CALIMA

On-the-fly radiation and thermo-chemistry of dust and PAHs in galaxy formation simulations

Ramses User Meeting, Yonsei University, 2026

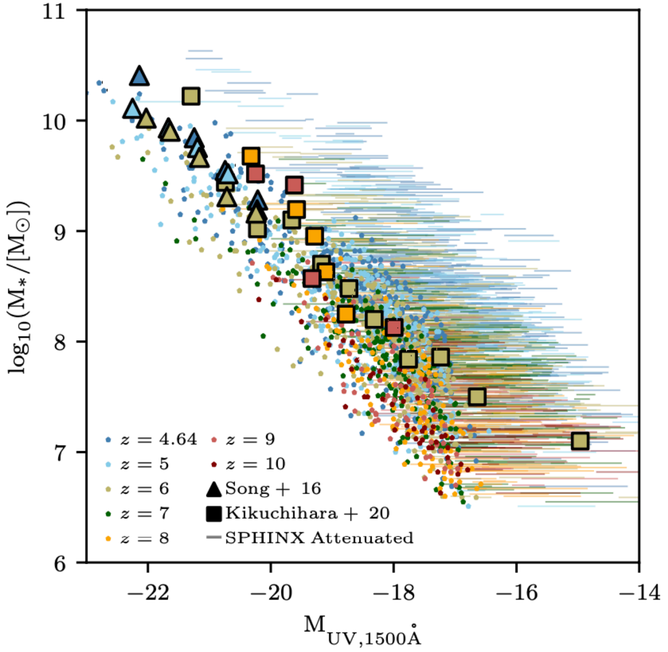
Curro Rodríguez Montero - KICP, University of Chicago

With Yohan Dubois and Harley Katz

The failures of models in the JWST era

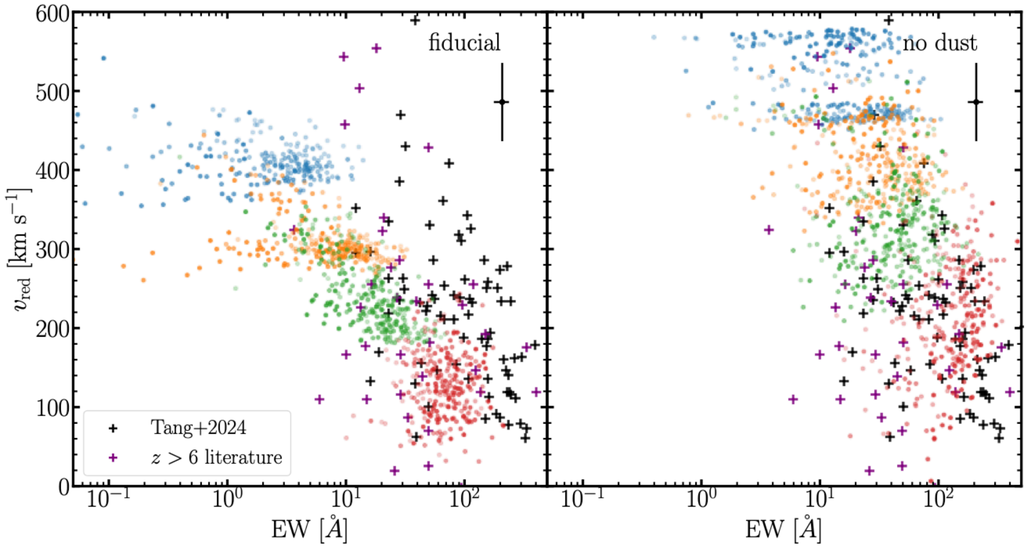
UV-calibrated simulations have too **massive** and/or too **dusty** galaxies

Katz+2023

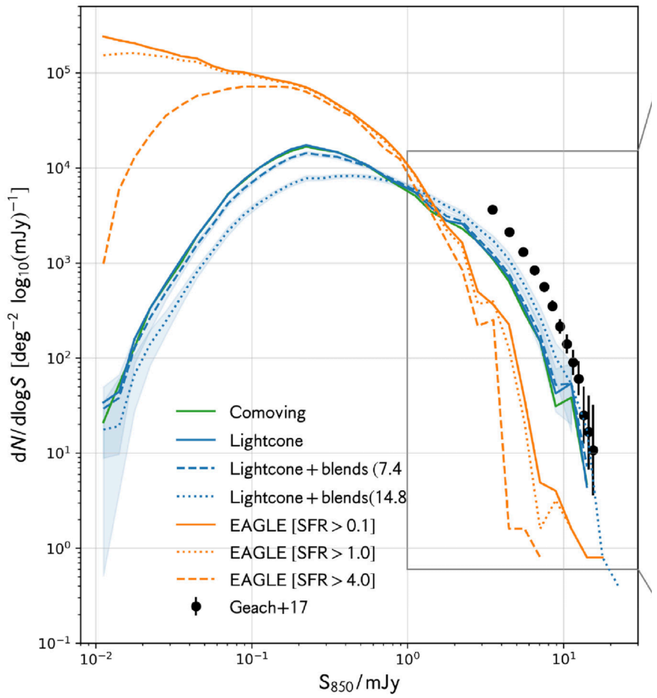


Simple dust models **incapable of predicting Lya** observables, even with additional physics

Yuan+2025



Lovell+2021



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

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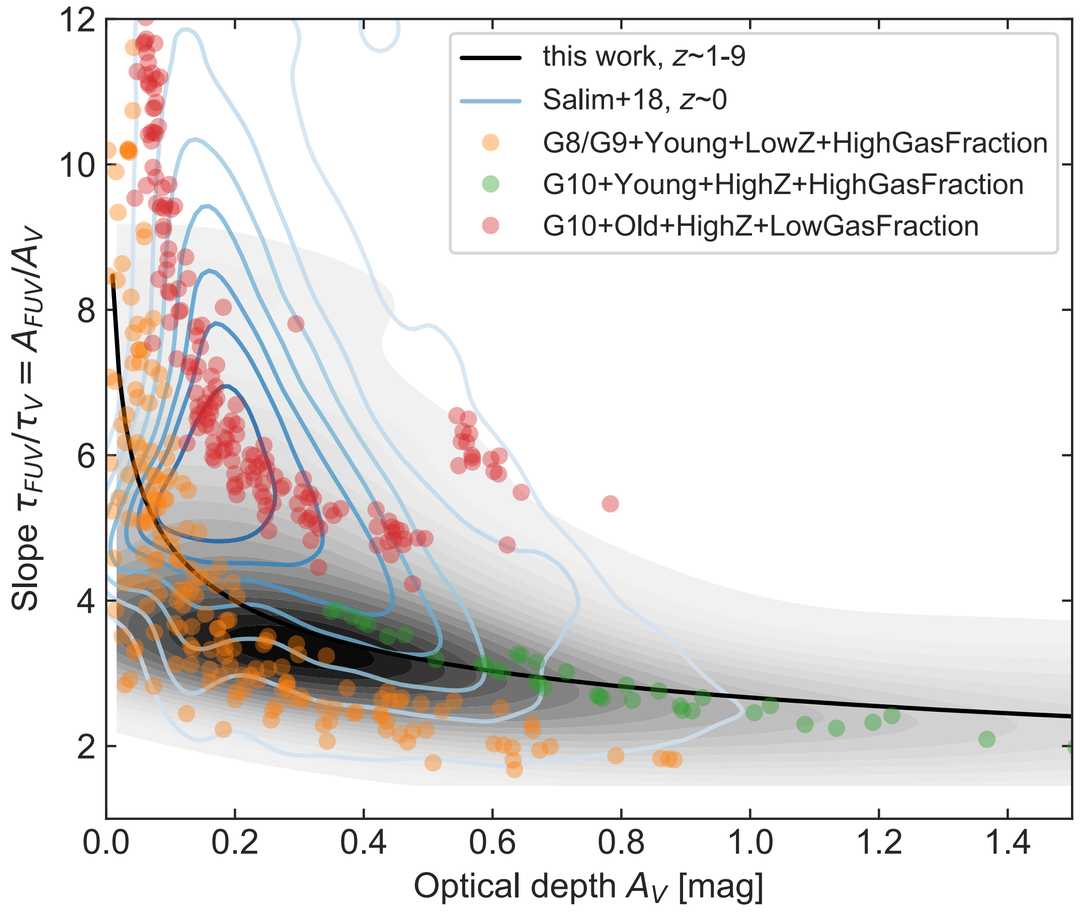
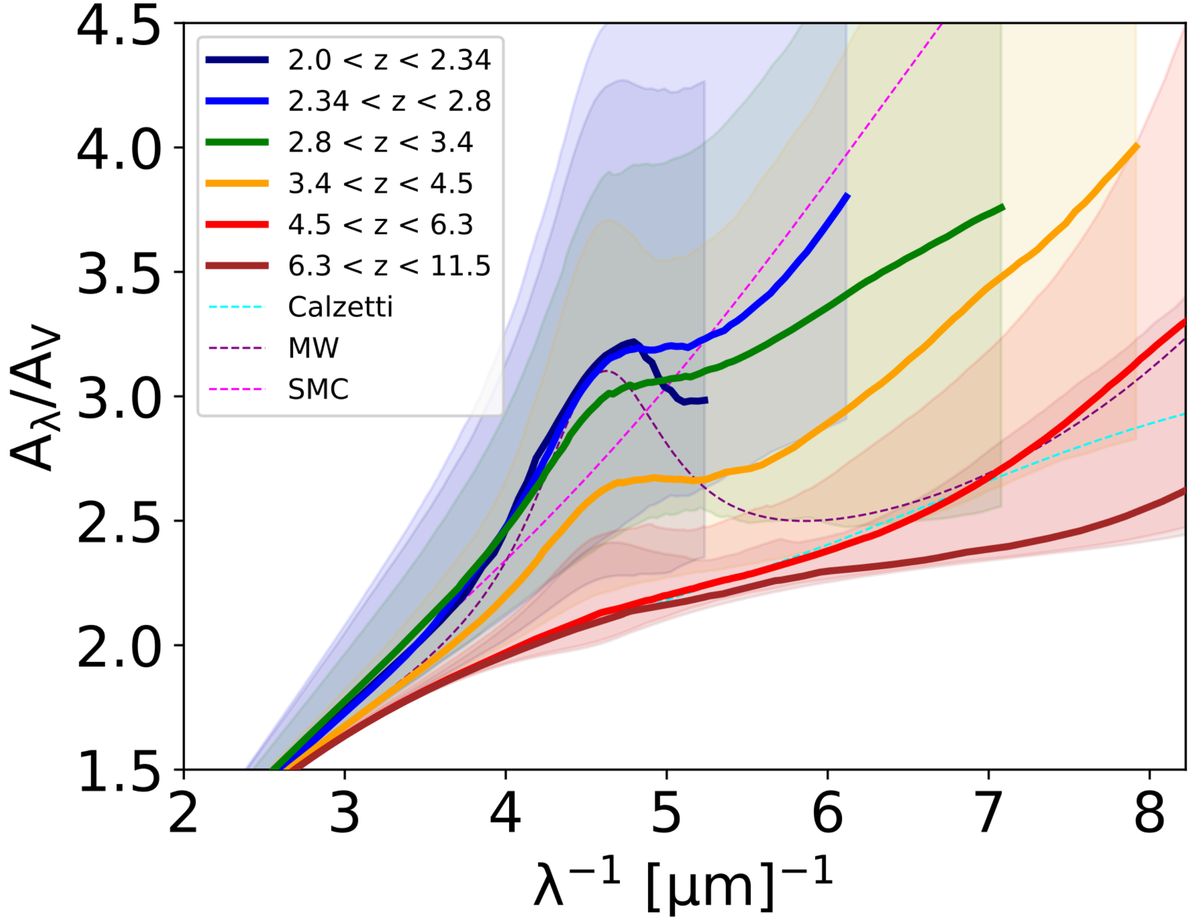
Dust properties change across cosmic time

