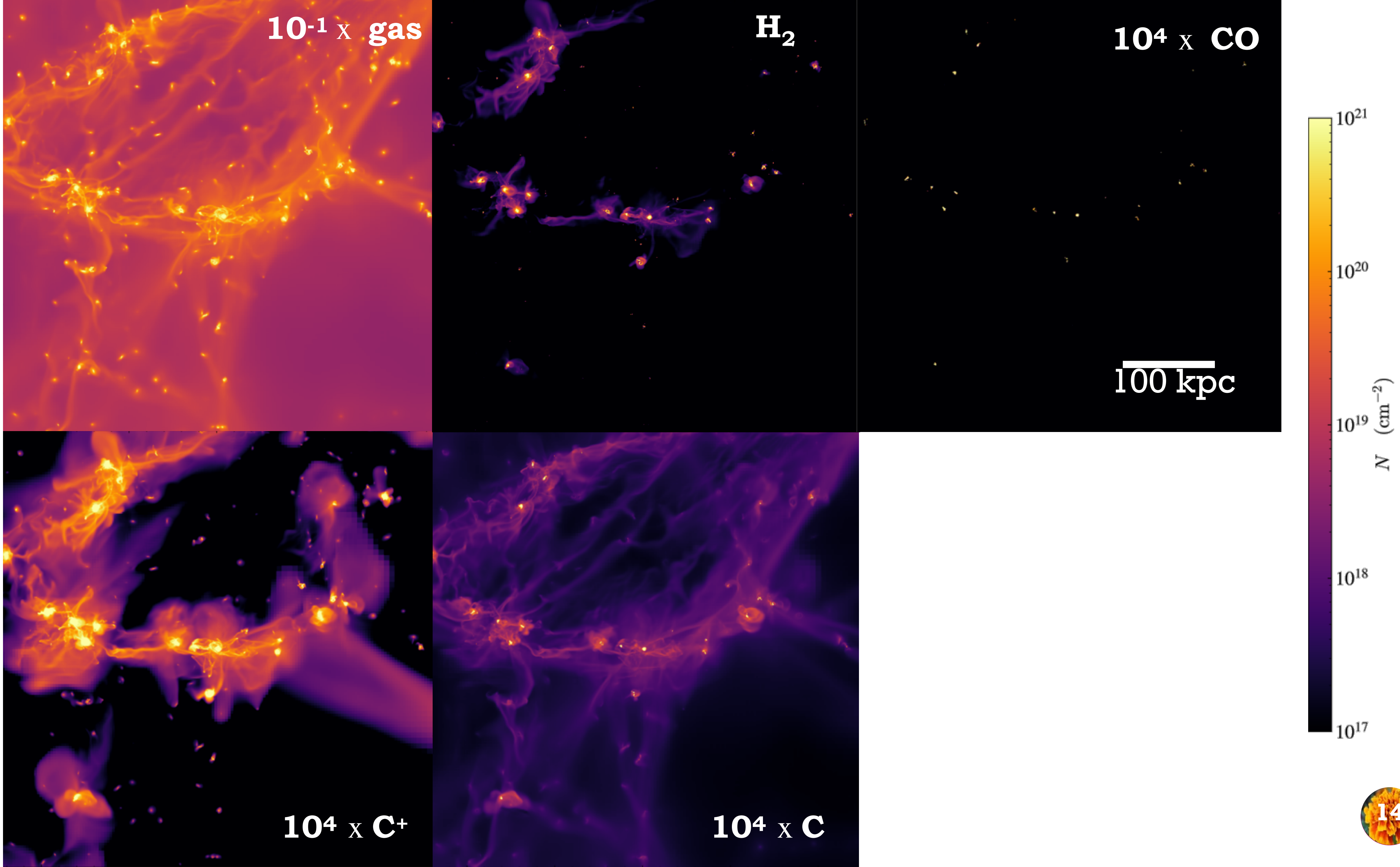
THE MARIGOLD SUITE

Simulation	L_{box} (Mpc)	N_{DM}	Δx^{min} (pc)	m_{DM} ($M_\odot$)	m_* ($M_\odot$)
M25	25	1024^3	32	5×10^5	7×10^3
M50	50	1024^3	64	4×10^6	6×10^4

Large enough volume to study statistical properties of galaxies

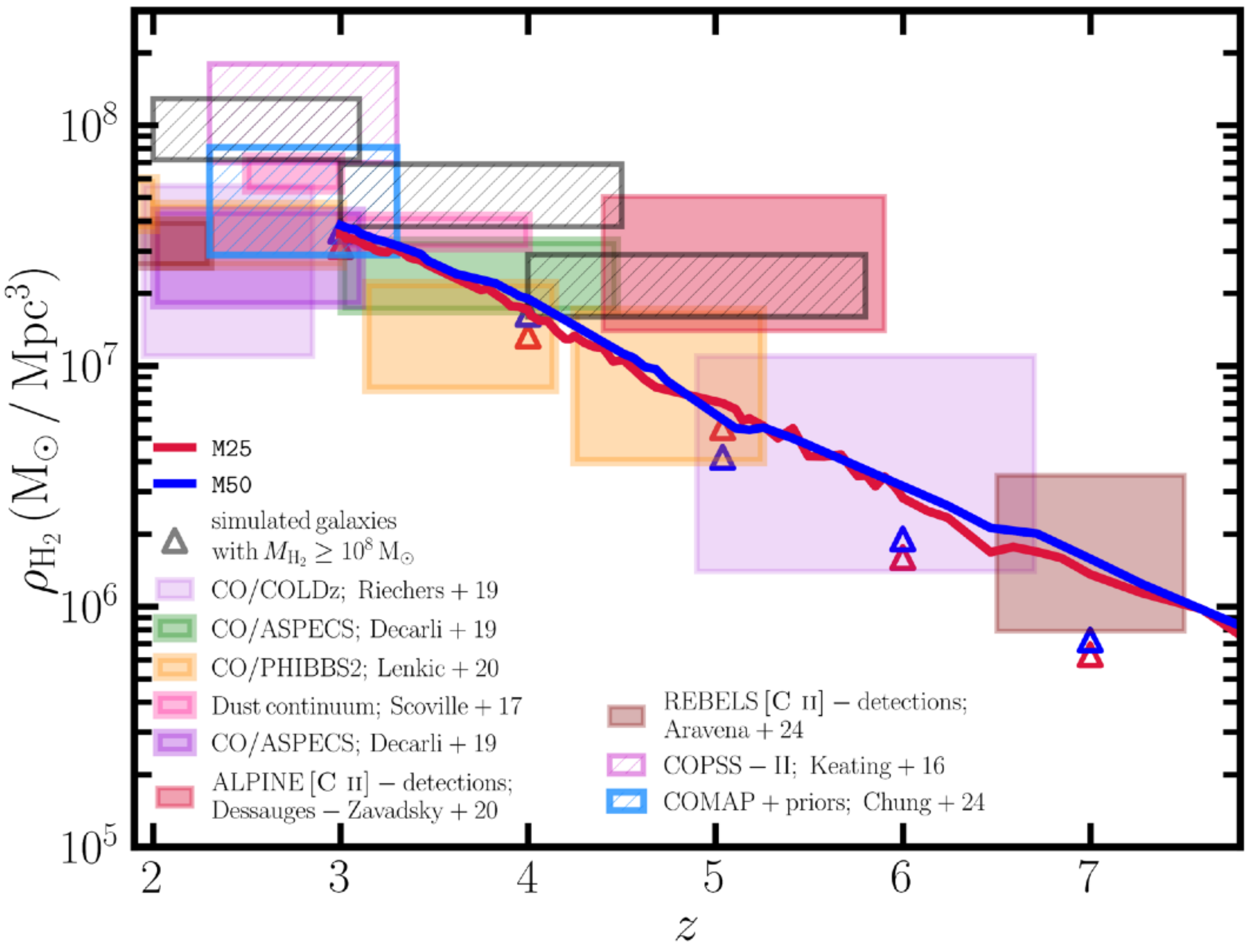
High spatial resolution to model chemistry and emission properties of galaxies

Sufficiently low particle mass to resolve low-mass galaxies



10^{-1} x gas
H_2
10^4 x CO
100 kpc
10^4 x C^+
10^4 x C
10^{21}
10^{20}
10^{19}
10^{18}
10^{17}
N (cm^{-2})

