



DUSTY | PRISM

Predicting the evolution of dust and PAHs across
cosmic time for PRIMA with radiation-hydrodynamics

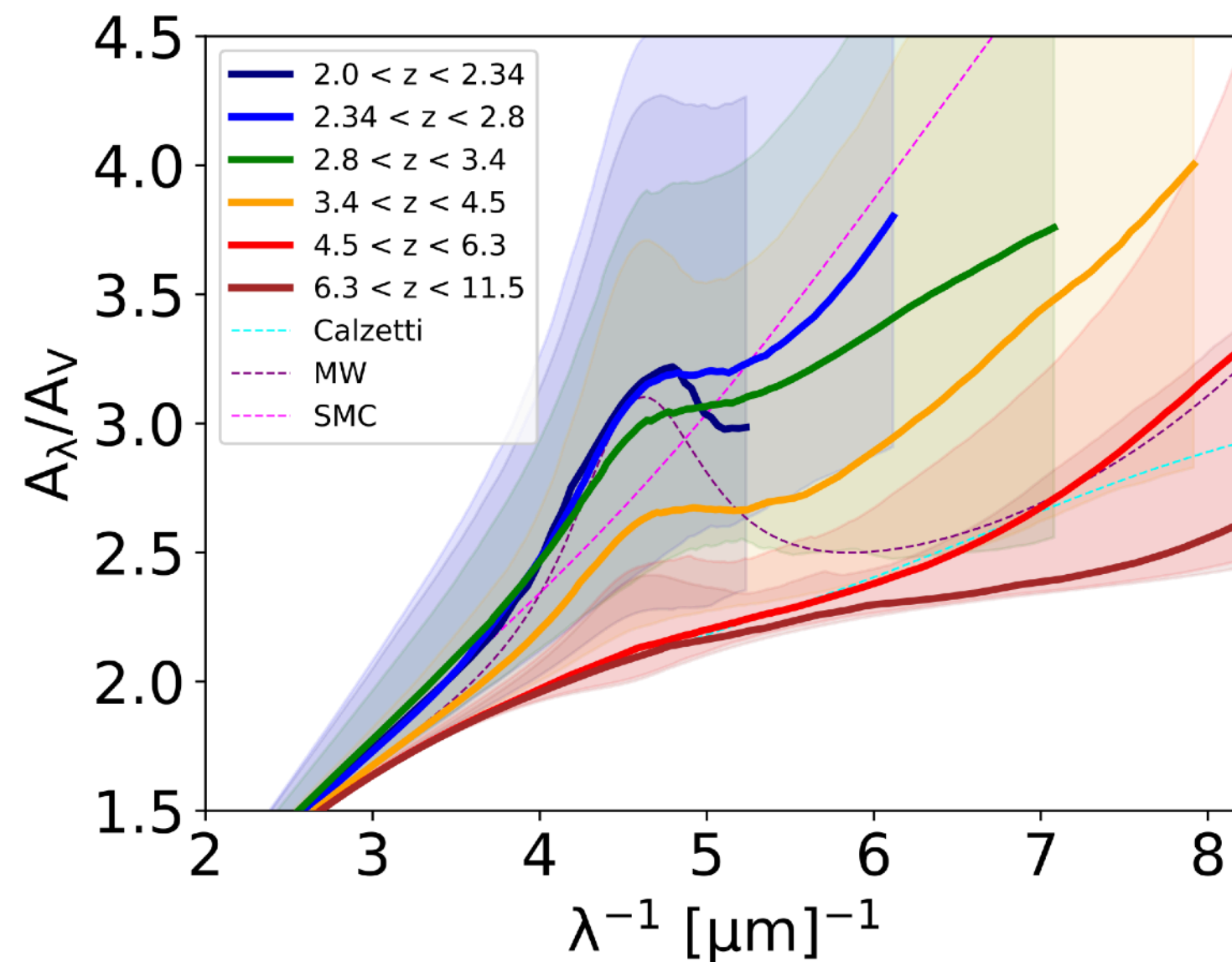
Francisco (Curro) Rodríguez Montero – Dusting Off the Secrets of the COSMOS with PRIMA IR Space Telescope

1. The need for forward modelling

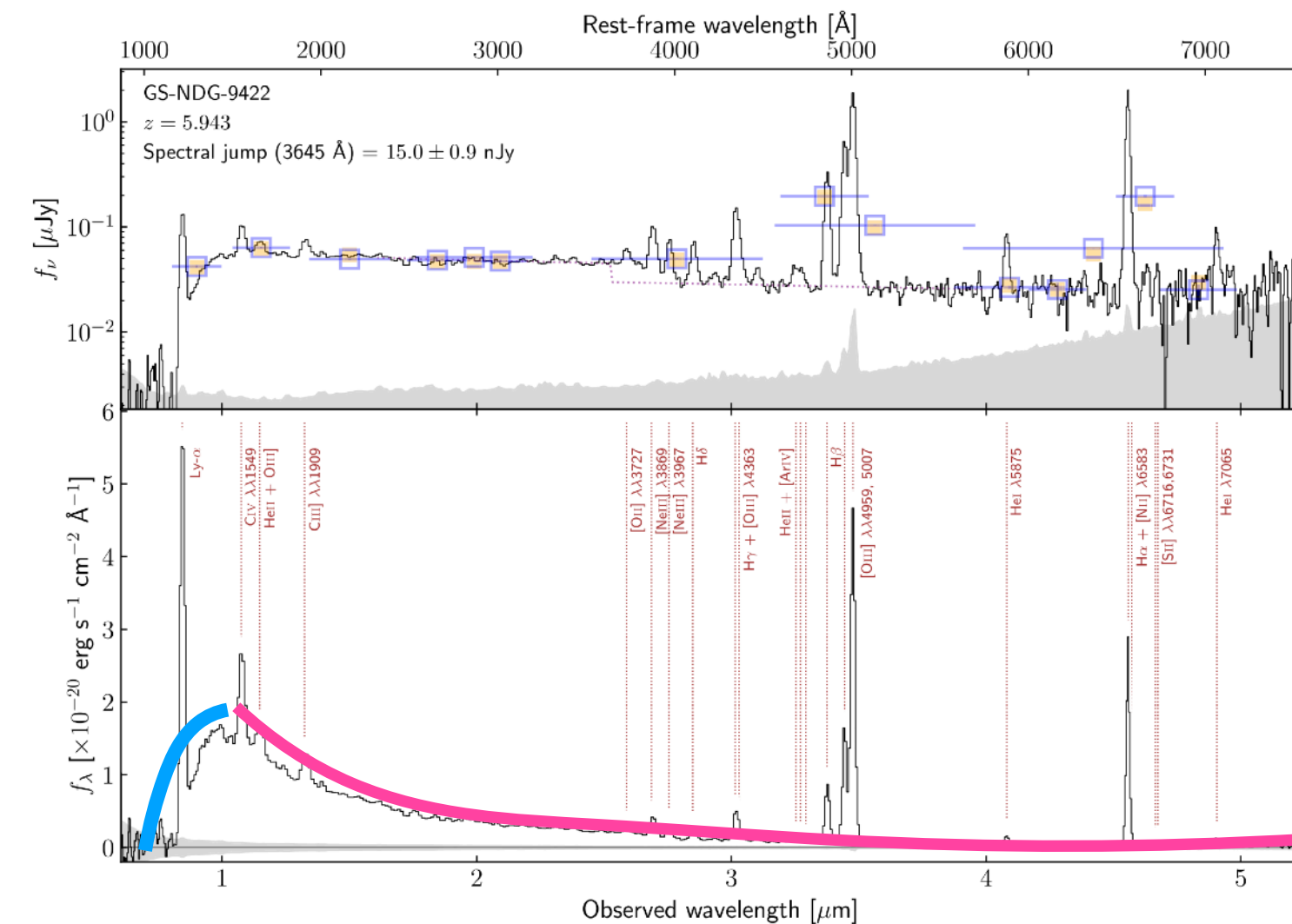
Cameron+2024

Studying galaxy formation at **all redshifts** relies heavily on **SED modelling**...

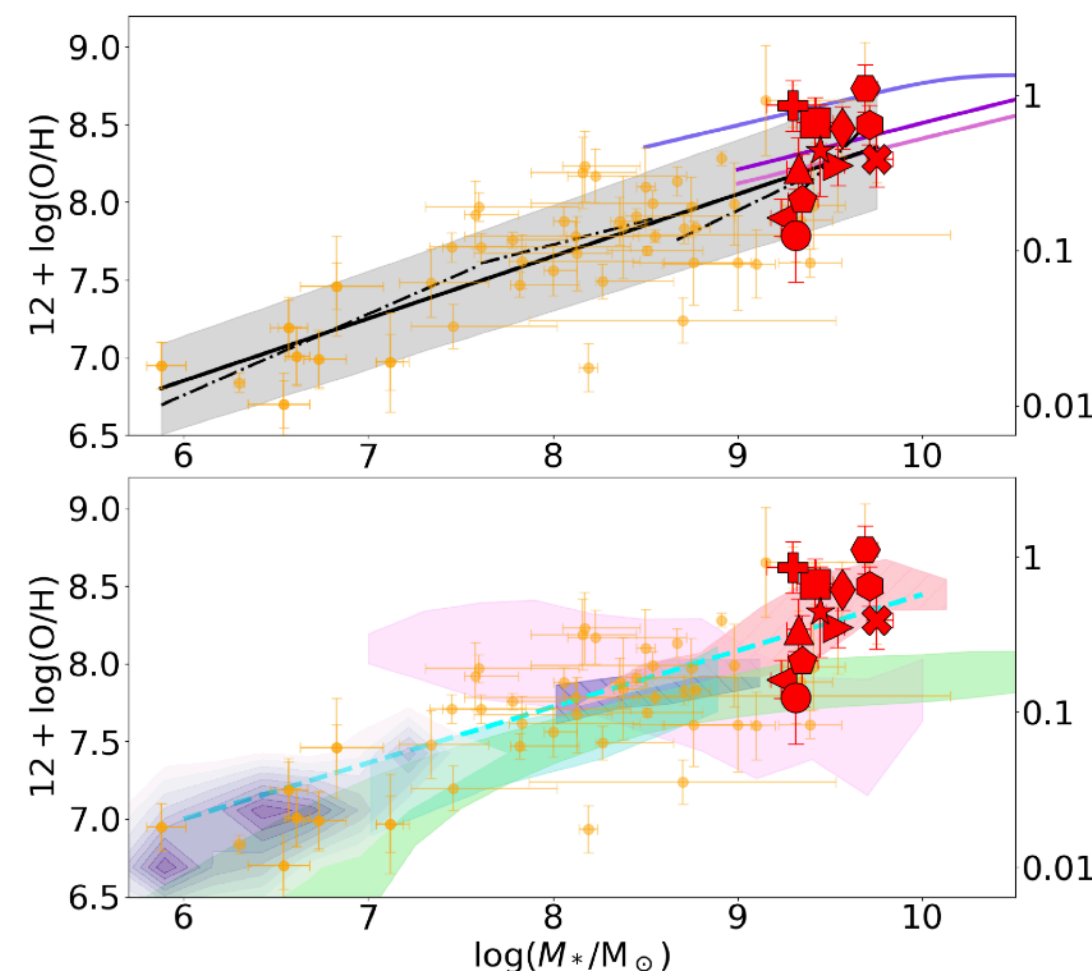
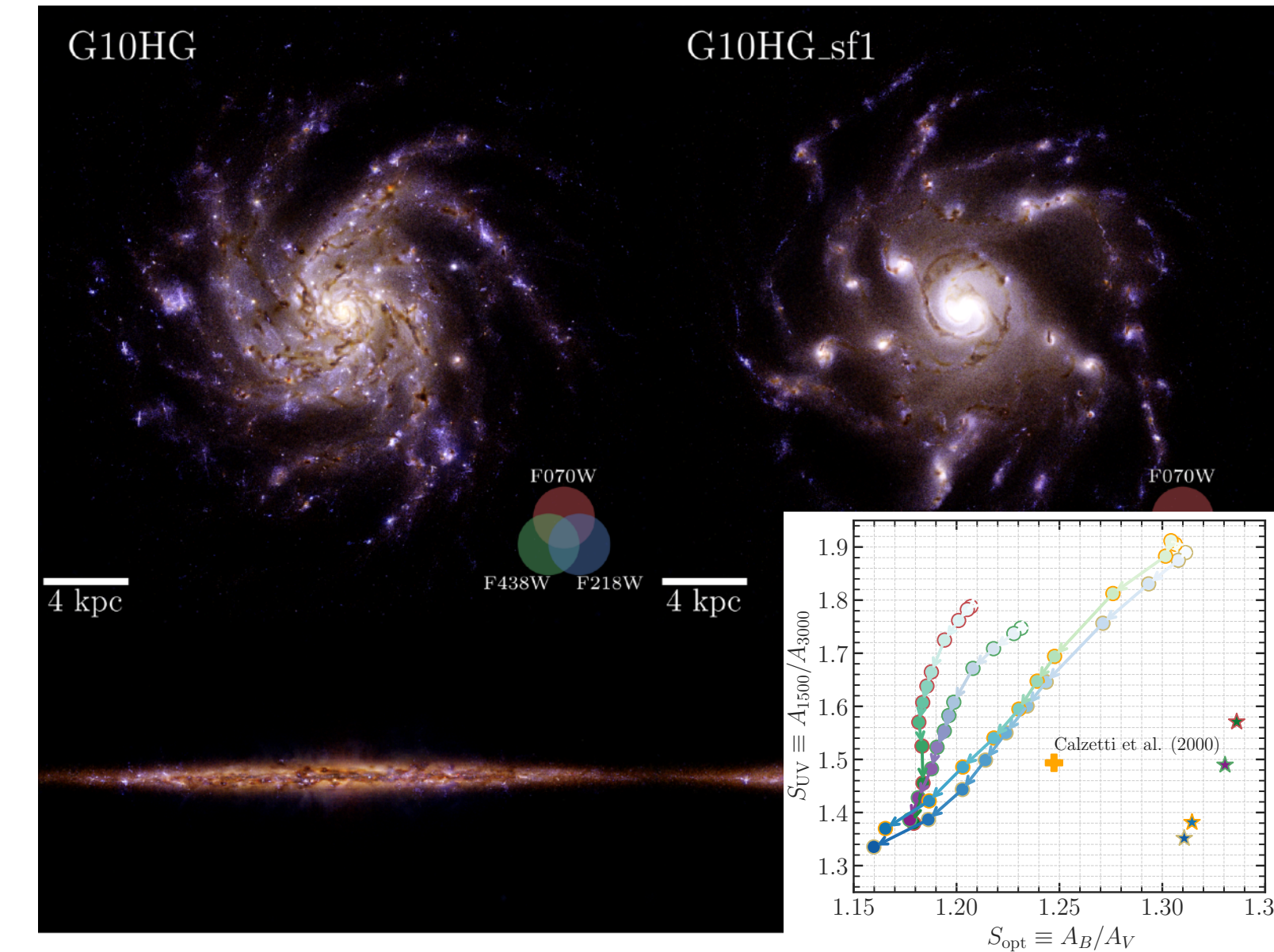
...but these rely on **unclear assumptions** and **extrapolations**



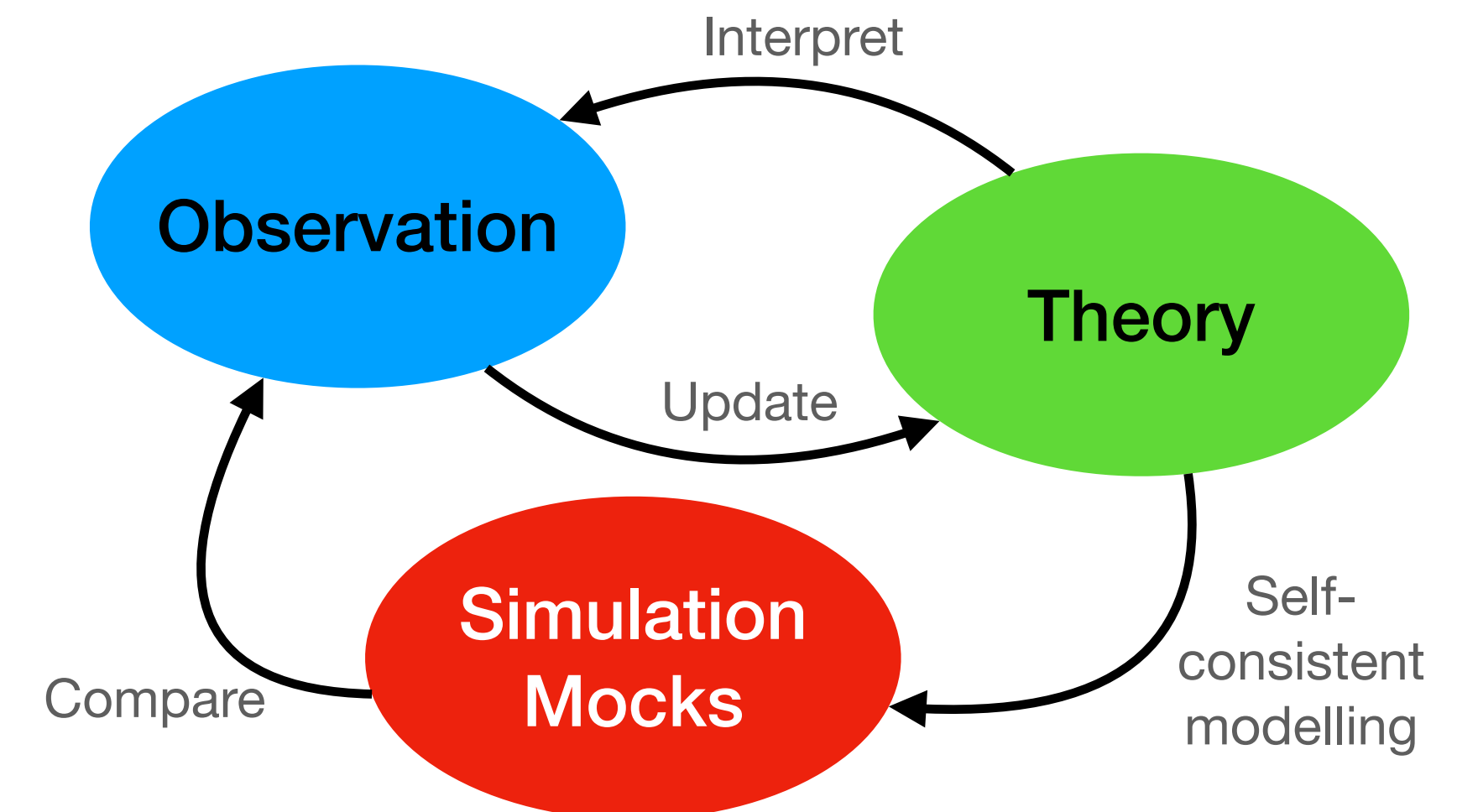
Markov+2024



Dubois, RM, in prep.

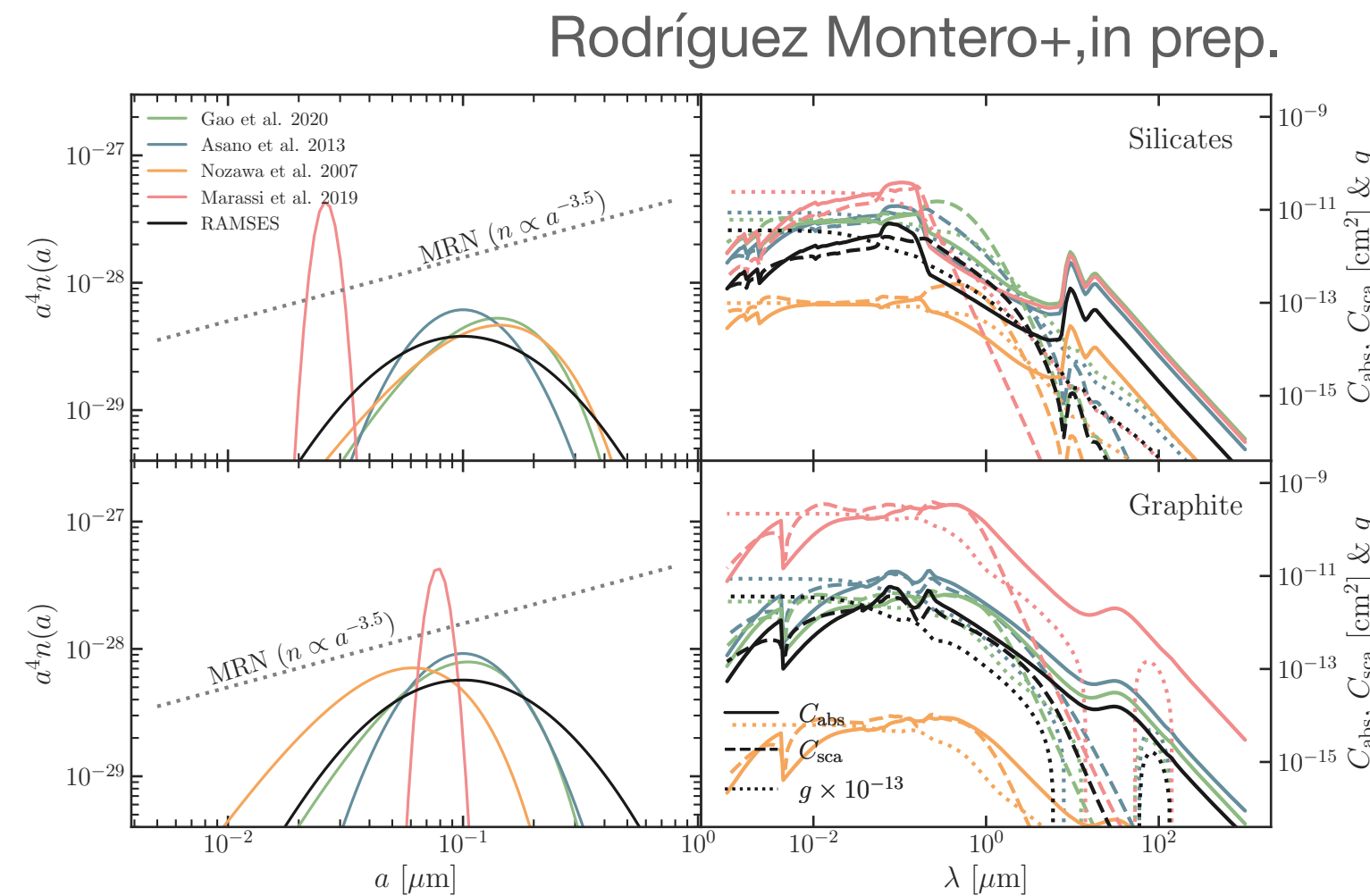
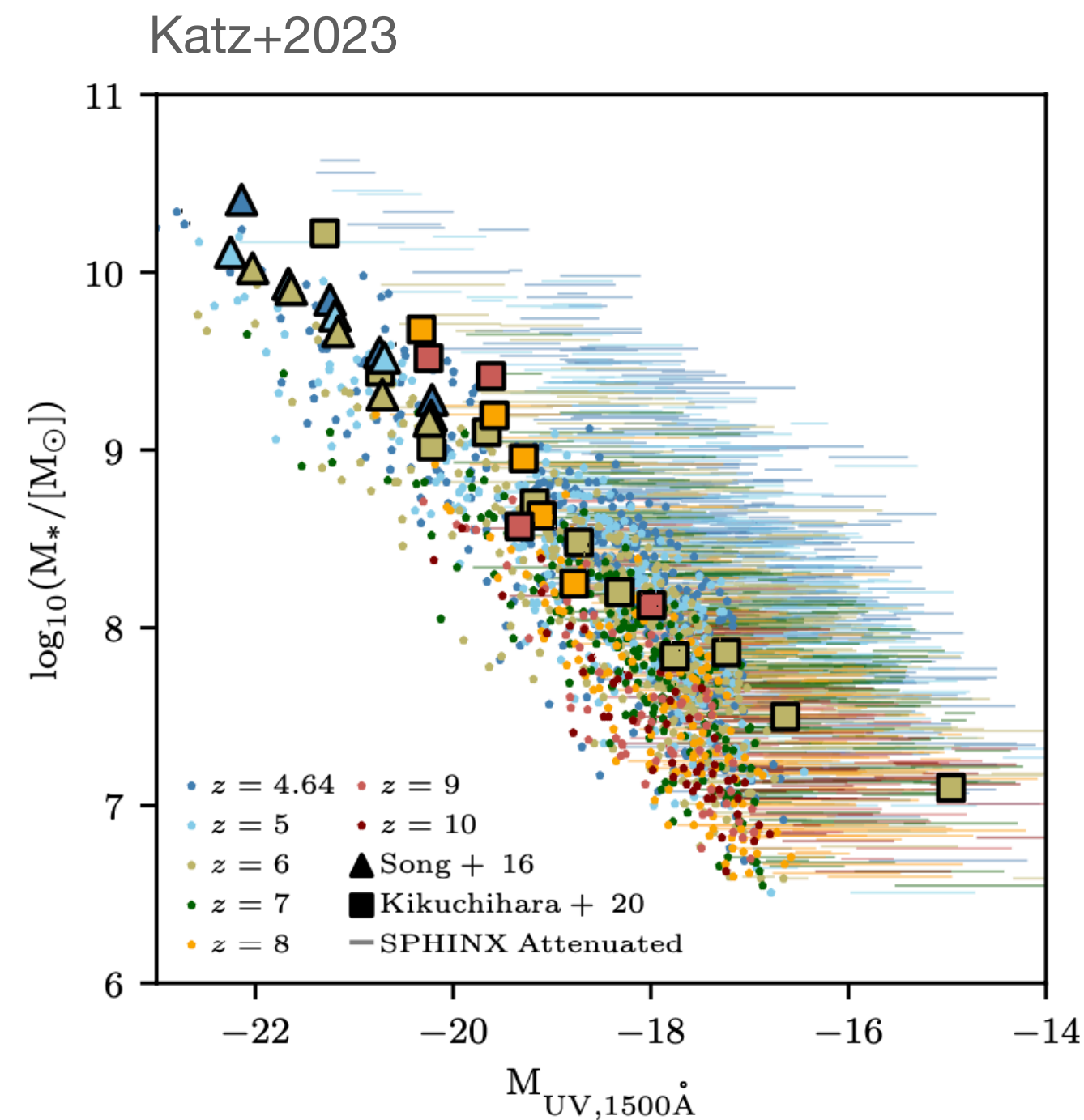


Rowland+2025



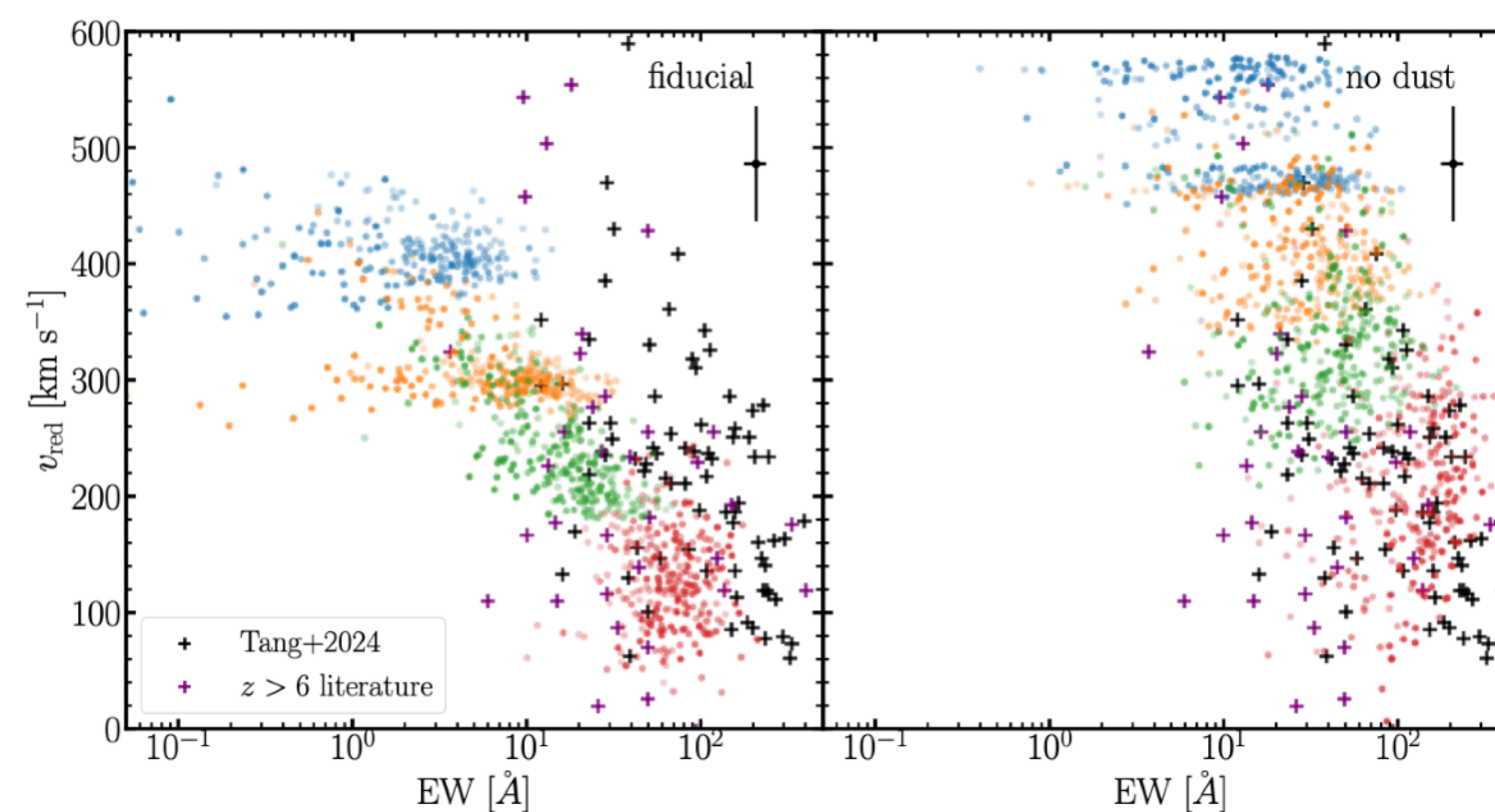
2. Why an on-the-fly dust model

UV-calibrated simulations have too **massive** and too **dusty** galaxies

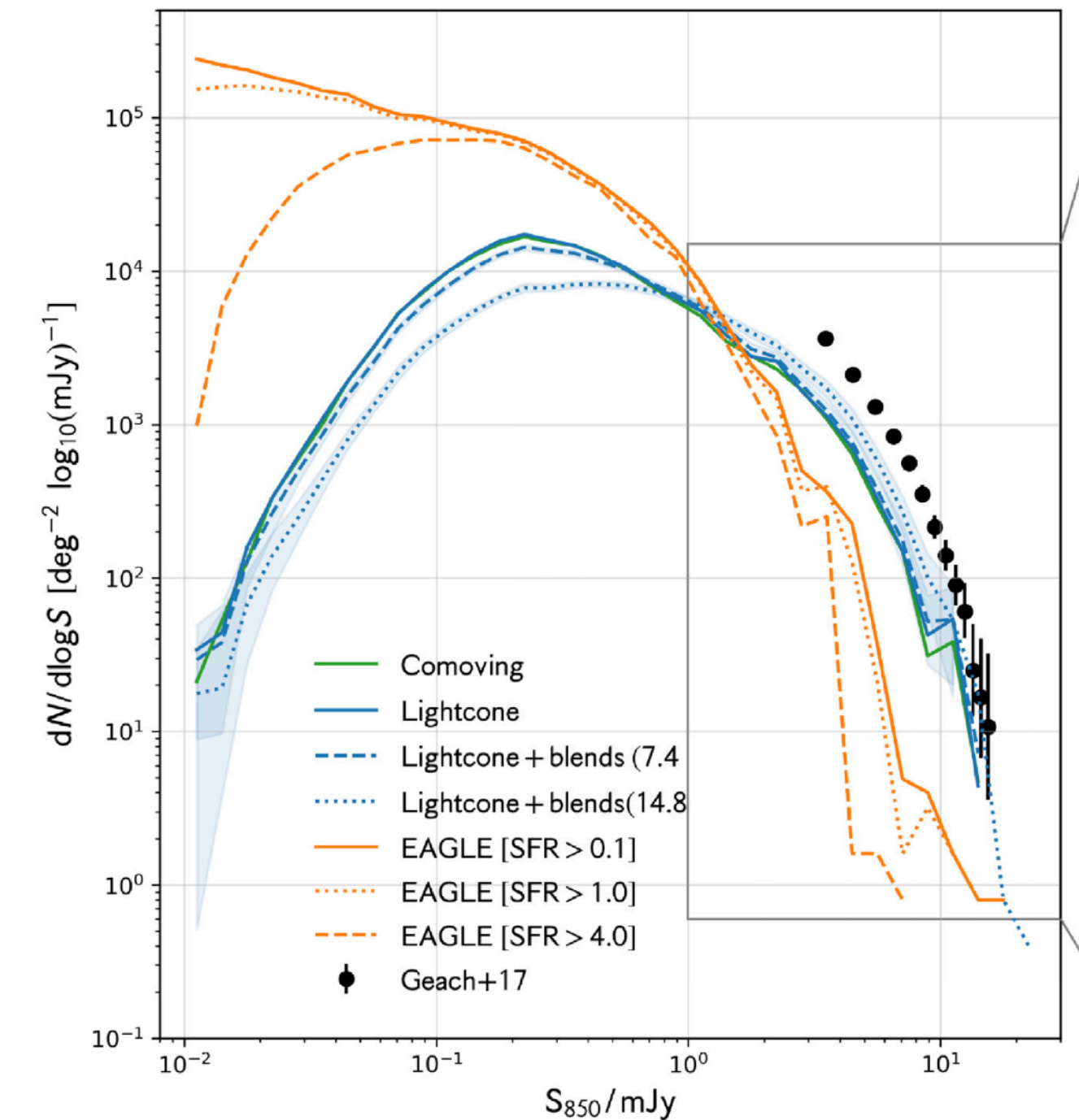


Simple dust models **incapable of predicting Ly α** observables, even with additional physics