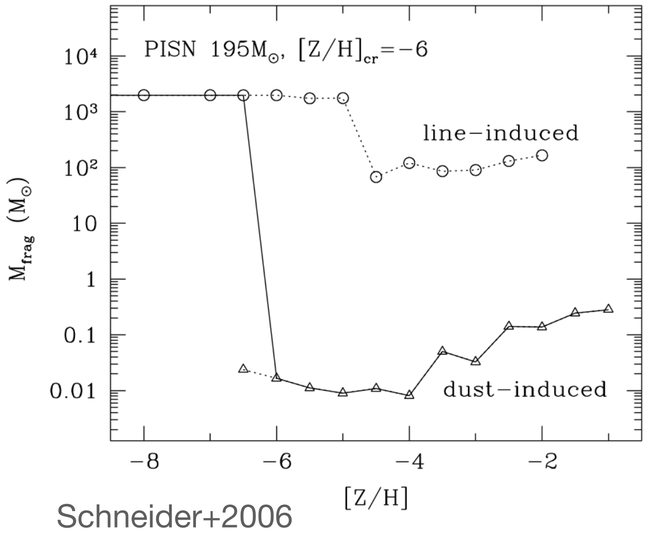


Shivaei+2026



Markov+2024

Why I can't get away with post processing?



Schneider+2006

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

Cloud fragmentation enriched by Pop III

Radiation pressure

Elemental abundances and enrichment

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

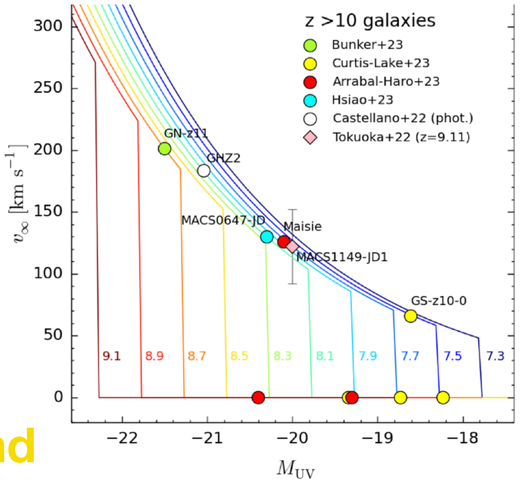
Ionisation properties of HII regions

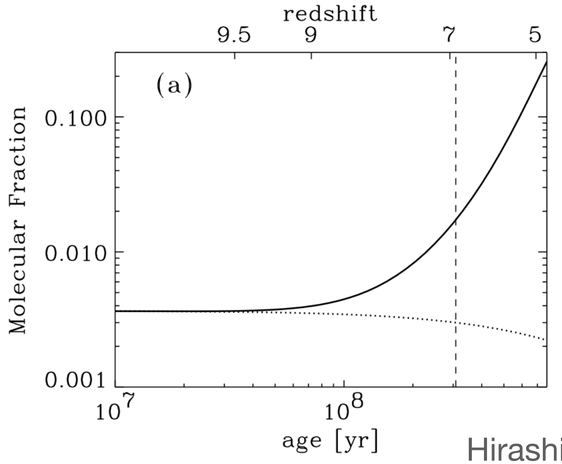
Photo-electric heating

Shielding from UV radiation

Molecule catalysis

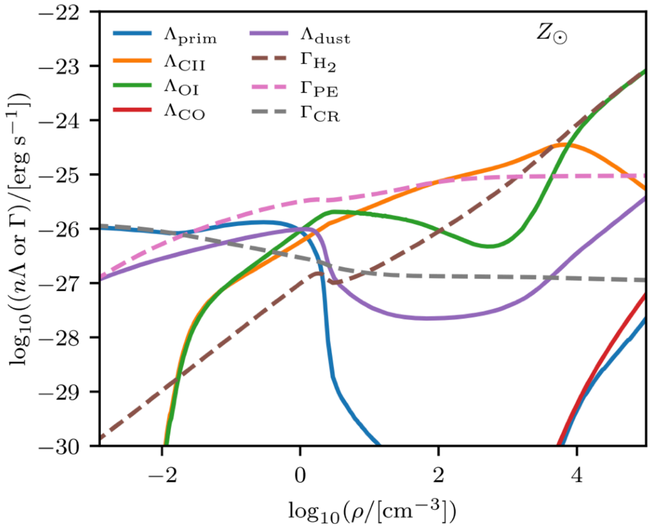
Ferrara2024





Hirashita&Ferrara2001

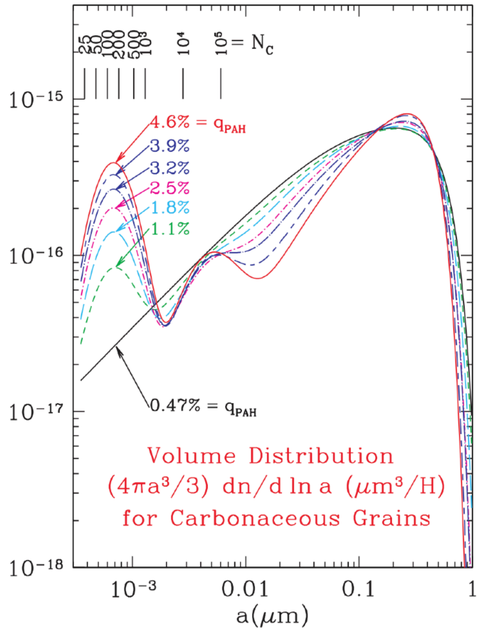
Katz,RM+2022



Why can’t I get away with post processing?

Diffuse ISM grain properties

- Fixed grain size distribution
- Fixed composition
- Mean ISRF
- Solar metallicity environment
- Low SFRs

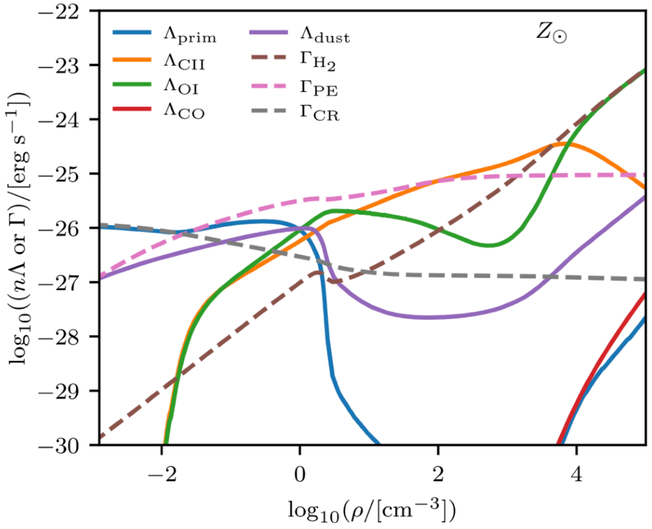


Draine&Li2007

Dust thermo-chemistry

- H_2 formation
- CO formation
- Photo-electric heating
- Extinction
- Ion recombination
- Radiation pressure
- …

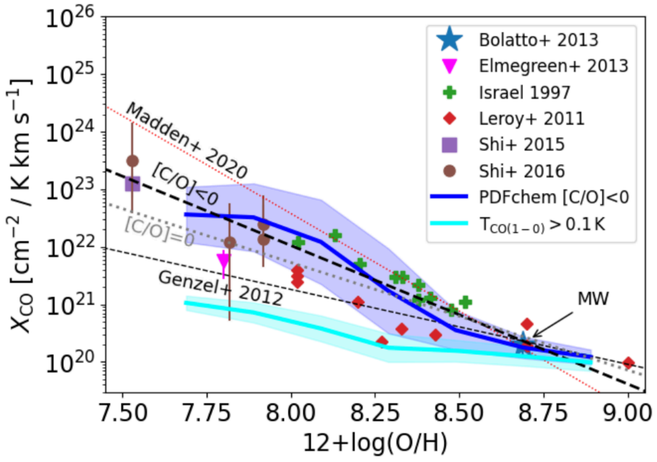
Katz,RM+2022



Modelling and observables

- CO-H_2 conversion factors
- Attenuation curves
- IR emission
- Stellar masses
- Depletions/metallicity
- HII region properties
- …

Bisbas+2025



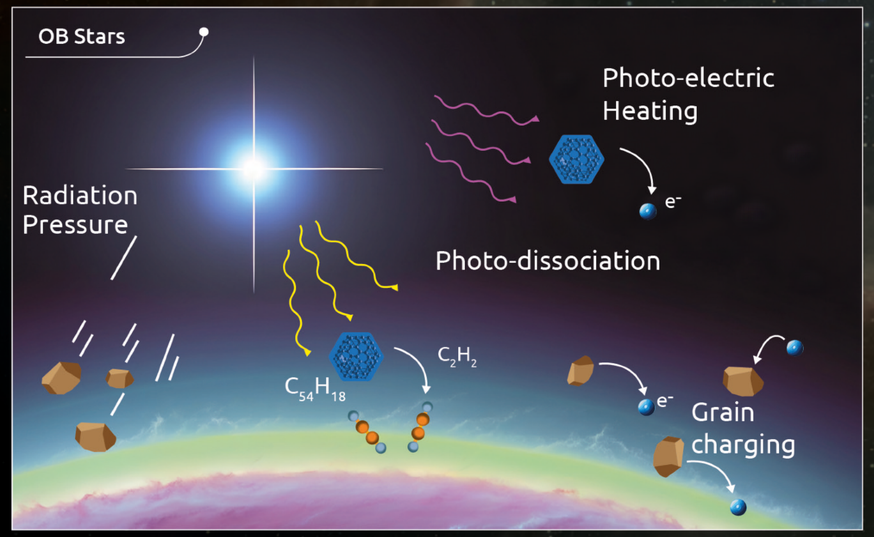
CALIMA

CALIMA 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.