COSMIC MOLECULAR GAS DENSITY

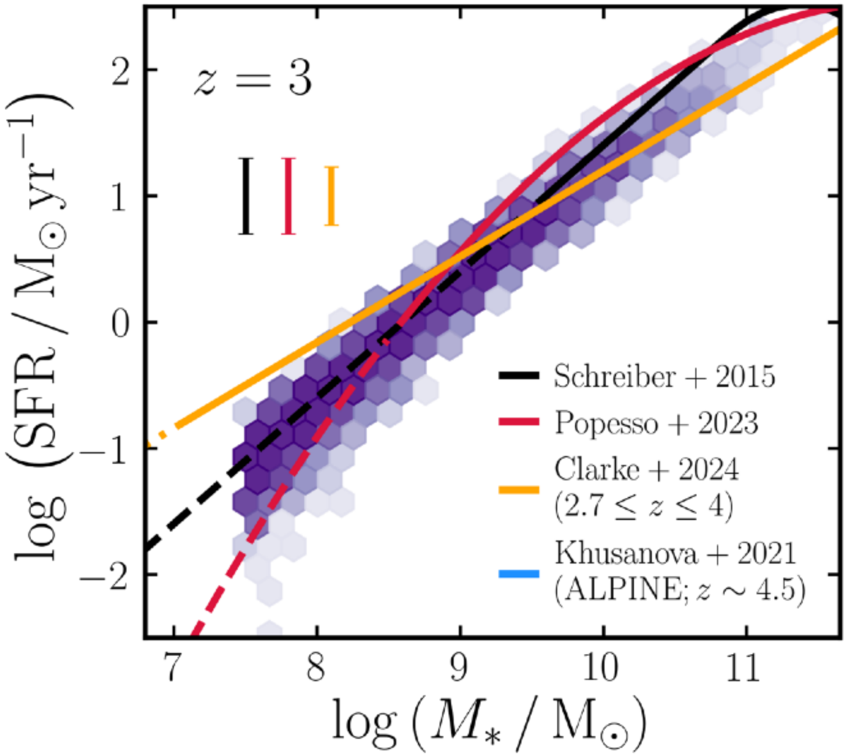


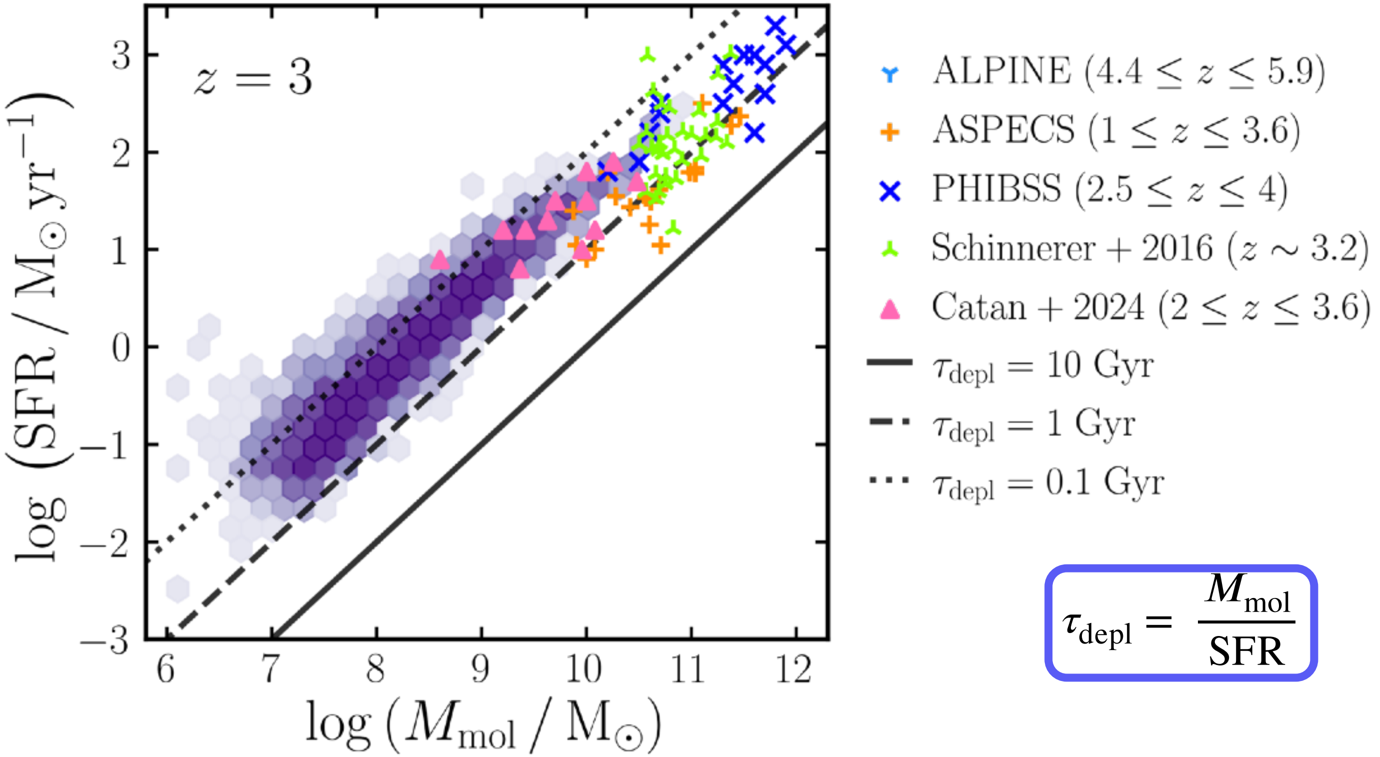
- Simulated ρ_{H_2} consistent with observational constraints
- Low-mass galaxies dominate the cosmic H_2 budget at z>7

