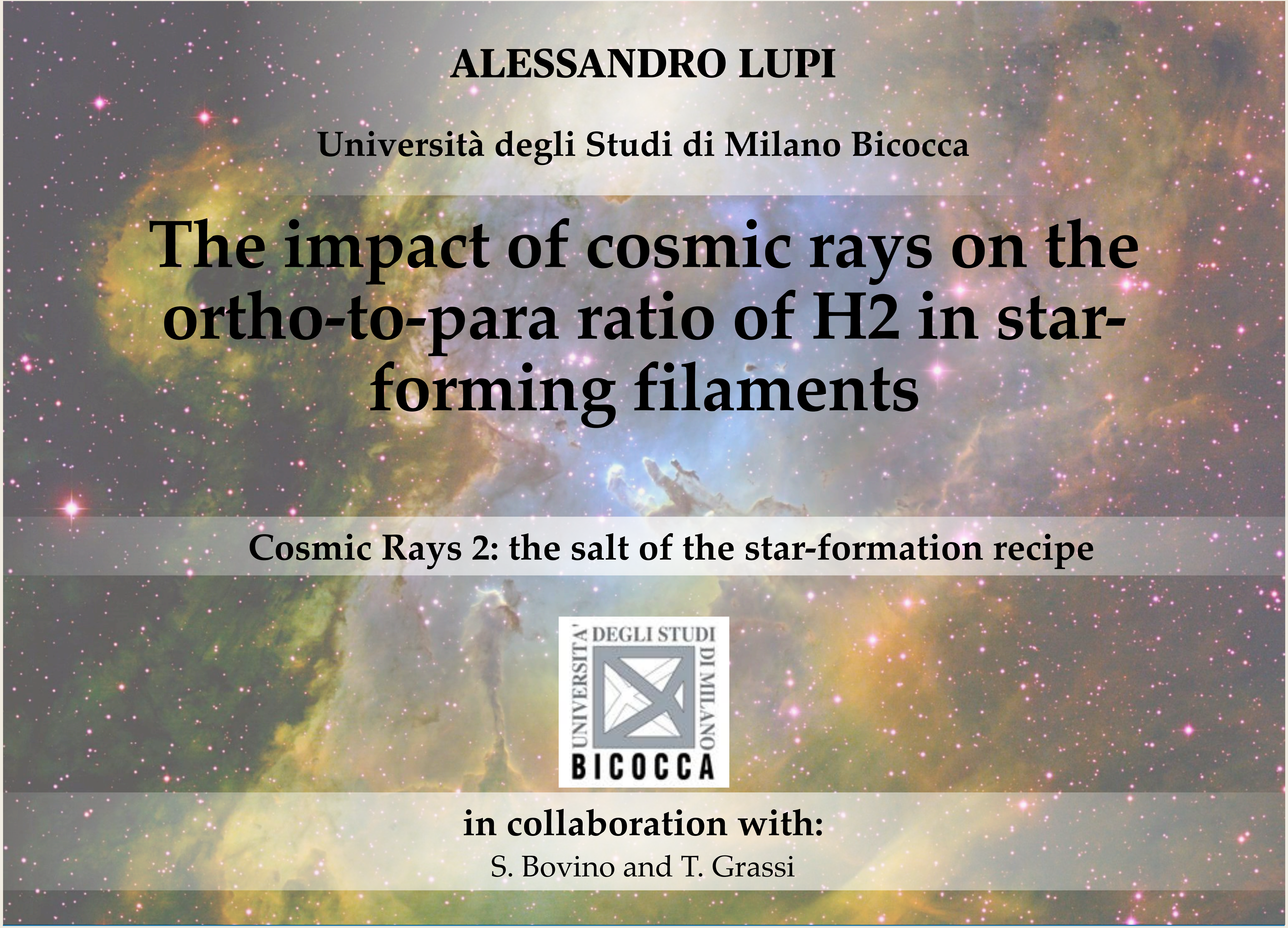

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The impact of cosmic rays on the ortho-to-para ratio of H2 in star-forming filaments