PDR AND THE MOLECULAR PHASE

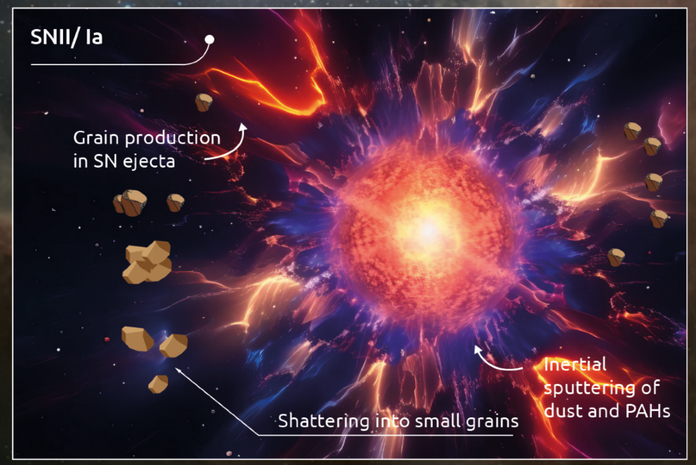
The high gas density of molecular clouds allows for a rich and fast thermochemistry, the formation of molecules and the growth of dust. Dust and PAH properties quickly evolve as the gas transitions from the ionised HII gas, to the photo-dissociation region, into the molecular and ice regime

HII REGIONS

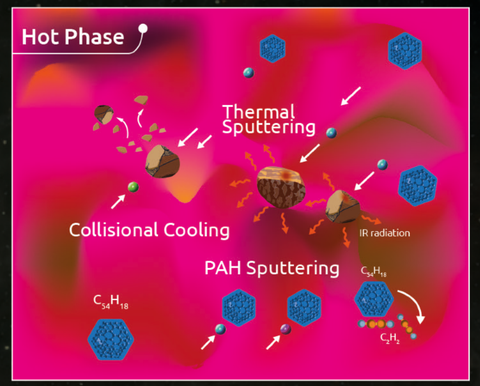


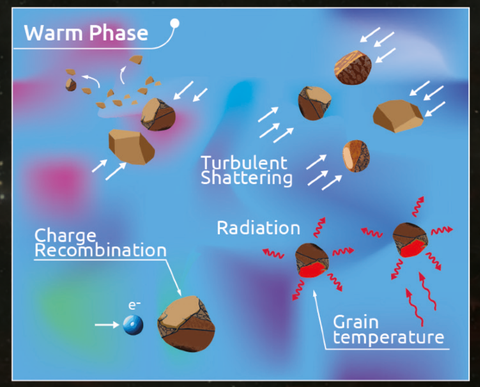
SEEDING AND DESTRUCTION BY STARS

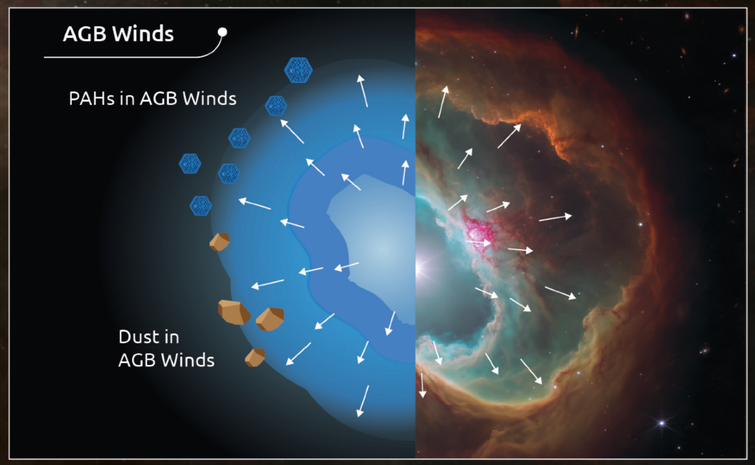
Stellar processes can both inject fresh dust and molecules to the ISM, as well as destroy the dusty material already present in it



THE TURBULENT DIFFUSE ISM







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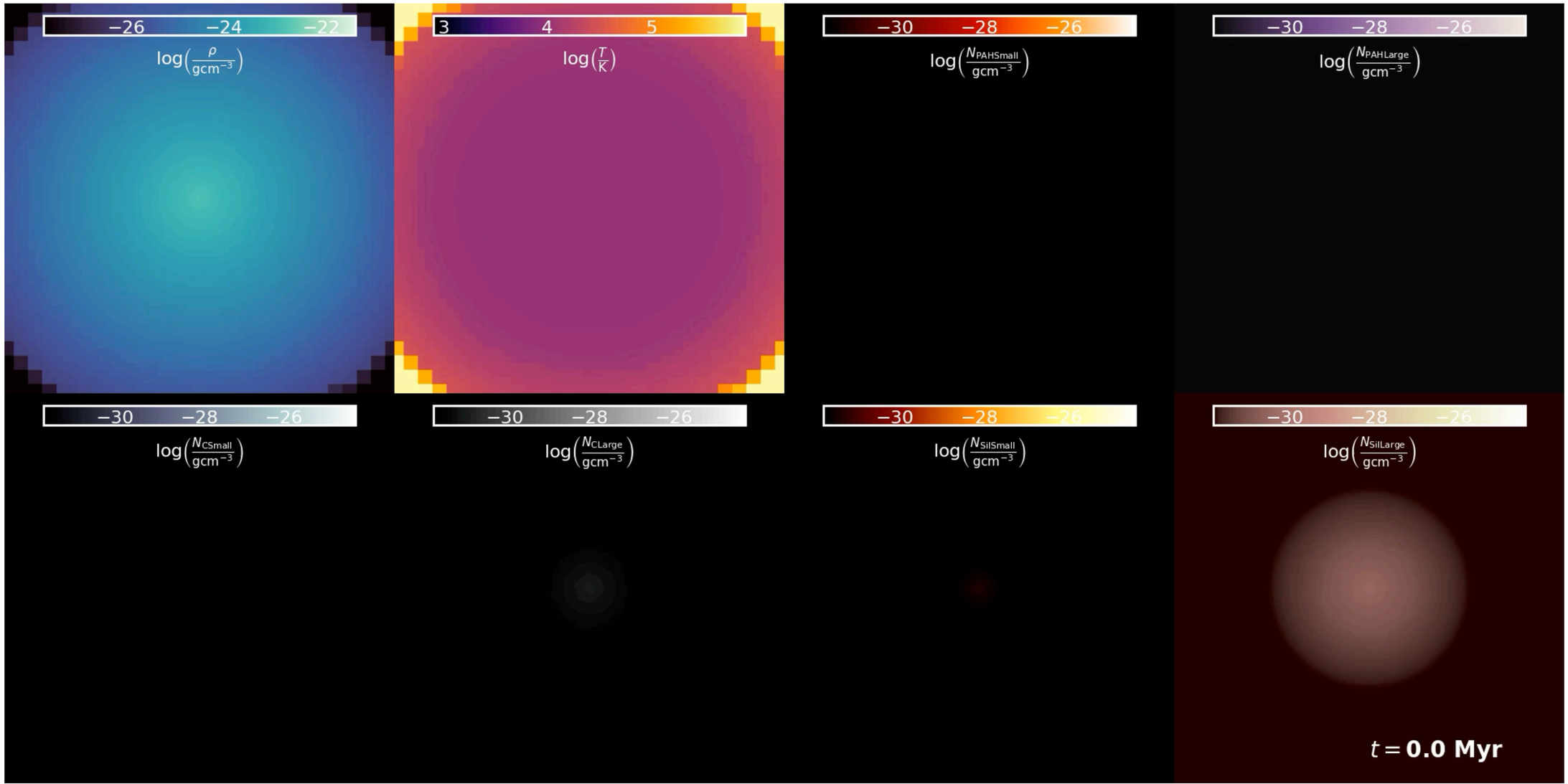
Molecules, dust and PAHs connected to galaxy formation