STATISTICAL PROPERTIES OF GALAXIES

Distribution of simulated galaxies aligns with empirical relations

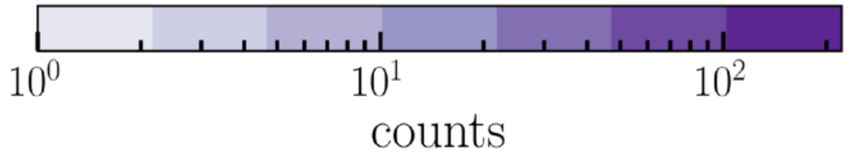
MARIGOLD





$$\tau_{\mathrm{depl}} = \frac{M_{\mathrm{mol}}}{\mathrm{SFR}}$$

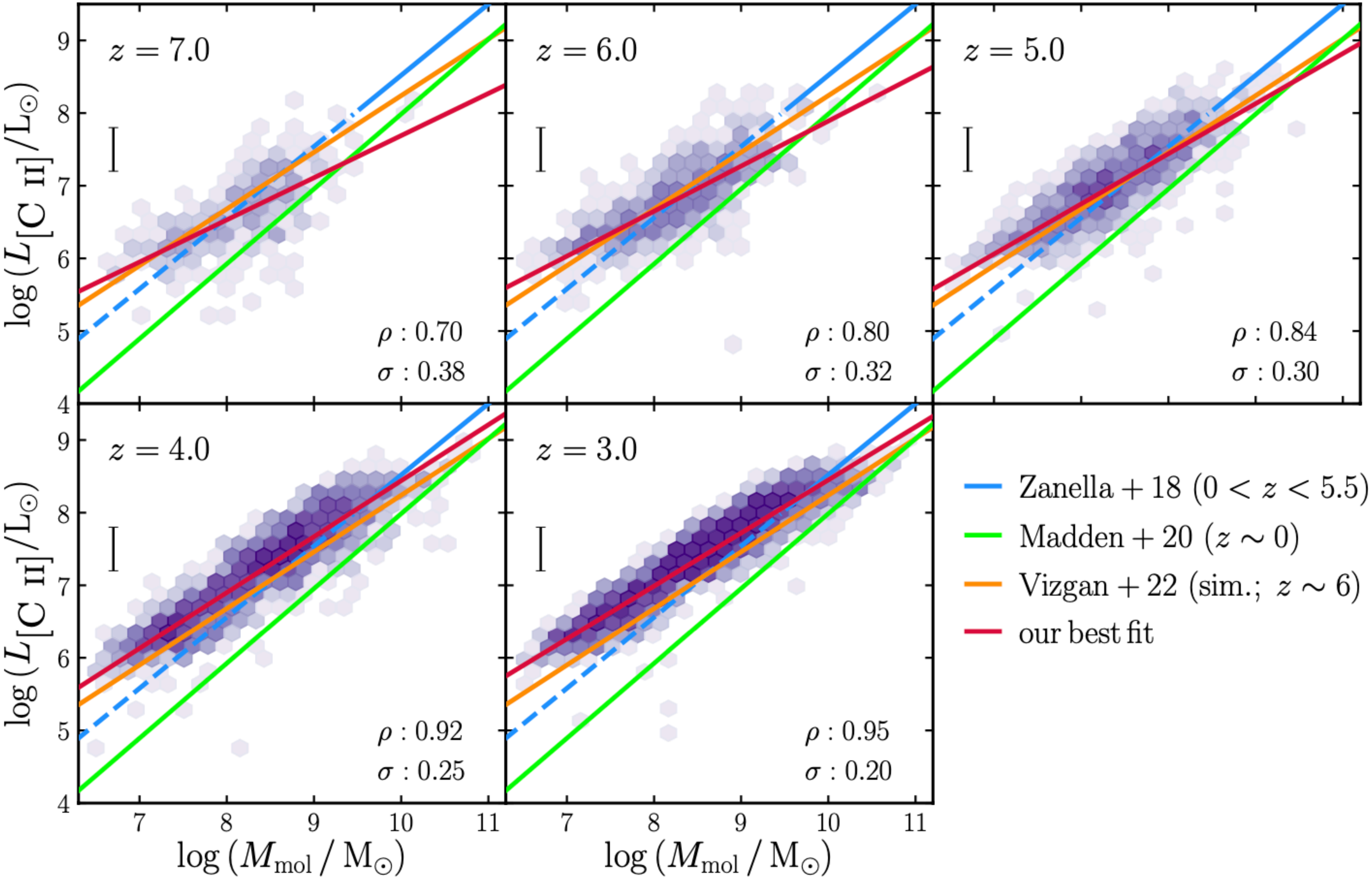
Main-sequence relation



Schmidt-Kennicutt relation

[CII]-M_{mol} RELATION: LINE RADIATIVE TRANSFER

The correlation is weak at high redshifts and strengthens over time



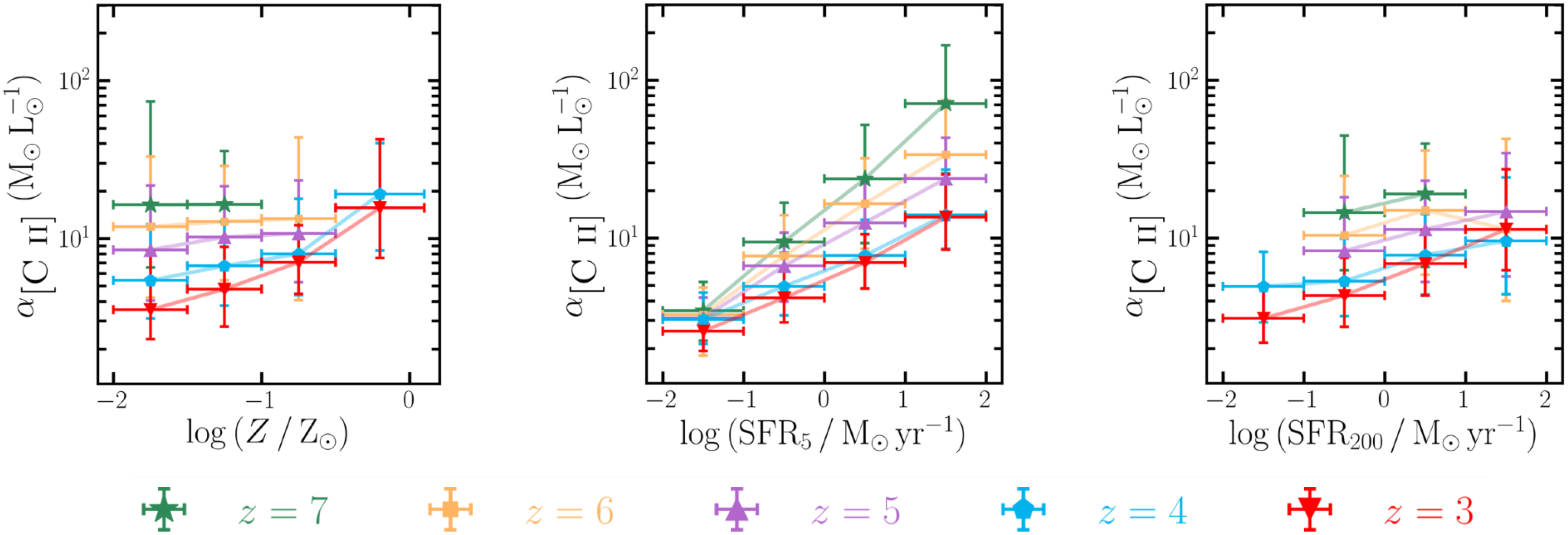
RT: Optically thick

$$\alpha_{[CII]} = \frac{M_{mol}}{L_{[CII]}}$$

The numerical factor used to convert the observed [CII] luminosity to a molecular gas mass

in MARIGOLD galaxies

How does $\alpha_{[CII]}$ change with galaxy properties?

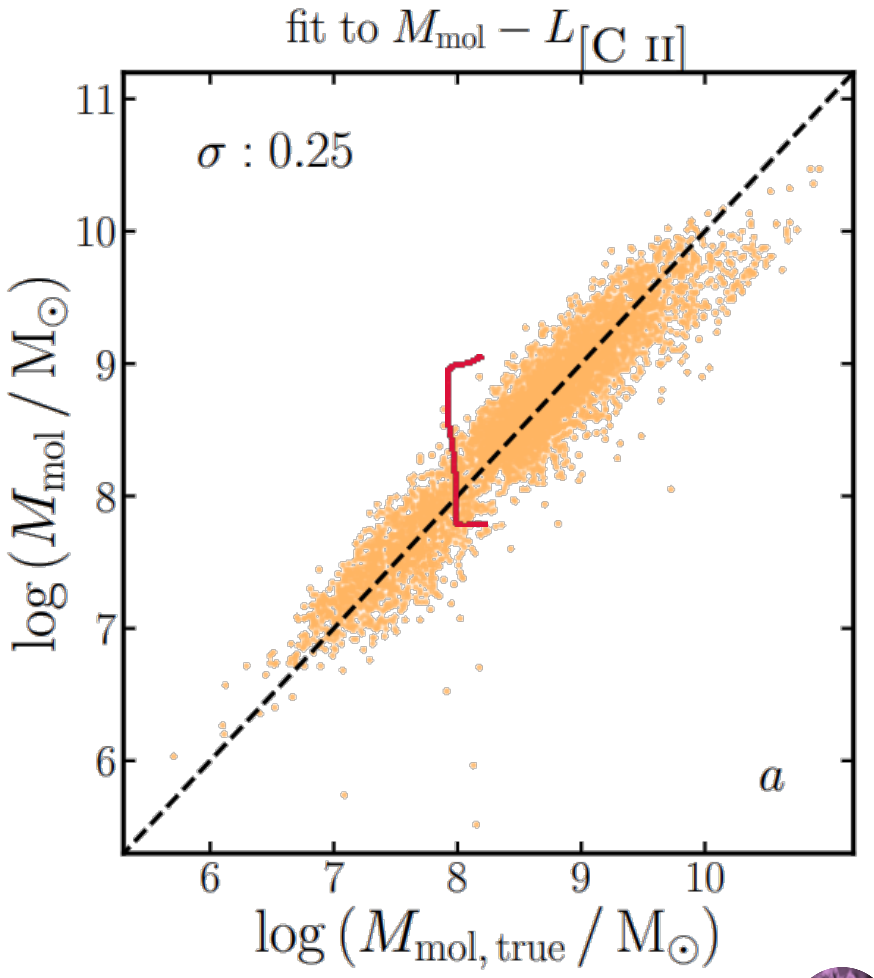


$$\alpha_{[CII]} = f(Z,\ \mathrm{SFR}_5, \mathrm{SFR}_{200})$$

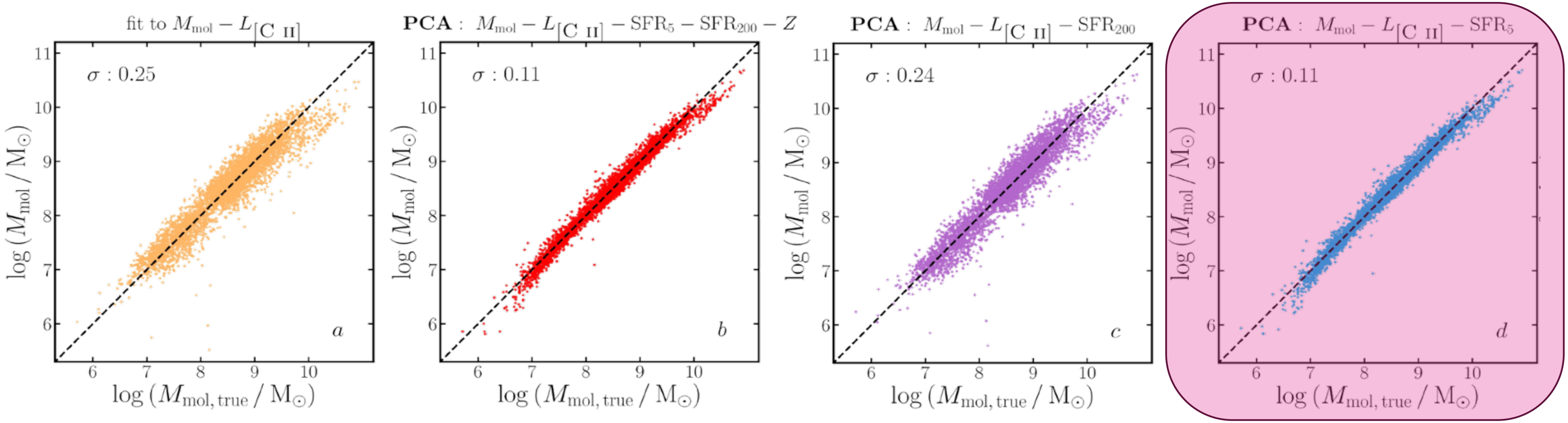
If $\alpha_{[CII]}$ depends on other galaxy properties, can we do a better job at predicting M_{mol} from $L_{[CII]}$?