Yuan+2025

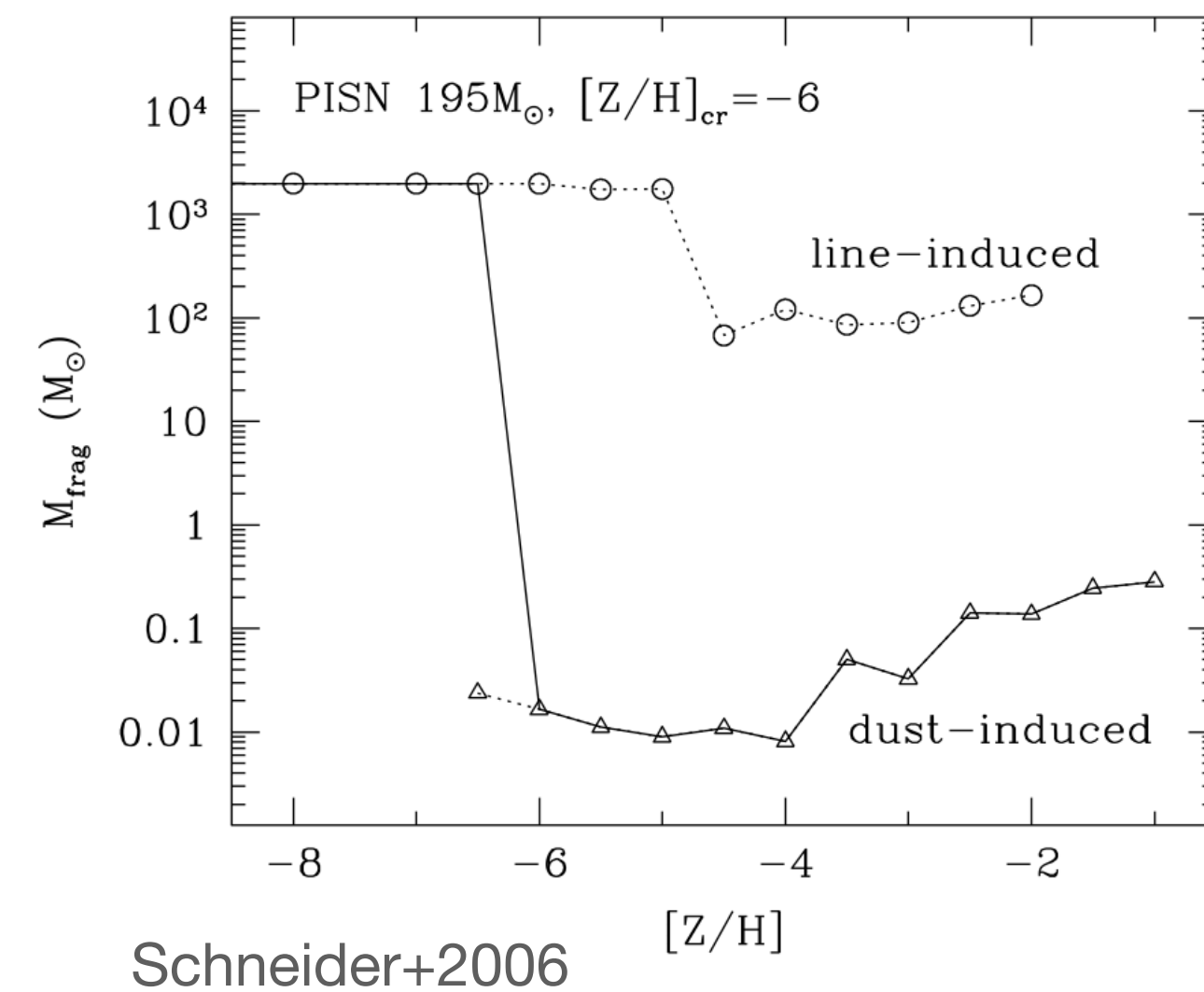


Lovell+2021



Dust modelling needs to go hand in hand with **ISM modelling**

2. Why an on-the-fly dust model



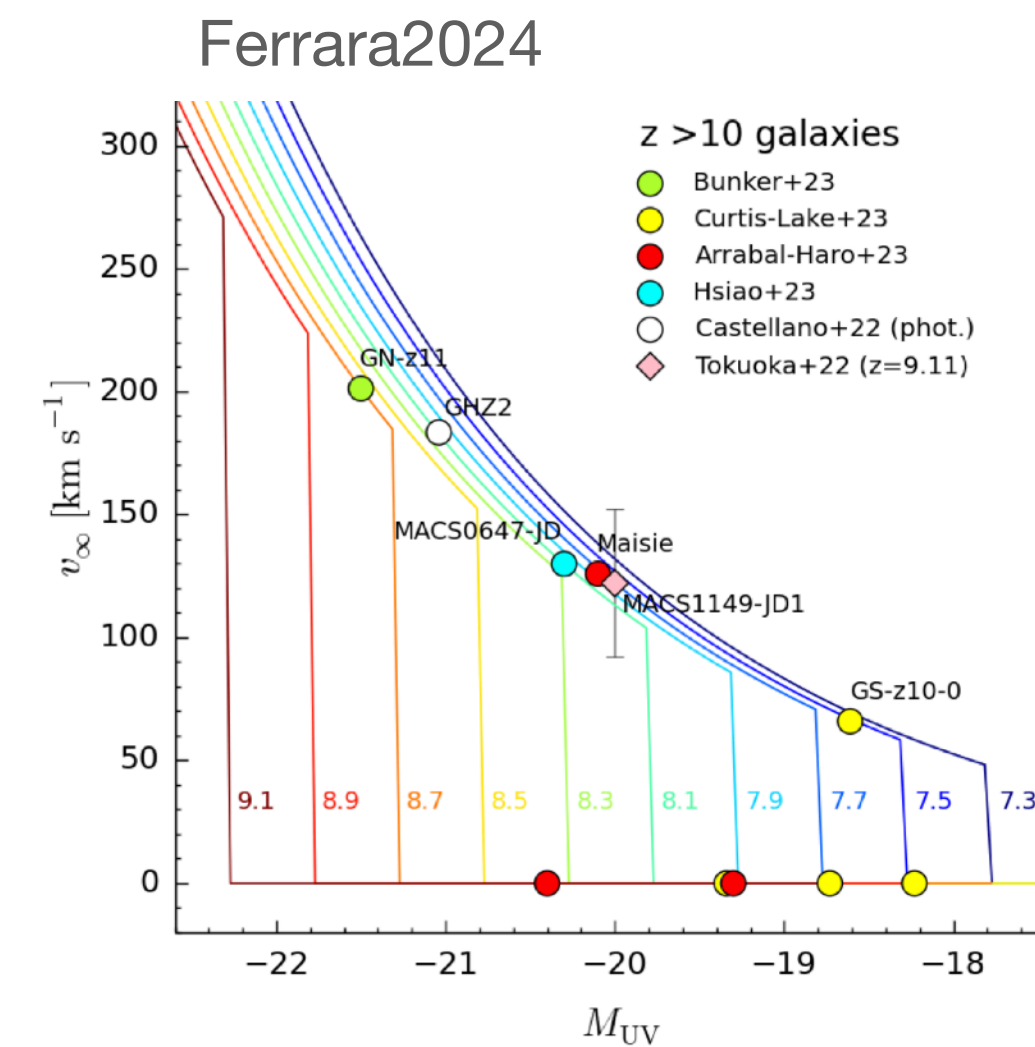
Dust physics have **timescales similar to fundamental ISM**, making **post-processing challenging**

Cloud fragmentation enriched by Pop III

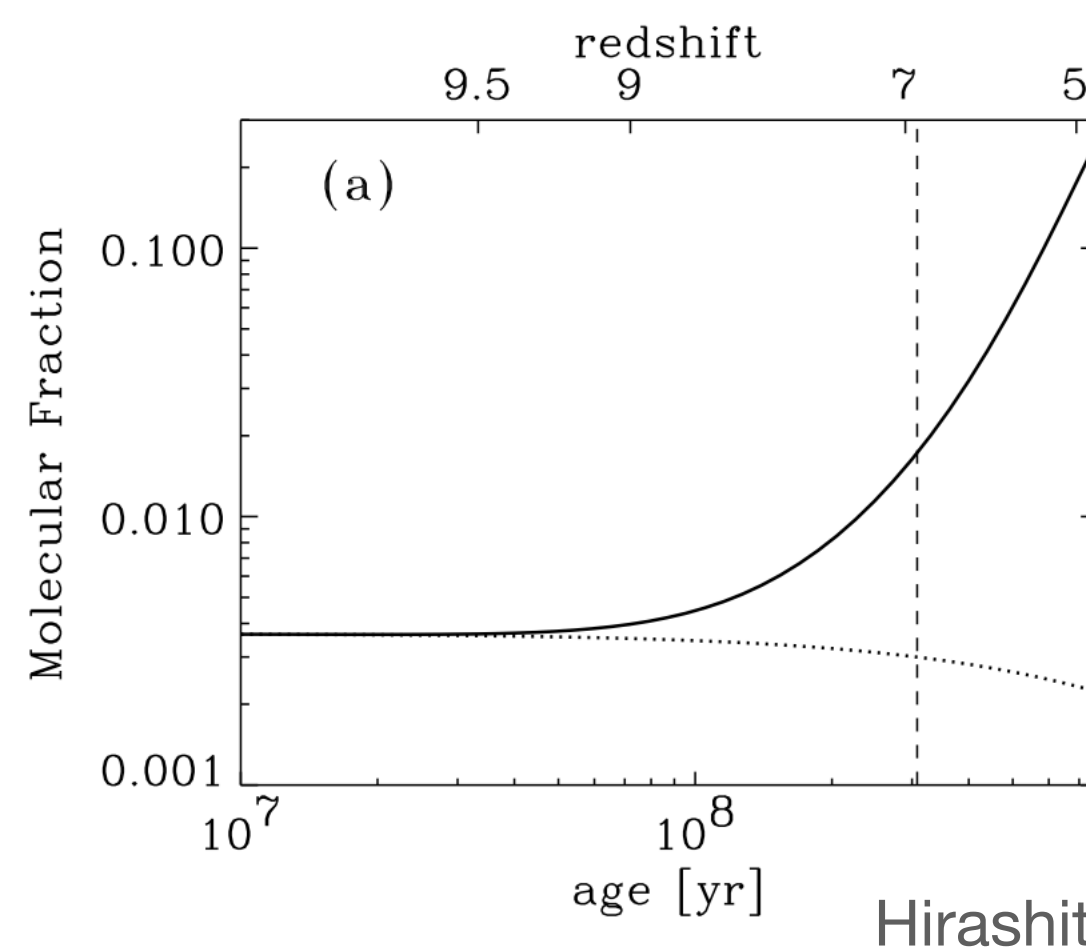
Radiation pressure

Just ~1% of the ISM mass, but a lot of influence!

Elemental abundances and enrichment



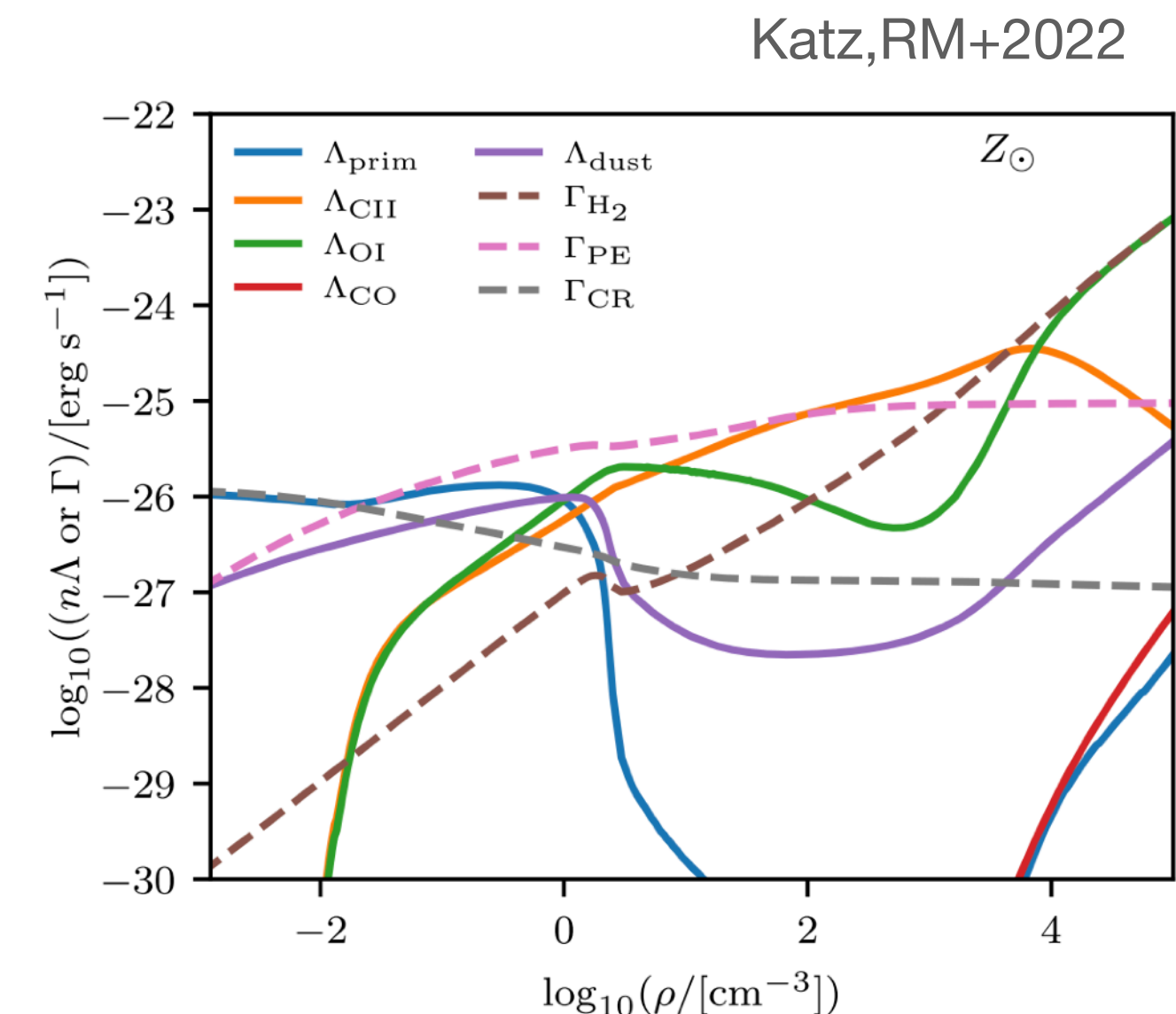
Ionisation properties of HII regions



Shielding from UV radiation

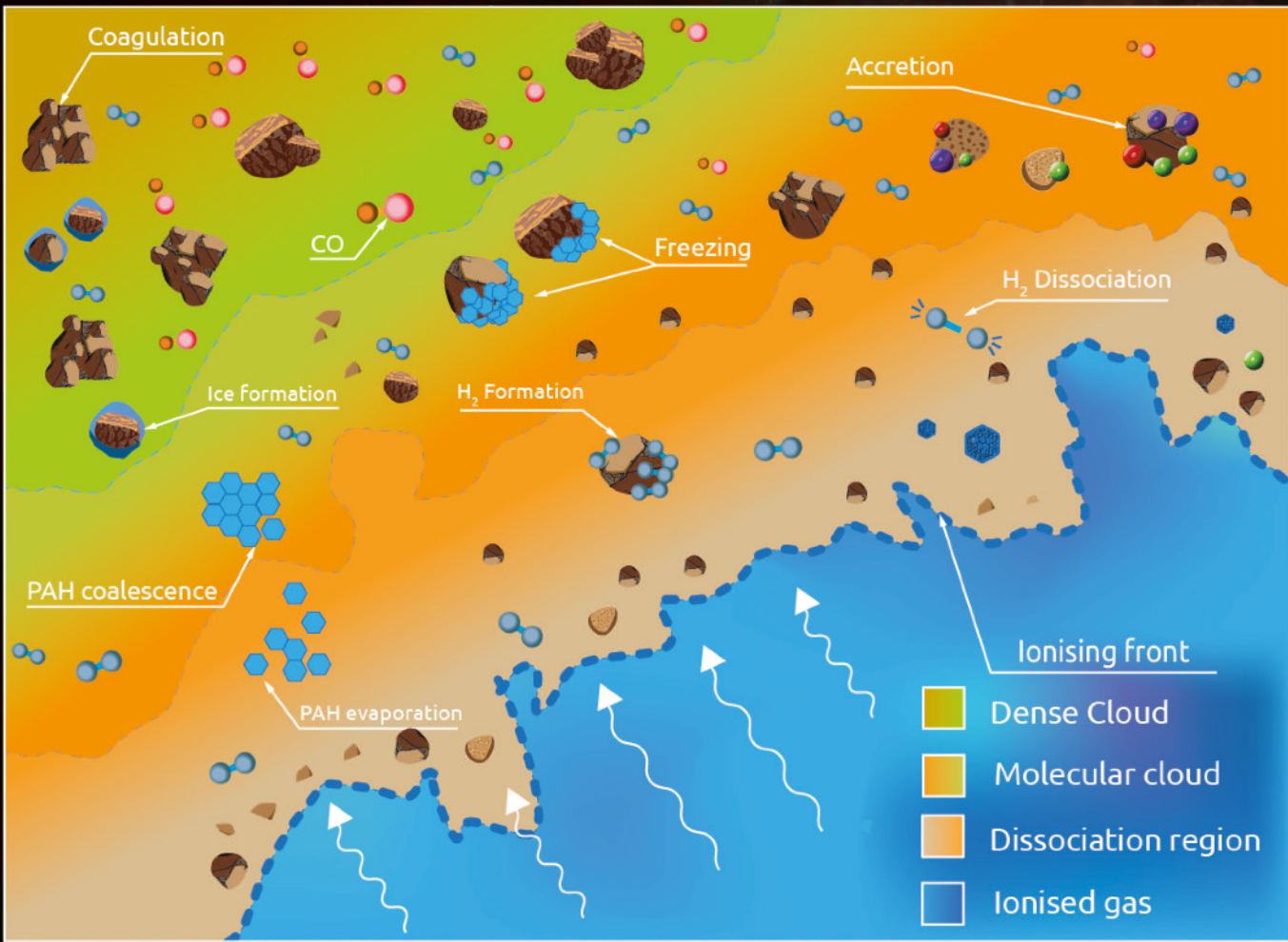
Photo-electric heating

Molecule catalysis



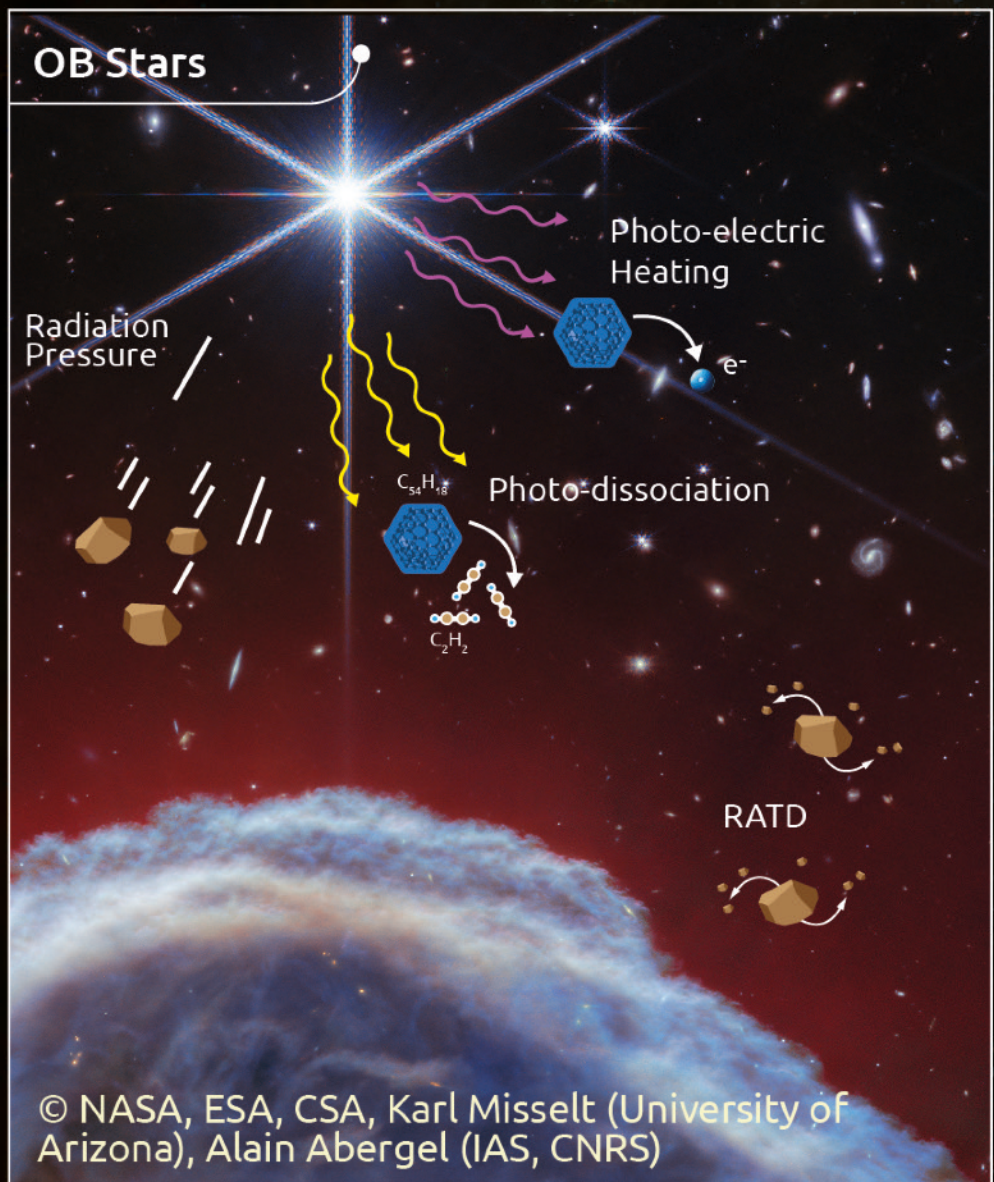
3. Introducing Dusty-PRISM

PDR and the Molecular Phase



The high gas density of molecular clouds allows for a rich and fast thermochemistry, the formation of molecules and the growth of dust. Dust and PAH properties quickly evolve as the gas transitions from the ionised HII gas, to the photo-dissociation region, into the molecular and ice regime

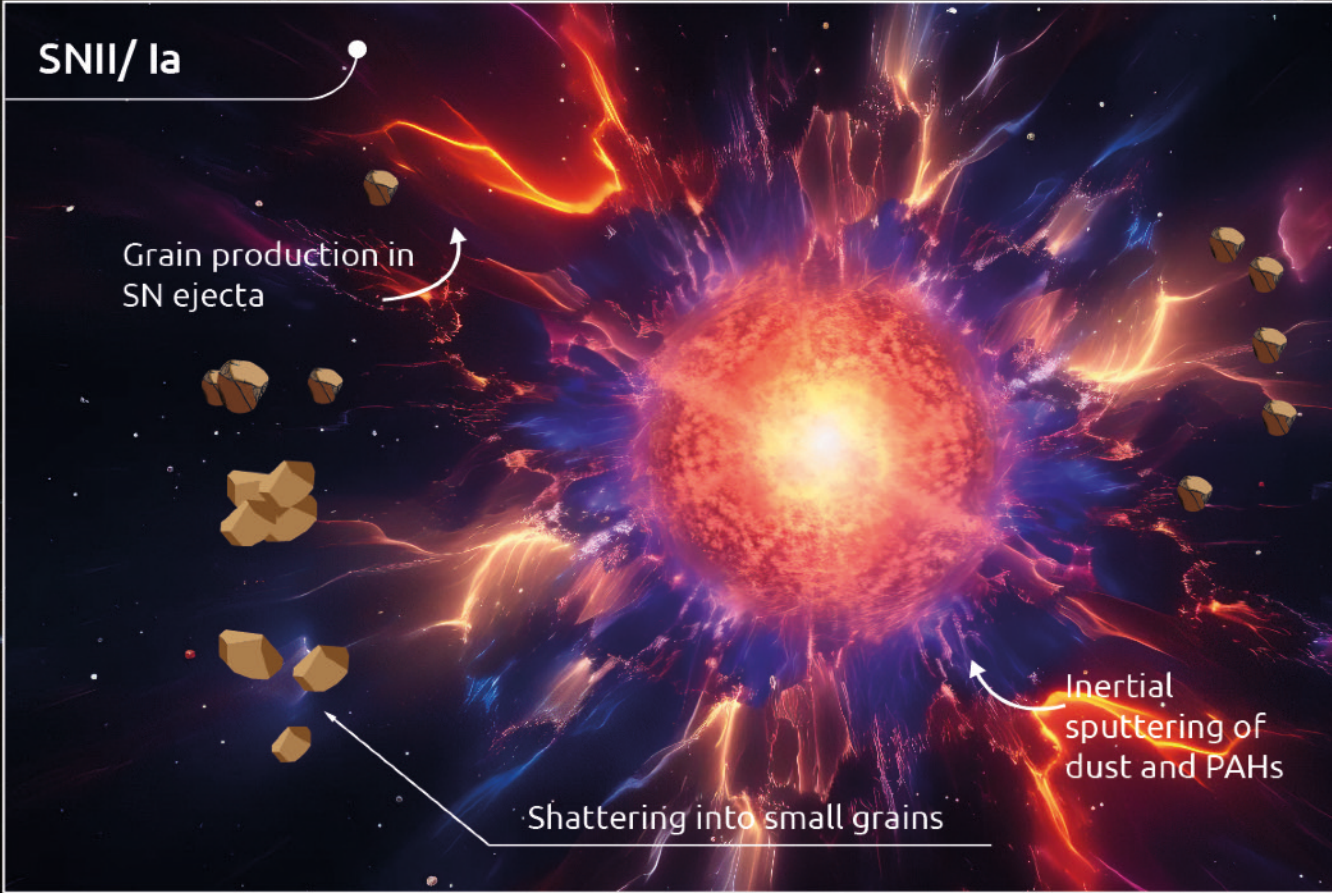
HII regions



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SEEDING AND DESTRUCTION BY STARS