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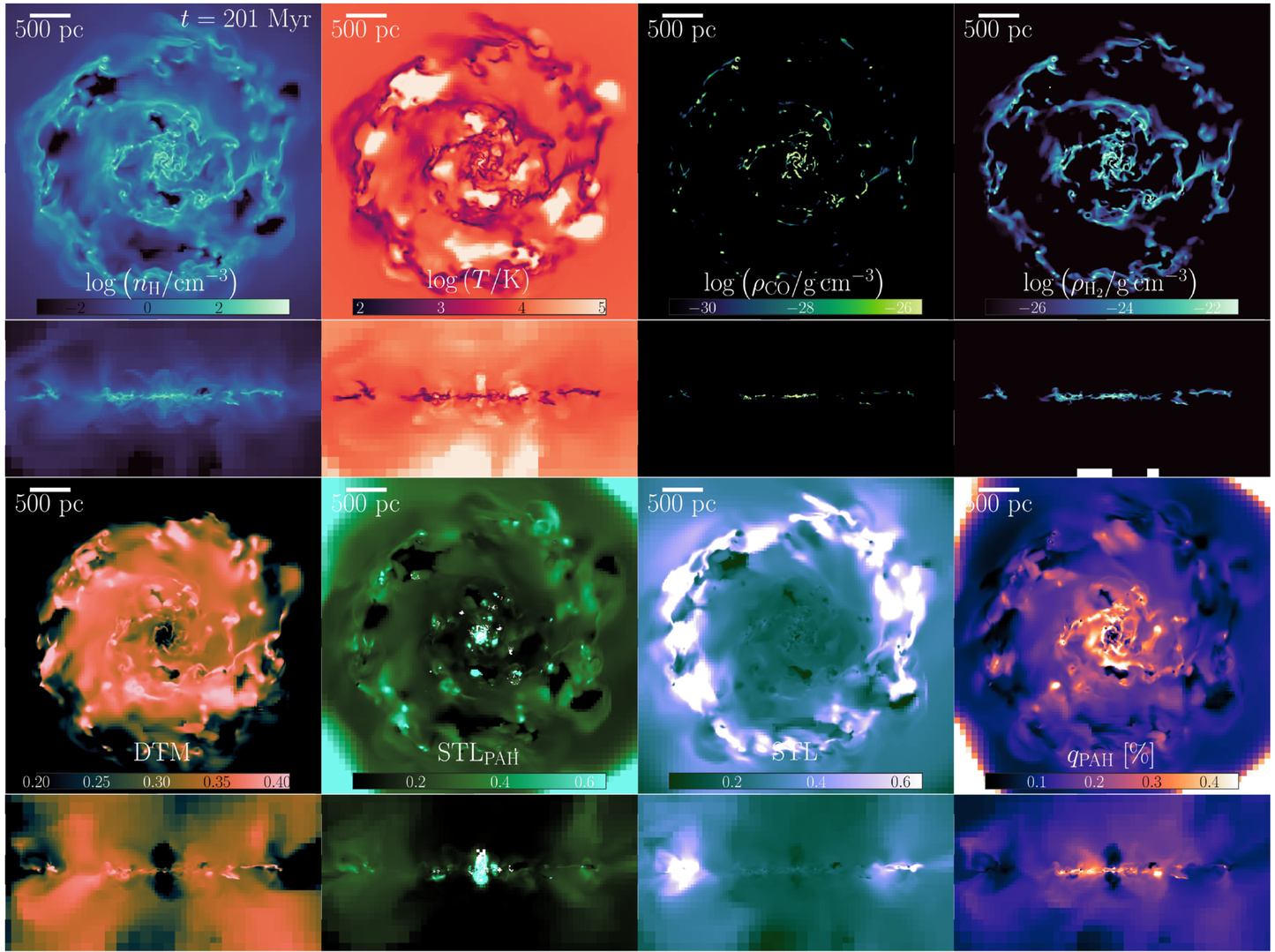
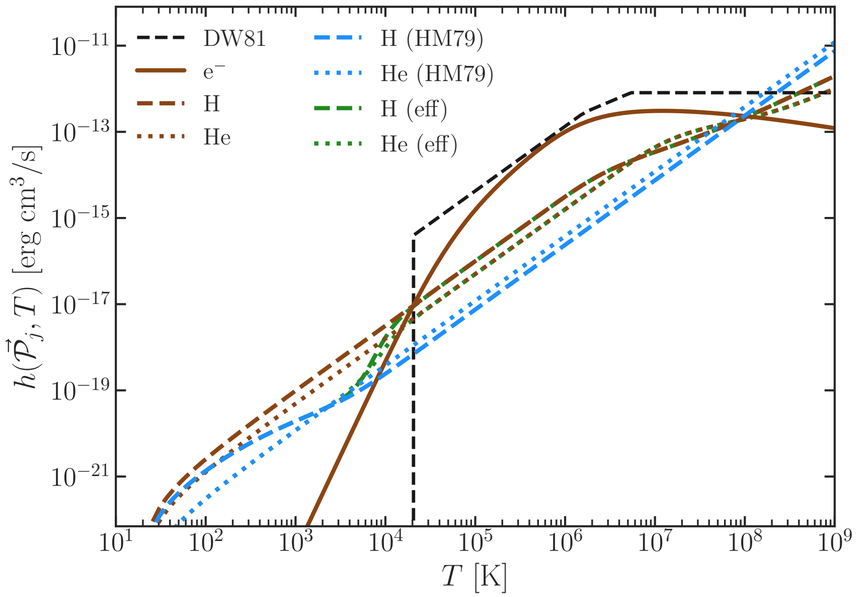


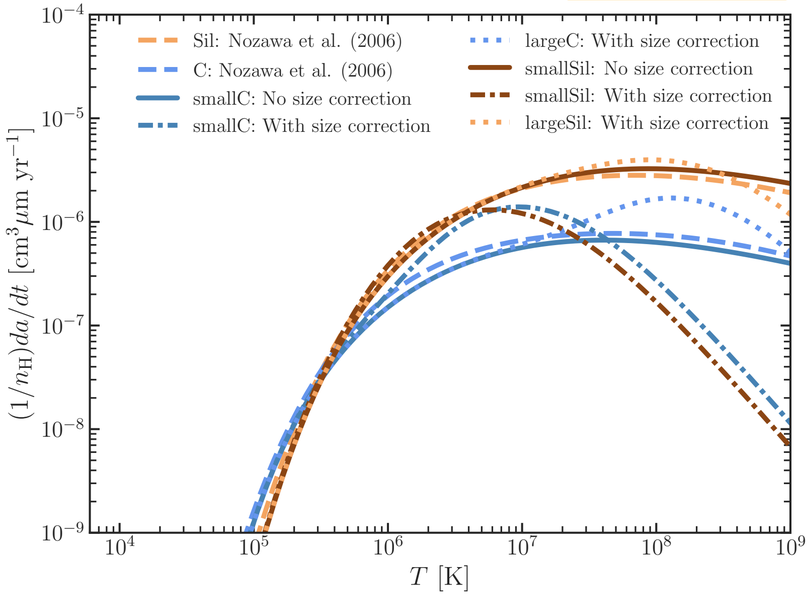
CALIMA

Flexible and self-consistent dust thermo-chemistry

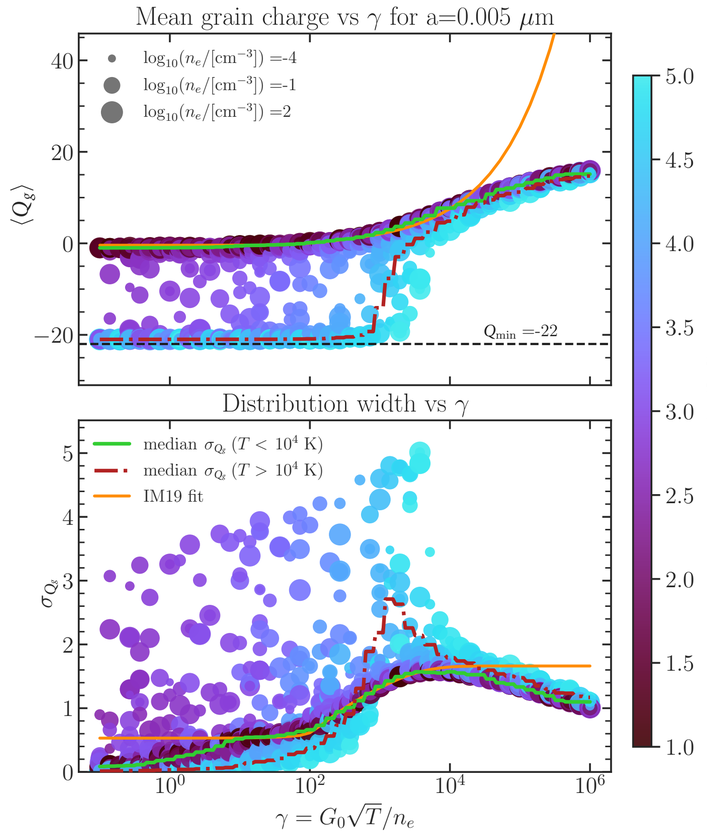
Collisional cooling



Sputtering



Grain charging

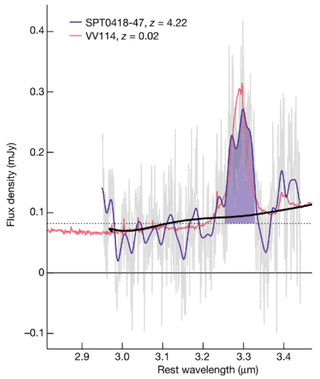


- Update ion interactions (~40 yr old)
- Grain charging directly related to local RF
- Variable molecular hydrogen formation
- Grain-assisted recombination
- Local extinction properties

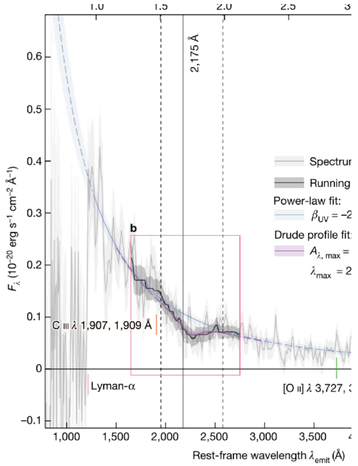
CALIMA

PAHs as the molecular regime of the dusty ISM

Spilker+2023



Witstok+2023



Shivaei+2024

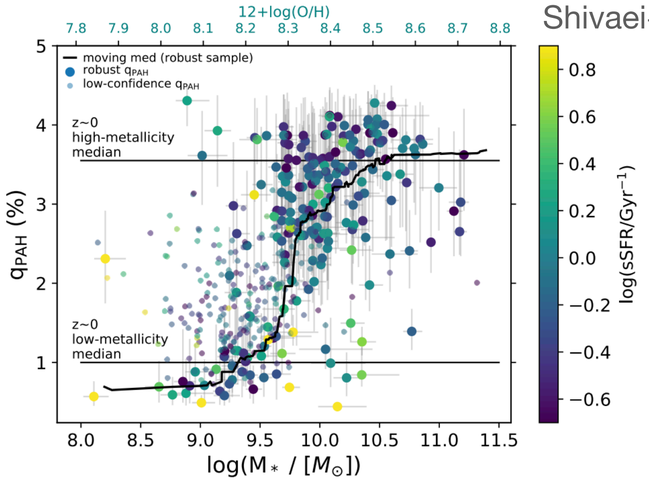
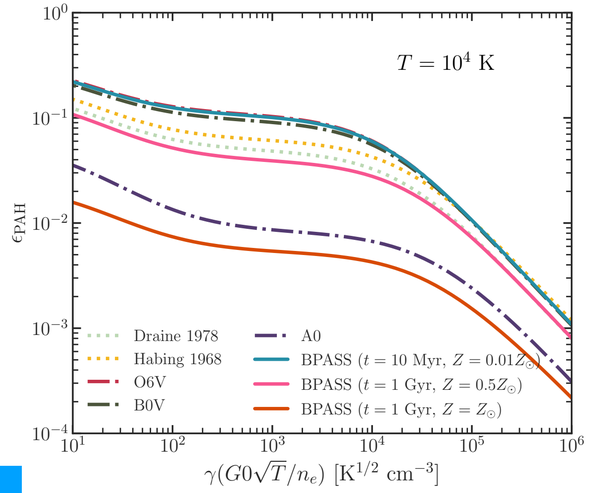
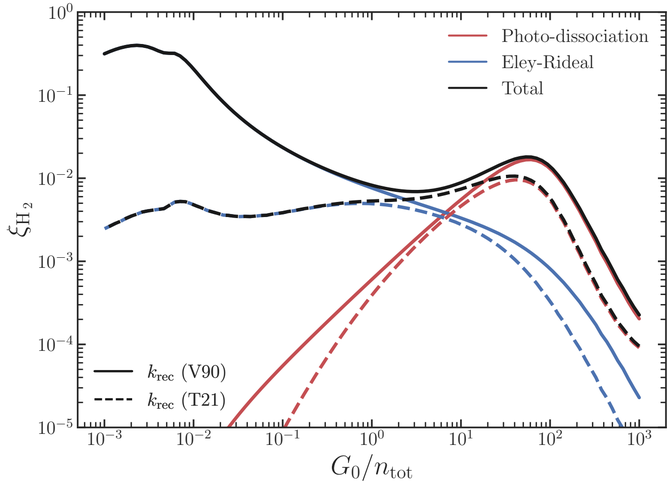