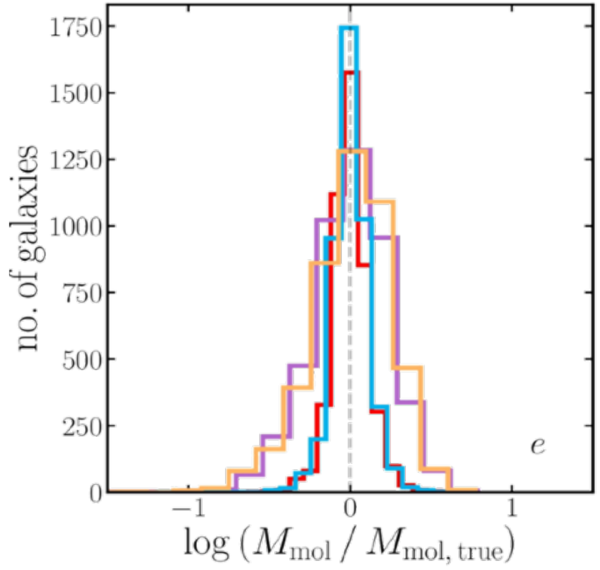
In other words, can we reduce this scatter?

=> PCA in the 5D parameter space:
$M_{mol} = f(L_{[CII]},\ Z,\ SFR_5, SFR_{200})$



PERFORMANCE OF PCA-BASED RELATIONS

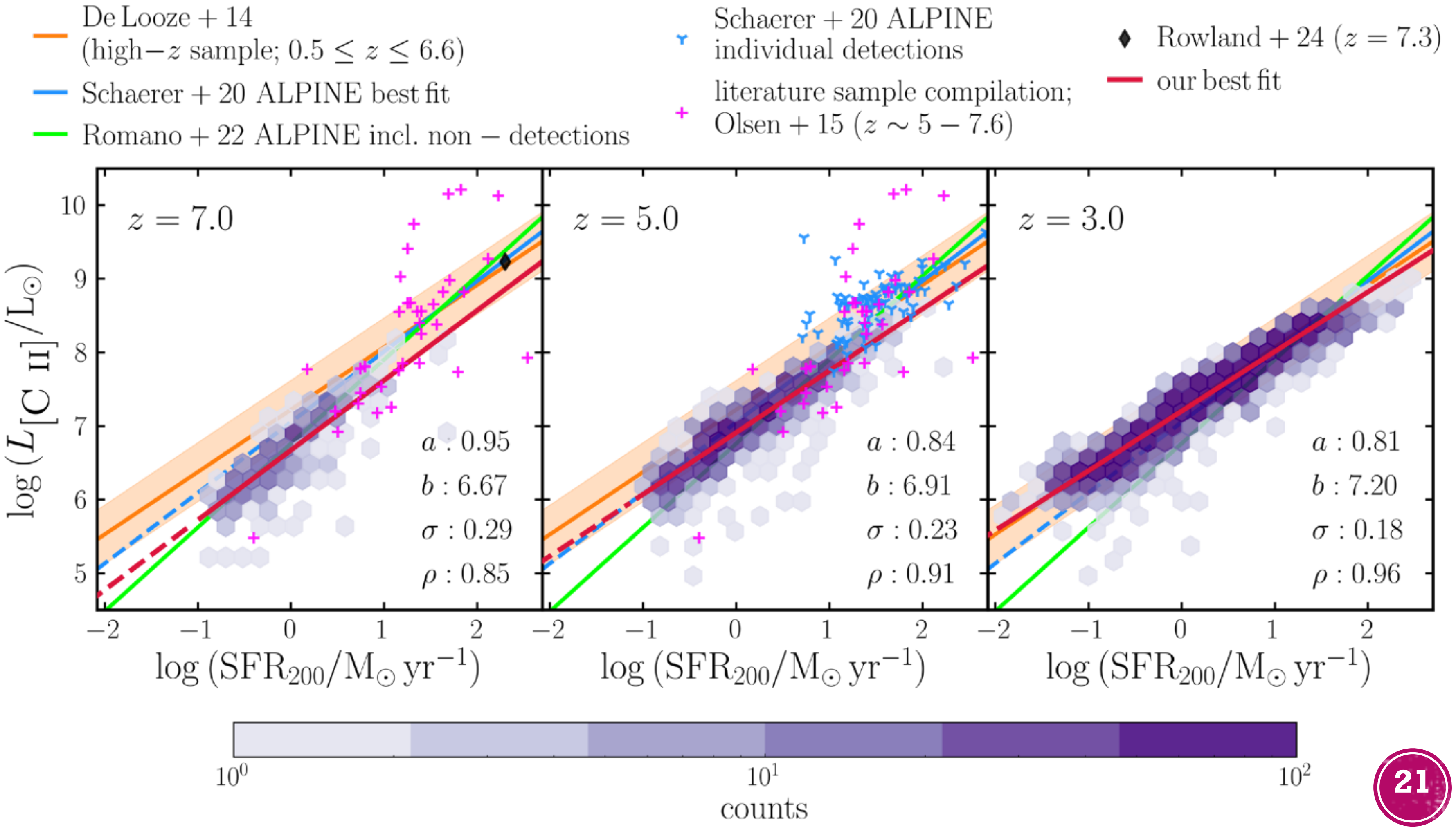




Three variable PCA-based relation: $M_{\rm mol}(L_{[\rm C\,ii]},\ {\rm SFR}_5)$ provides an excellent approximation of the true $M_{\rm mol}$, with ≈2.3x higher accuracy compared to a two-variable $M_{\rm mol}(L_{[\rm C\,ii]})$

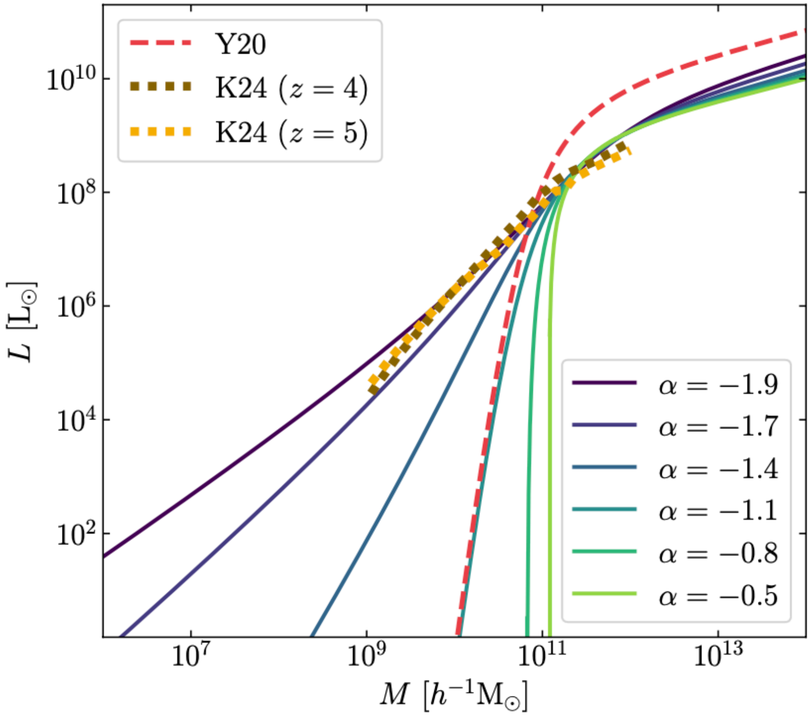
[CII]-SFR RELATION

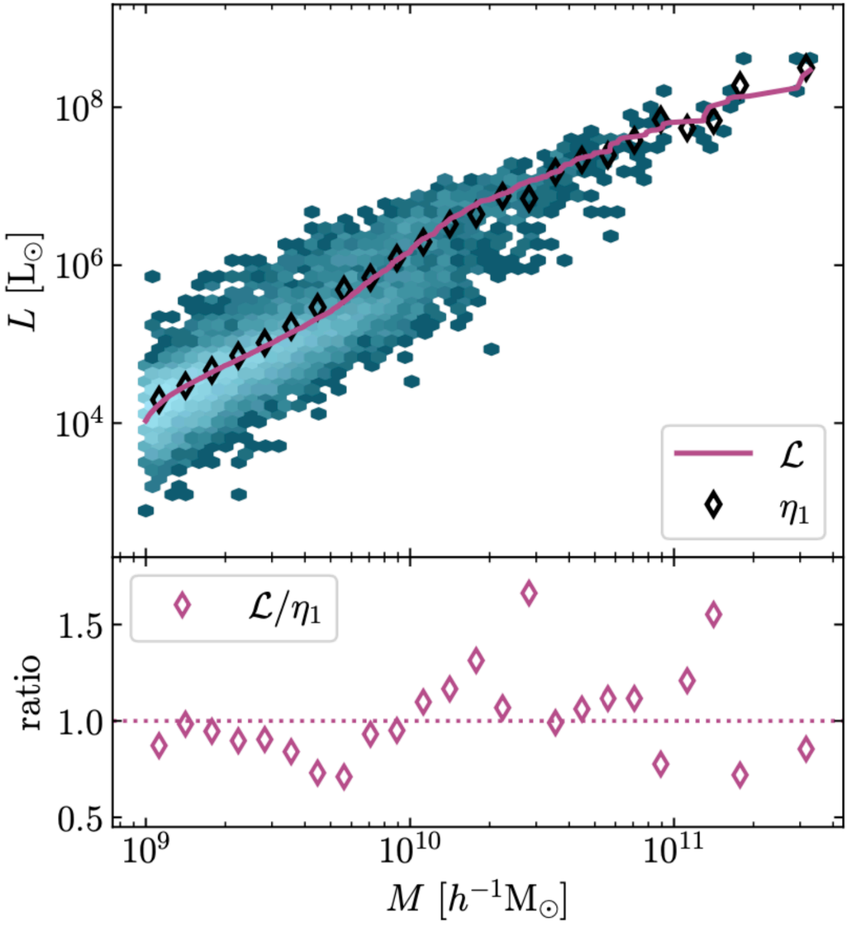
- ➢The correlation is strong at all redshifts
- ➢Strong evolution in the intercept --- > ~0.5 dex in 1.4 Gyr