Cosmic Rays 2: the salt of the star-formation recipe

in collaboration with:
S. Bovino and T. Grassi

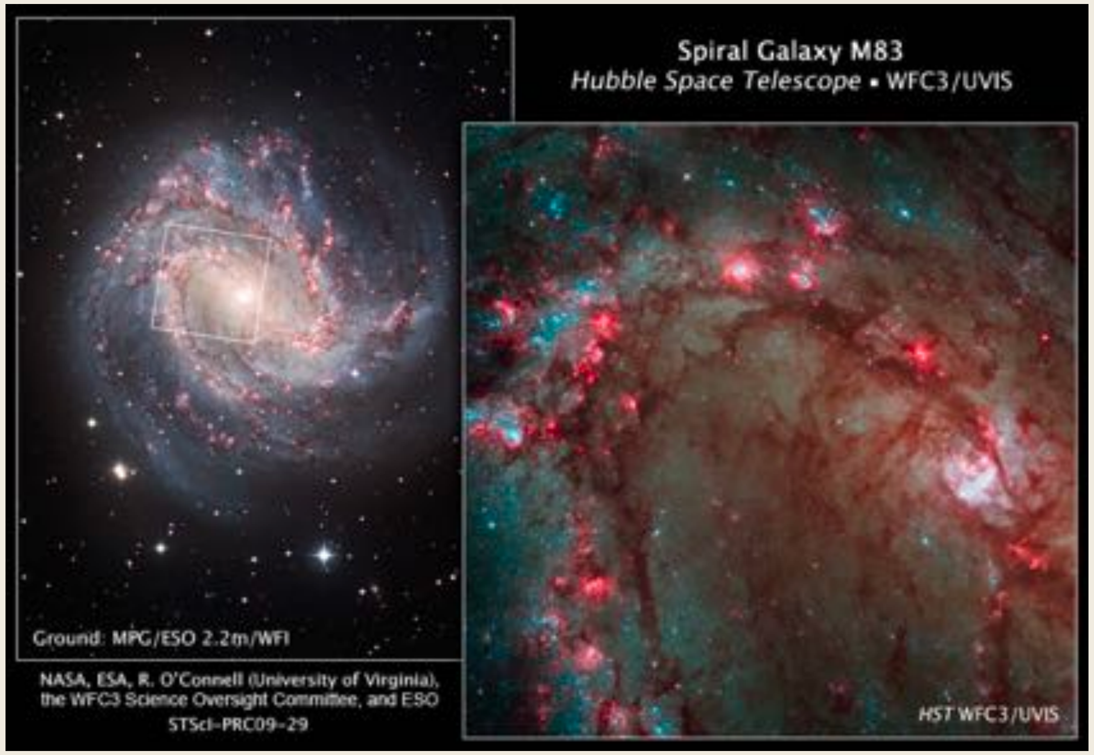
Florence (Italy)

November 8th, 2022

Introduction

Star formation commonly occurs in molecular clouds, dense and cold regions forming out of the interstellar medium of galaxies

Credit: NASA



While a general agreement has been reached on the typical properties of MCs

$$\mathscr{M} \gg 1,\ n_{\mathrm{H_{tot}}} \gtrsim 100\,\mathrm{cm^{-3}},\ T \ll 100\,\mathrm{K},\ \alpha_{\mathrm{vir}} \sim 1-2$$