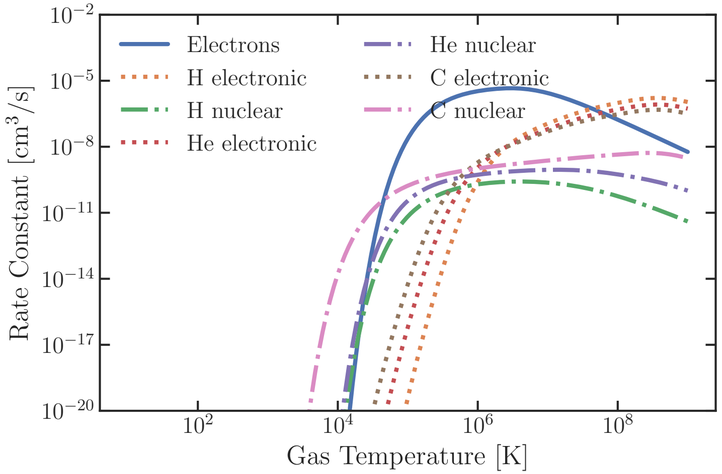
Photo-electric heating



H_2 formation

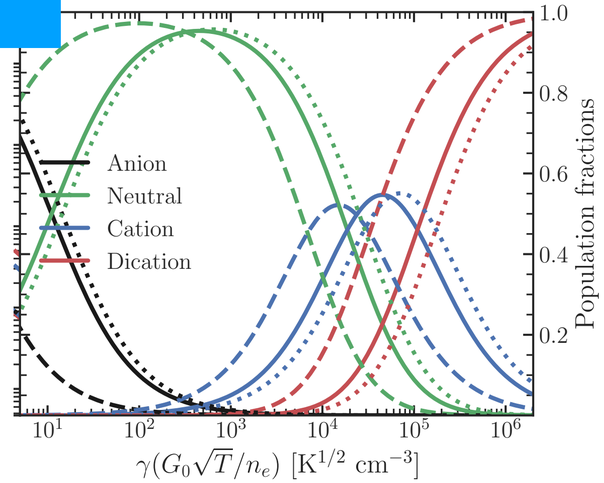


Sputtering



PAH bottom-up formation

Omont+2025

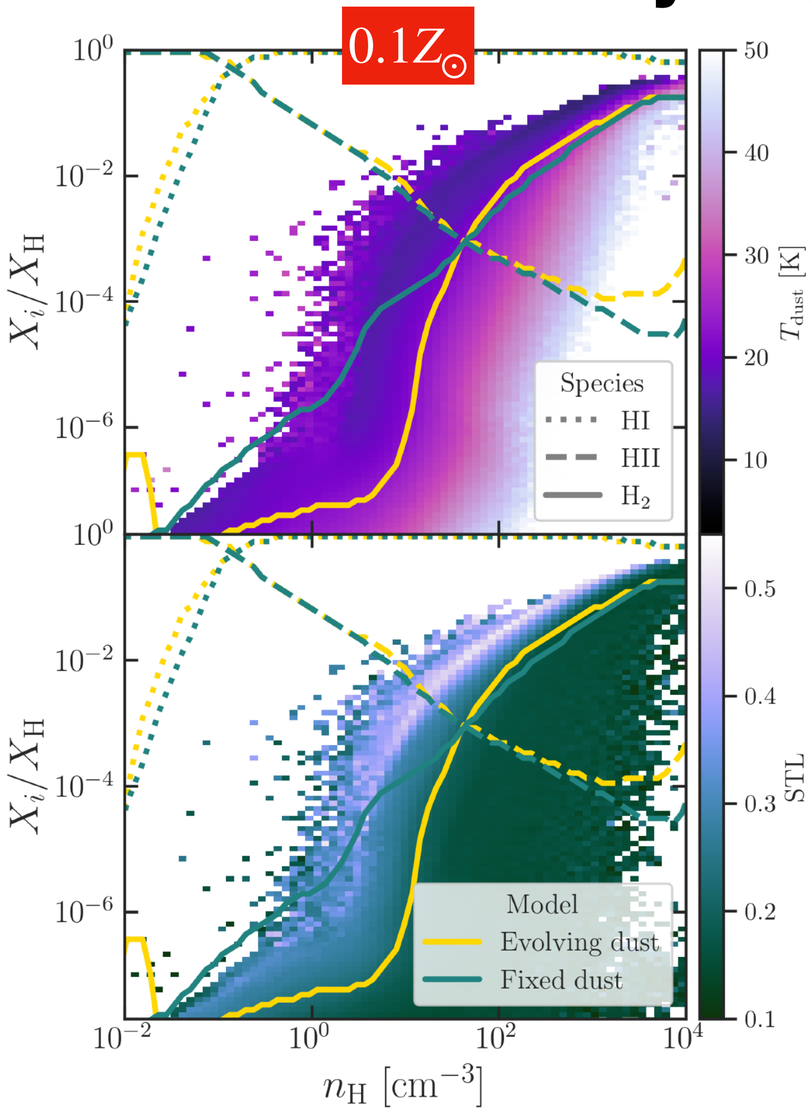


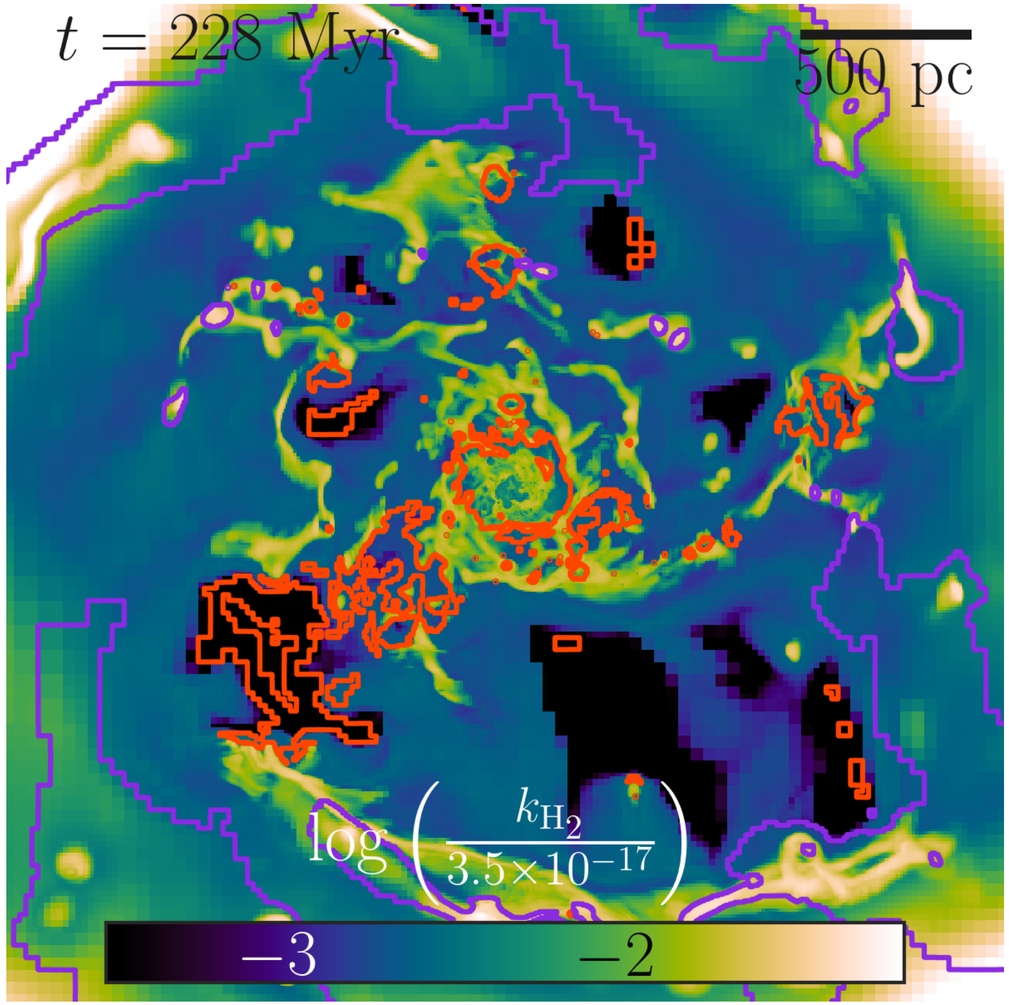
CALIMA

The role of dust in molecular hydrogen and CO formation

Dust temperature

Small-to-large mass ratio