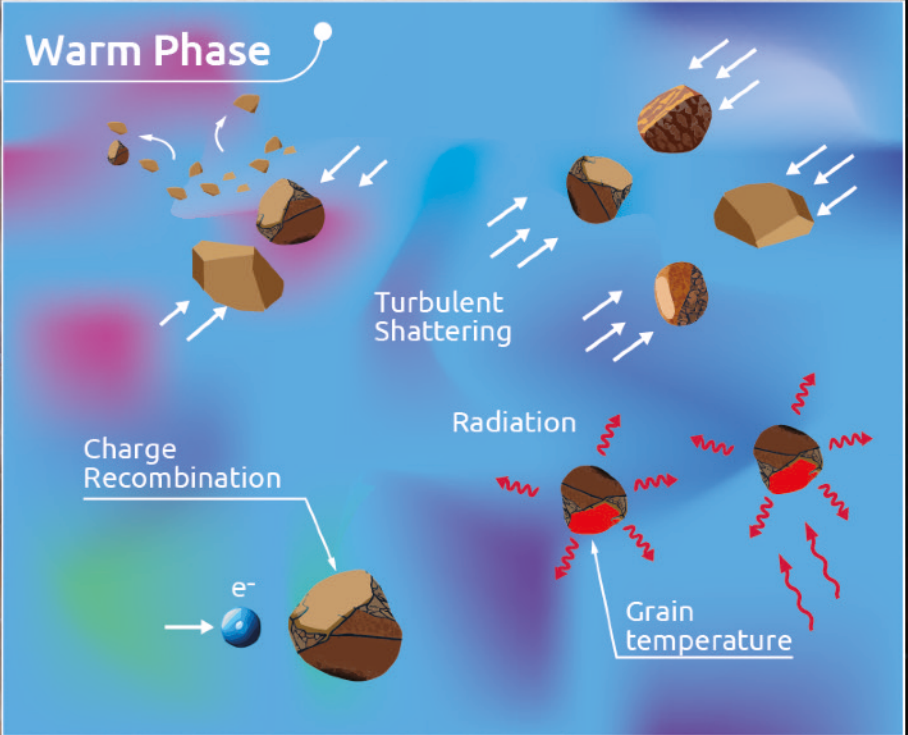
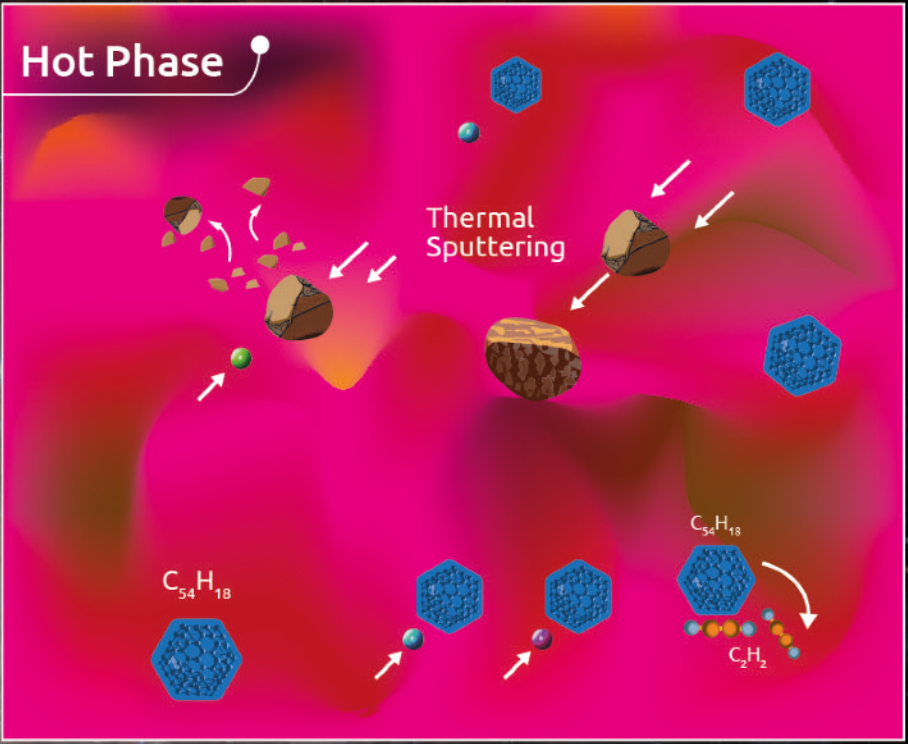
Stellar processes can both inject fresh dust and molecules to the ISM, as well as destroy the dusty material already present in it



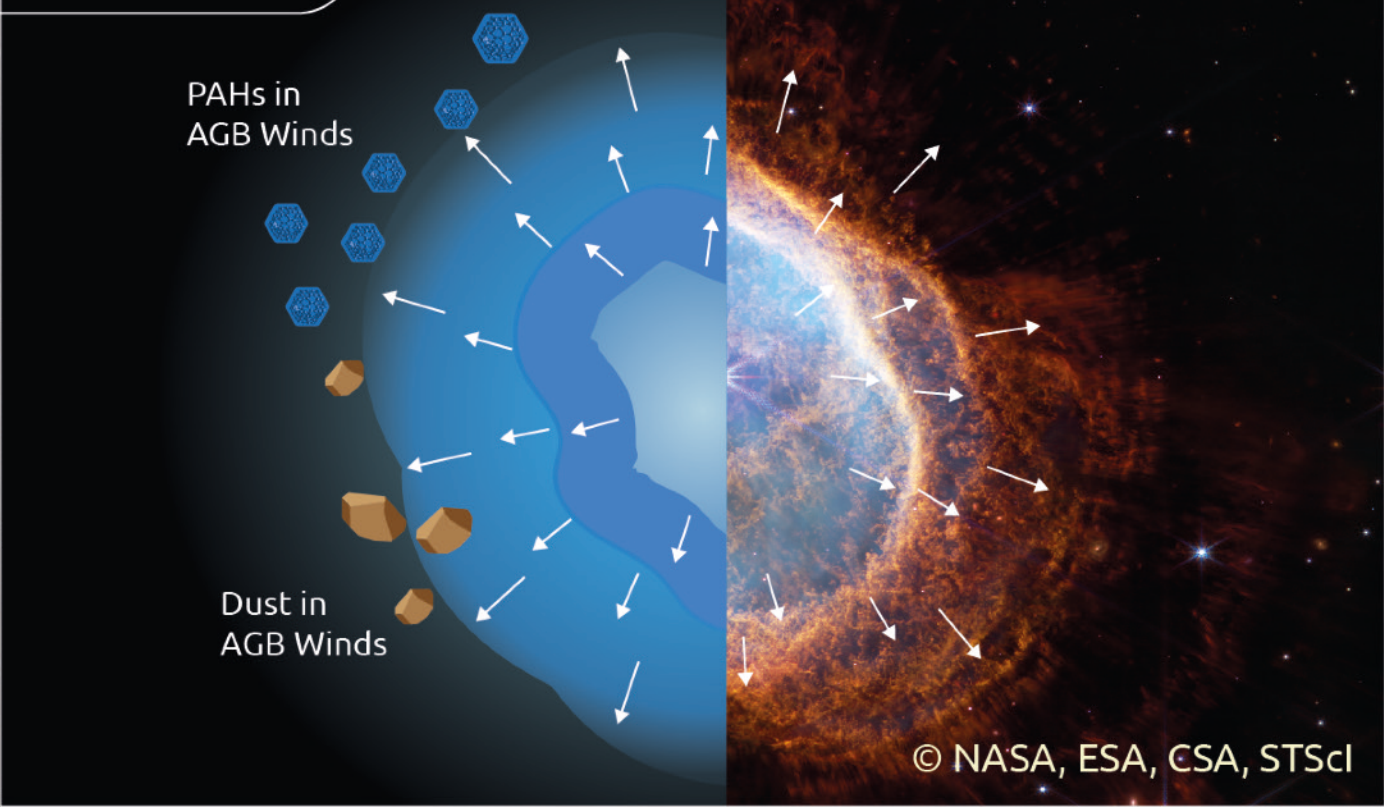
DUSTY|PRISM

From the first thermonuclear reaction in the early Universe, the condensation of metals into dust has played a fundamental role in the evolution of galaxies and how observe them today. Dusty-PRISM is a major step forward in our understanding of chemical enrichment of galaxies and their observables. It allows the tracking of the most relevant dust species, their seeding, growth, destruction and influence on the thermochemistry of the ISM. All while being fully coupled to non-equilibrium chemistry with on-the-fly radiation hydrodynamics.

THE TURBULENT DIFFUSE ISM



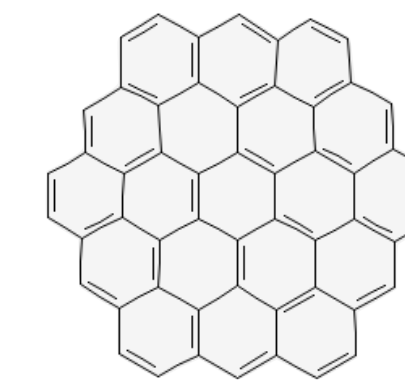
AGB Winds



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3. Introducing Dusty-PRISM

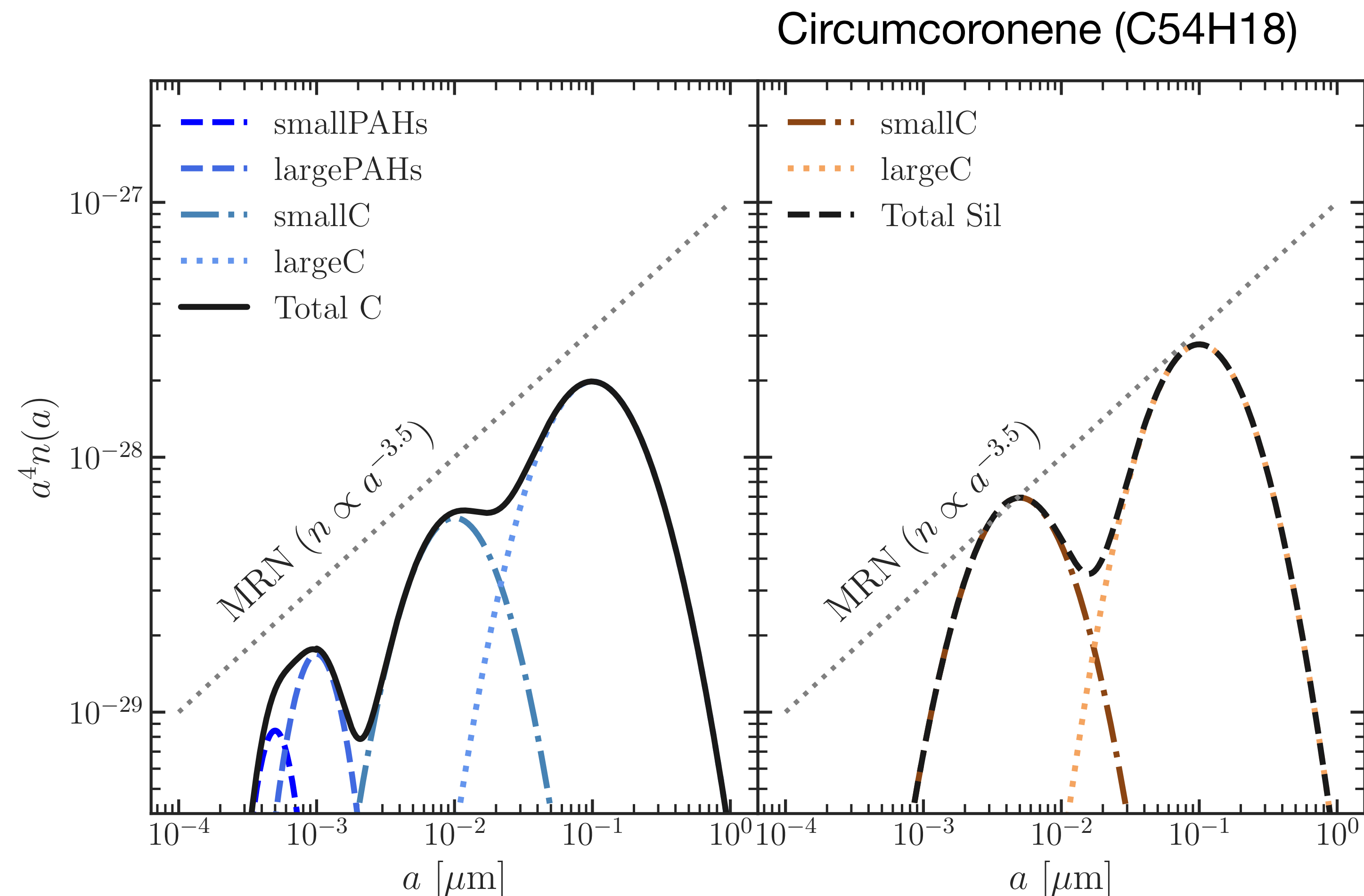
Extending the GSD into the molecular regime



Why smalls AND large?

- Strong polarisability = strong bonding between aromatic planes
- Clusters may be the carrier of the mid-IR plateau
- Variation in band ratios
- Link between molecules and amorphous grains

	s [g cm ⁻³]	N_C	a_0 [μm]	a_{\min} [μm]	a_{\max} [μm]
small PAHs	2.0	54	5×10^{-4}	3×10^{-4}	1×10^{-3}
large PAHs	2.0	418	1×10^{-3}	3×10^{-4}	9×10^{-3}
small C	2.2	-	1×10^{-2}	1×10^{-3}	1×10^{-1}
large C	2.2	-	1×10^{-1}	5×10^{-3}	1.0
small Sil	3.3	-	5×10^{-3}	5×10^{-4}	1×10^{-1}
large Sil	3.3	-	1×10^{-1}	5×10^{-3}	1.0



3. Introducing Dusty-PRISM

Building a dynamical, molecular ISM

Implementation in the RAMSES code:
radiation transfer hydrodynamics code with magnetic fields and cosmic ray transport

ISM Physics

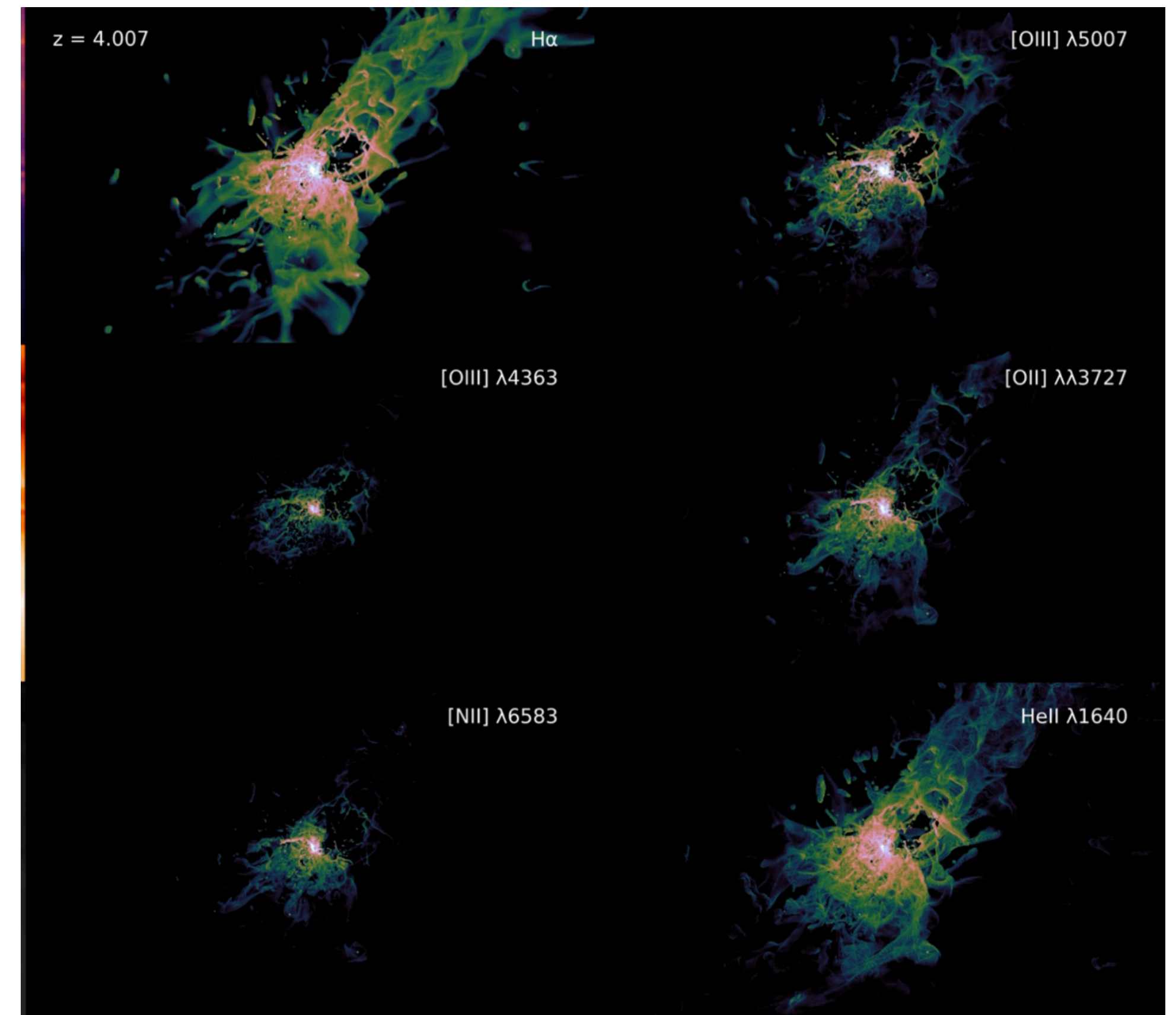
- M1 multi-band on-the-fly radiation transfer
- Full non-eq chemistry network tracking the population of ~150 ions, H₂ and CO
- H/He and metal cooling
- H₂ heating and cooling
- Photo-heating
- Photo-electric heating
- Charge transfer
- Cosmic ray heating

Dust physics

- 6 grain species
- Tracking of ice formation
- Turbulent model for shattering and coagulation
- Size-dependent sputtering and collisional cooling
- H₂ formation
- RAT-D
- Sublimation
- Charge-mediated accretion
- Recombination cooling and photoelectric heating

diffusion length

(Gas-dust fully coupled)
$$L_D = 5 \left(\frac{a_{\text{gr}}}{0.1 \mu\text{m}} \right) \left(\frac{n}{1 \text{cm}^{-3}} \right)^{-1} \left(\frac{\sigma_{\text{gr}}}{c_s} \right) \text{pc}$$



3. Introducing Dusty-PRISM

Coupling to on-the-fly multi-bin RT and non-eq chemistry

(Optical properties based on the NASA AMES PAH Database)

Photo-electric heating (PEH)

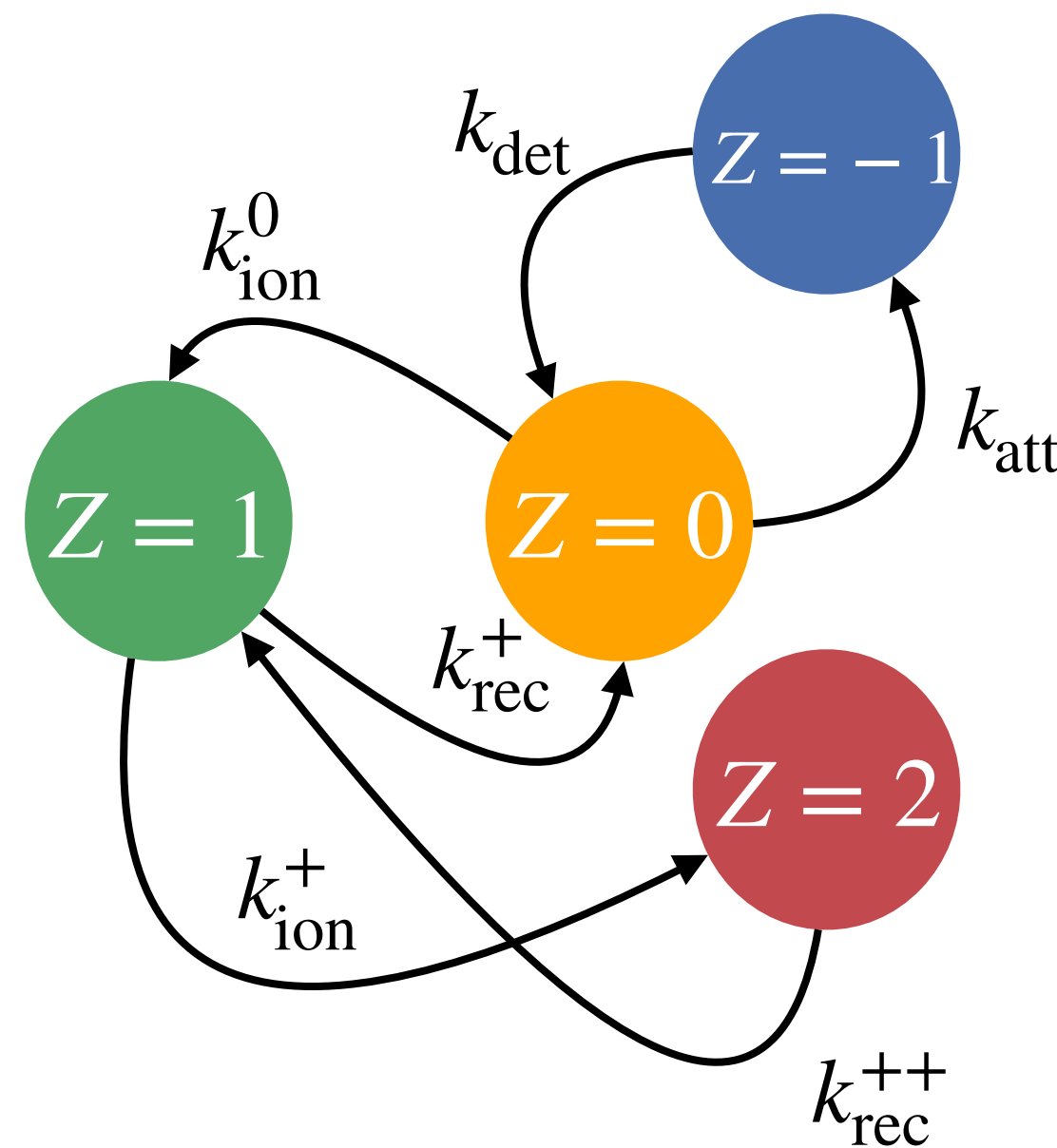
Consider at every position and time:
 Photo-ionisation
 + Recombination
 + Electron attachment
 + Electron detachment

Self-consistent local heating!!

Photo-dissociation

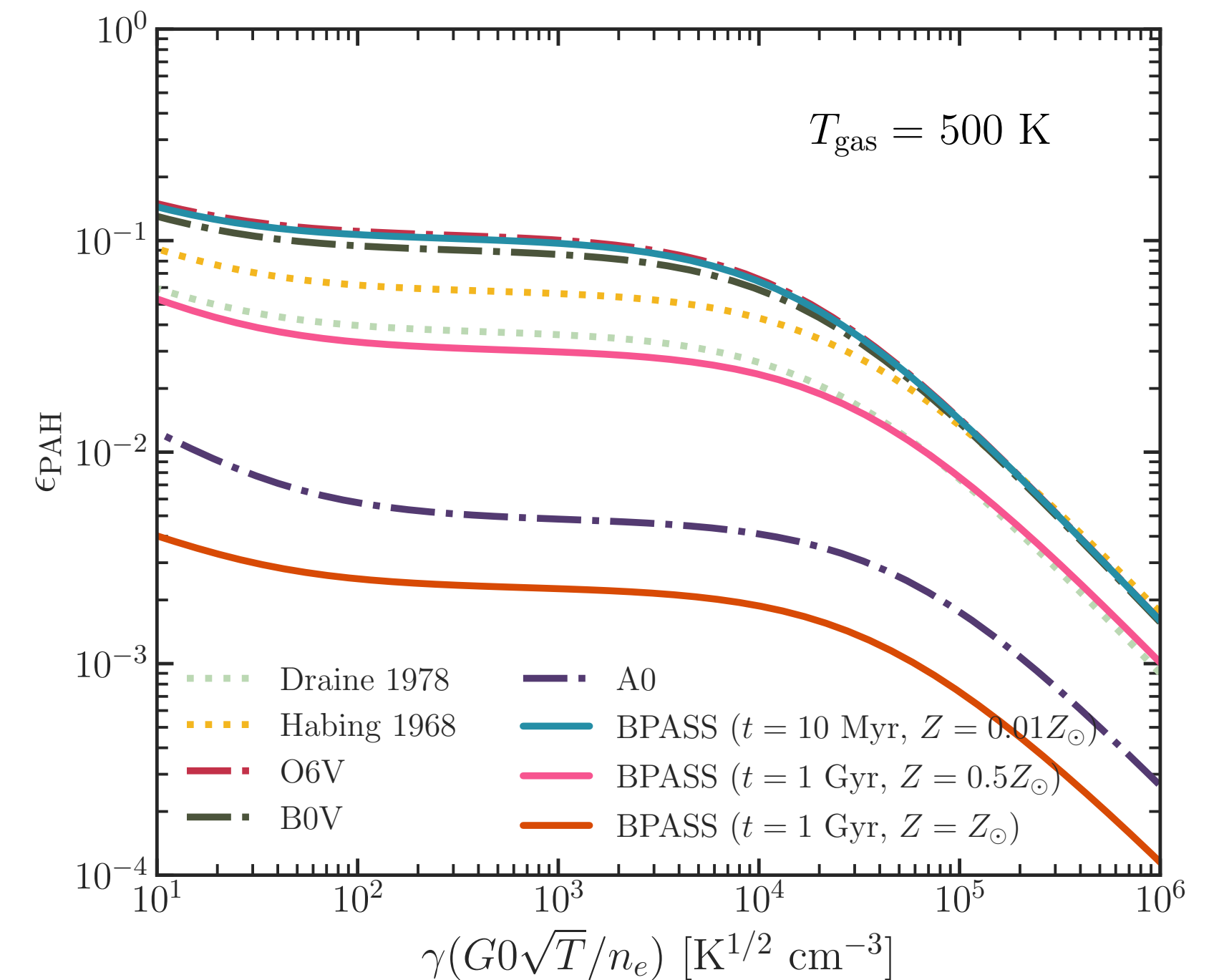
$$P_{\text{diss}}^{\text{C}_2\text{H}_2}(E) = \frac{k_{\text{diss}}^{\text{C}_2\text{H}_2}(E)}{k_{\text{diss}}^{\text{C}_2\text{H}_2}(E) + k_{\text{IR}}/(n_{\text{max}} - 1)}$$

$$R_{\text{diss}}^{\text{C}_2\text{H}_2}(G_0) = \int_{6\text{ eV}}^{13.6\text{ eV}} \chi_{\text{dH}} \sigma_{\text{PAH}}(E) P_{\text{diss}}^{\text{C}_2\text{H}_2}(E) \frac{F(E)}{E} dE$$



Only for de-hydrogenated PAHs!

(For the diffuse ISM
 $\sim 4.7 \times 10^{-17} [\text{s}^{-1}]$, $\sim 10\times$
 faster than Allain+1996)



PEH depends on the shape of the spectrum, which is not considered in state-of-the-art ISM models (Wolfire+2003, Bialy & Sternberg 2019, Kim+22)