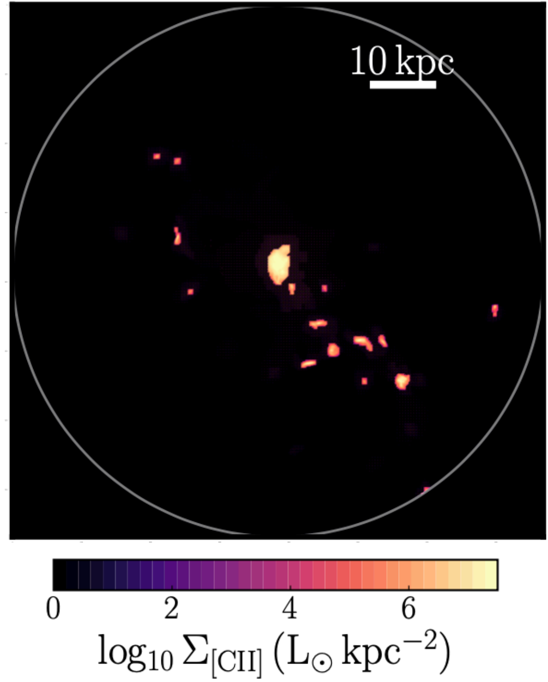


MARIGOLD & LIM

- Our results can be used together with Halo Abundance Matching (HAM) to populate large Nbody simulations for LIM purposes:
- 1 halo - 1 galaxy
- No scatter in LF_{C+} at fixed mass
- CLF: $\phi(L|M,z)$ monotonic function







(Elena Marcuzzo's talk, tomorrow)

CONCLUSIONS

- ➢HYACINTH – a sub-grid model for hydrogen and carbon chemistry in hydro simulations.

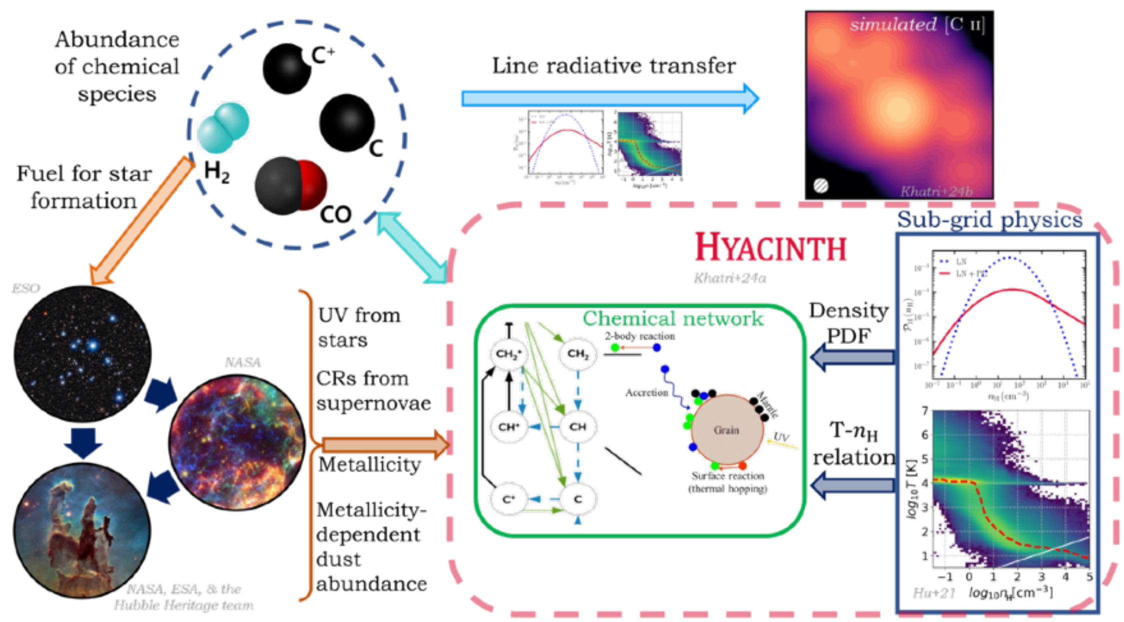
- ➢HYACINTH can be used as a post-processing tool

- ➢The MARIGOLD simulations – cosmological simulations for tracing molecular gas & C-related species in galaxies.

- ➢ Simulated cosmic H_2 density in agreement with observational estimates.

- ➢[C ii] – $M_{\rm mol}$ correlation
  - Evolves over time
  - Is sensitive to SFR

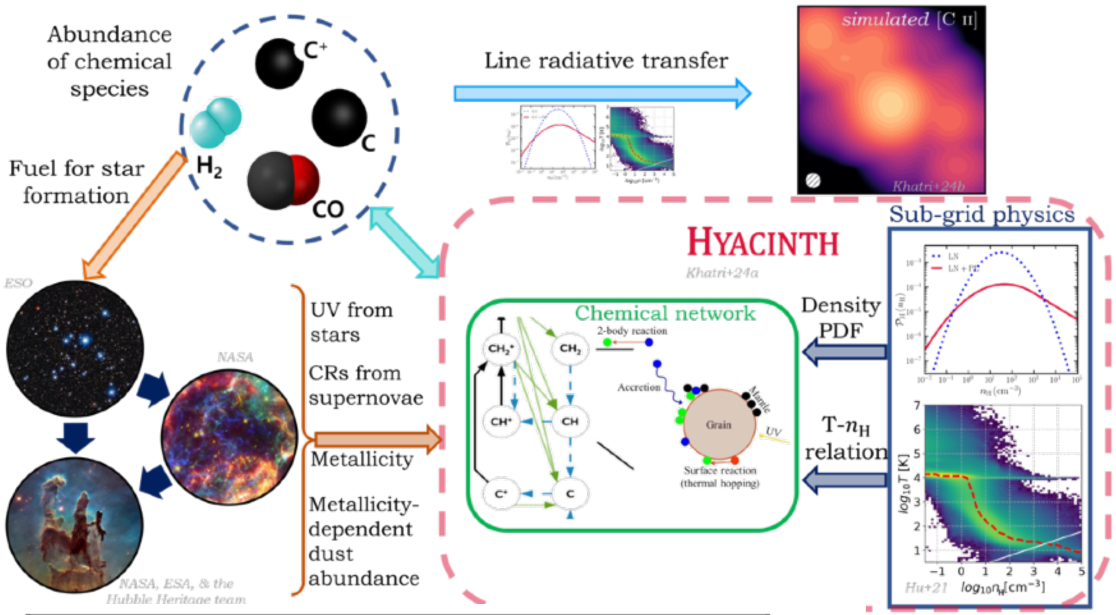
Modelling molecular gas and its tracers with HYACINTH

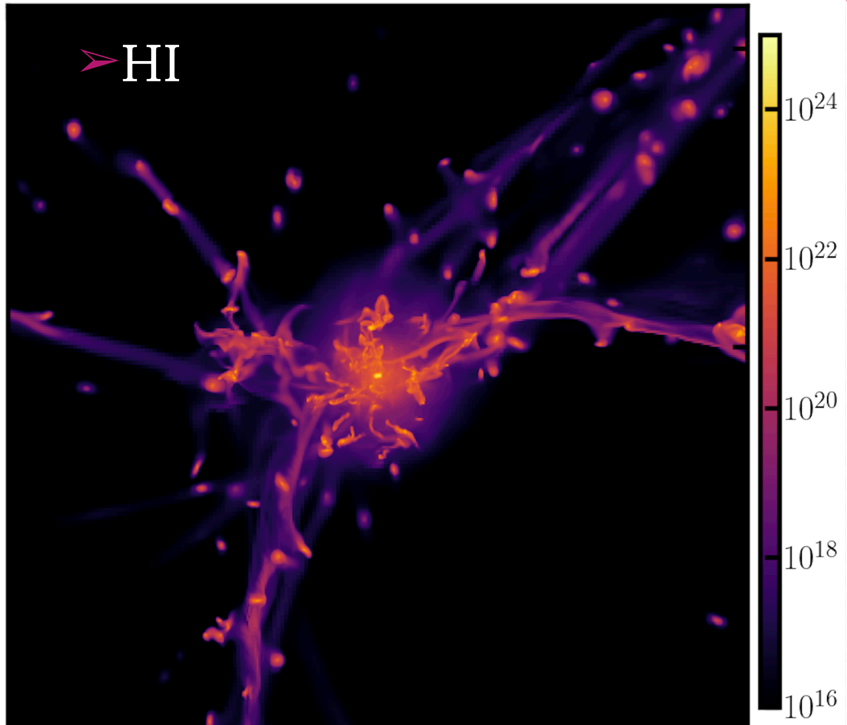


THE FUTURE:

- ➢ The future is bright! ☺
- ➢ CO analysis: RT -> line emission & LF -> LIM
- ➢ Include neutral and ionized hydrogen (HI & HII) within HYACINTH
- ➢ Include massive galaxies' contributions -> Constrained Realizations & zoom-ins
- ➢ …

Modelling molecular gas and its tracers with HYACINTH





Trehan+25 in prep

25

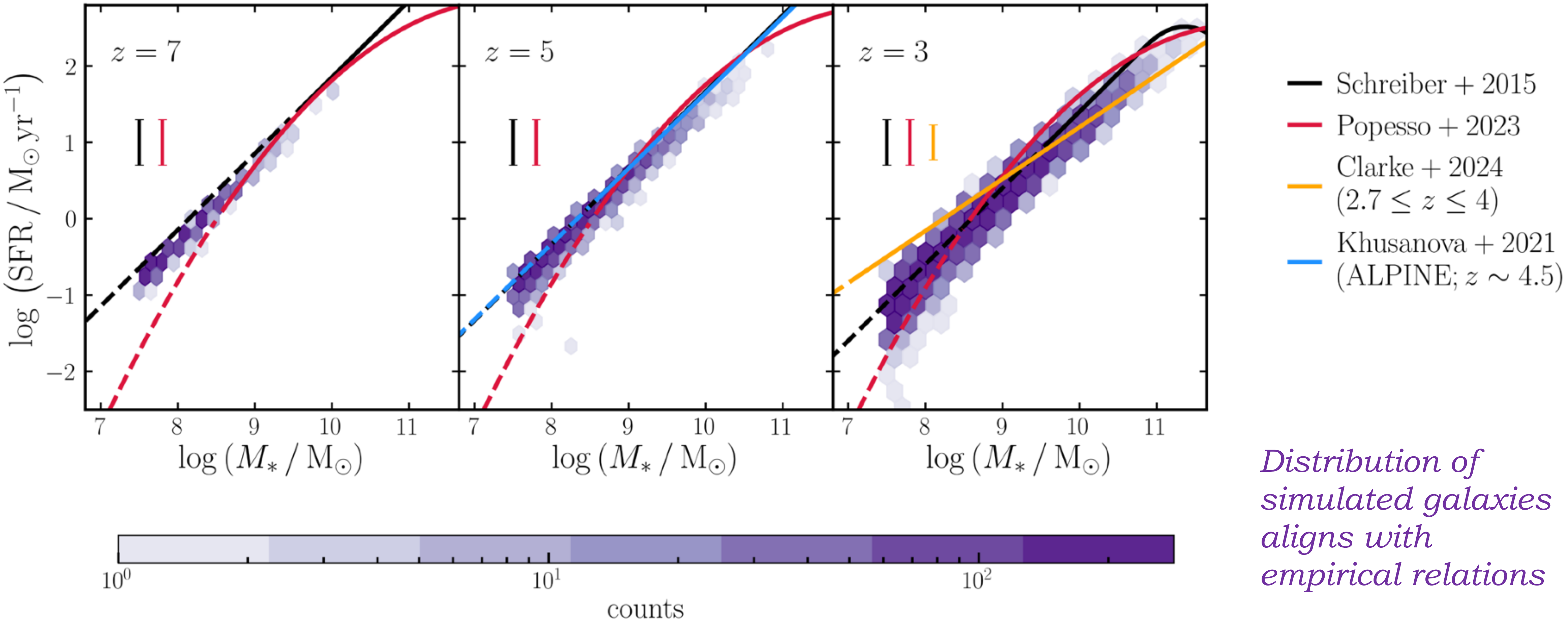
BACKUP

Table 2: Best-fit parameters to the LF for the DPL function given in Eq. (2).

z	$\log(\phi_* \,/\, \mathrm{Mpc}^{-3}\,\mathrm{dex}^{-1})$	$\log(L_* \,/\, \mathrm{L}_\odot)$	α	β	$\Delta\mathrm{DIC}^{(a)}$	$\Delta\mathrm{DIC}^{(b)}$
7	$-1.84^{+0.15}_{-0.15}$	$6.44^{+0.10}_{-0.11}$	$-1.54^{+0.06}_{-0.05}$	$-2.75^{+0.08}_{-0.09}$	105	107
6	$-1.26^{+0.12}_{-0.12}$	$6.20^{+0.10}_{-0.10}$	$-1.24^{+0.06}_{-0.06}$	$-2.30^{+0.04}_{-0.05}$	222	223
5	$-1.52^{+0.13}_{-0.13}$	$6.72^{+0.11}_{-0.11}$	$-1.42^{+0.03}_{-0.03}$	$-2.31^{+0.05}_{-0.05}$	159	161
4	$-0.91^{+0.08}_{-0.07}$	$7.03^{+0.04}_{-0.04}$	$-1.28^{+0.01}_{-0.01}$	$-2.57^{+0.05}_{-0.05}$	449	451
3	$-1.00^{+0.08}_{-0.08}$	$7.37^{+0.04}_{-0.04}$	$-1.22^{+0.01}_{-0.01}$	$-2.65^{+0.05}_{-0.05}$	174	176

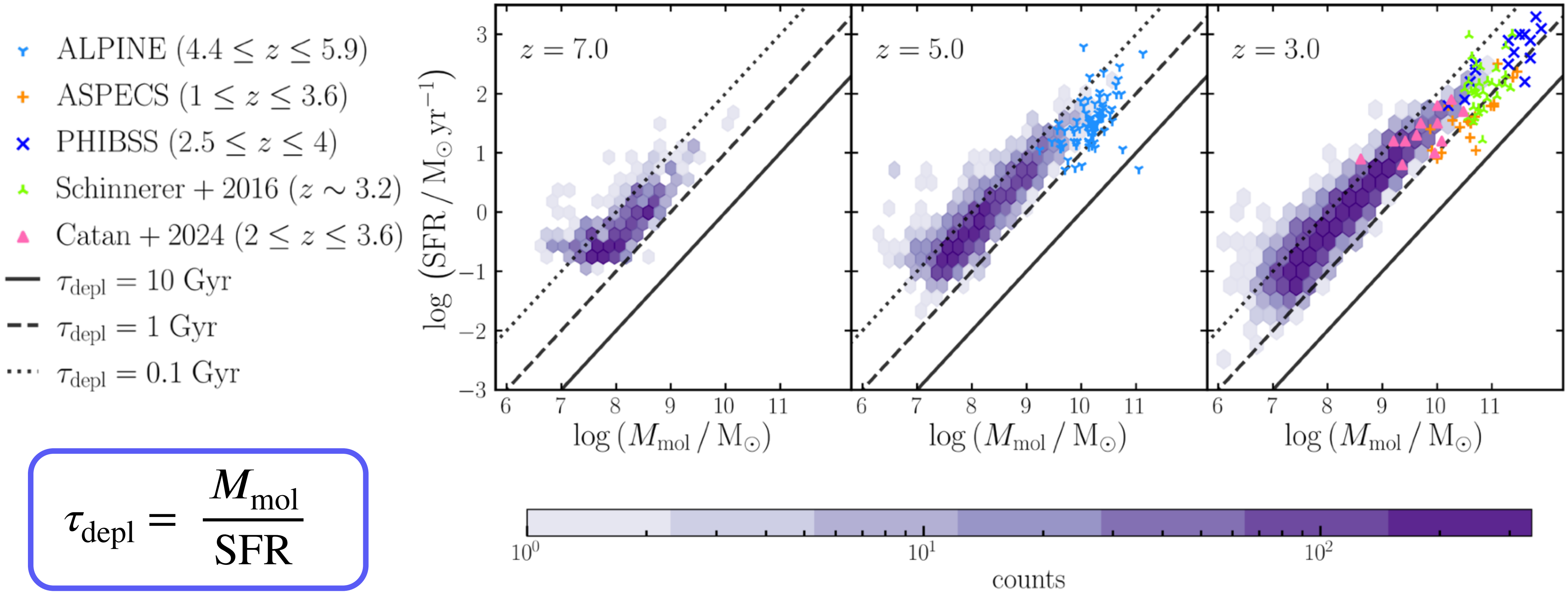
Notes. The last two columns show the values of $\Delta\mathrm{DIC}^{a}$ and $\Delta\mathrm{DIC}^{b}$ between the Schechter function and the DPL (see text).