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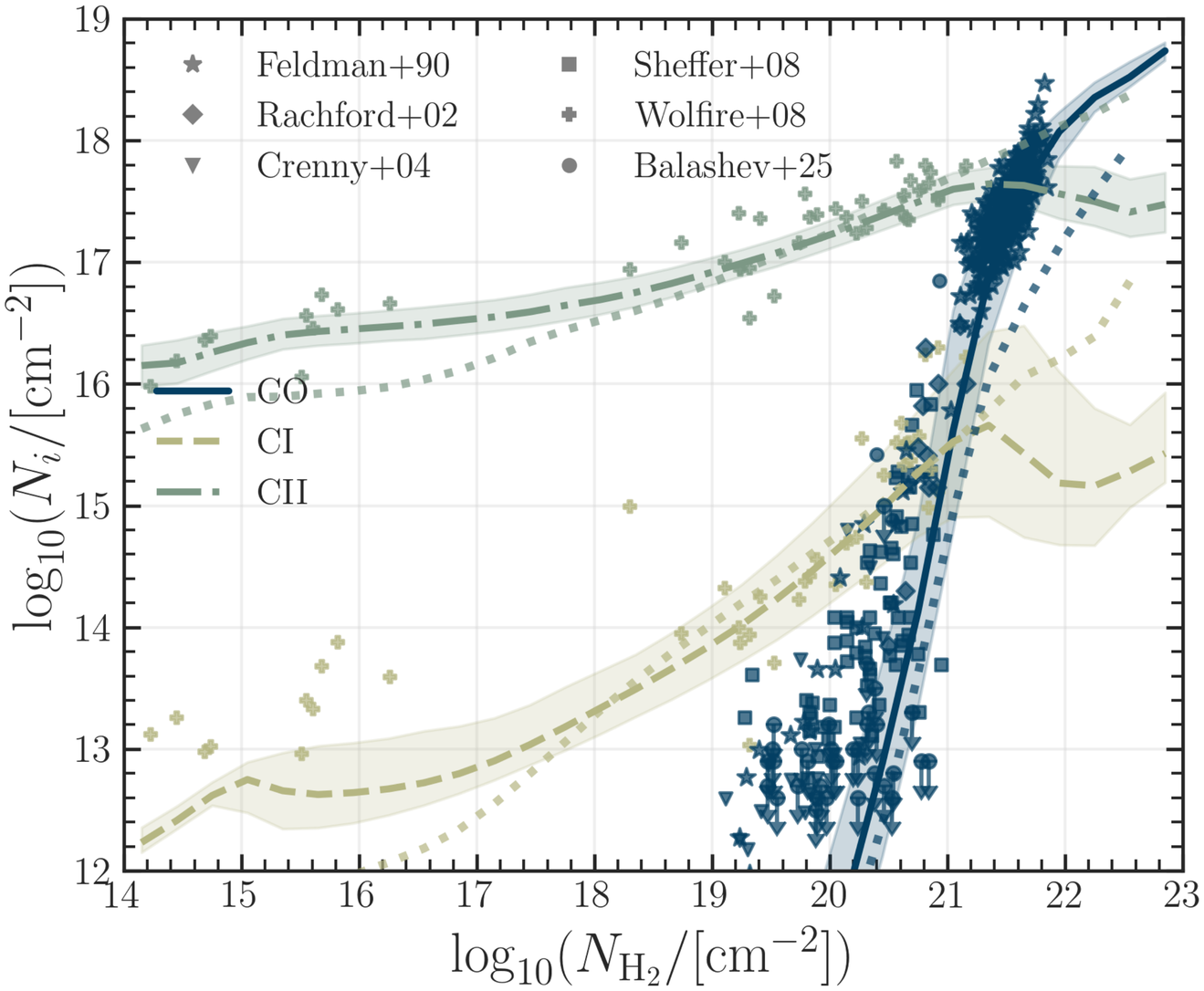

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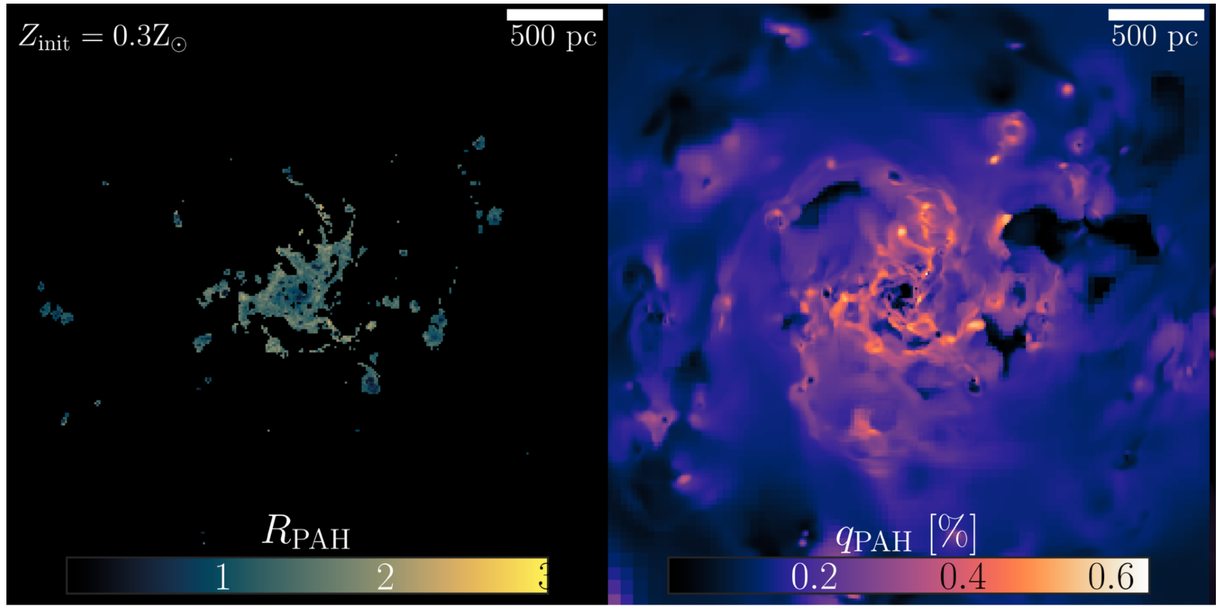
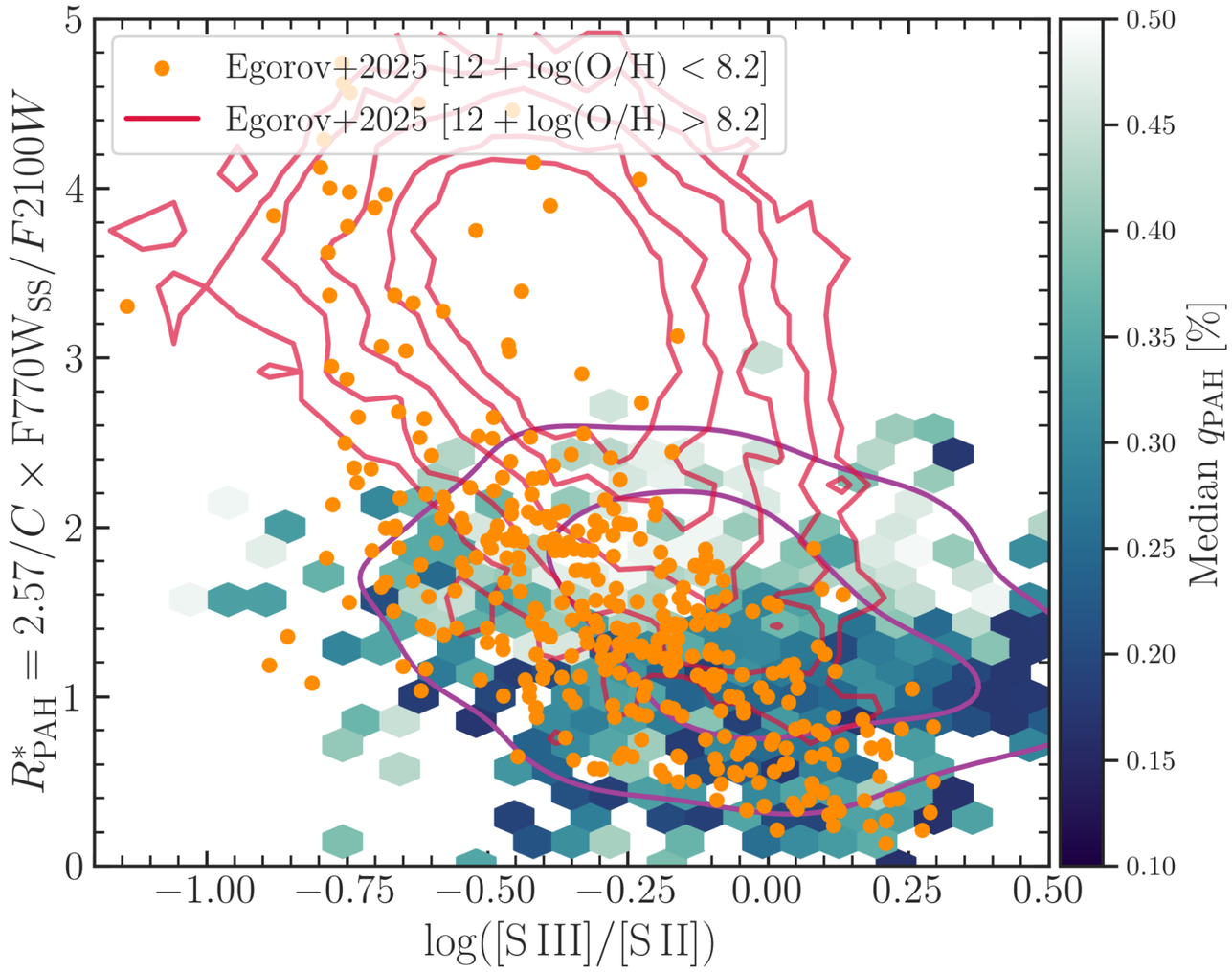
The destruction of PAHs within HII regions





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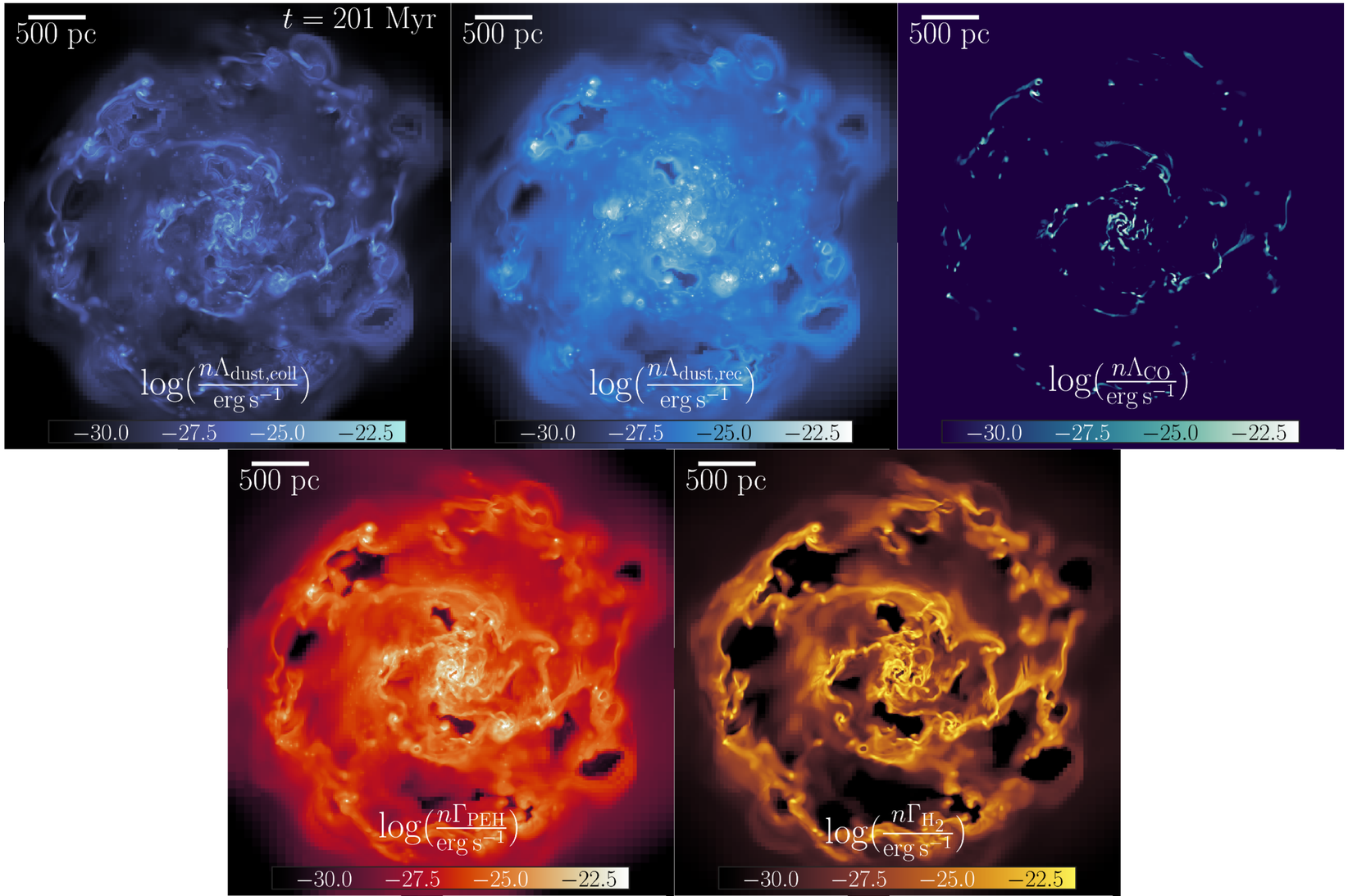
Heating and cooling in the presence of evolving dust and PAHs