3. Introducing Dusty-PRISM

Thermal and non-thermal destruction

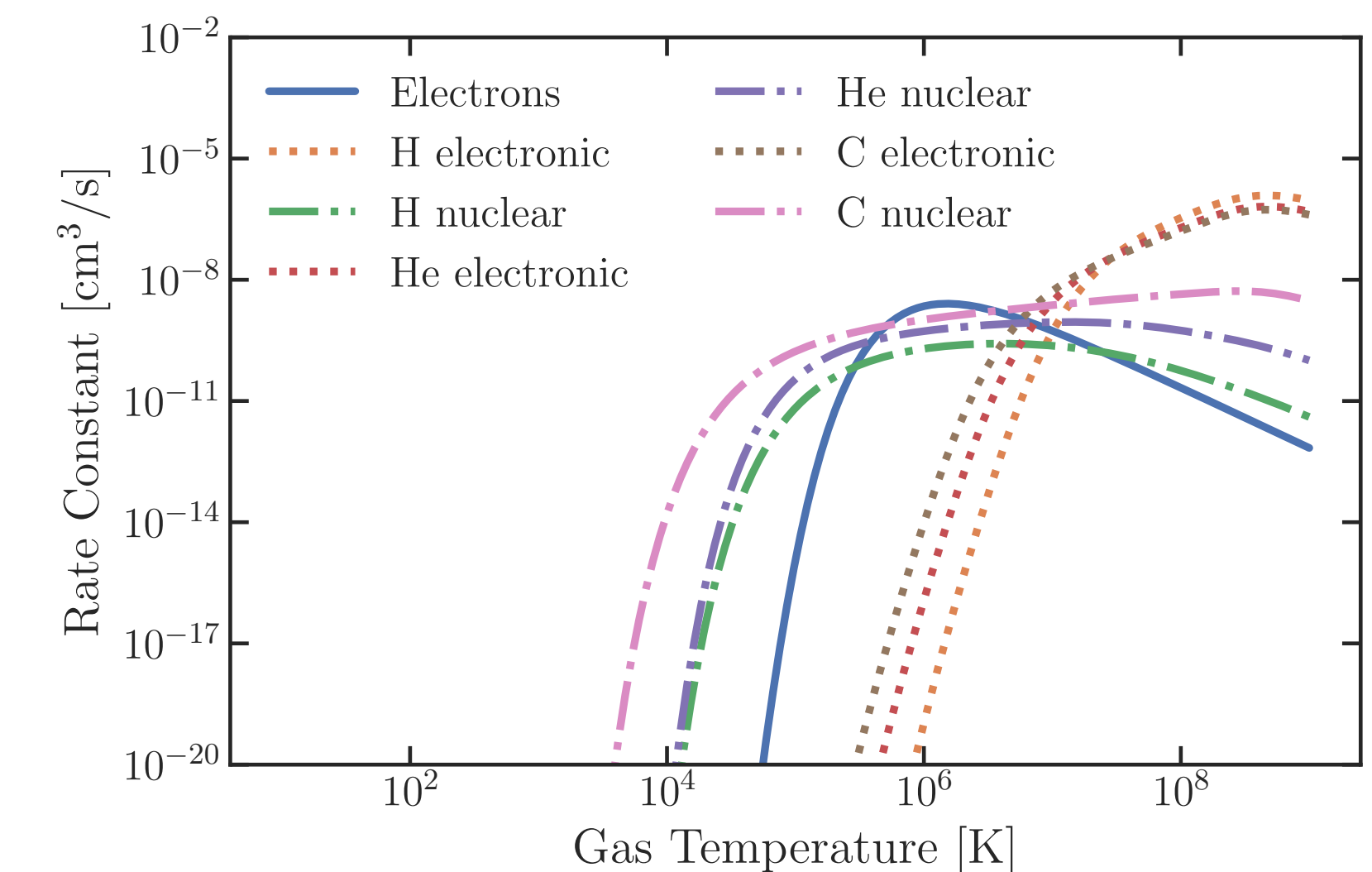
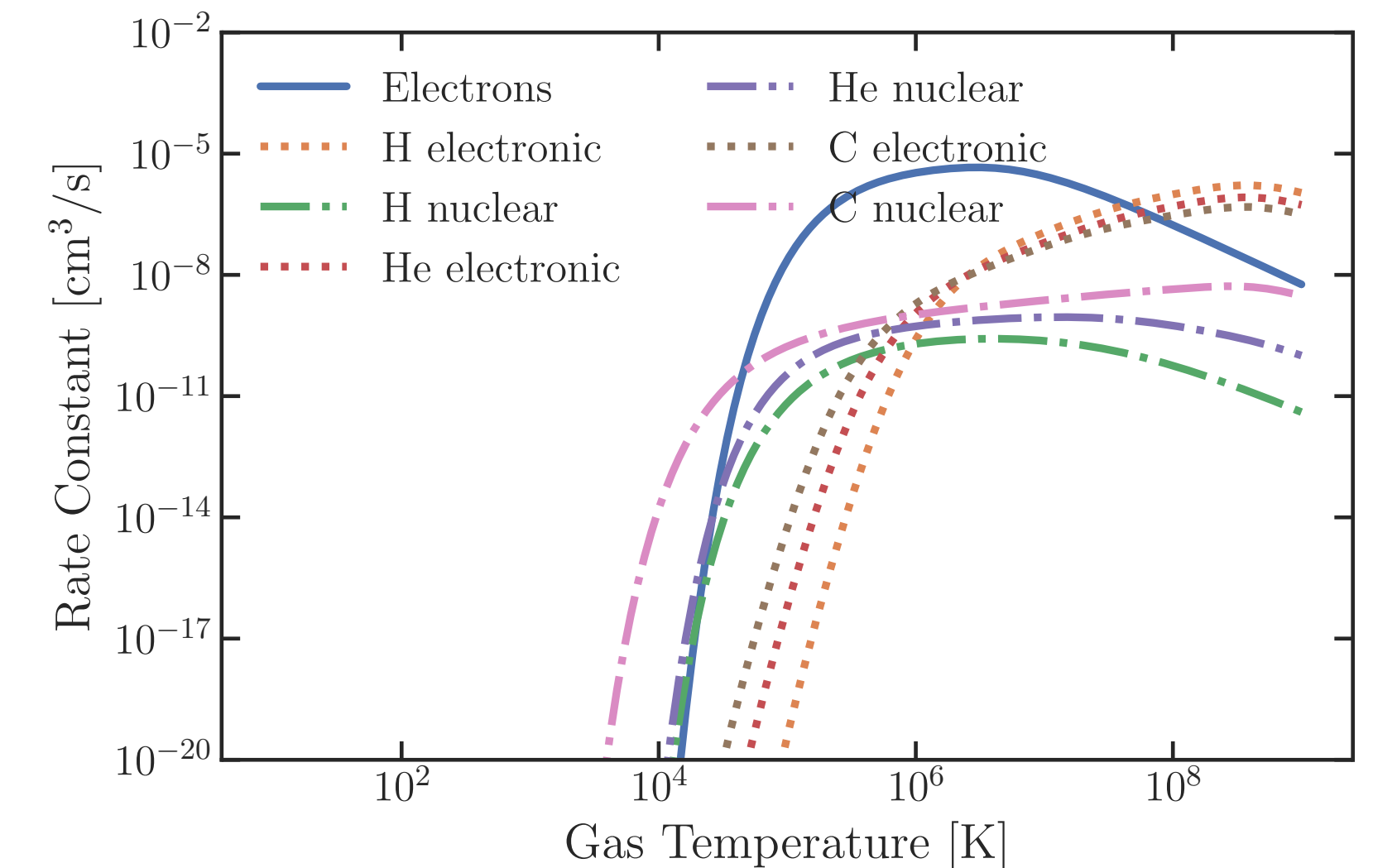
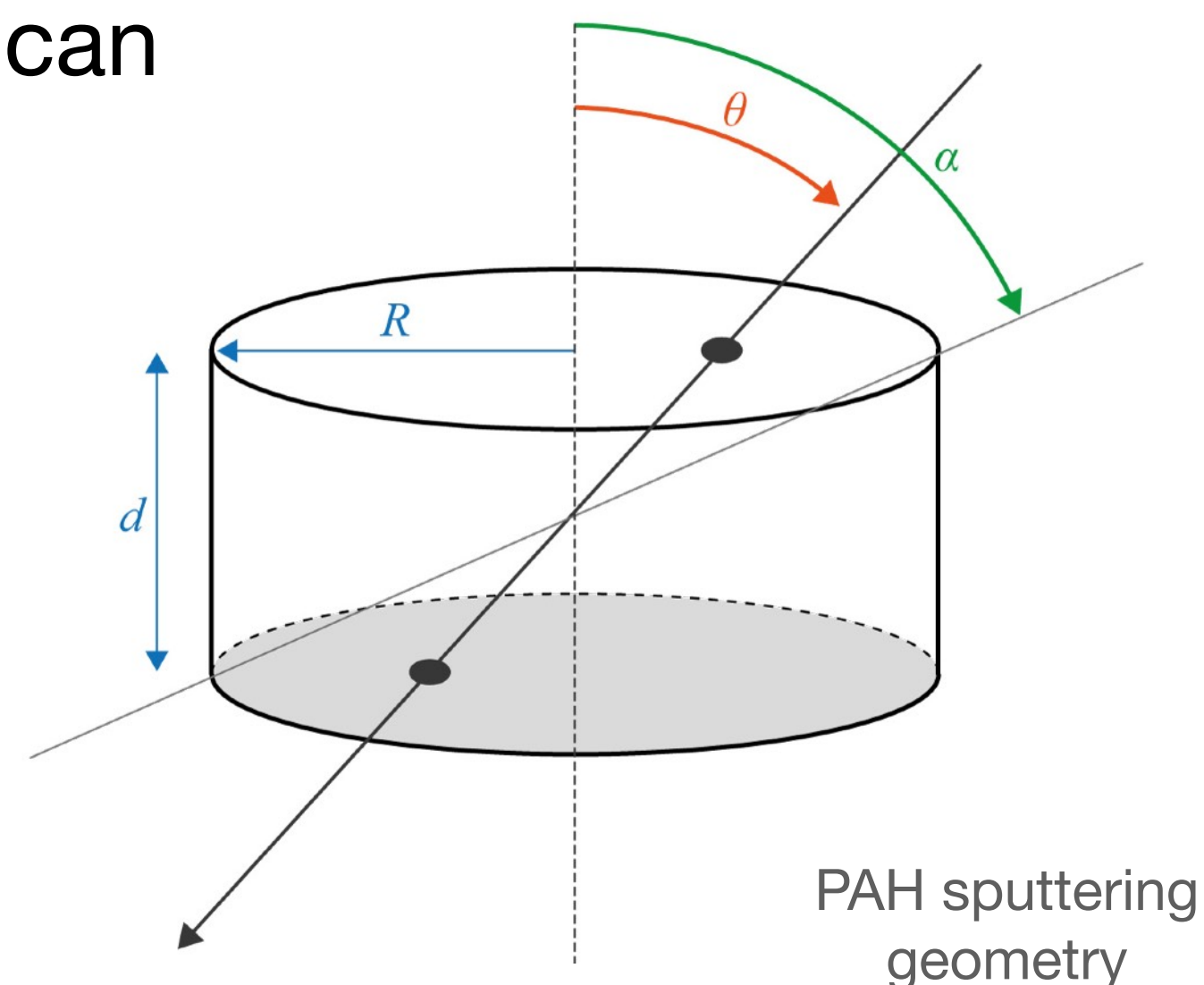
We follow also the RRKM theory as for photo-dissociation + data from the work of Micelotta+2010a

Collisions are dominated by e⁻, H, He and C

We consider sputtering when acetylene (C₂H₂) dissociation is achieved

Upon collision, the excited state can decay via:

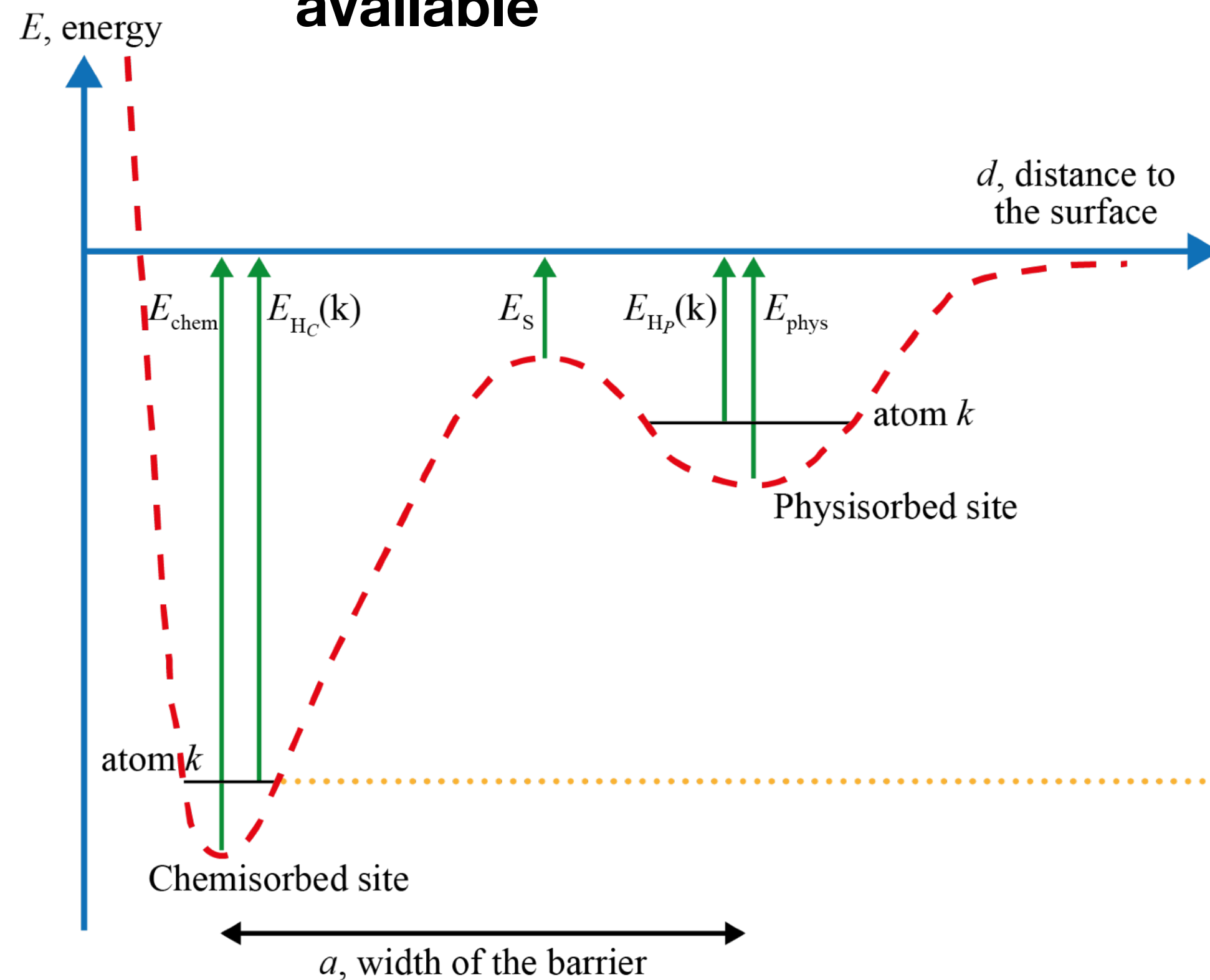
- IR emission
- Ionisation
- Thermionic emission
- Fragmentation



3. Introducing Dusty-PRISM

PAHs as a chemical catalyst

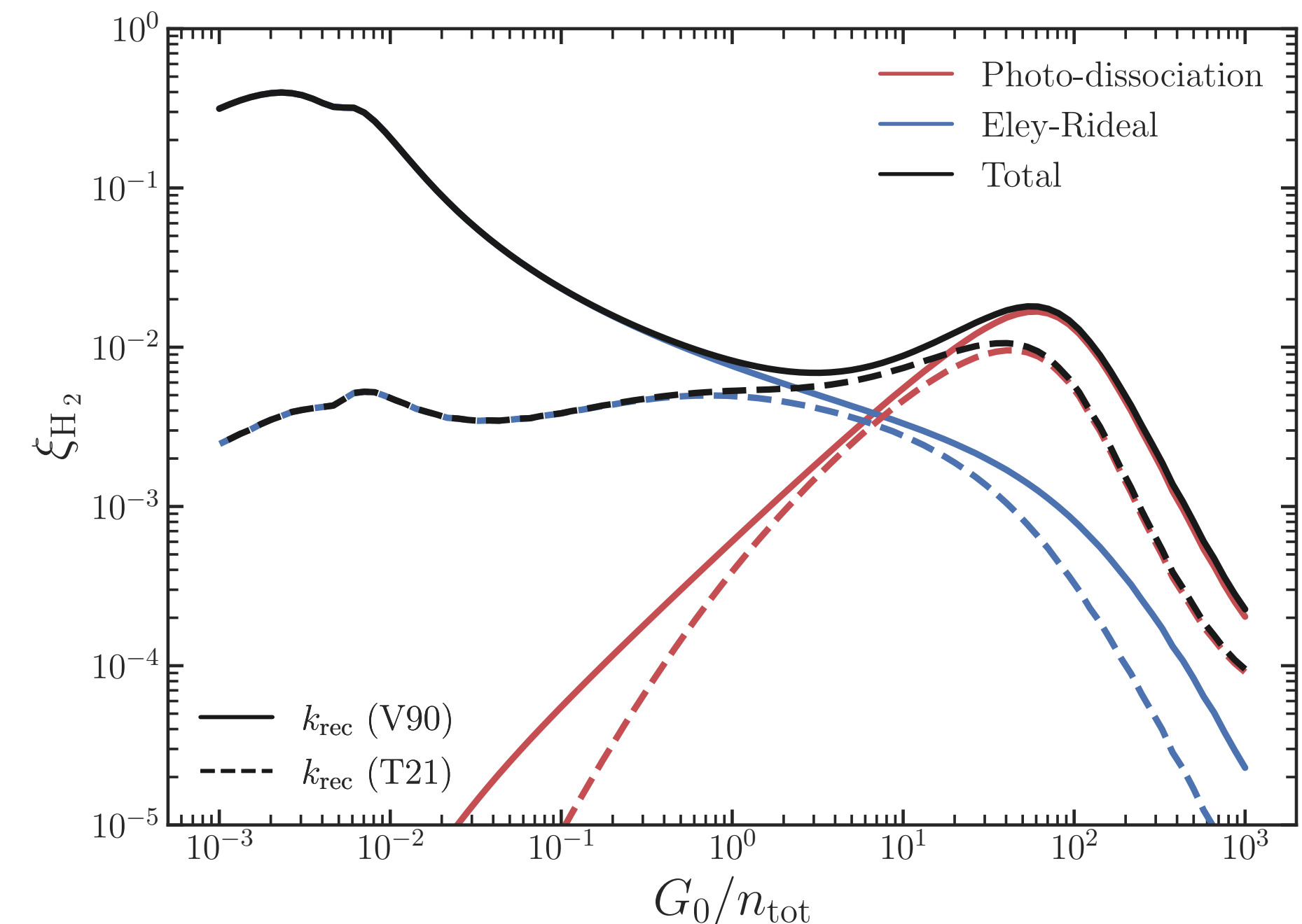
Beyond ~ 20 K, physisorbed site **no longer available**



Large **drop in H_2 formation efficiency**, in stark contrast to observations of PDRs (Habart+2003b, Allers+2005)

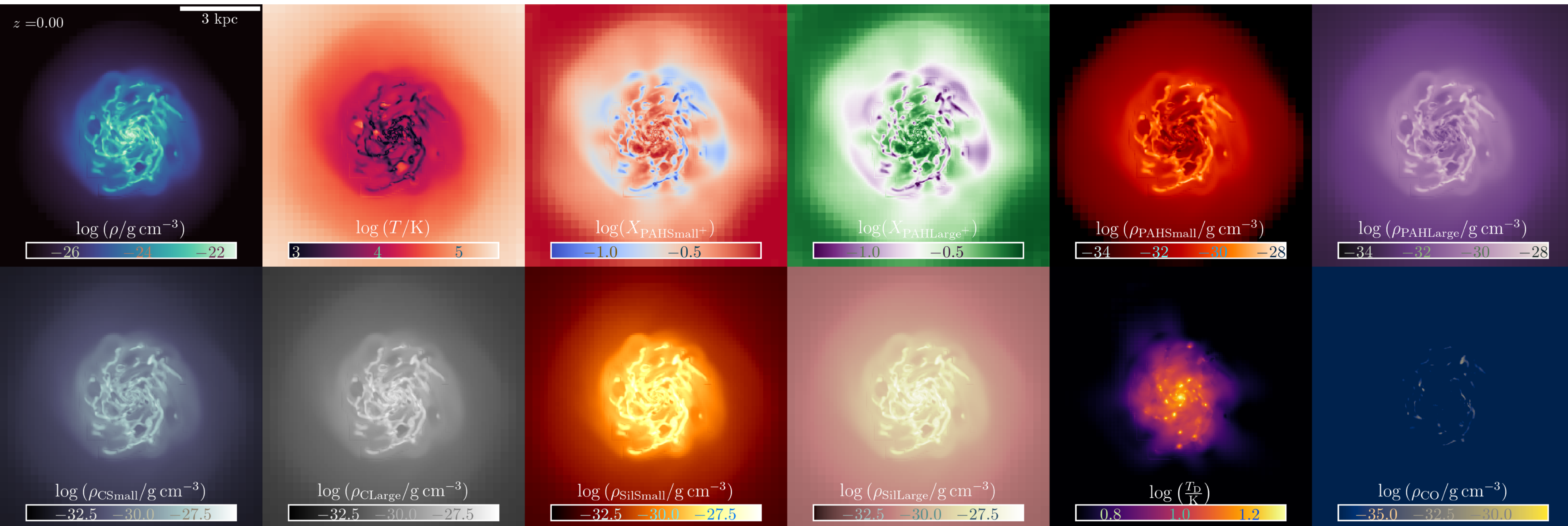
We consider:

- H covalent bond then abstracted by another H
- Photo-desorption of H_2 by a super-hydrogenated PAH



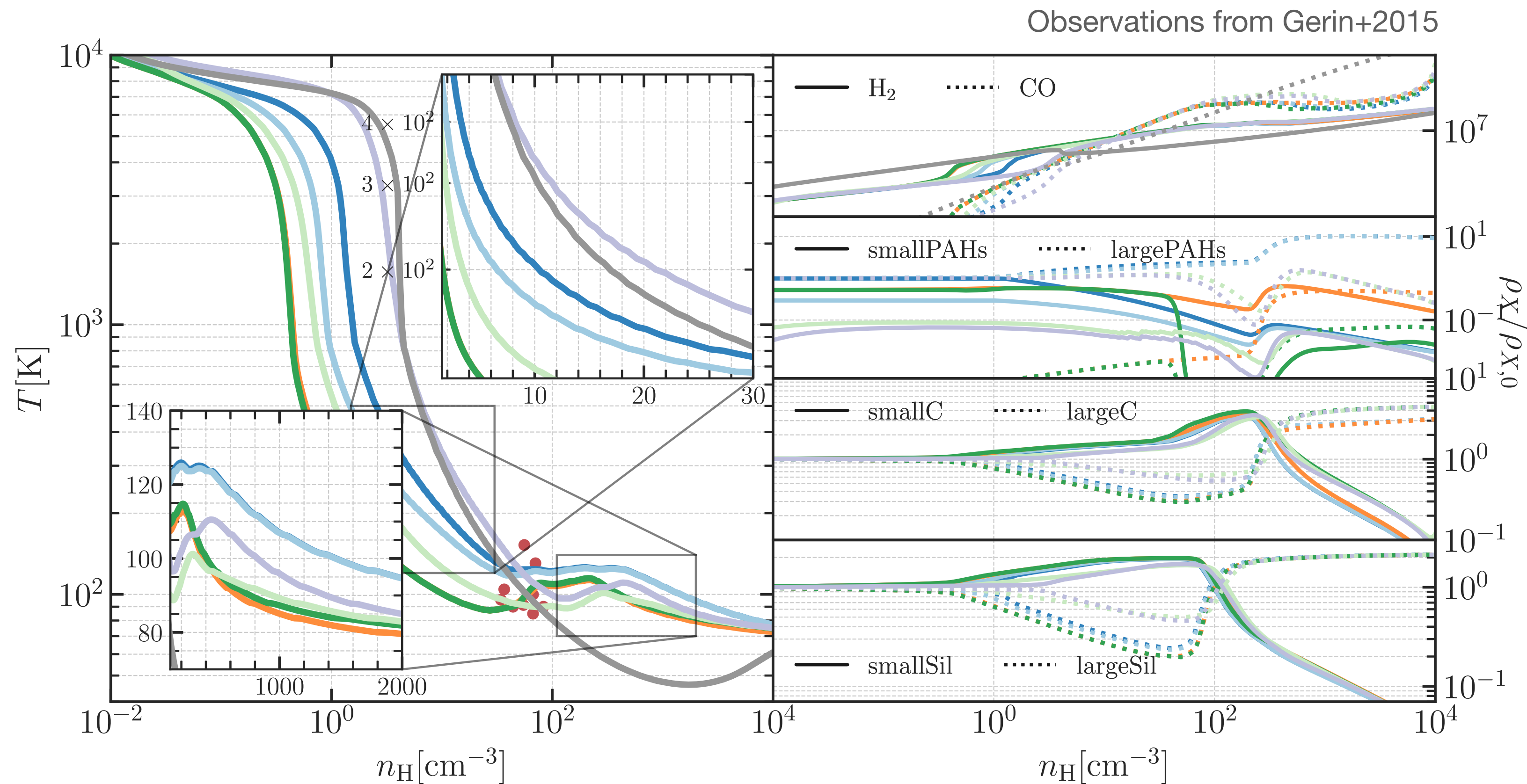
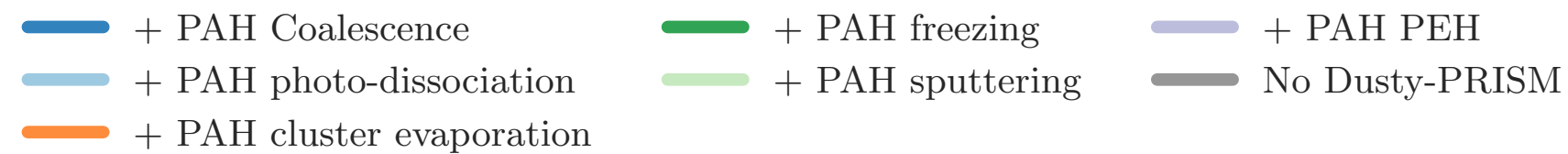
3. Introducing Dusty-PRISM

G8 simulation: low metallicity, dwarf galaxy



3. Introducing Dusty-PRISM

How different PAH processes affect the equilibrium curve in the ISM



- Fix PAH fraction predicts too much heating
- Photo-dissociation reduces the abundance in the diffuse gas and close to the cooling instability
- Cluster evaporation allows for higher small PAH abundance, but little effect in the cooling
- Similar for freezing
- Sputtering destroys PAHs that could be forming H₂, hence less cooling
- Consistent PE Heating recovers the cooling instability of the no-dust simulations

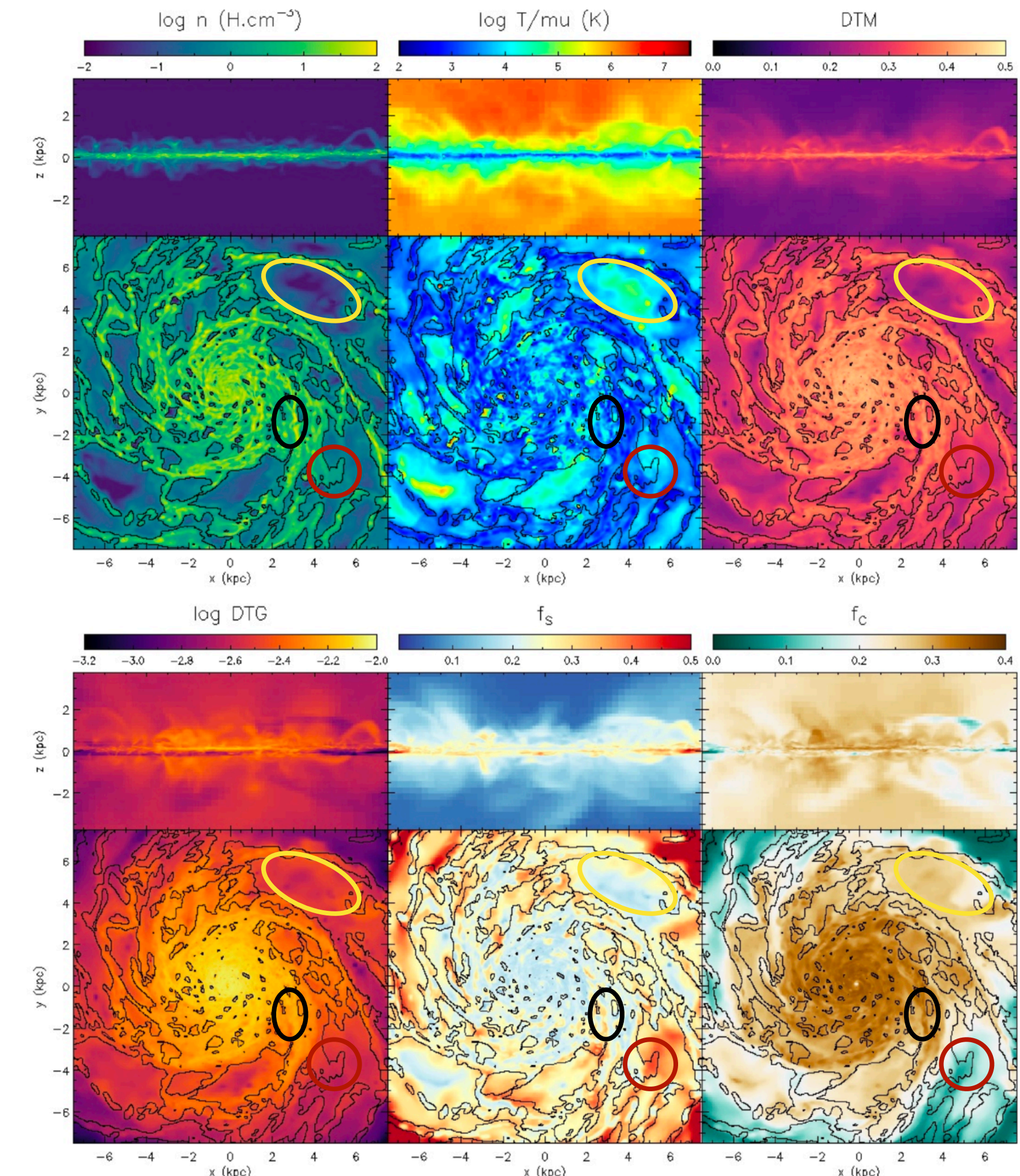
4. What gives rise to the extinction curve of the Local Group?