MAIN-SEQUENCE OF STAR-FORMING GALAXIES



Distribution of simulated galaxies aligns with empirical relations

SFR-M_{MOL} RELATION IN MARIGOLD GALAXIES

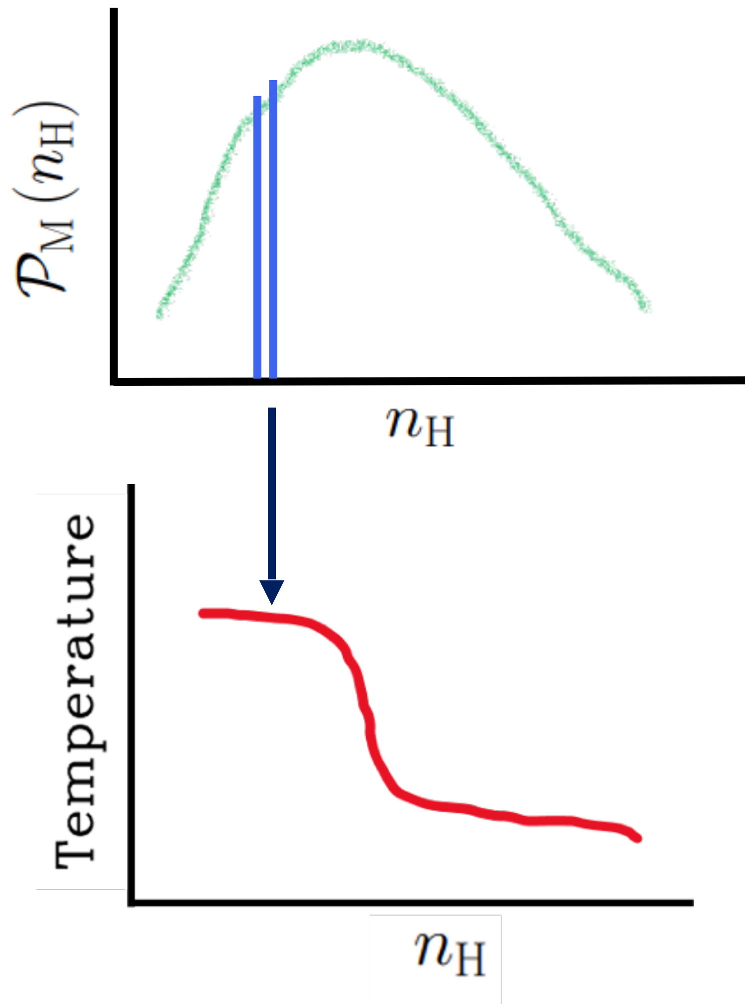


$$\tau_{depl} = \frac{M_{mol}}{\mathrm{SFR}}$$

Most simulated galaxies have τ_{depl} = 0.1-1 Gyr – similar to observed galaxies

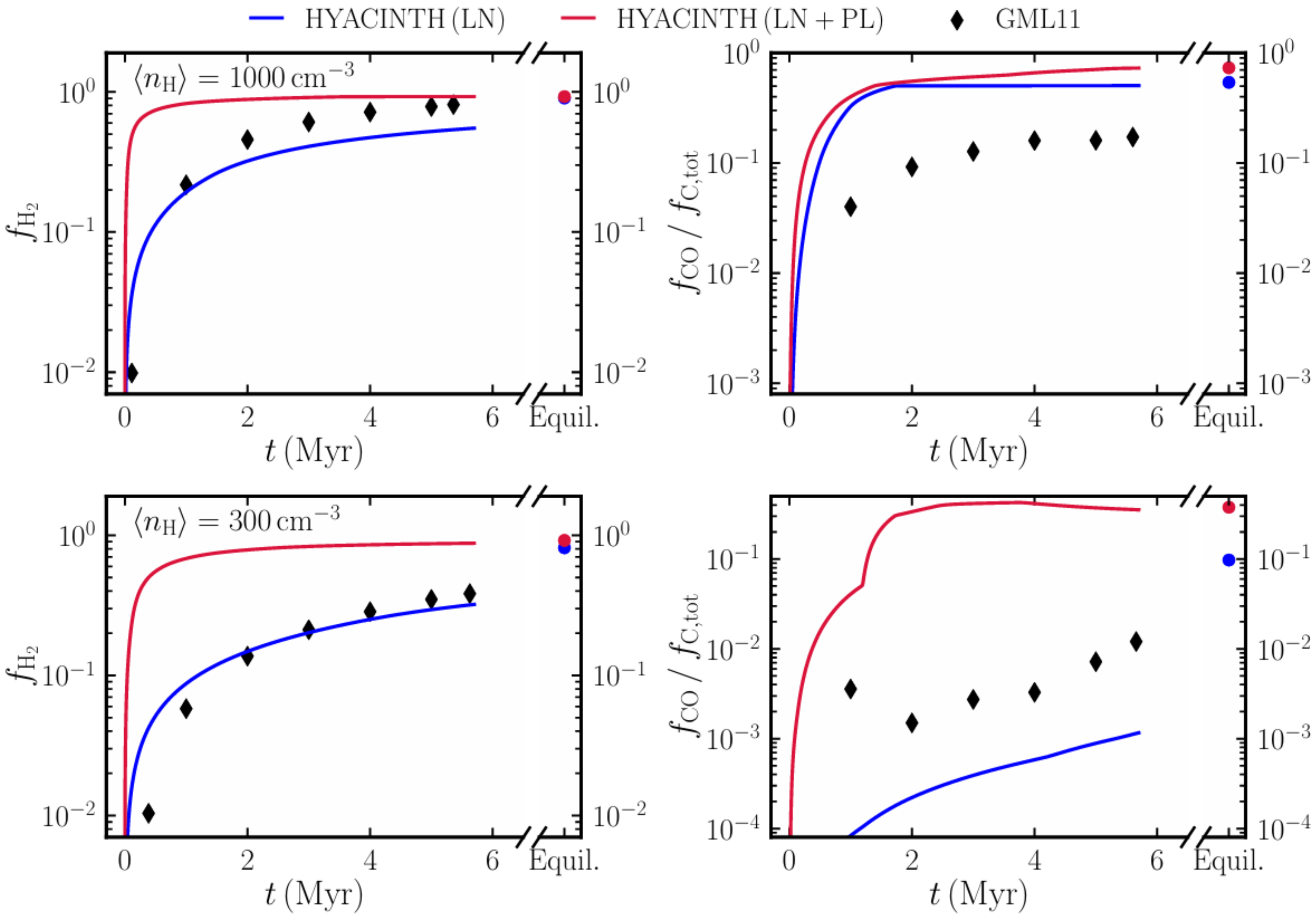
REACTION RATE CALCULATION

- Compute reaction rate at a given n_{H}
- For temperature-sensitive reactions – read out the T corresponding to a given n_{H} using the $T - n_{\mathrm{H}}$ **relation**
- Integrate over n_{H} weighing by the **PDF** to obtain the cell-level reaction rate
- Repeat for all reactions in the network