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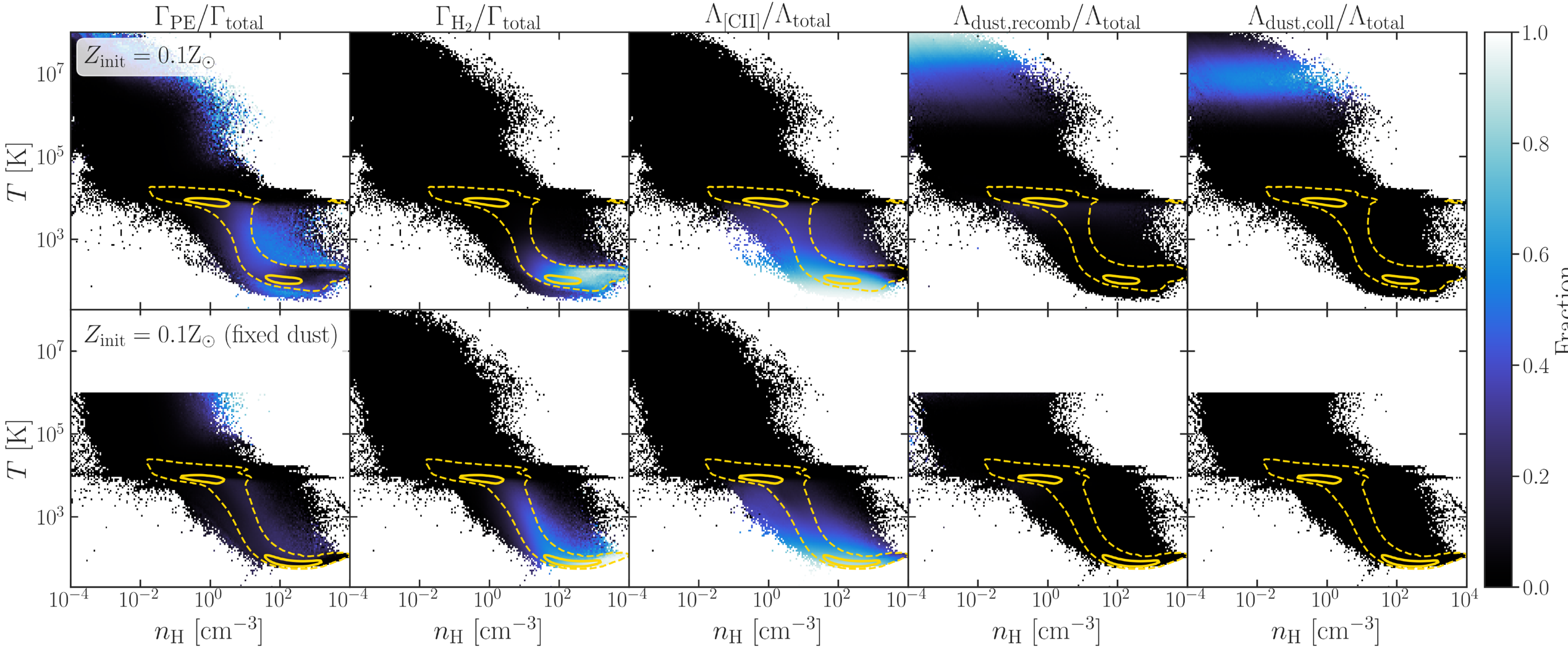

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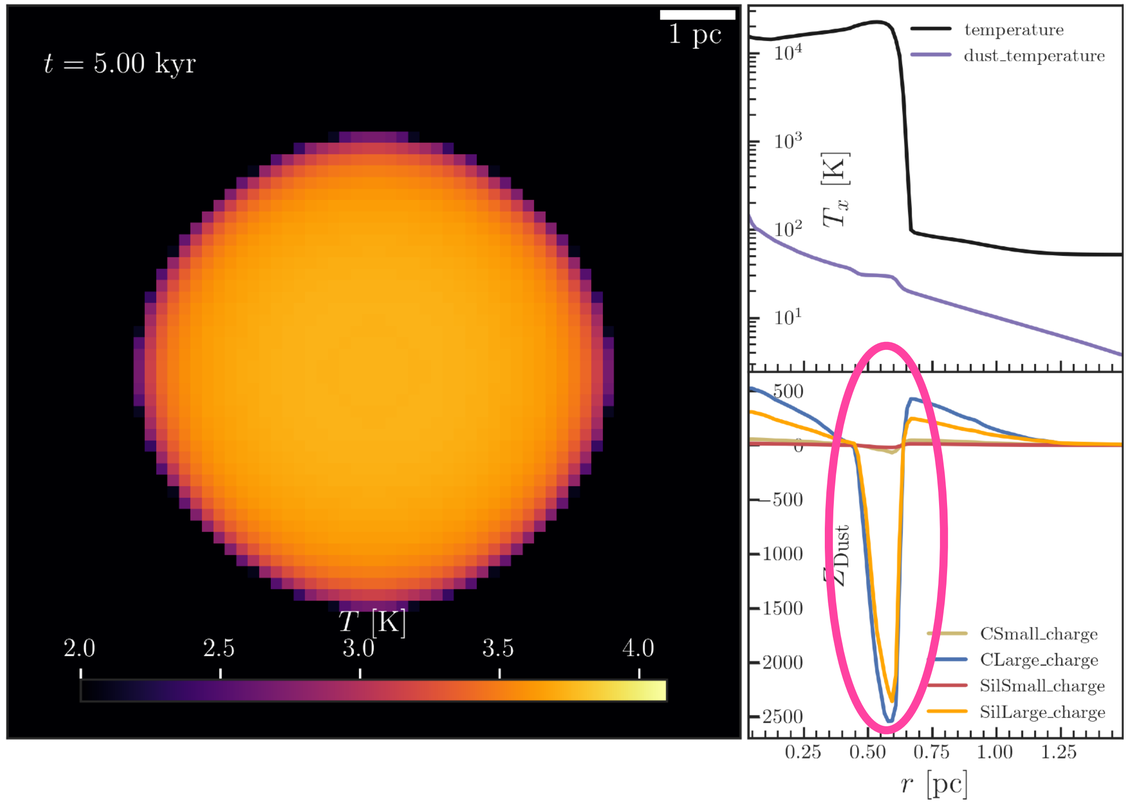
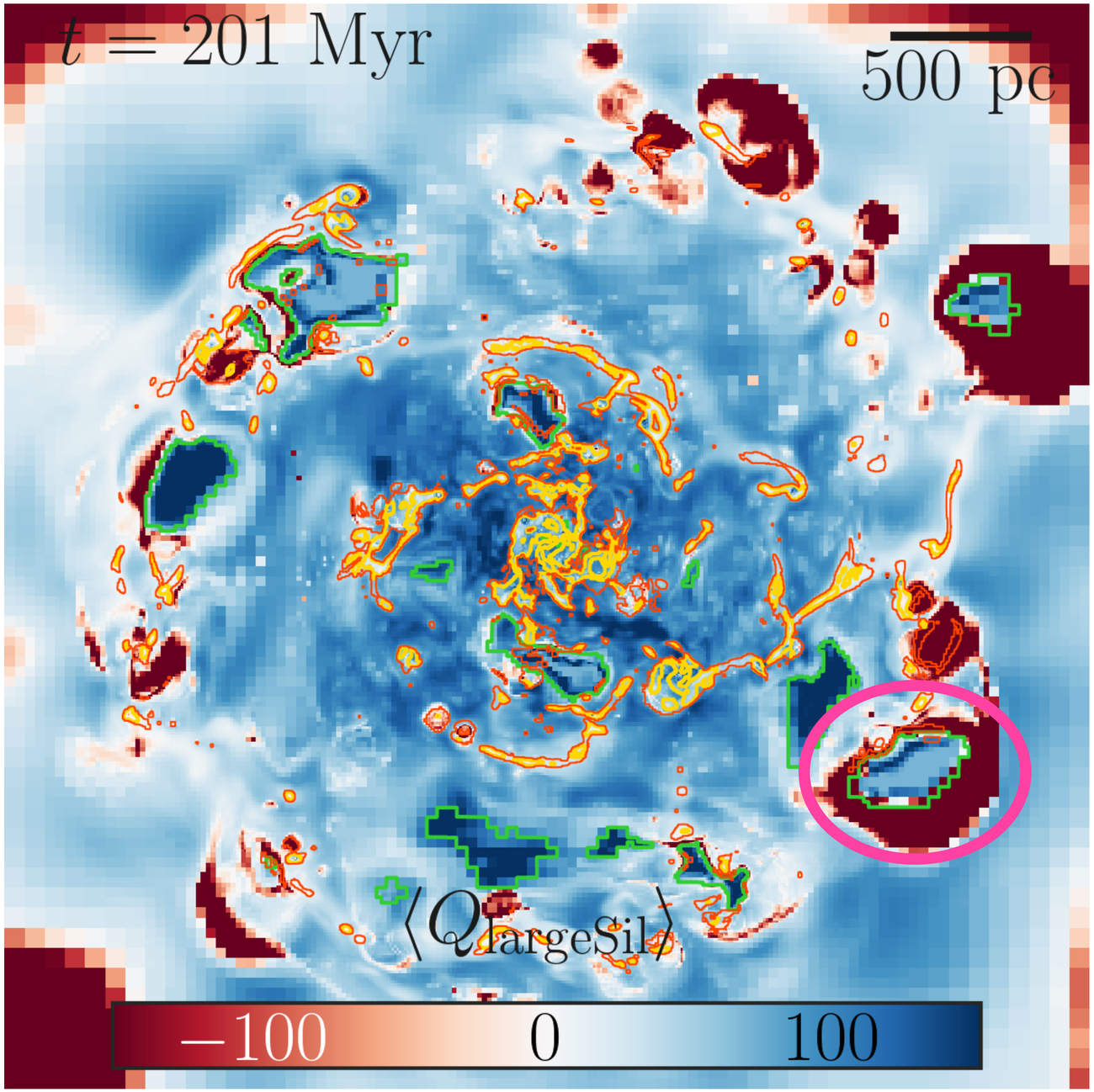
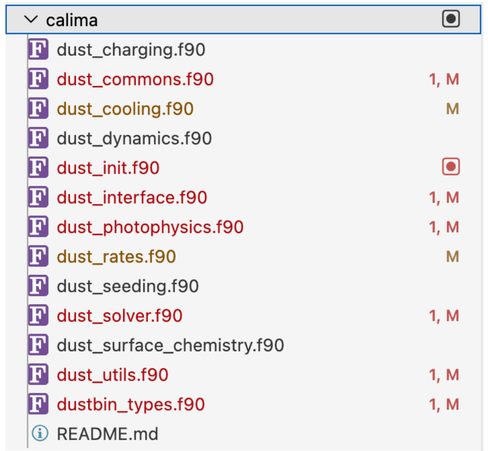