The G8, G9 and G10 suite of isolated galaxy simulations

- Hydro simulations with adaptive mesh refinement code **RAMSES** (Teyssier 02)
- **Isolated disc** initial conditions
- **Halo mass** $10^{10}, 10^{11}, 10^{12} M_{\text{sun}}$
- **Stellar mass** $2 \times 10^8 M_{\text{sun}}, 2 \times 10^9 M_{\text{sun}}, 2 \times 10^{10} M_{\text{sun}}$ (B/D=0.2)
- Disc **gas fraction** 10 or 50%
- Initial $\langle Z_{\text{gas}} \rangle = [0.1, 0.3, 0.8, 1.6] Z_{\text{sun}}$
- Initial **Solar composition** of elements
- 10^6 star particles + 10^6 DM particles
- Mass resolution ($8 \times 10^3 M_{\text{sun}}$) + Jeans length refinement
- $\Delta x_{\text{min}} = 20 \text{ pc}$ (also 10, 40, 80 pc)
- *Initial stars do not contribute to the overall feedback/metals/dust*

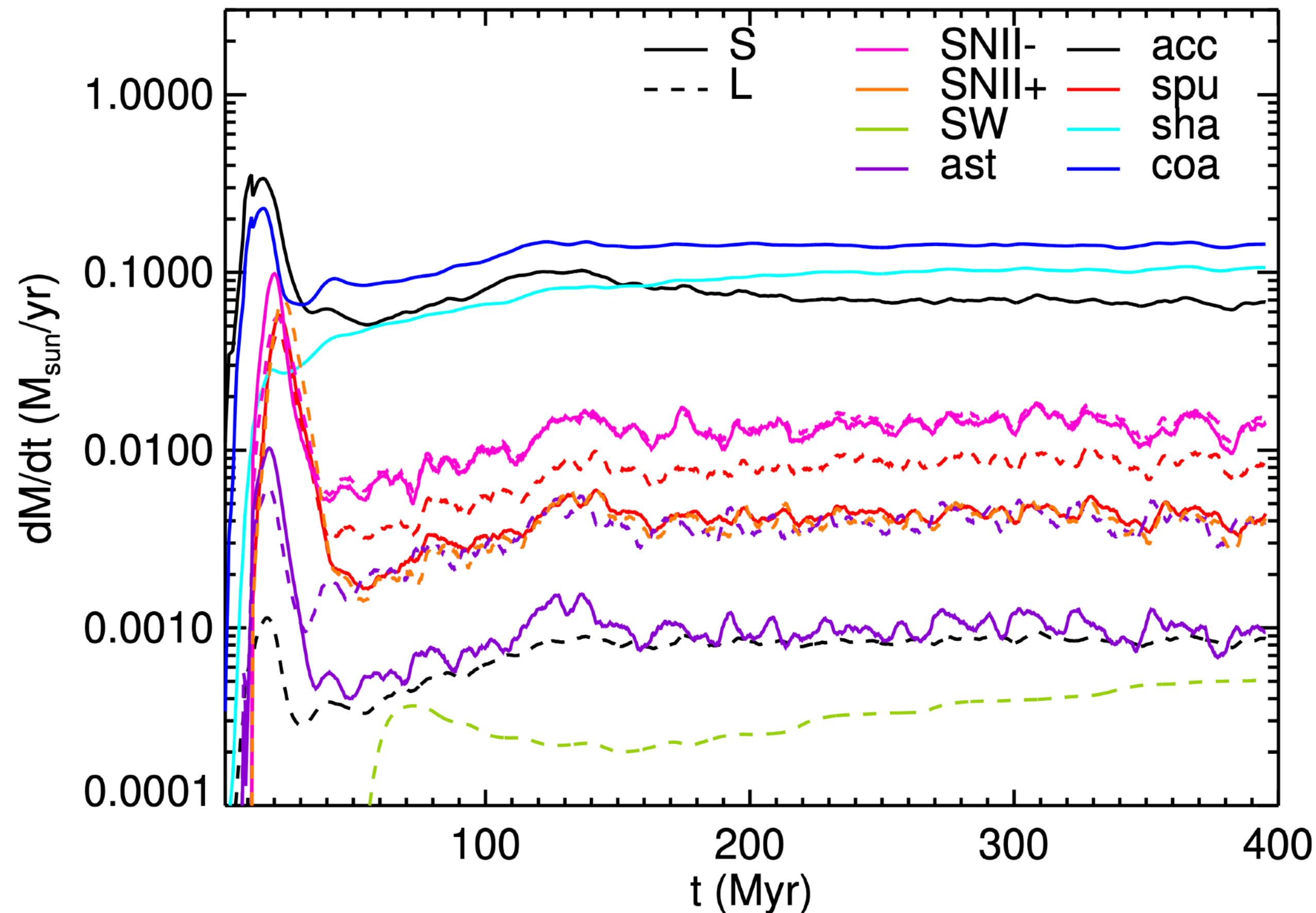
- Gas cooling down to $T_{\text{min}} = 10 \text{ K}$
- Star formation with $\dot{\rho}_{\star} = \epsilon_{\text{ff}} \rho_g / t_{\text{ff}}$ and gravo-turbulent efficiency: $\epsilon_{\text{ff}} = f(\mathcal{M}_{\text{turb}}, \alpha_{\text{vir}})$
- SNI feedback + SNIa+ stellar winds

Dubois, RM+2024



4. What gives rise to the extinction curve of the Local Group?

The G8, G9 and G10 suite of isolated galaxy simulations

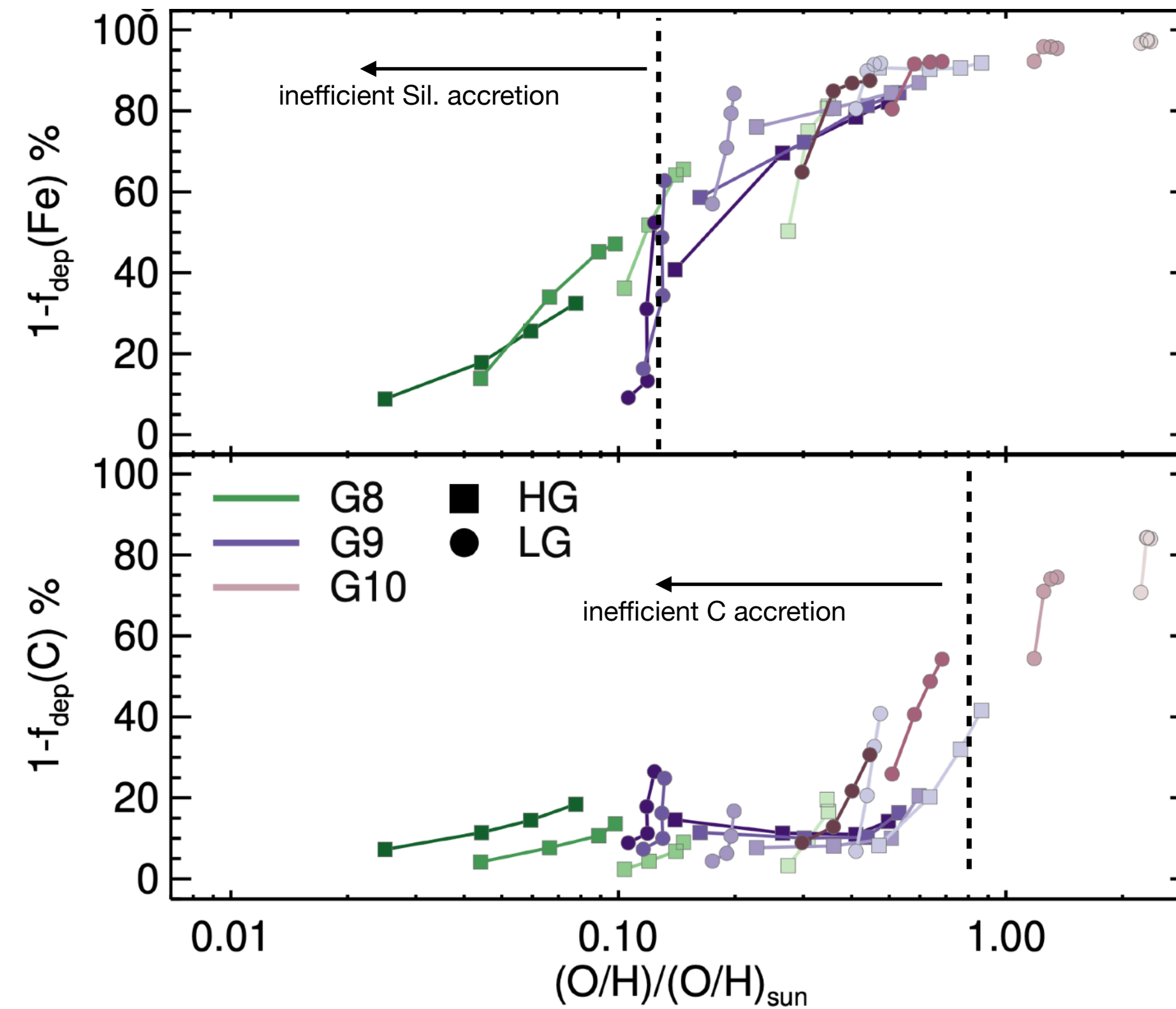
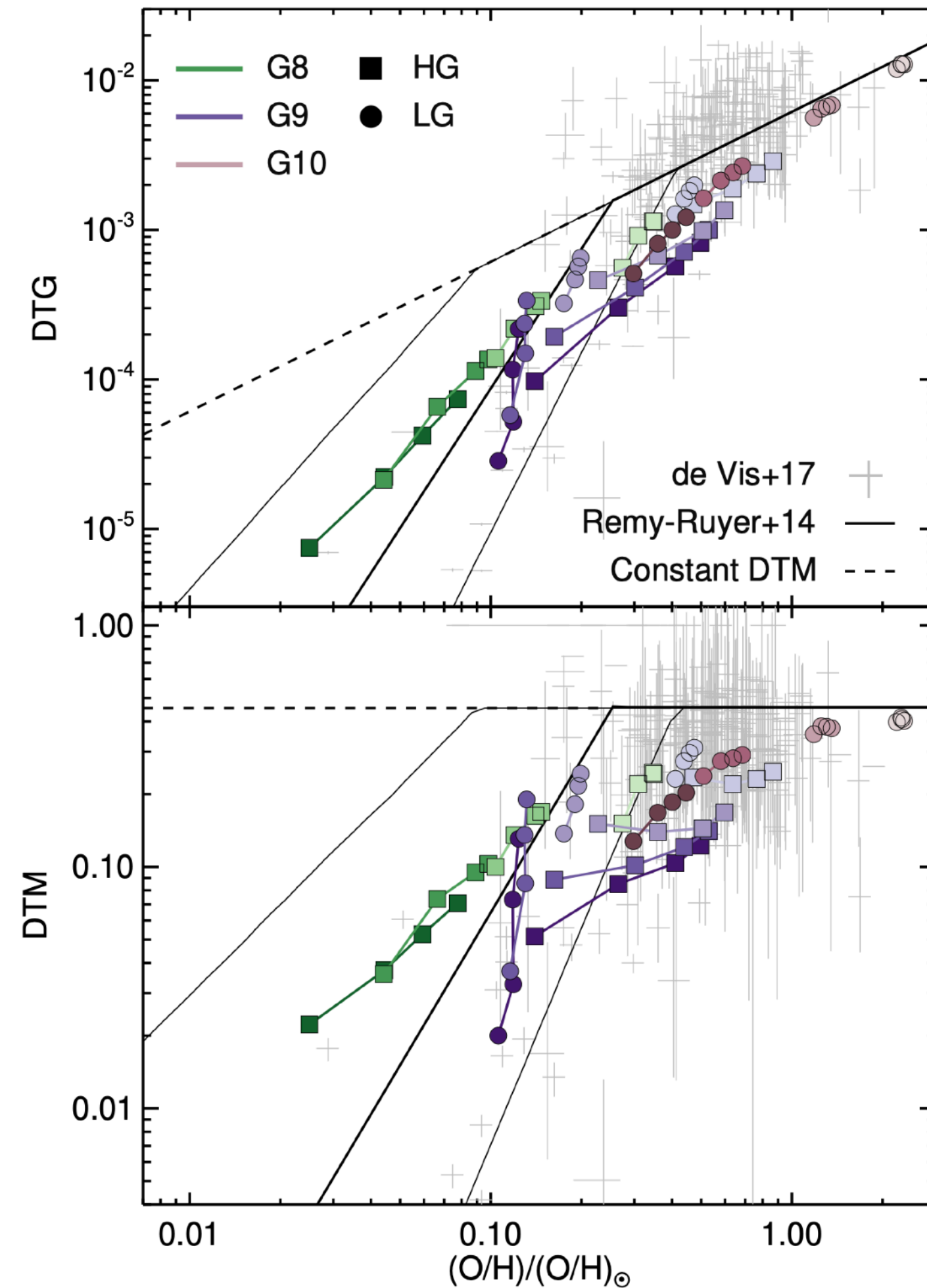


$t_{\text{acc,Sil}} \simeq 2 \text{ Myr}$ $\bar{n} \simeq 30 \text{ H cm}^{-3}$ **MW-like galaxy**
 $t_{\text{acc,C}} \simeq 10 \text{ Myr}$ $\mathcal{M} = \sigma_{\text{turb}}/c_s \simeq 3$ $M_{\text{halo}} = 10^{12} M_{\text{sun}}$
 $t_{\text{ff}} \simeq 8 \text{ Myr}$ $f_{\text{gas}} = 10\%$

- Accretion from ISM on grains (small grains) more efficient than stellar ejecta
- Coagulation and shattering very strong
 ➡ shape the size distrib.
- Direct destruction by SNII is the dominant destruction process
- Astration and AGB winds negligible

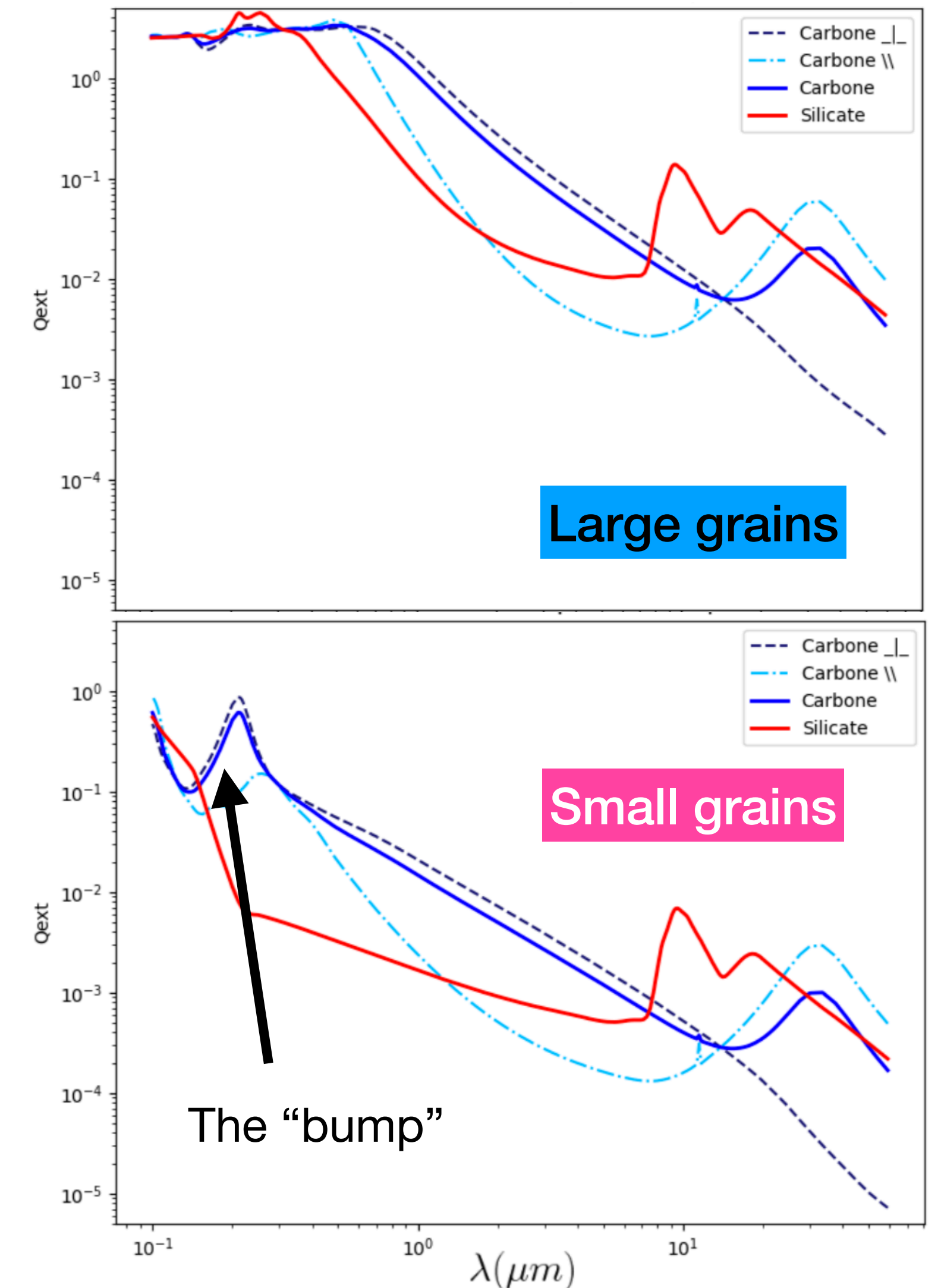
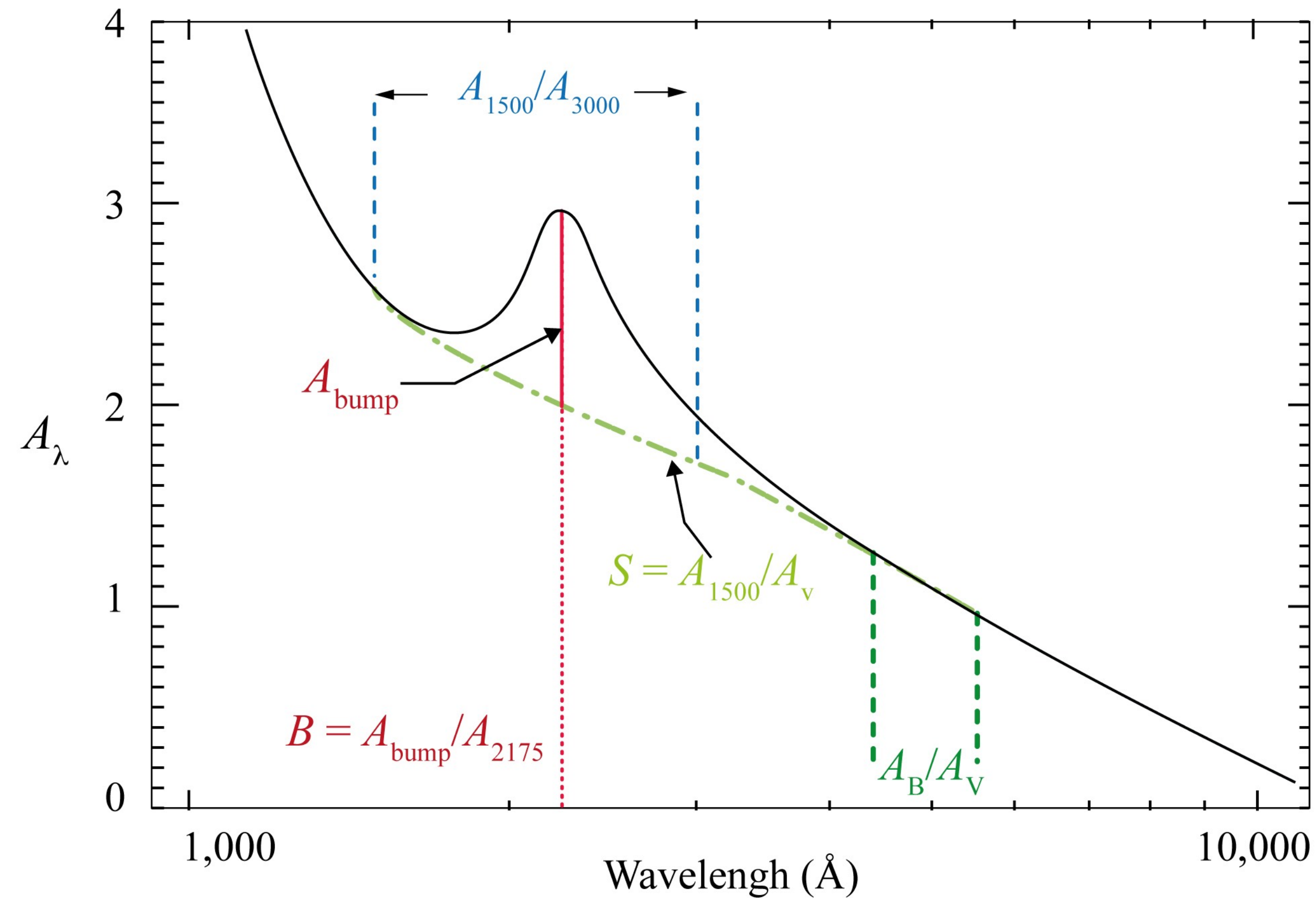
4. What gives rise to the extinction curve of the Local Group?

DTM/DTG variation with metallicity



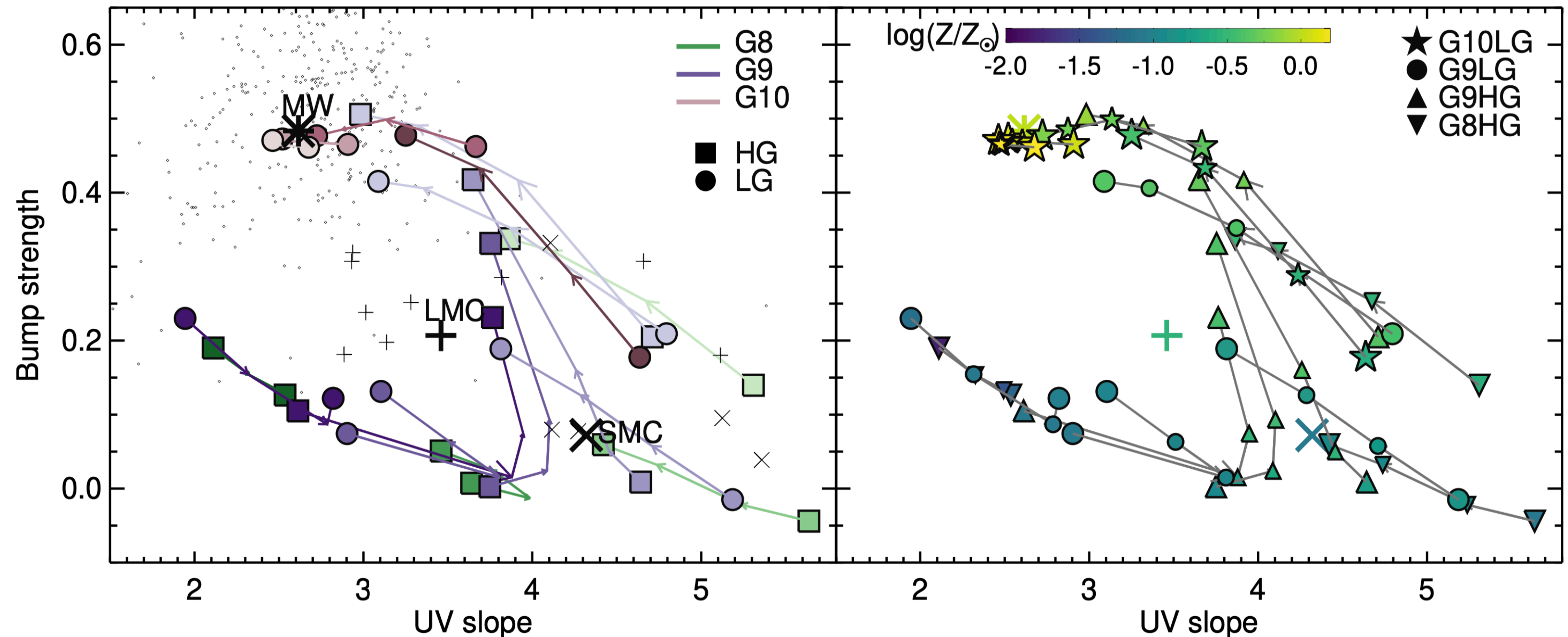
4. What gives rise to the extinction curve of the Local Group?

Evolution of extinction curve parametrisation



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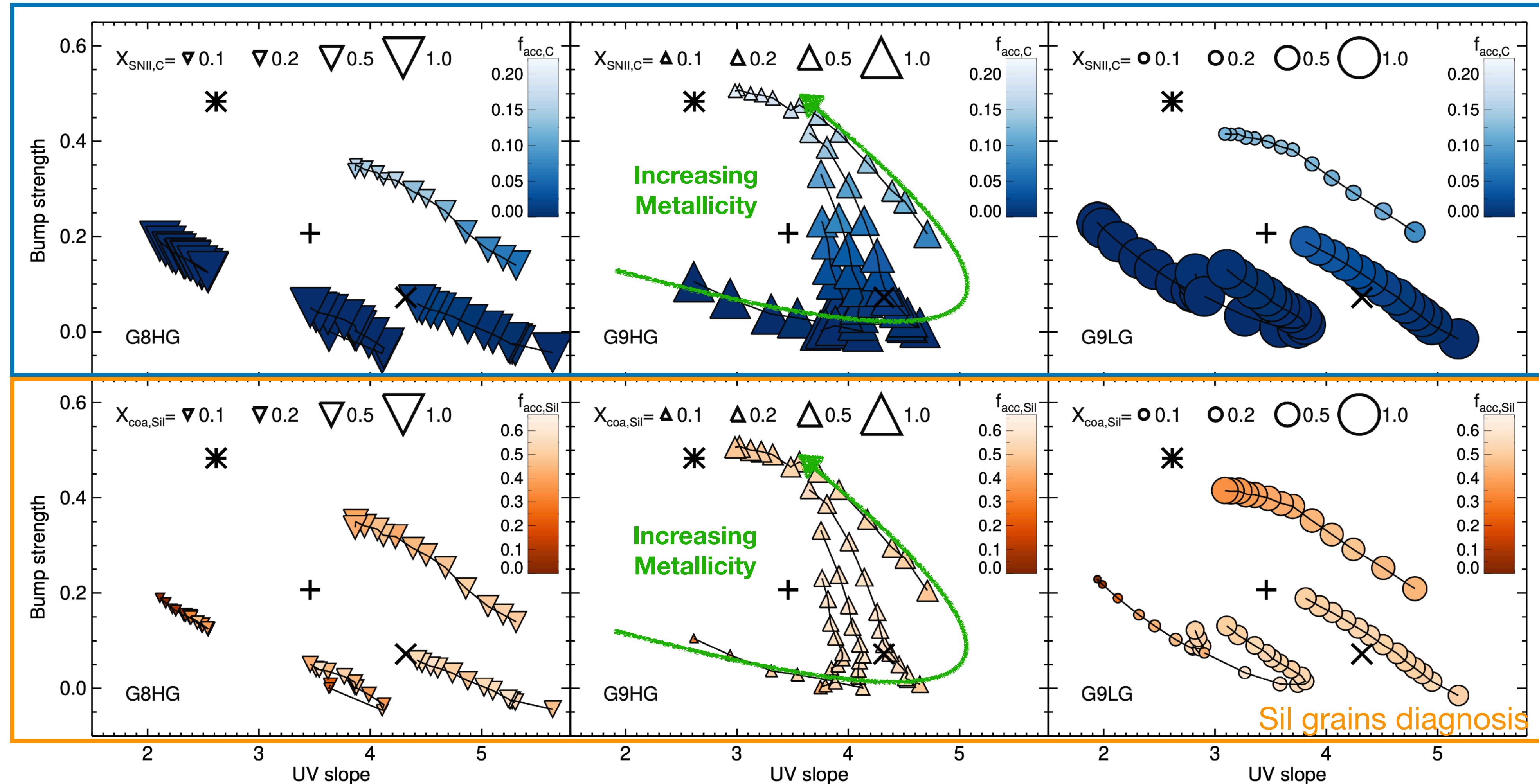
Evolution of extinction curve parametrisation



4. What gives rise to the extinction curve of the Local Group?

Evolution of extinction curve parametrisation

C grains diagnosis

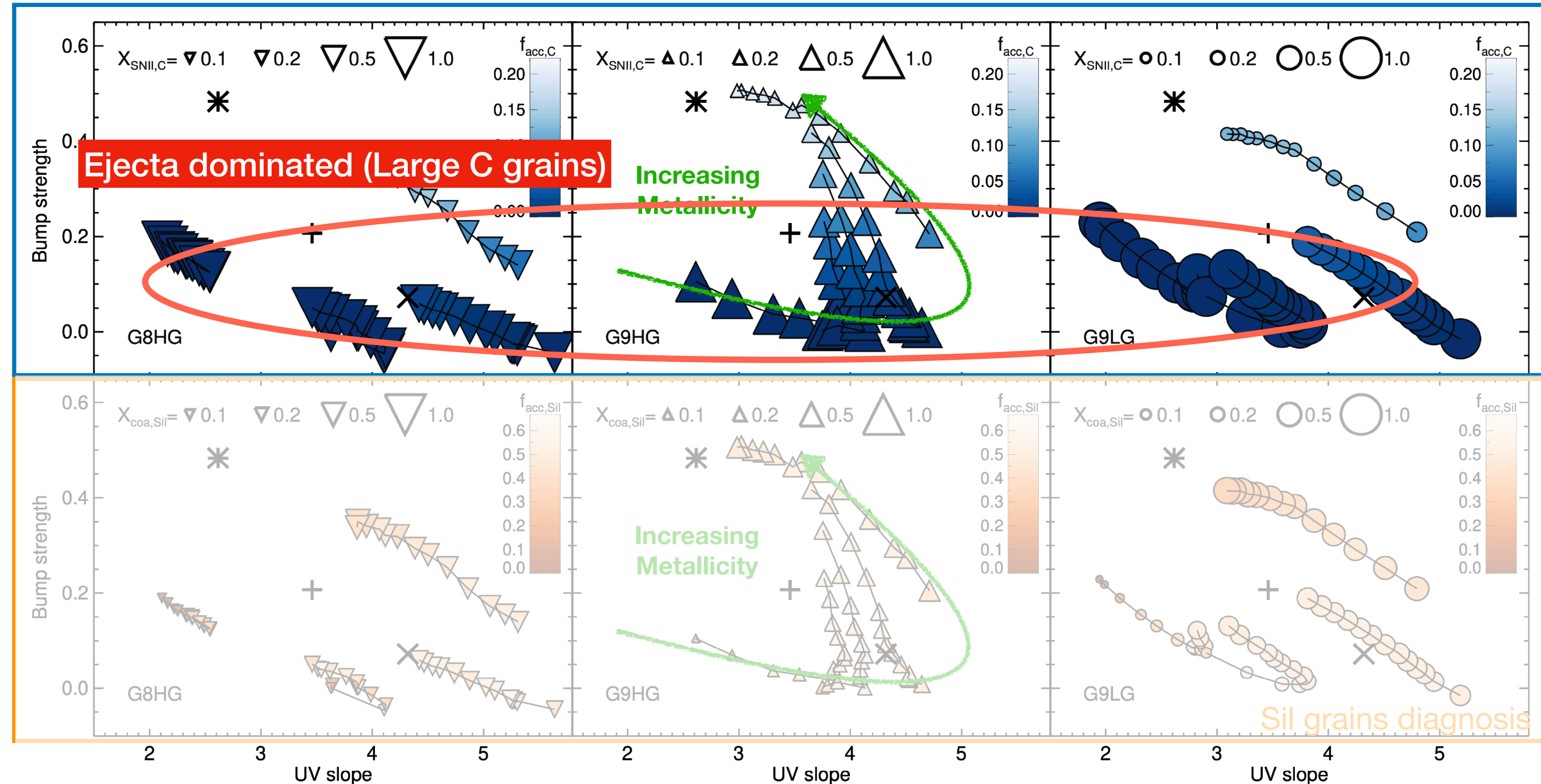


Si grains diagnosis

4. What gives rise to the extinction curve of the Local Group?

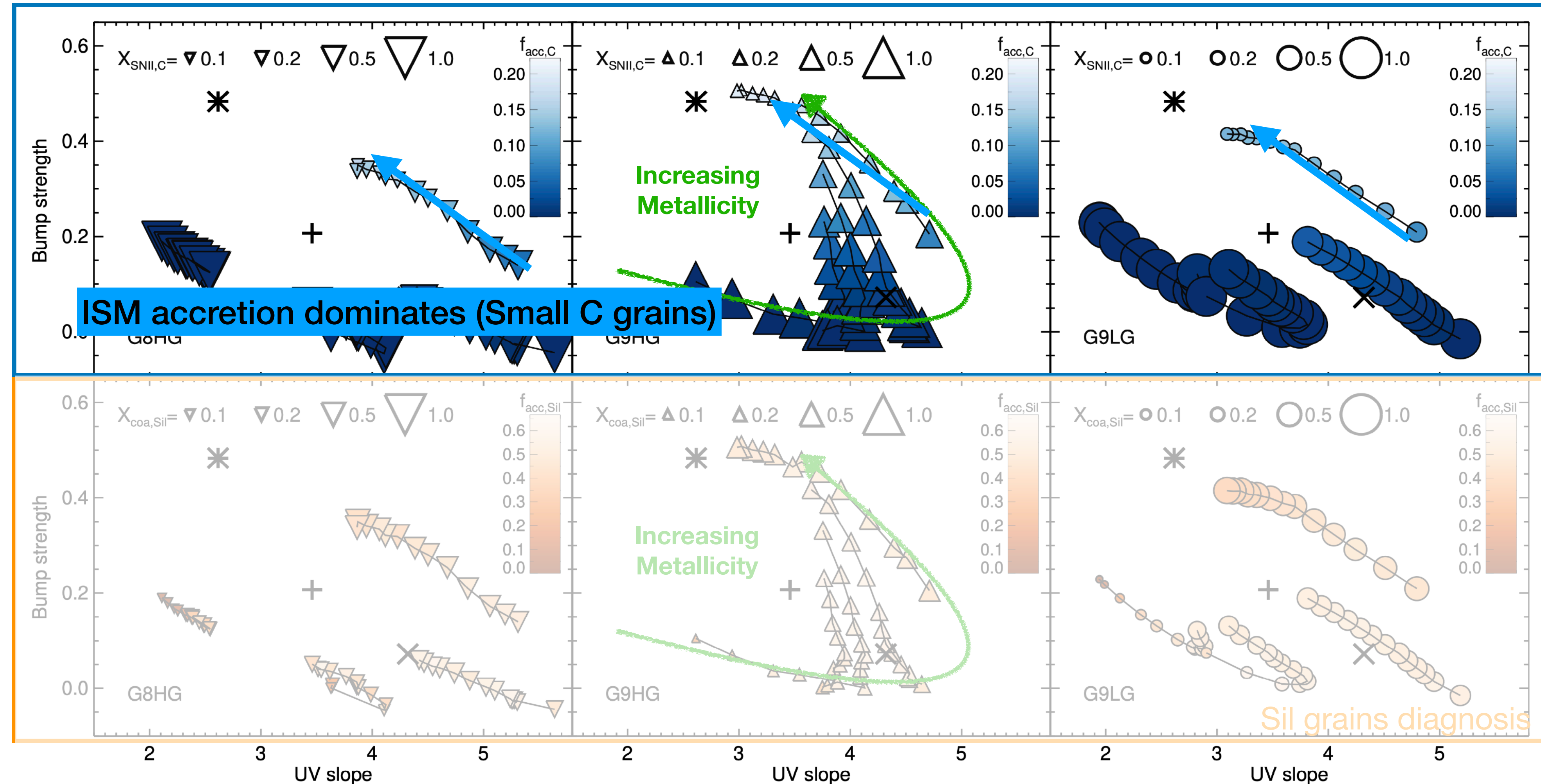
Evolution of extinction curve parametrisation