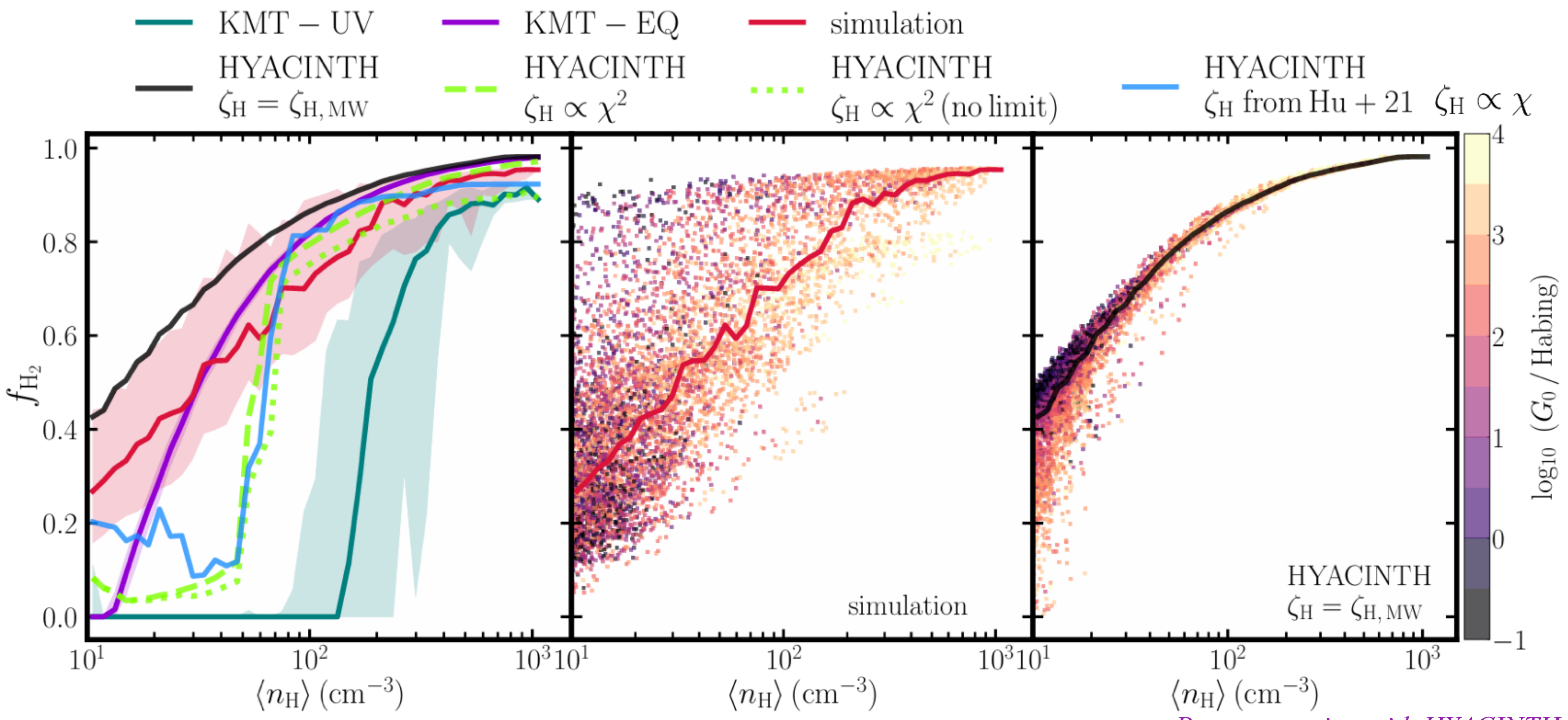


HYACINTH captures the effect of microscopic (i.e., unresolved) density fluctuations on the macroscopic (i.e., on resolved scales) chemical abundances.

Comparison of dynamically-evolve abundances with Glover & Mac Low 2011

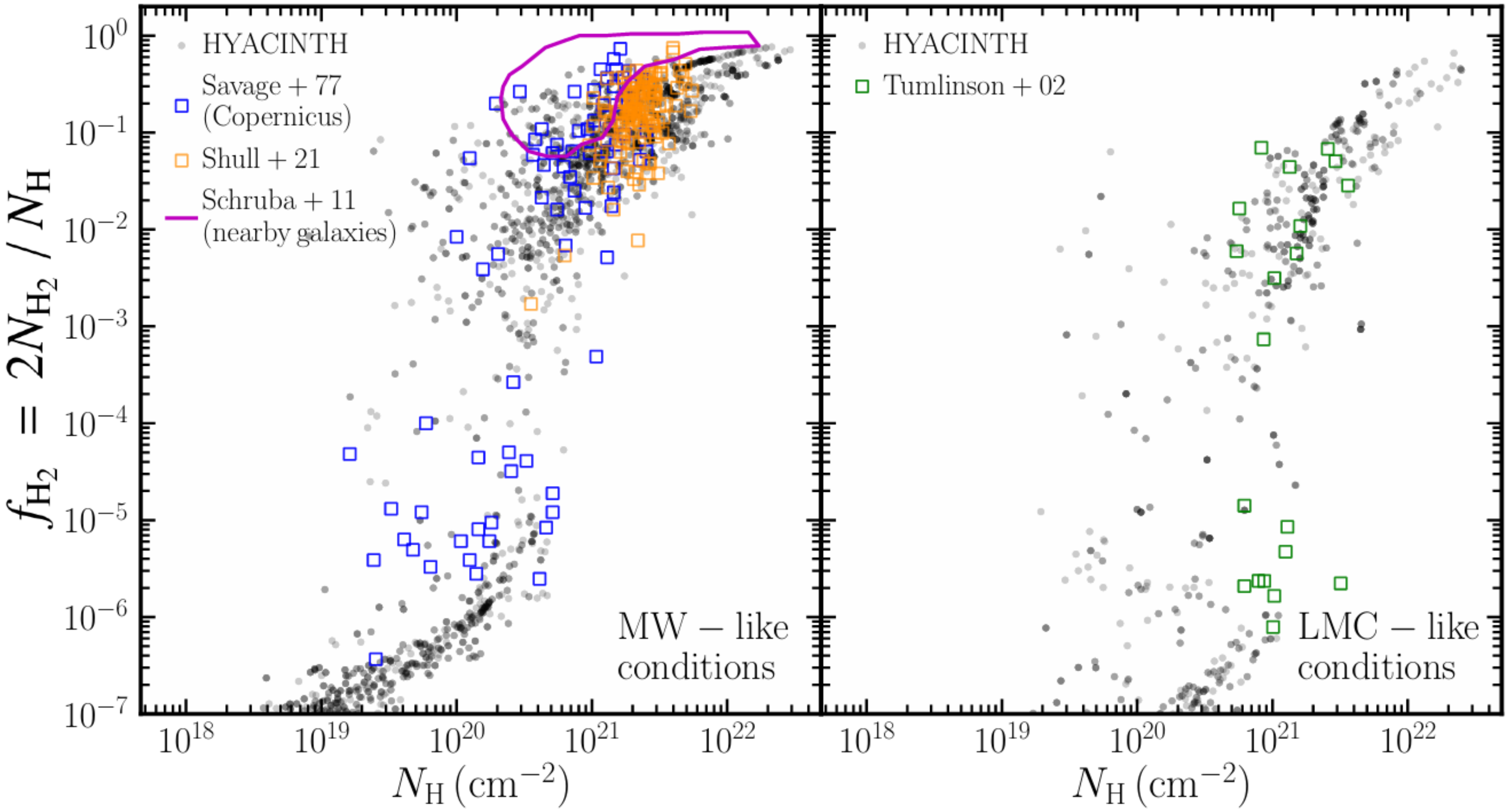


COMPARISON OF APPROACHES



Post-processing with HYACINTH

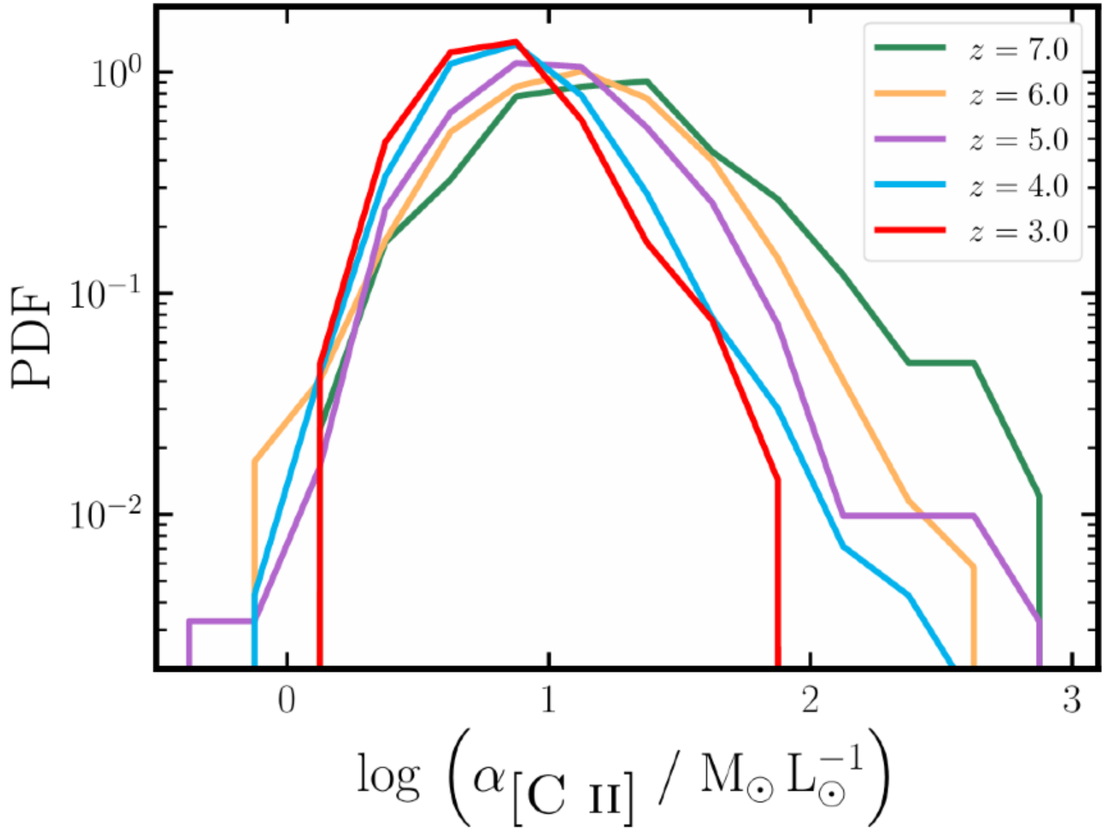
COMPARISON WITH OBSERVATIONS



Post-processing with HYACINTH

THE CONVERSION FACTOR $\alpha_{[CII]}$

Distribution of $\alpha_{[CII]}$



$$\alpha_{[CII]} = \frac{M_{mol}}{L_{[CII]}}$$

The numerical factor used to convert the observed [CII] luminosity to a molecular gas mass