CALIMA for the RAMSES community

In the public RAMSES:



Re-designed self-contained modules, with minimal interaction points

CALIMA can now be run with:

HD/MHD

Growth, destruction and evolution of grains can be tracked, and accreted metals modify classic cooling curves (see Dubois+2024)

RT

The effect of local dust properties are directly propagated into the radiative transfer (e.g. Dusty-SPHINX)

RTZ

Full model, considers the individual ion thermochemistry to modify the full interaction of radiation, gas and dust/PAHs

CALIMA for the RAMSES community

README

pyCALIMA

pyCALIMA is a research codebase for modeling dust and PAH microphysics used in RAMSES simulations. It combines grain-size distributions, radiation, charging, sputtering, collisional cooling, and PAH-specific photophysics into reusable Python modules plus export scripts that generate simulation-ready tables.

Related References

- RAMSES repository: https://github.com/ramses-organisation/ramses
- CALIMA model paper: https://ui.adsabs.harvard.edu/abs/2026arXiv260221790R/abstract

The new version moves away from fixed number of bins and grain compositions

pyCALIMA allows for easy computation od run-time tables for many more compositions:

Olivine, metallic Iron, Pyrrhotite, Fayalite, Troilite, Enstatite, Quartz, Forsterite, Silicon Carbide, Alumina, etc.

This is all coupled to fast (numba powered) dust chemistry solvers to post-processed simulations and get a 0th-order approximation for the local grain size distribution

Talk to me if you'd like access to the repo!

Conclusions

- Many questions remains as to the evolution of dust in the early Universe
- CALIMA provide the framework to explore the evolution of the ISM across cosmic time from first principles
- Live dust modelling results in non-trivial interactions with radiation, the molecular ISM and the thermochemistry
- CALIMA is now a portable theoretical framework that can be used in many versions of future RAMSES simulations as well as in post-processing

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THANK YOU

Curro Rodríguez Montero - RUM2026

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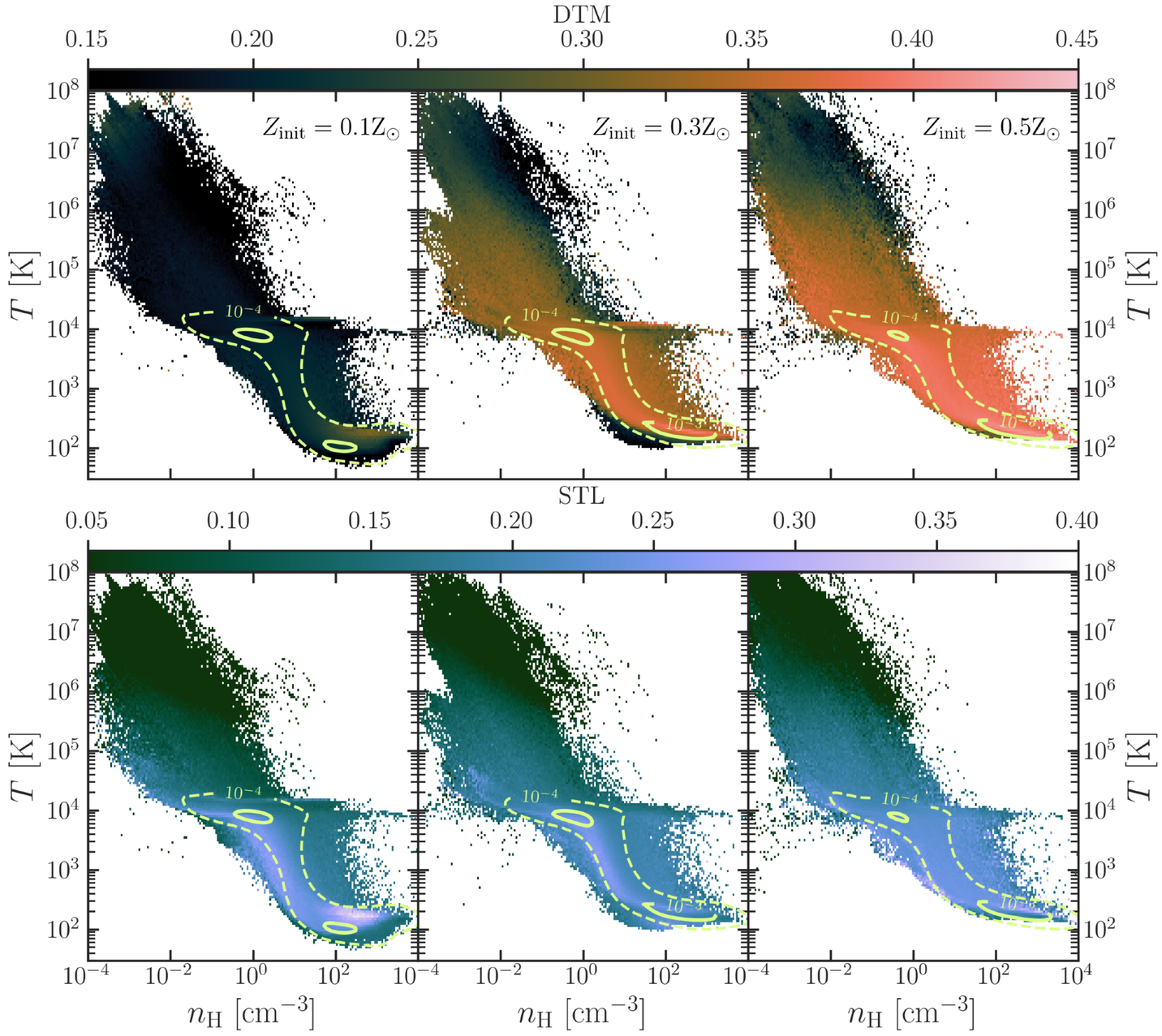
The dust content of different phases of the ISM



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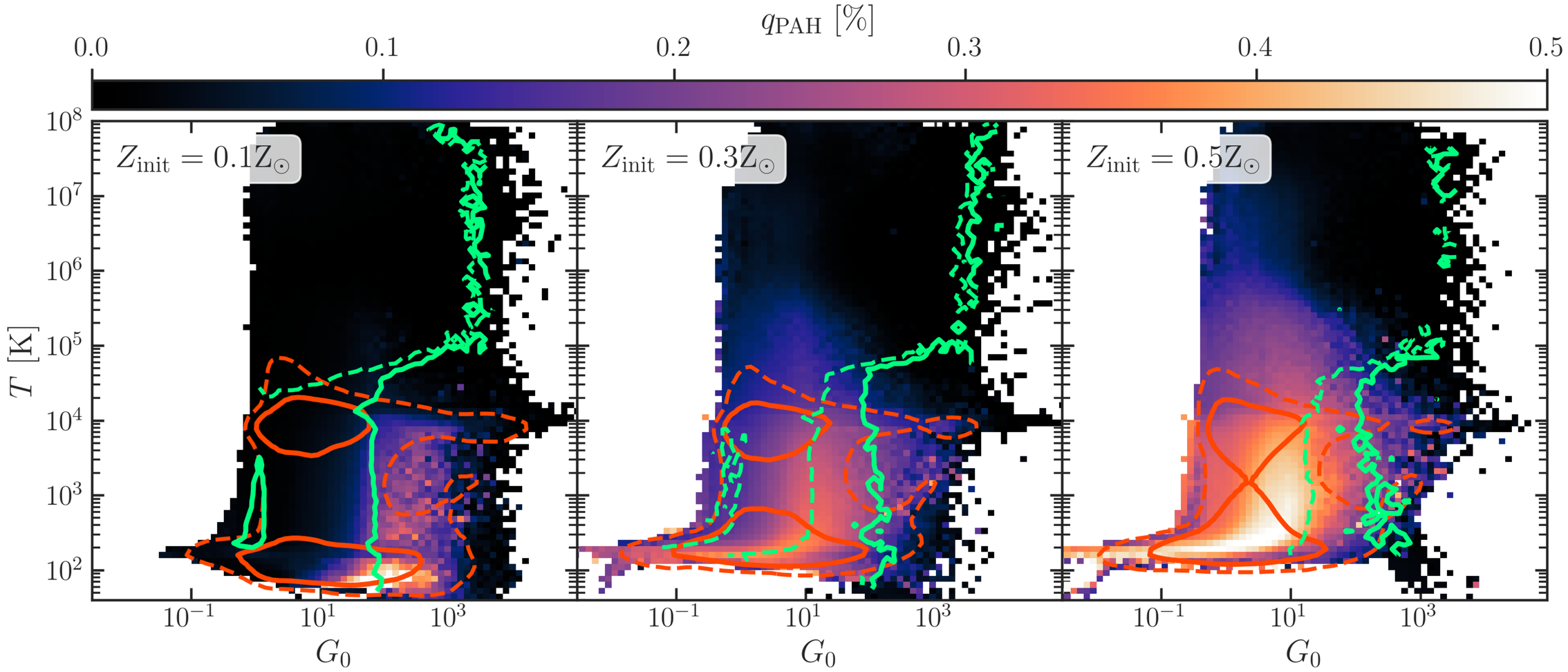

CALIMA

The influence of dust modelling on the thermochemistry of the ISM