C grains diagnosis



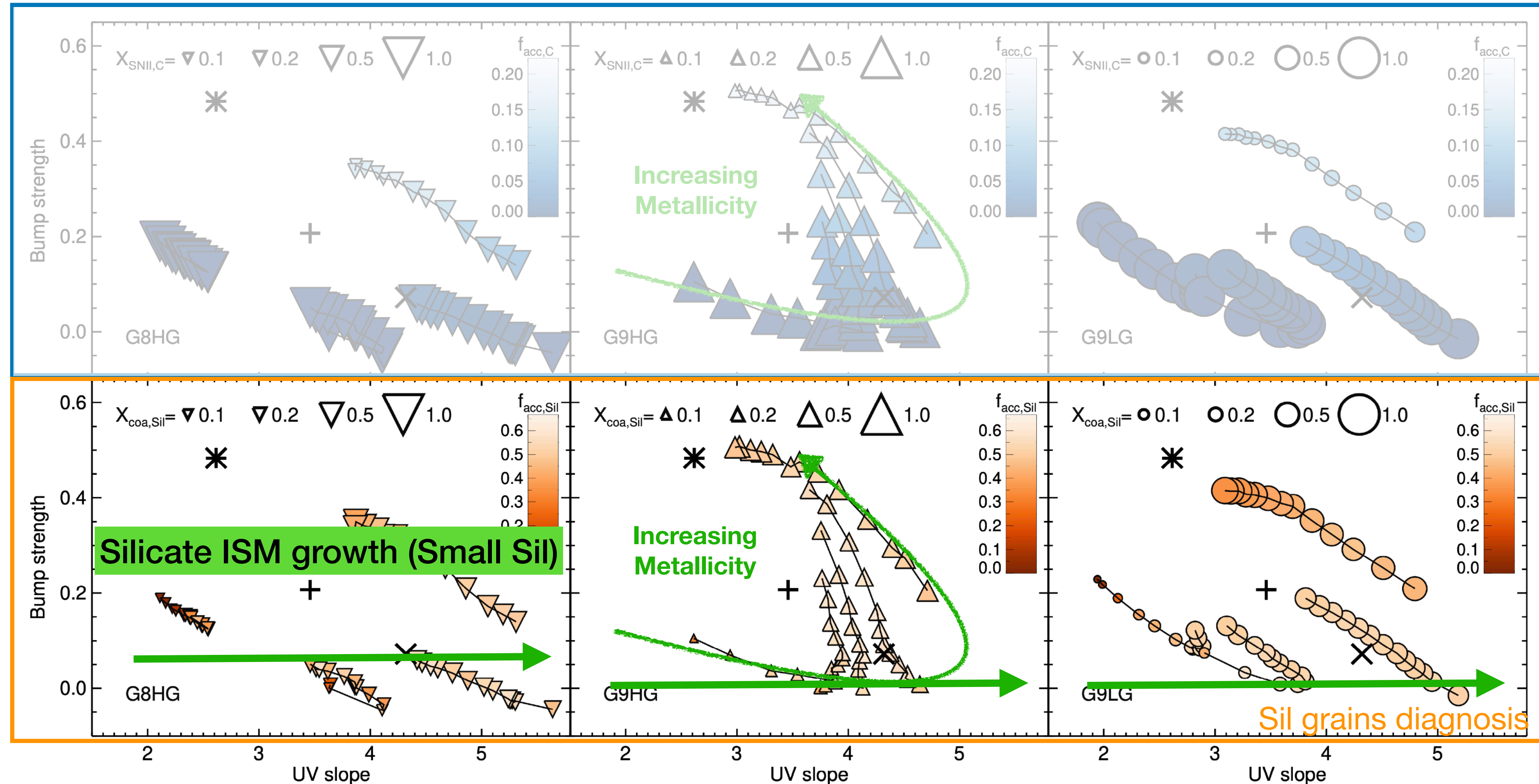
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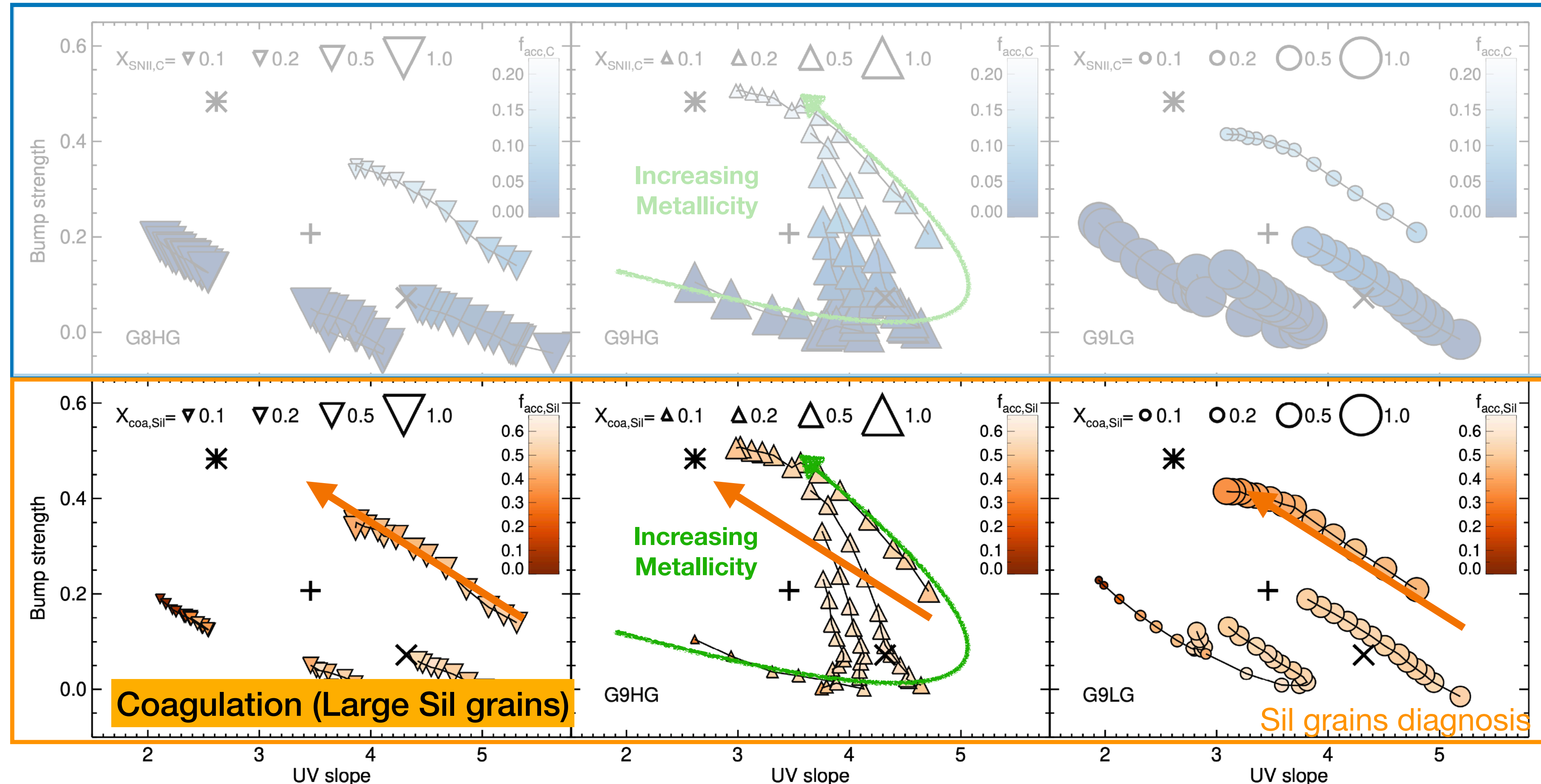
Evolution of extinction curve parametrisation



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Evolution of extinction curve parametrisation

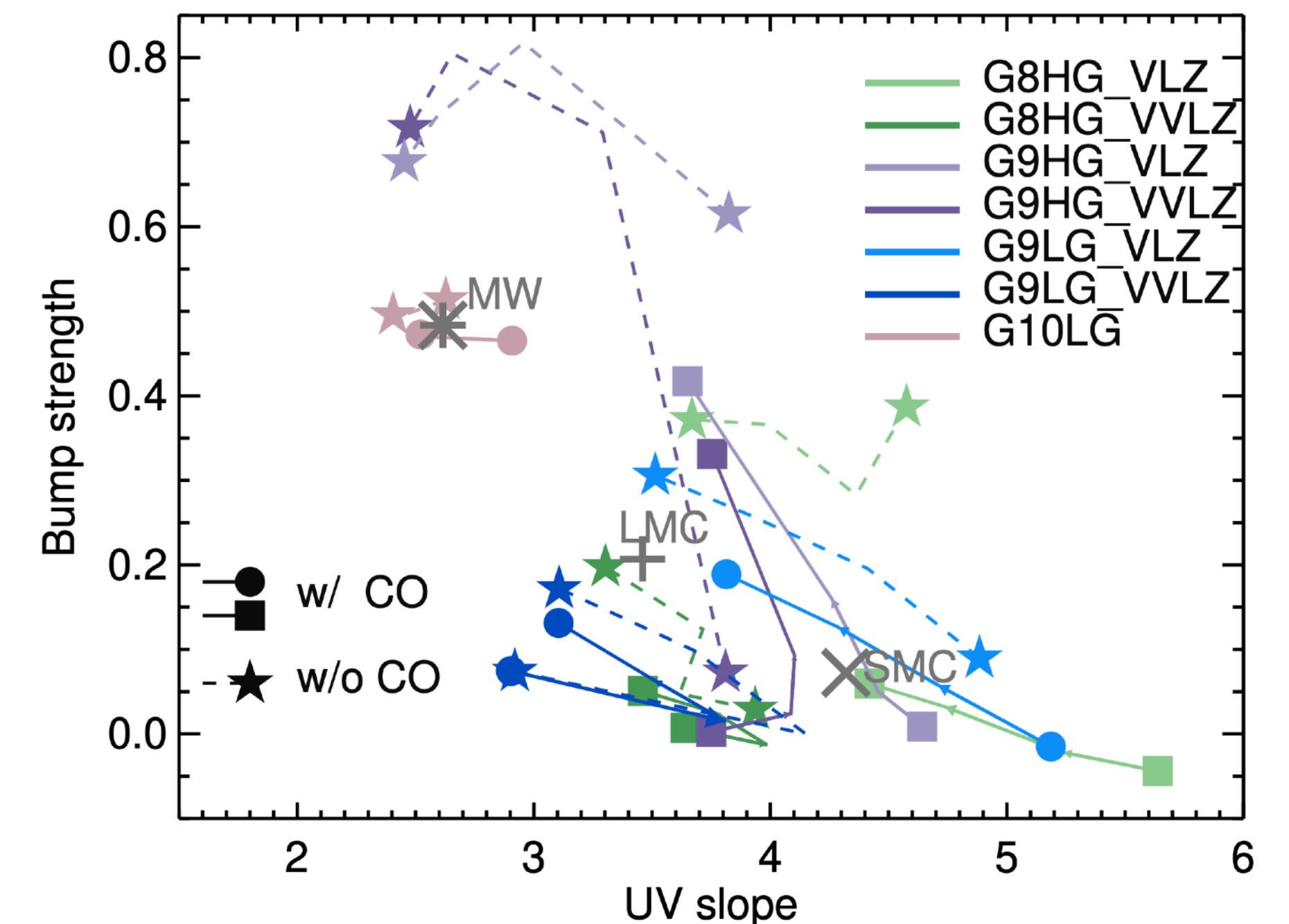
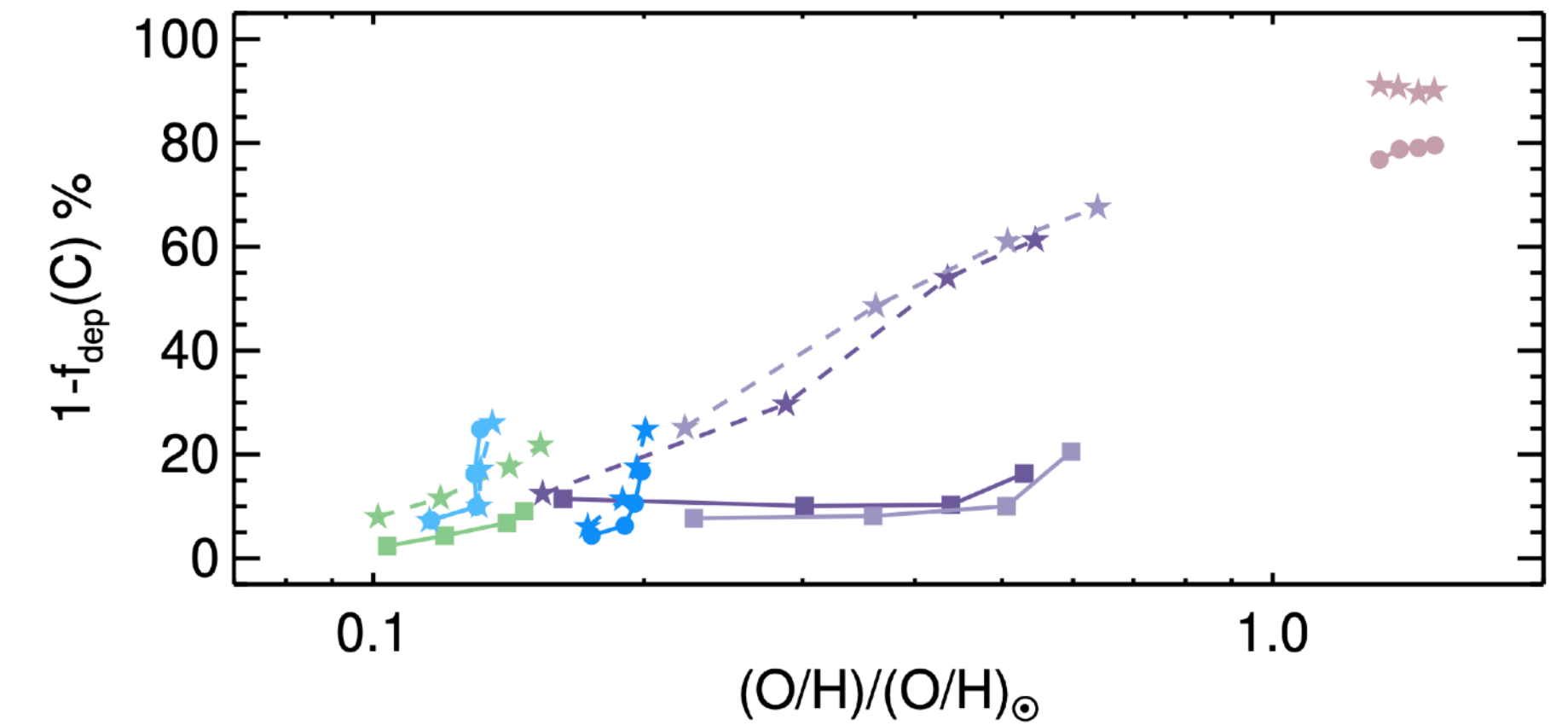
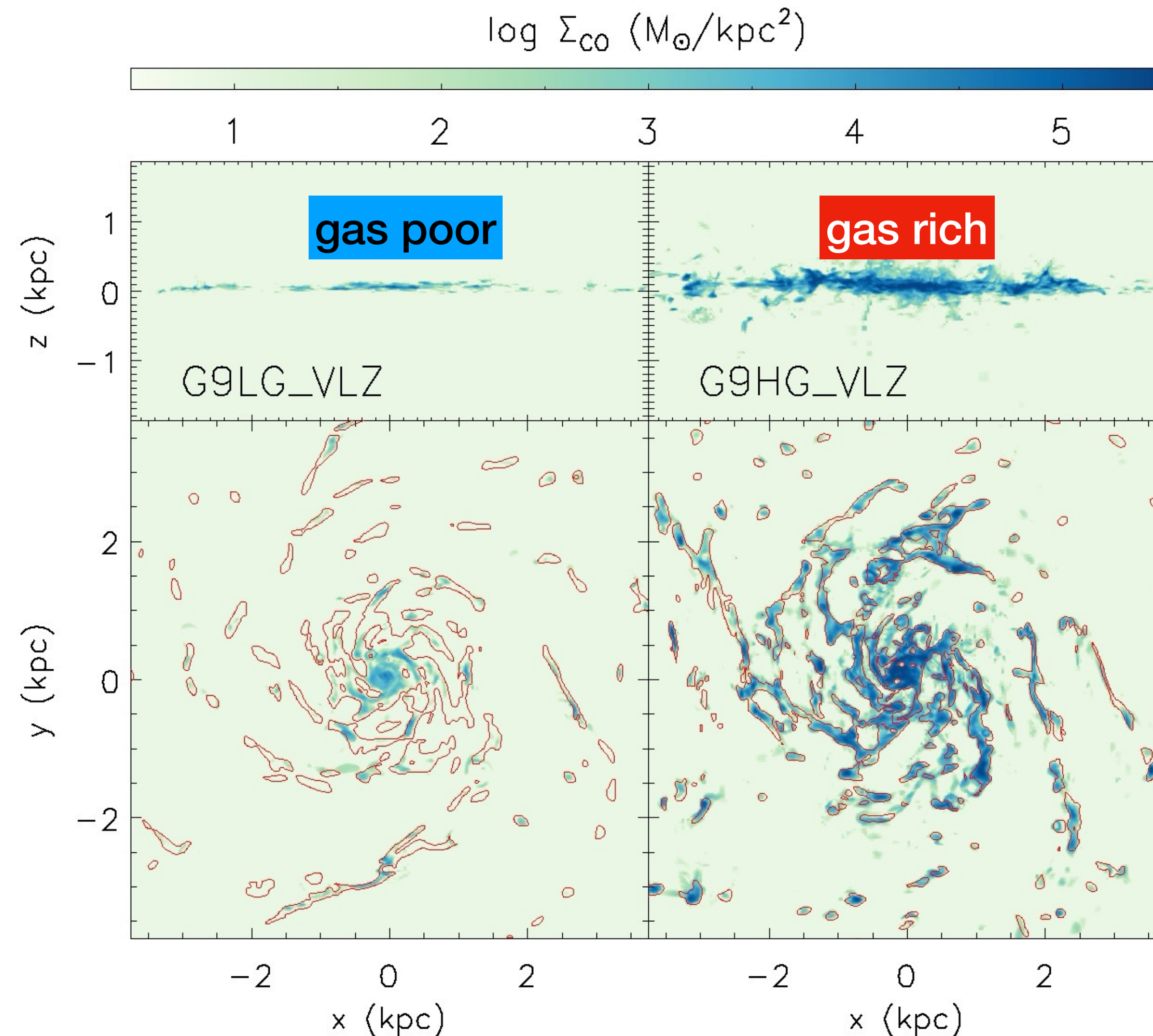
C grains diagnosis



Sil grains diagnosis

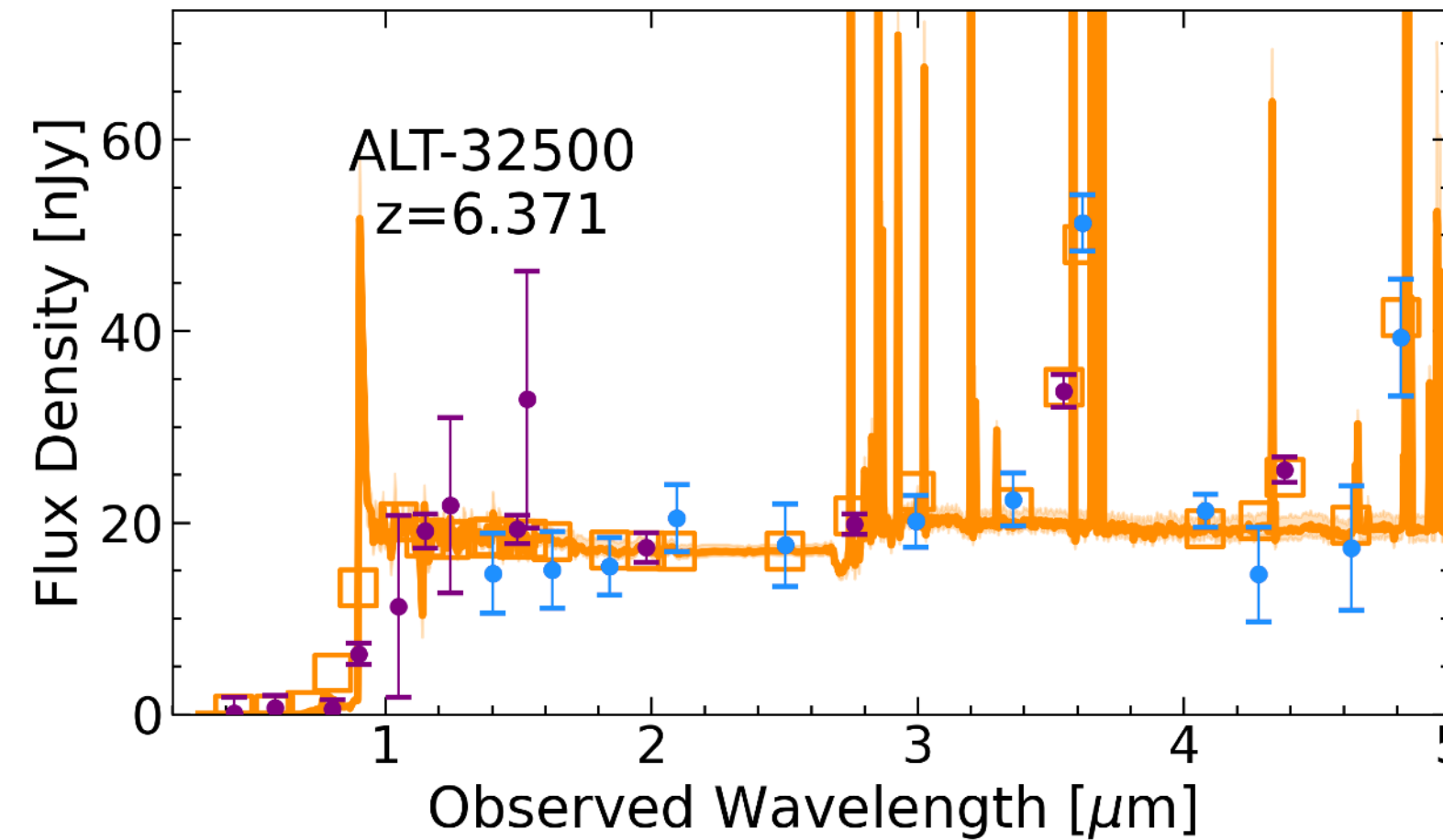
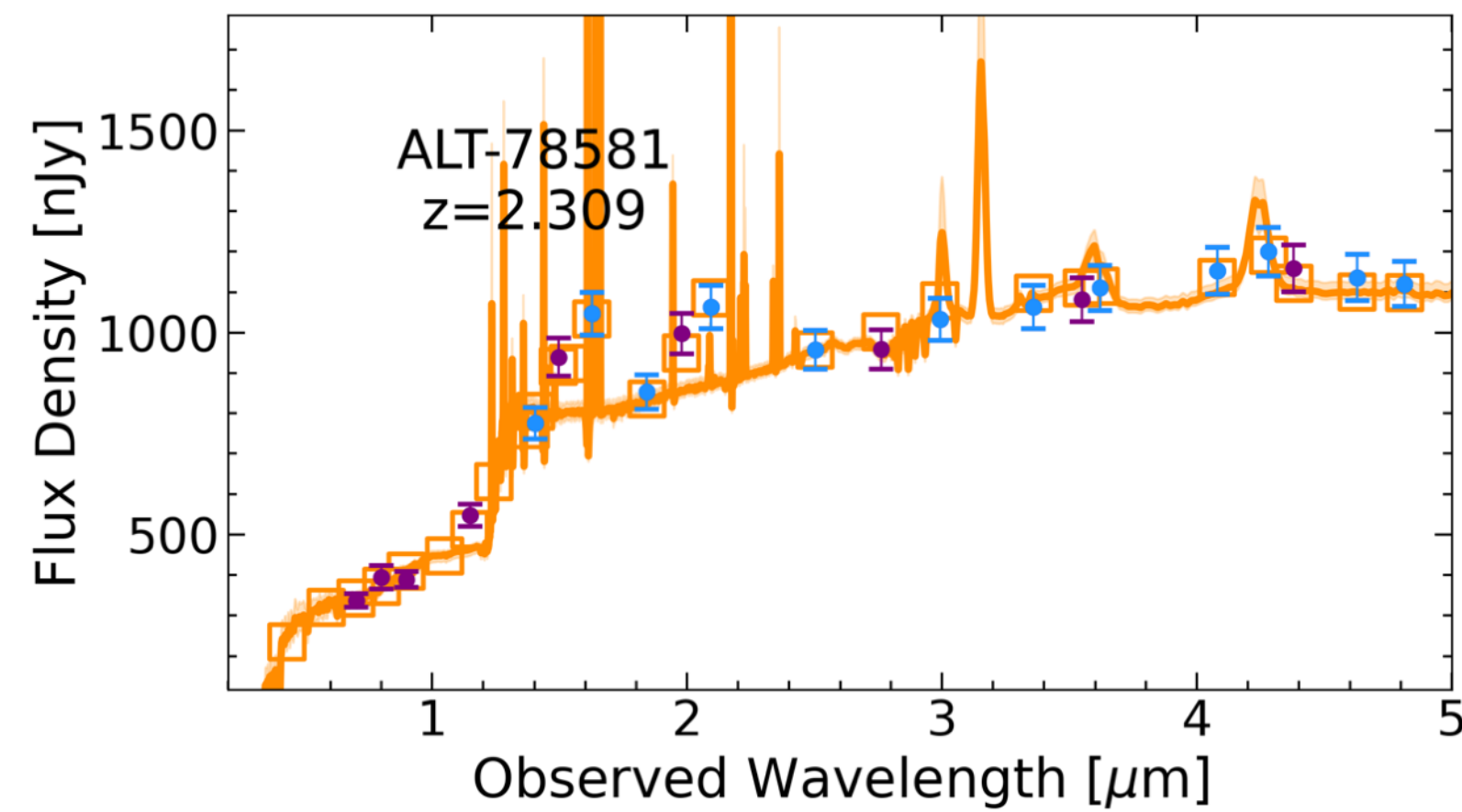
4. What gives rise to the extinction curve of the Local Group?

The need for CO formation

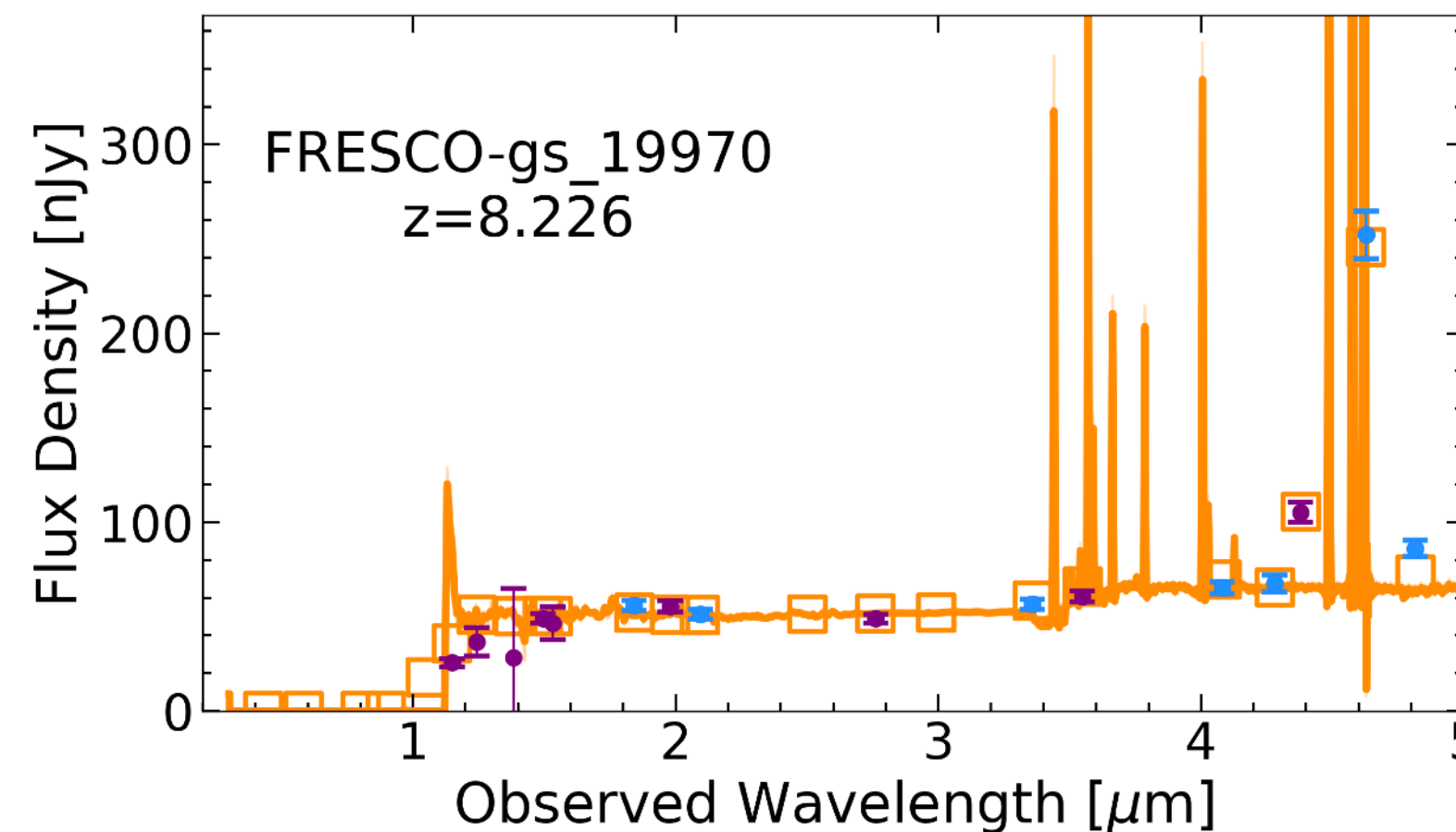
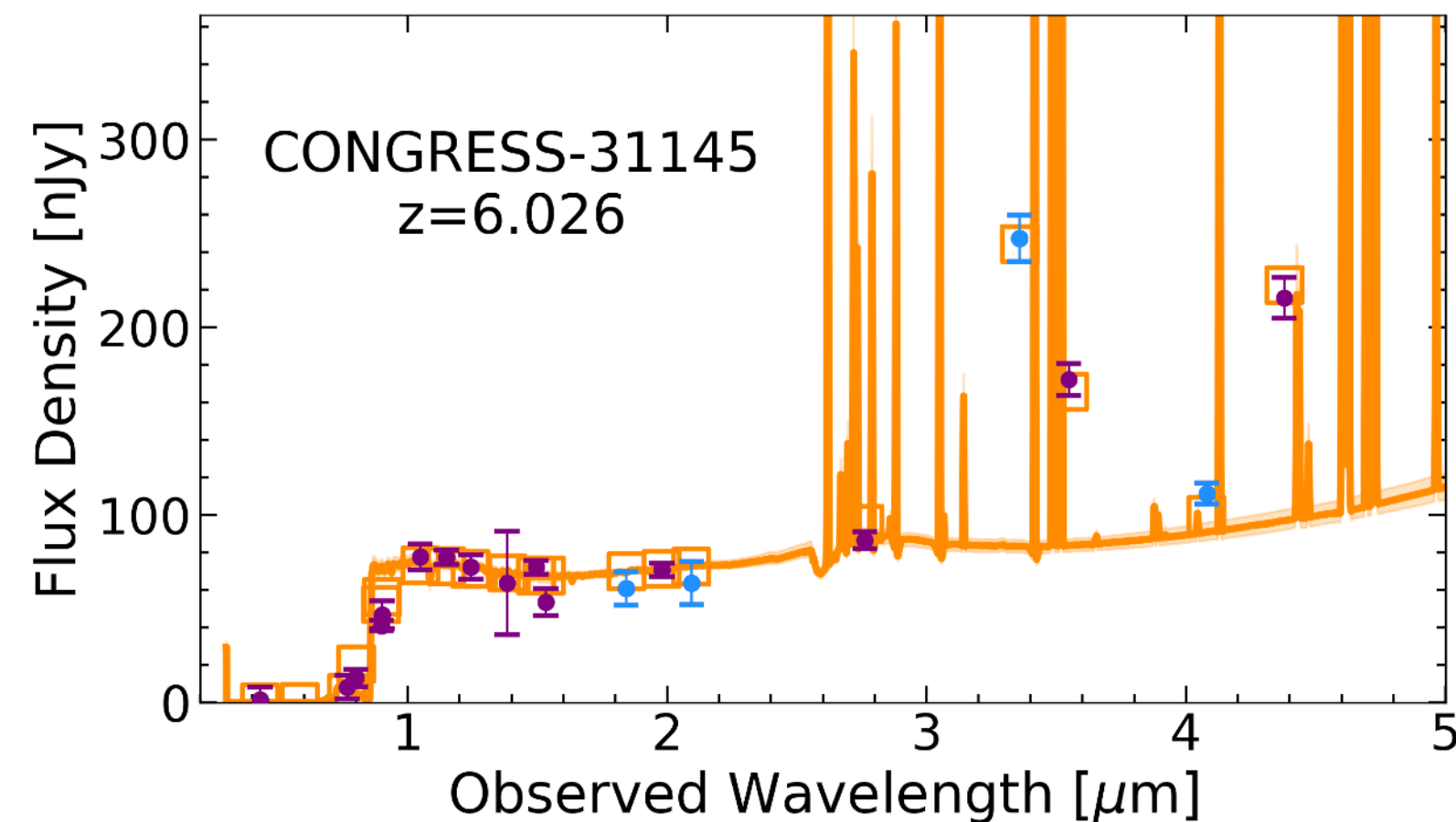


5. Predicting attenuation curves across cosmic time

Three large grism campaigns: **FRESCO** (PI: Oesch), **ALT** (PIs: Matthee, Naidu), **CONGRESS** (PIs: Egami, Sun)



(Plot credits: Irene Shivaiei)



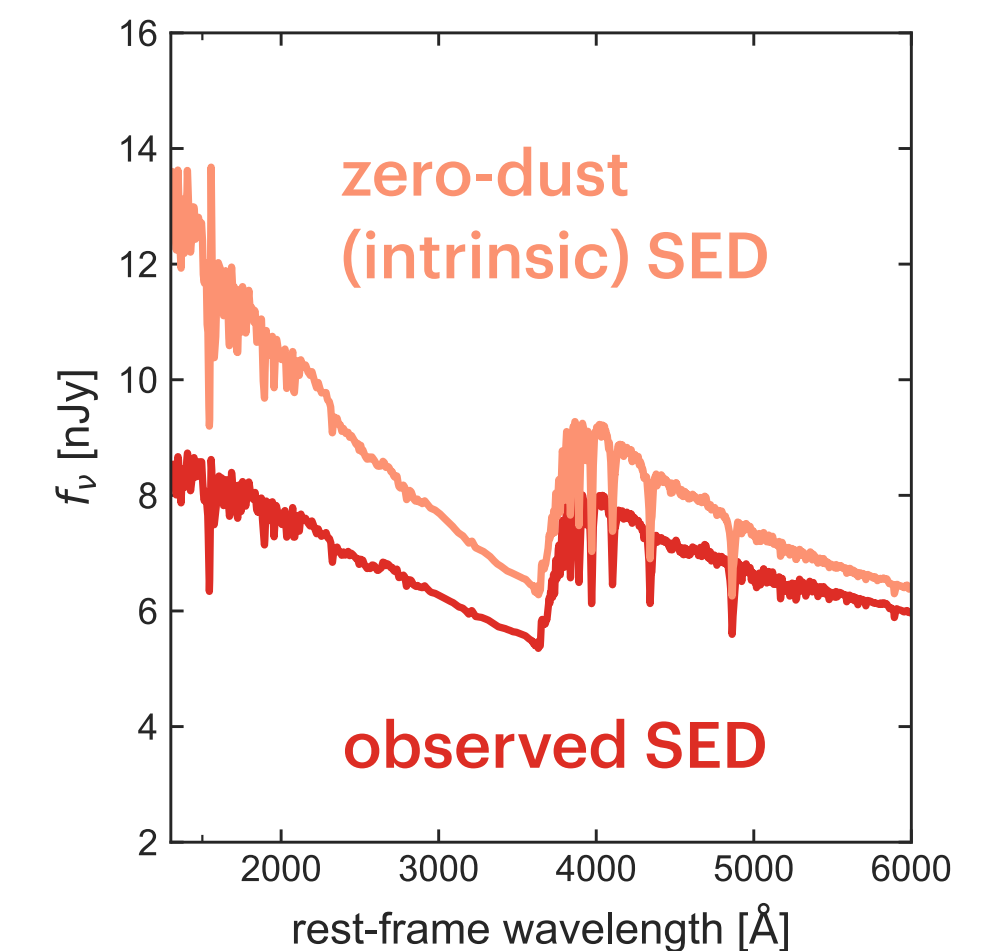
- Two component dust model (Charlot & Fall 2000): Birth-cloud and diffuse ISM dust

$$\hat{\tau}_{\lambda}(t') = \begin{cases} \hat{\tau}_{\lambda}^{\text{BC}} + \hat{\tau}_{\lambda}^{\text{ISM}} & \text{for } t' \leq t_{\text{BC}}, \\ \hat{\tau}_{\lambda}^{\text{ISM}} & \text{for } t' > t_{\text{BC}}, \end{cases}$$

- Flexible attenuation curve slope for the ISM dust

$$k_{\lambda, \text{mod}} = k_{\lambda, \text{Cal}} \frac{R_{V, \text{mod}}}{R_{V, \text{Cal}}} \left(\frac{\lambda}{5500 \text{\AA}} \right)^{\delta} + D_{\lambda},$$

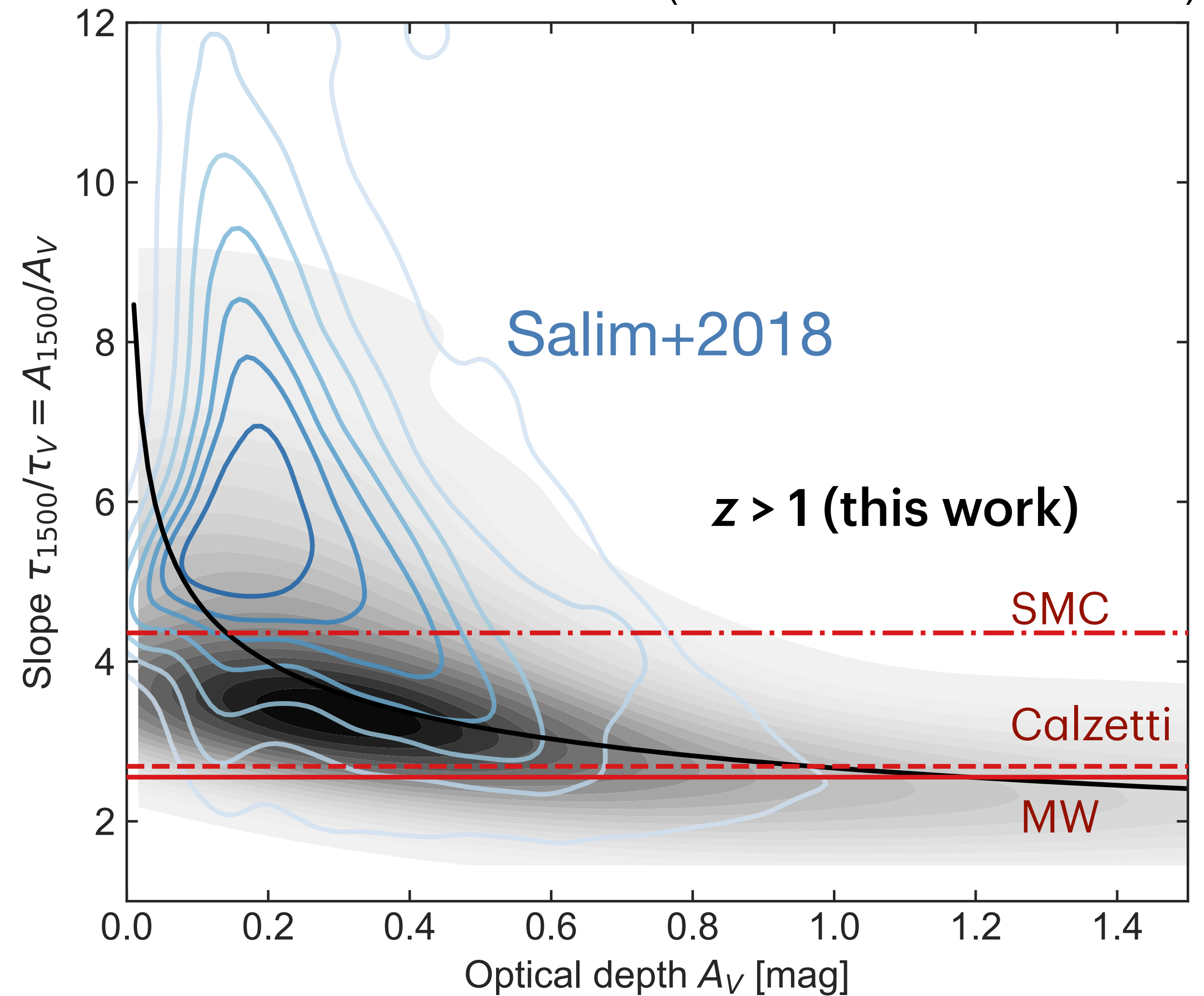
$$L_{\lambda, \text{obs}}(t) = L_{\lambda, 0}(t) 10^{-0.4 A_{\lambda}}$$



5. Predicting attenuation curves across cosmic time

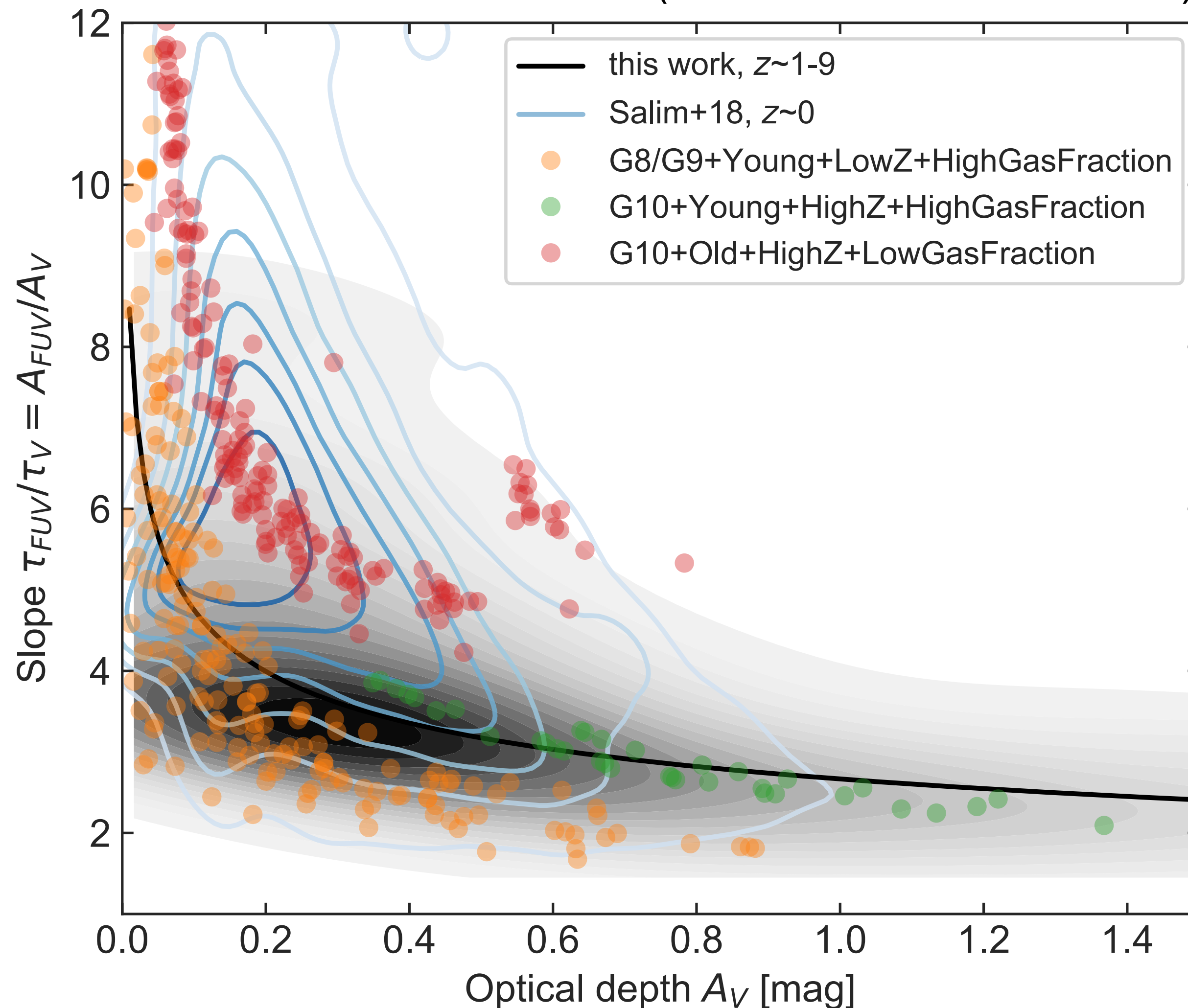
(Plot credits: Irene Shivaiei)

Shallower slopes at fixed optical depth



5. Predicting attenuation curves across cosmic time

(Plot credits: Irene Shivaiei)



Dusty-PRISM suite of isolated disks, post-processed with SKIRT

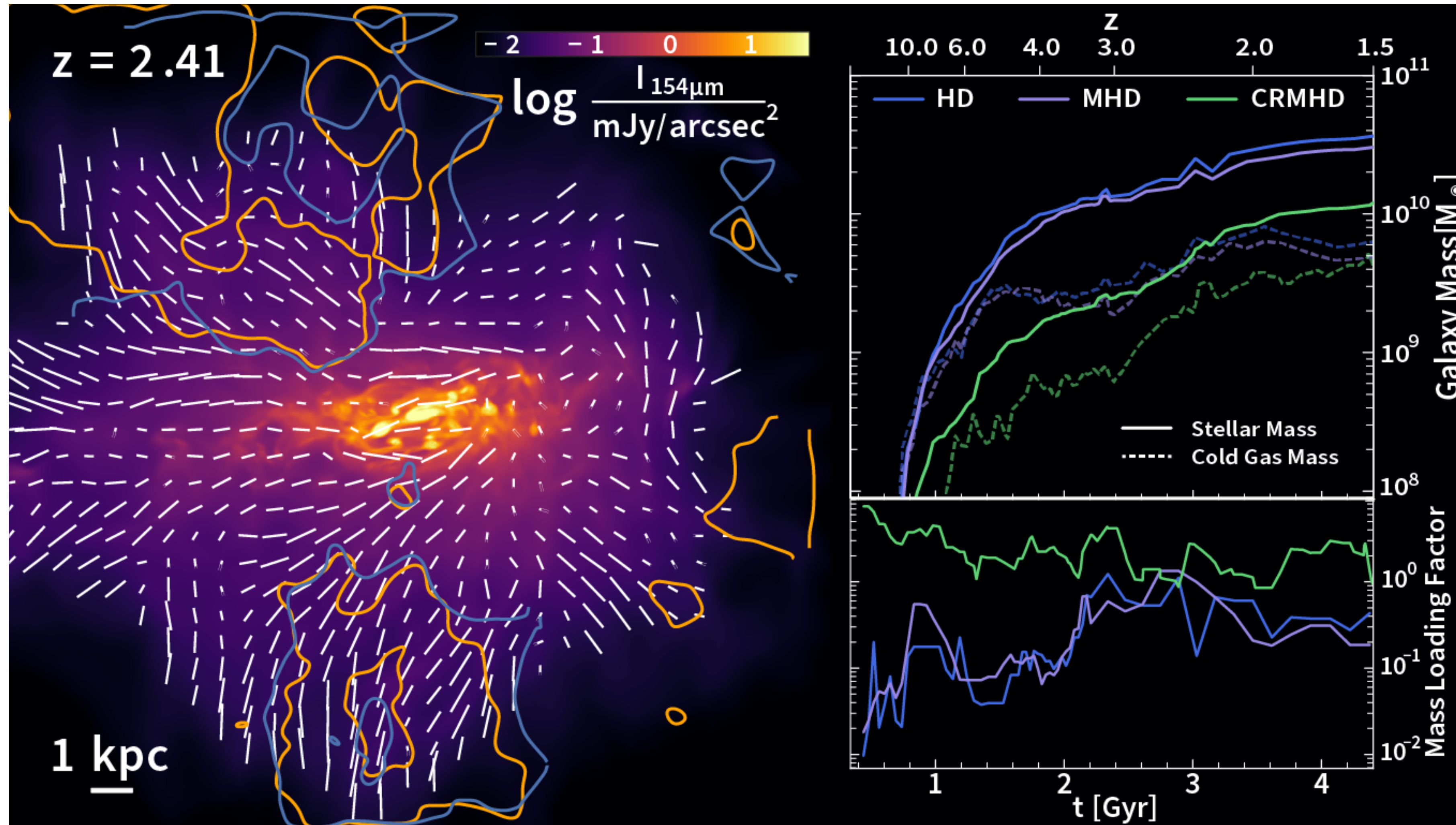
Two channels for dust production:

- ★ ISM growth (metal accretion from gas phase) - small grains
- ★ Stellar origin (SN ejecta) - large grains

>> dominant primordial stellar dust

(Inefficient gas accretion, dominant large dust grain population originating from SN ejecta)

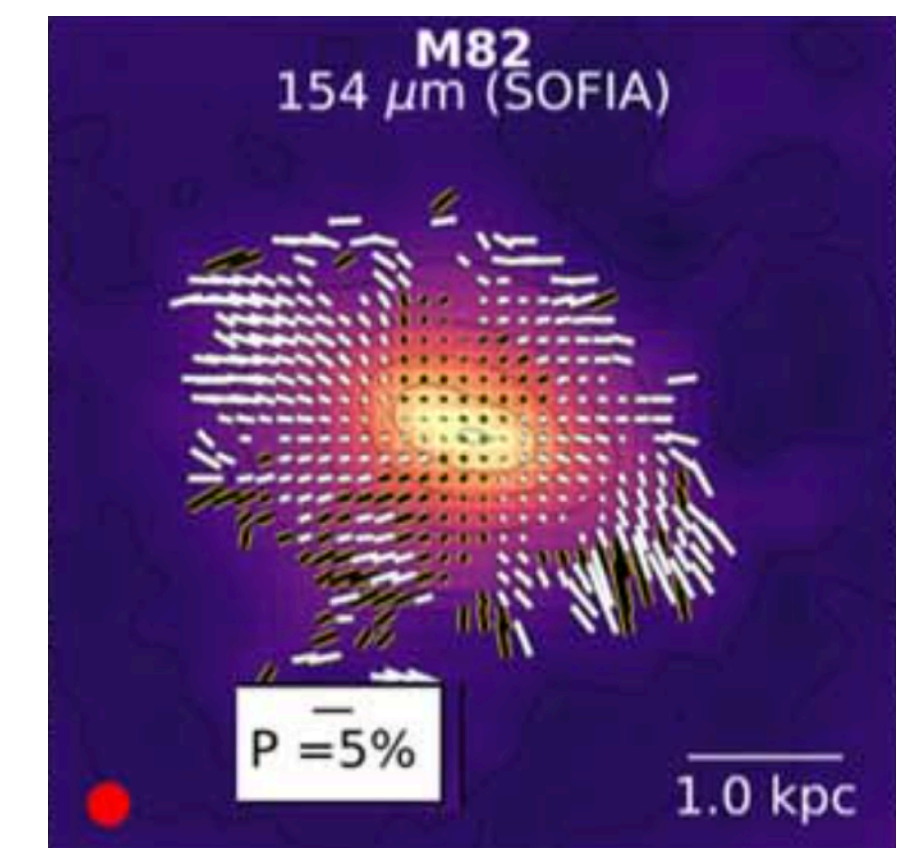
6. Dusty outflows in starburst galaxies



Adding CRs decreases the stellar mass by ~ 1 dex at high redshift and a factor 4 at lower redshift

Large depletion of cold gas compared to HD and MHD (lower star formation efficiency)

High mass loading outflows in the presence of CRs, which are cooler and observed in **FIR polarised emission**



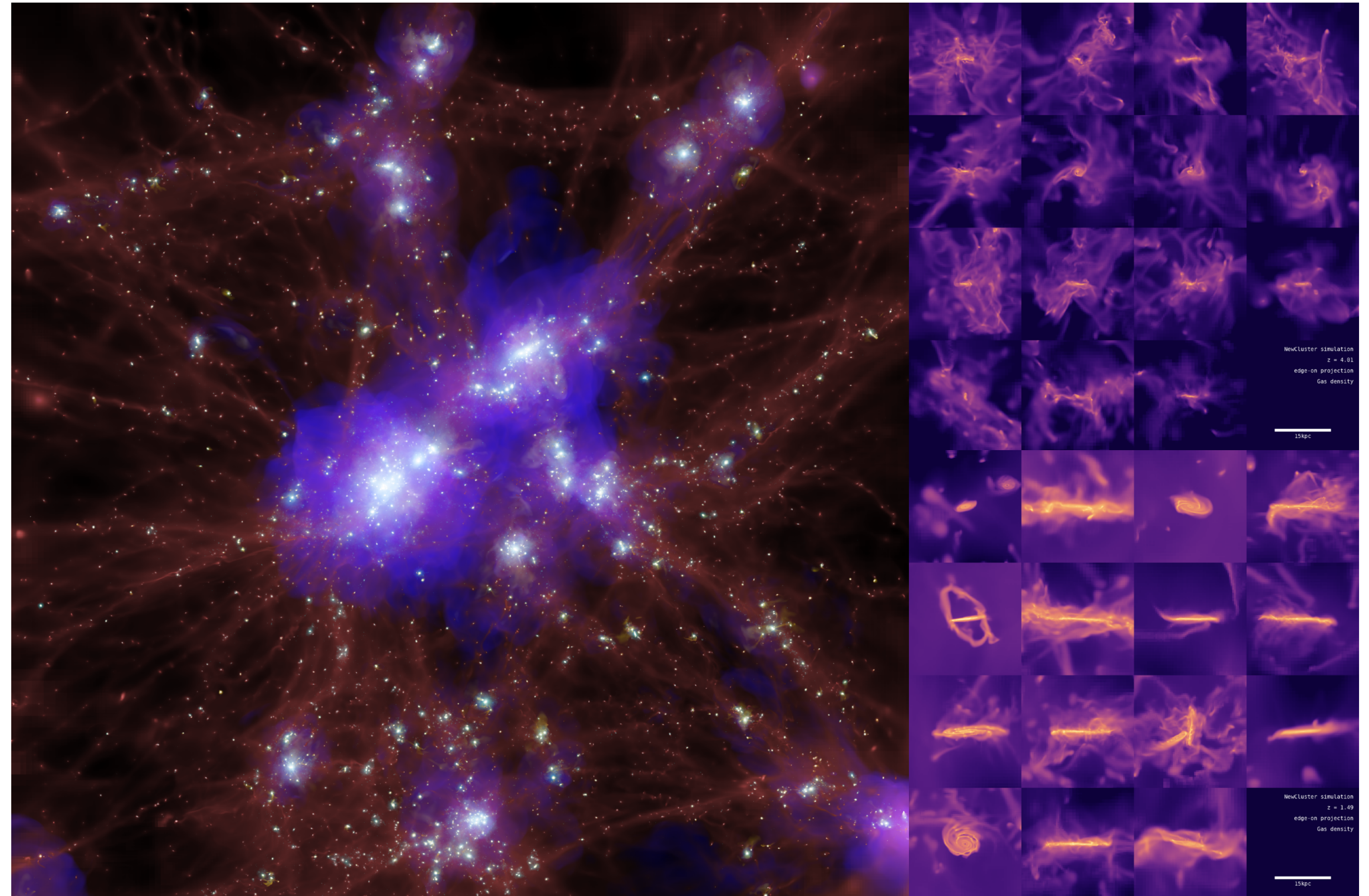
Lopez-Rodriguez2023

7. Ongoing projects using Dusty-PRISM

NewCluster

NewCluster simulation (Han, Yi+, in prep.)

Massive halo zoom-in simulation with <100 pc spatial resolution including the new dust model

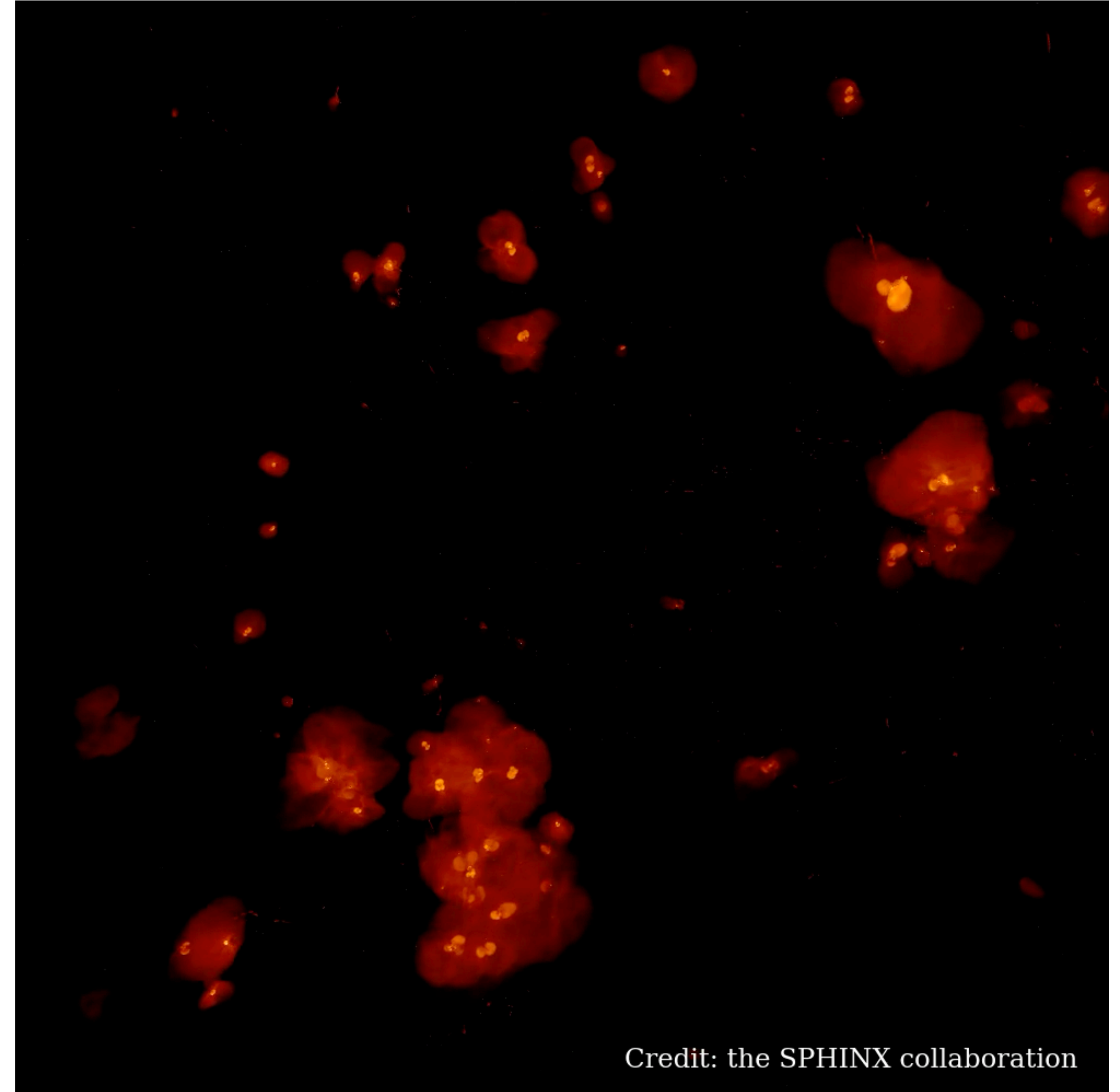


7. Ongoing projects using Dusty-PRISM

Dusty-SPHINX

Reionisation-era cosmological simulation with resolved ISM, radiation transfer and multi-grain dust evolution

PI: Dubois, RM, Rosdahl



Credit: the SPHINX collaboration

8. Conclusions

- A new model of dust and chemistry evolution for galaxy and ISM simulations
- Multiphase ISM can help in constraining dust+PAH physics
- We can reproduce Local Group extinction curves
- SMC-like curves arise from inefficient gas accretion onto C grains (LMC) and also onto Sil grains (SMC) due to lower metallicity
- Low metallicity, young galaxies can reproduce observations at high-z
- Dust + additional physics (CRs) results in more realistic galaxies

The synergy between Dusty-PRISM and future PRIMA observations

- Dusty-PRISM can be used from small-scale cloud predictions all the way to large cosmological volumes
- On-the-fly dust and PAH evolution allows for quantitative analysis of the spatial and temporal variability of dust properties and observables
- Multi-grain prescription and state-of-the-art stellar evolution models will provide an understanding of the evolution of dust properties with cosmic time
- Direct coupling with non-thermal physics (radiation, magnetic fields and cosmic rays) provides an unprecedented predictive power for galaxy formation models
- Trivially extendable to different dust models/properties

Very exciting times ahead!



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DiRAC

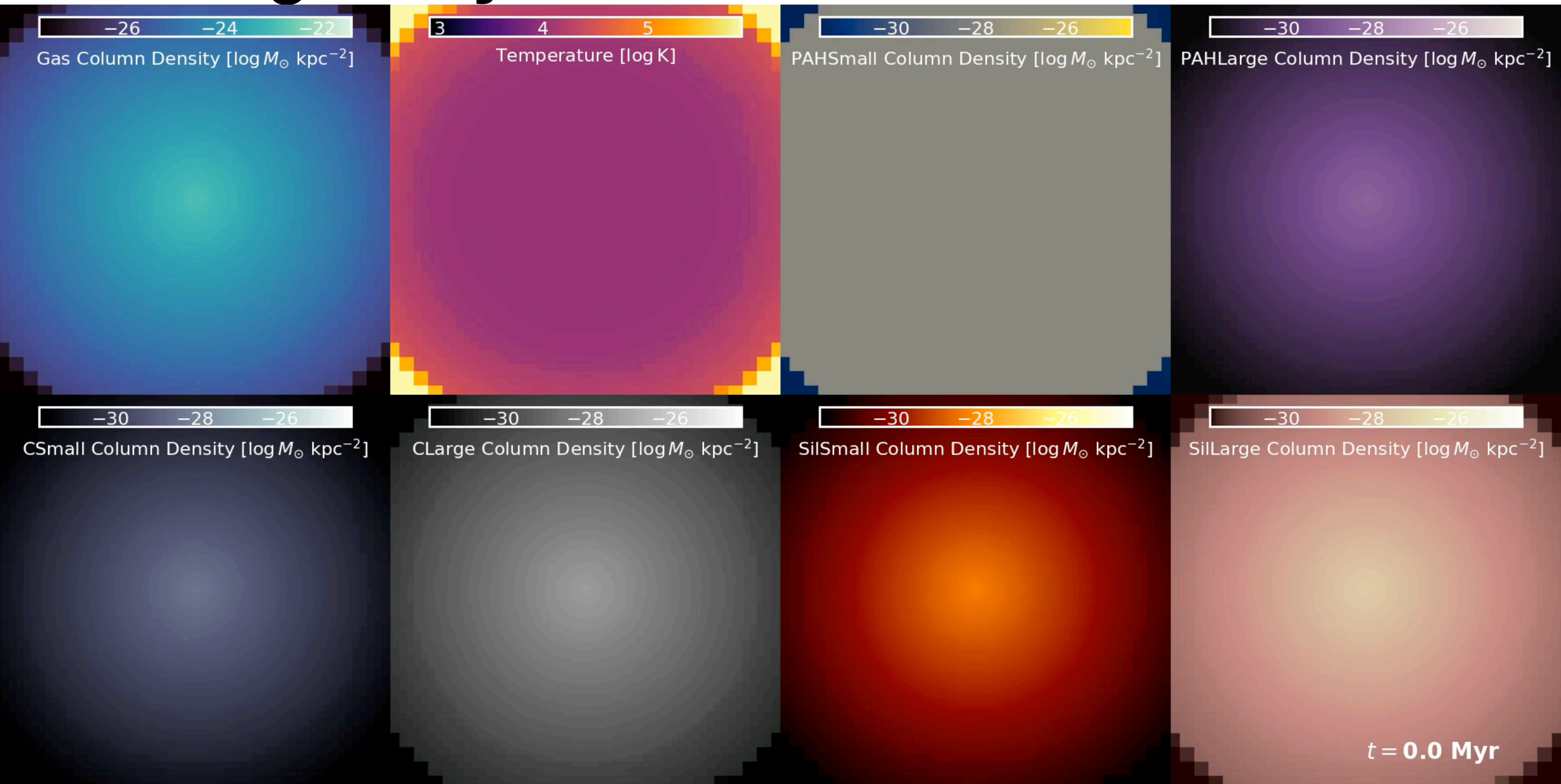


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THANK YOU

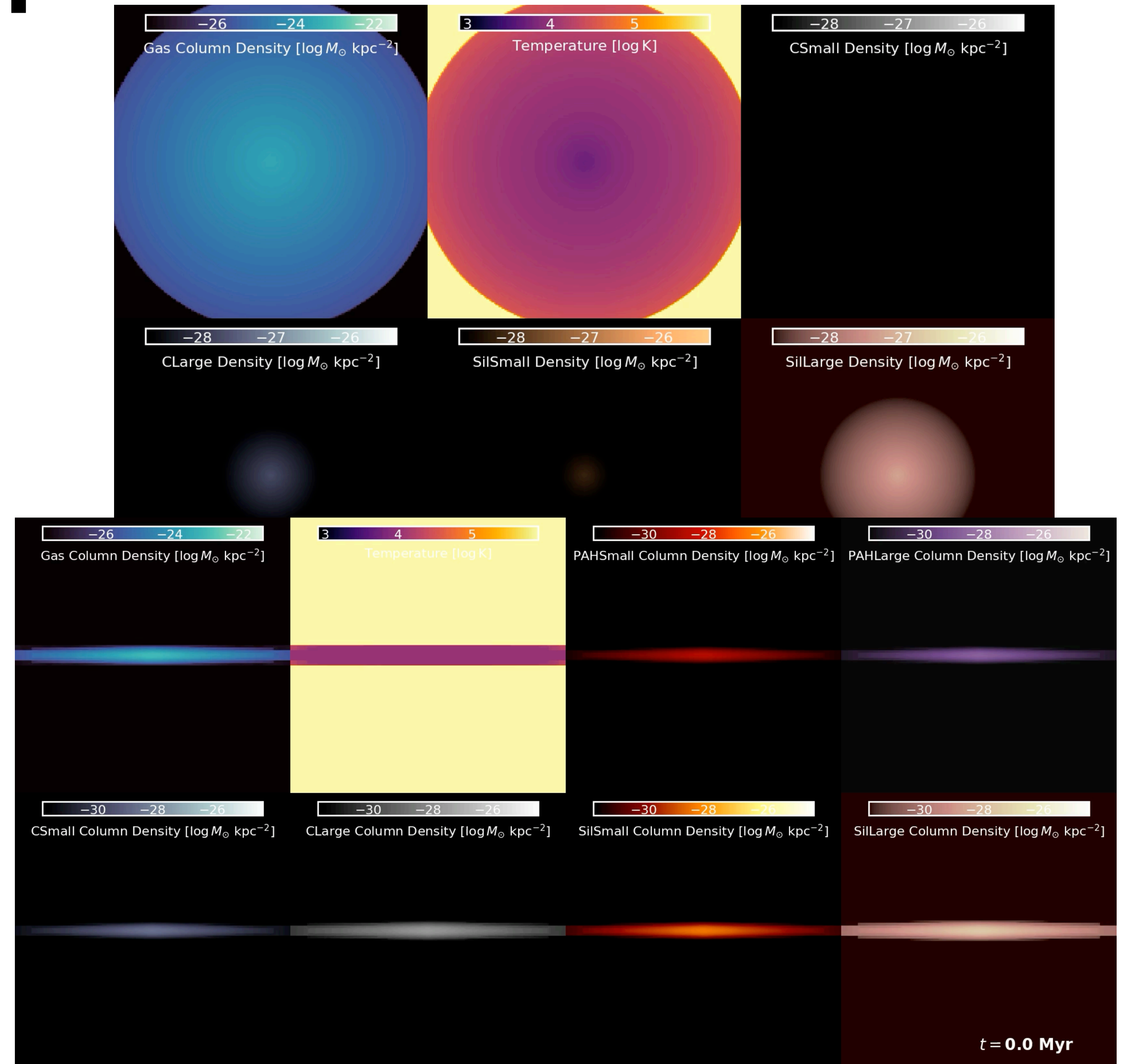
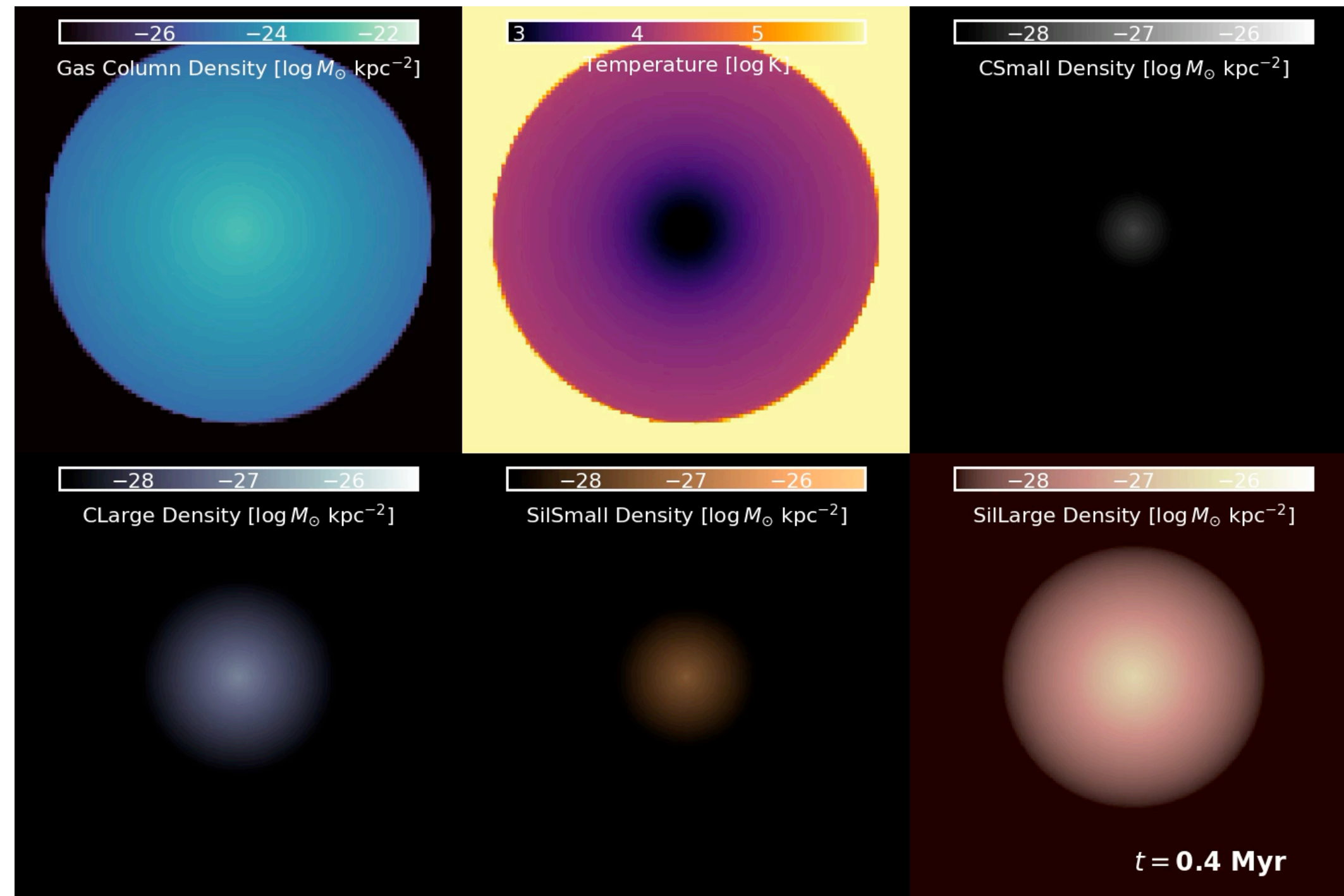
Francisco (Curro) Rodríguez Montero – Dusting Off the Secrets of the COSMOS with PRIMA IR Space Telescope

Testing Dusty-PRISM



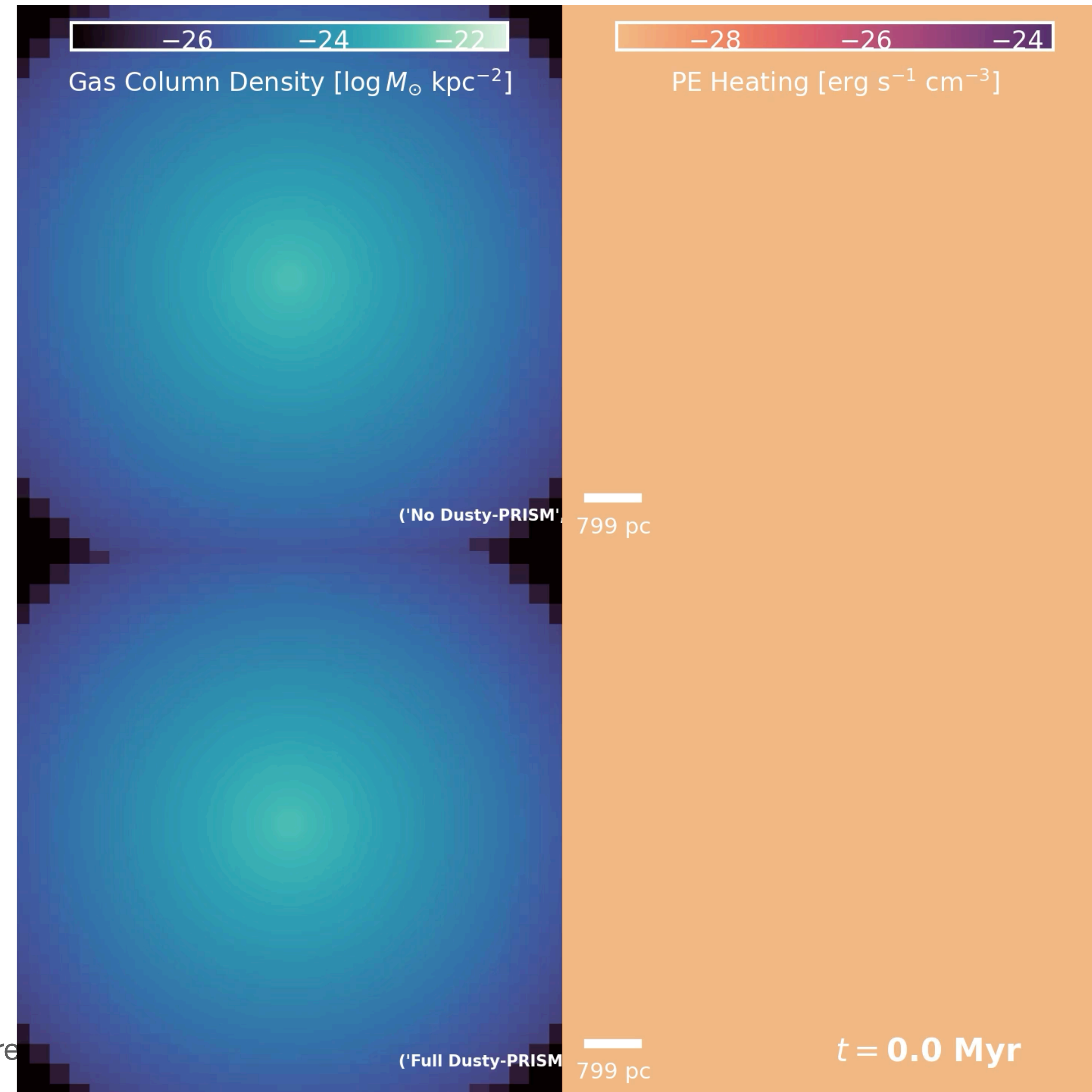
Testing Dusty-PRISM

Isolated galaxy simulations



Testing Dusty-PRISM

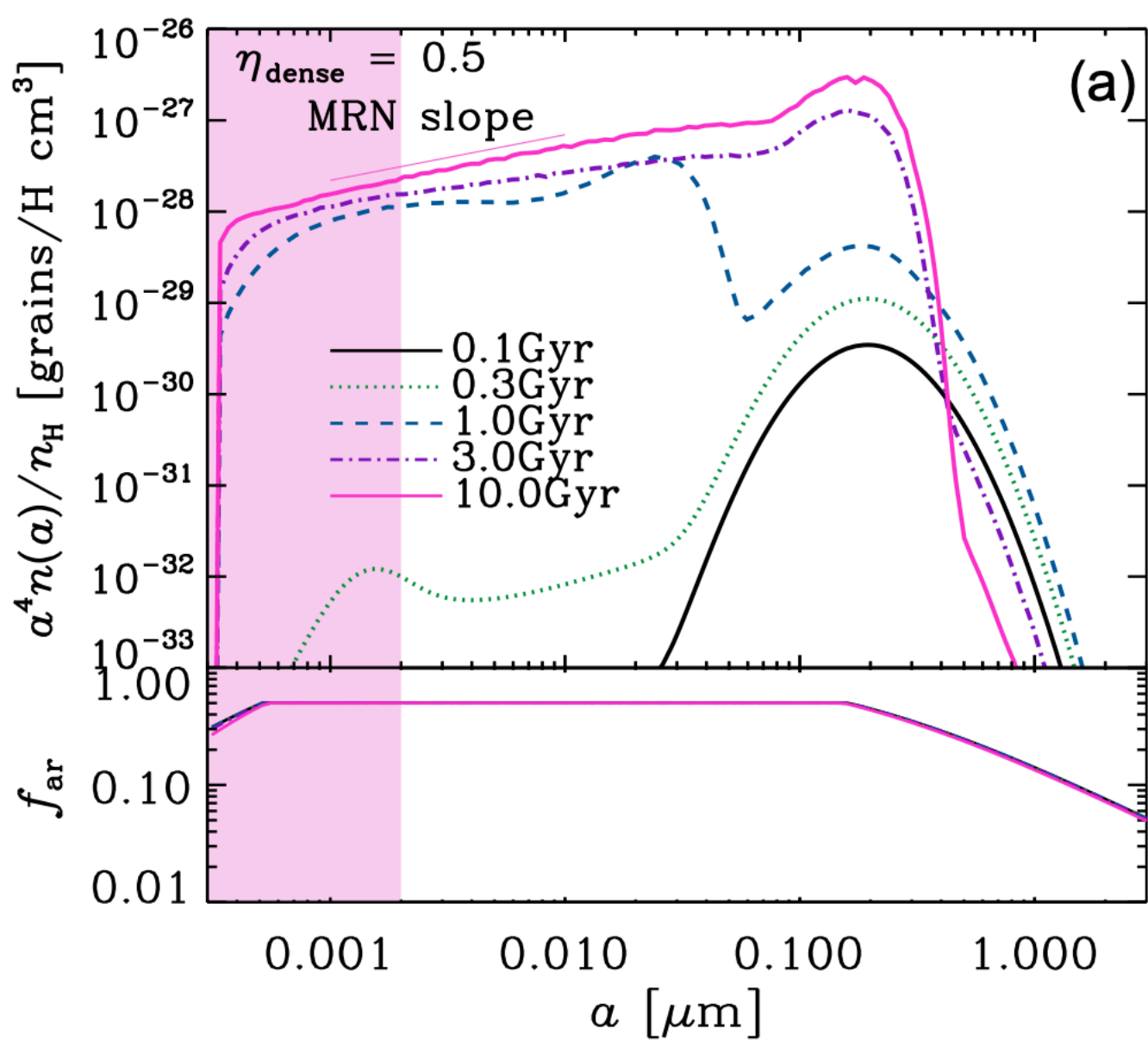
Photo-electric heating



...and what about?

Where do PAHs come from??

Shattering cascade and quick aromatisation?



Hirashita&Murga2020,
Narayanan+2023

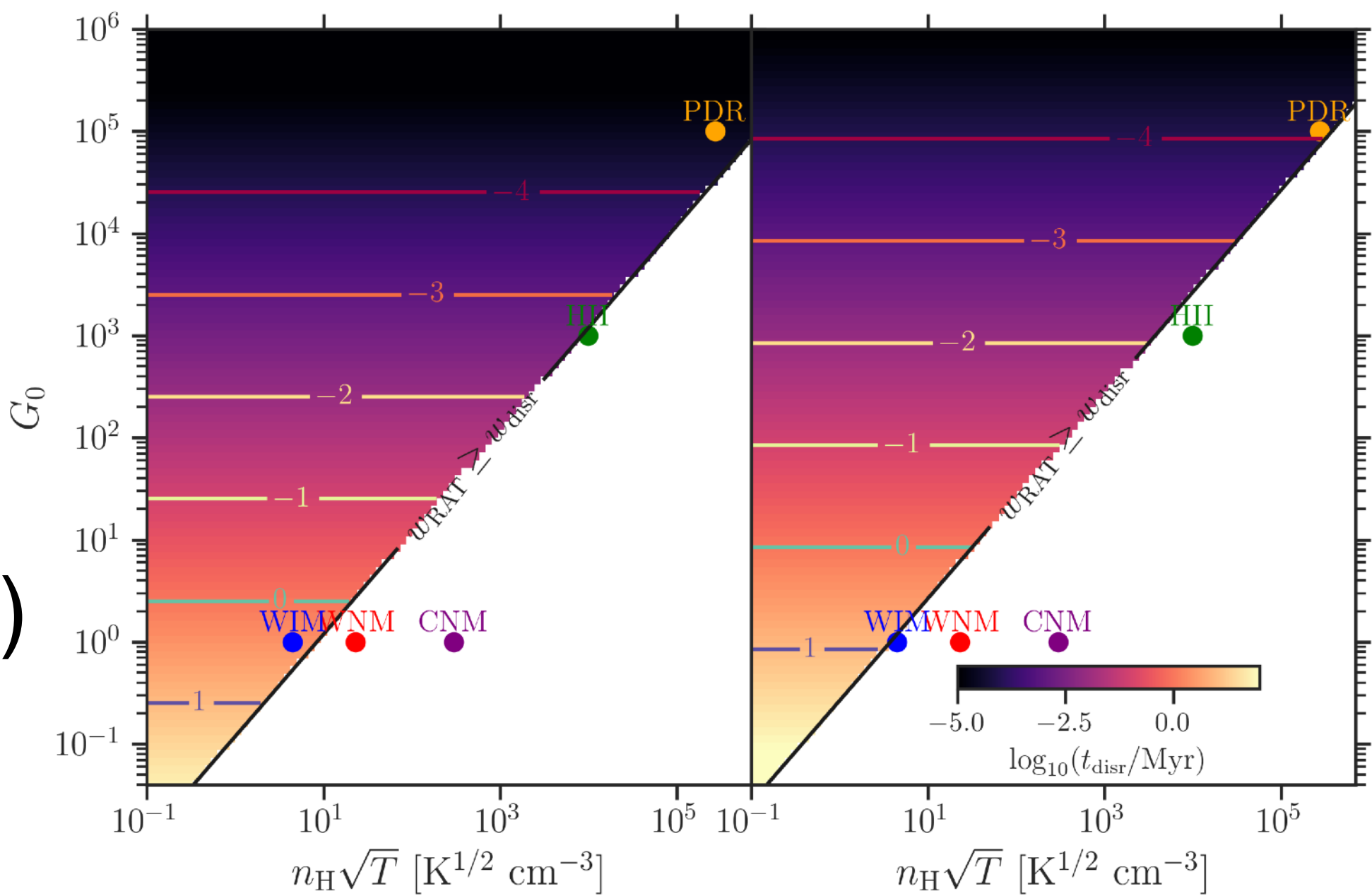
I propose we discuss
this the next few day ;)

Allamandola+1989

AGB winds?

Hoang+2021ab,Hirashi
ta&Hoang2020

Fragmentation during
radiative torque disruption?



Combustion-like reactions
in clouds?

Wang+97, Frenklach+02, Shukla+12,
Zhao+18ac,Kaiser+15, Gavilan Marin+20,
Cherchneff+1992, Gou2002
Francisco Rodriguez Montero - PRIMA Conference, Marseille 2025

Formation of
ethane (C₂H₆)
on dust ice
mantels

Formation of
acetylene
(C₂H₂)

Vinylacetylene

Graphene etching on dust
surface?

Formation of
benzene (C₆H₆)

Phenyl radical
(C₆H₅)

Naphthalene!!

Sub-grid turbulent model

$$\Delta V_{i,j}^B = \sqrt{\frac{8k_B T_{\text{gas}}(m_i + m_j)}{\pi m_i m_j}}.$$

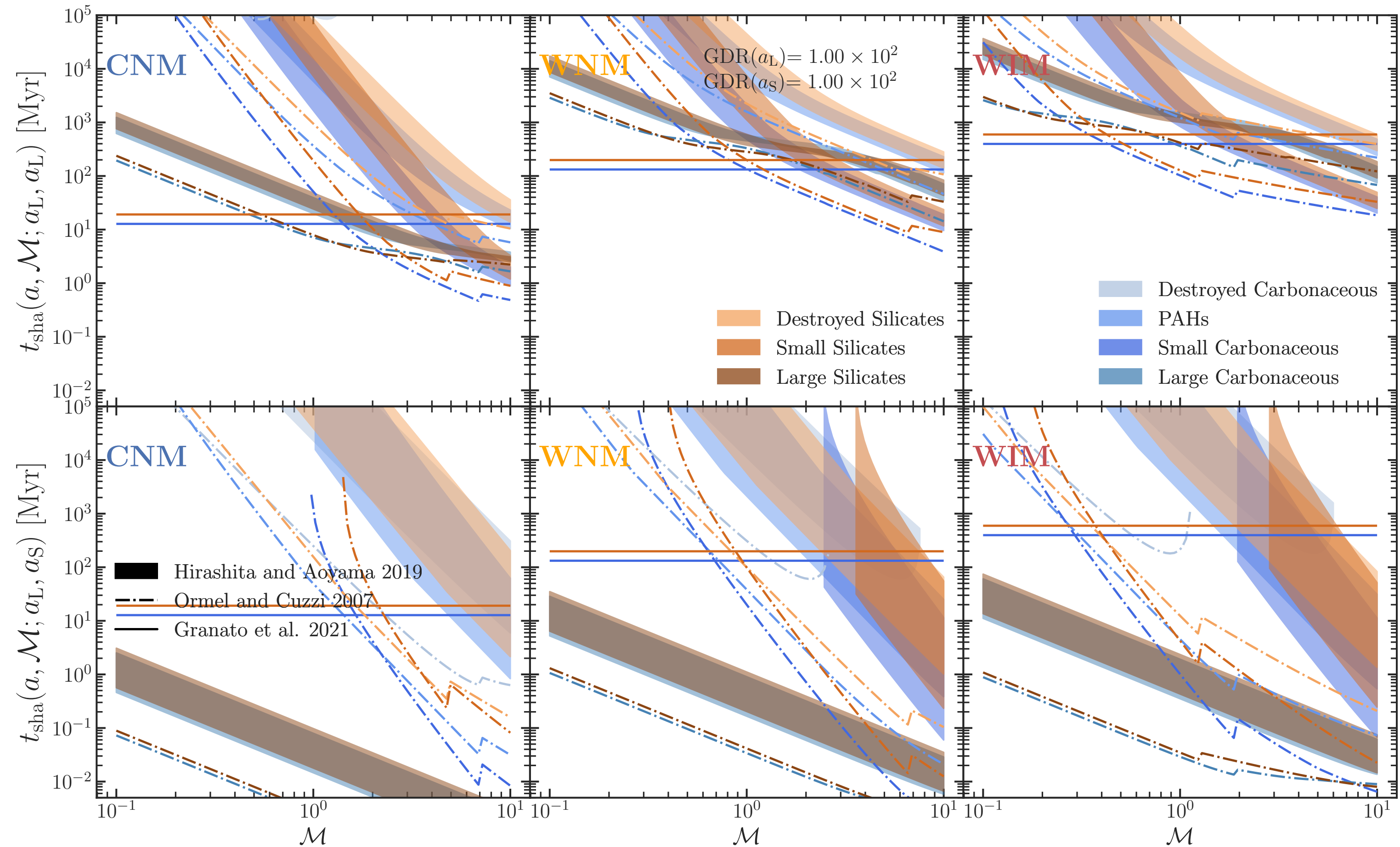
$$\Delta V_{i,j}^T = \begin{cases} \sqrt{\frac{3}{2}} \sigma \sqrt{\frac{St_i - St_j}{St_i + St_j}} \sqrt{\frac{St_i^2}{St_i + St_{\min}} - \frac{St_j^2}{St_j + St_{\min}}}, & \text{if } \tau_\eta > t_s^i, \\ \sqrt{\frac{3}{2}} \sigma \sqrt{f\left(\frac{St_j}{St_i}\right) St_i}, & \text{if } \tau_\eta \leq t_s^i < \tau_L, \\ \sqrt{\frac{3}{2}} \sigma \sqrt{\frac{1}{1+St_i} + \frac{1}{1+St_j}}, & \text{if } \tau_L \leq t_s^i, \end{cases} \quad (46)$$

with the function f given by

$$f(x) = 3.2 - (1+x) + \frac{2}{1+x} \left(\frac{1}{2.6} + \frac{x^3}{1.6+x} \right), \quad (47)$$

and $St_{\min} \equiv \tau_\eta / \tau_L = 1/\sqrt{\text{Re}}$. The final relative velocity is obtained by combining the Brownian and turbulent contributions:

$$\Delta V_{i,j} = \sqrt{(\Delta V_{i,j}^B)^2 + (\Delta V_{i,j}^T)^2}. \quad (48)$$



Testing Dusty-PRISM