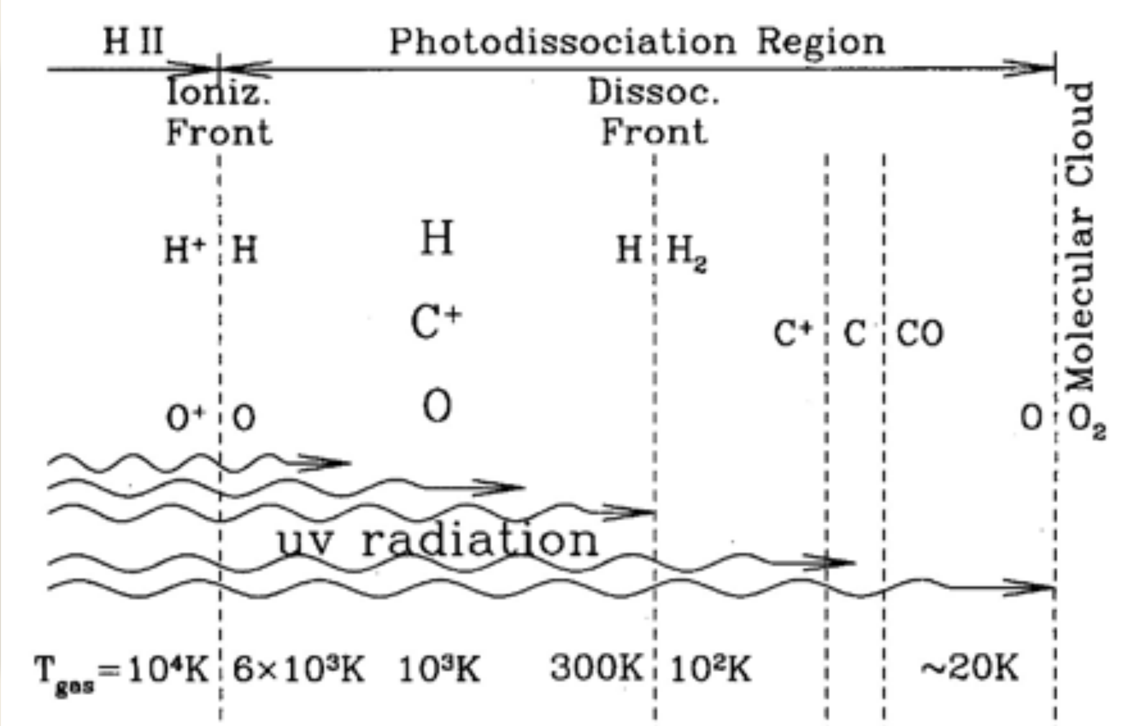
no clear consensus exists about the initial chemical conditions in filaments and cores.

In particular, the evolution of the ortho- and para- states of H_2 has crucial implications on the deuteration process, which affects the reliability of chemical clocks based on deuterated species (see, e.g. Bovino, Ferrada-Chamorro, Lupi et al. 2019, Bovino, Lupi, et al. 2021).

Theoretical modelling for molecular clouds

Standard approach:

- Isothermal equation of state (or strongly simplified analytic cooling function)
- Chemical modelling in post-processing, with no feedback on the gas dynamics (see Ferrada-Chamorro et al. 2021 for a discussion)
- Constant CRIR



Self-consistent approach:

- Non-equilibrium chemistry on-the-fly (for every resolution element, at each time-step), including at least 37 species (Grassi et al. 2017): $H, H^+, He, He^+, He^{++}, H_2, H_2^+, H^-, C^+, C, O^+, O, OH, HOC^+, HCO^+, CO, CH, CH_2, C_2, HCO, H_2O, O_2, H_3^+, CH^+, CH_2^+, CO^+, CH_3^+, OH^+, H_2O^+, H_3O^+, O_2^+, C^-, O^-, e^-$, plus G, G^-, G^+ (neutral and charged grains) => (more than 350 reactions, **including CR-induced ones**)
- Radiative cooling fully-dependent on the thermodynamic and chemical state of the gas, accounting for dust cooling, metal line cooling (CI, CII, OI), CO rotational cooling, chemical cooling and heating, H_2 roto-vibrational cooling, Compton cooling, continuum cooling, photoheating, **CR-induced heating**, photoelectric heating.

Modelling the H_2 ortho- and para- evolution

We need isomer-dependent chemistry (Sipilä et al, 2015, Bovino et al. 2019). In particular:

- H_2 formation (H^- and on dust grains), with initial OPR = 3
- H_2 ortho-to-para and para-to-ortho conversion in gas phase (collisions with H^+ and H_3^+)
- H_2 dissociation by stellar radiation (Draine flux plus shielding)

And possibly:

- H_2 ortho-to-para and para-to-ortho conversion on dust (Furuya et al. 2019), expected to further accelerate the decrease in OPR.

$$k_{\mathrm{op}} = k_{\mathrm{ads}}^{\mathrm{oH_2}} \eta_{\mathrm{op}},$$
$$k_{\mathrm{po}} = k_{\mathrm{ads}}^{\mathrm{pH_2}} \eta_{\mathrm{po}},$$

$$\eta_{\mathrm{op}} = \frac{t_{\mathrm{des}}}{t_{\mathrm{des}} + \tau_{\mathrm{conv}}} \frac{1}{1+\gamma},$$
$$\eta_{\mathrm{po}} = \frac{t_{\mathrm{des}}}{t_{\mathrm{des}} + \tau_{\mathrm{conv}}} \frac{\gamma}{1+\gamma},$$

$$\tau_{\mathrm{conv}} = 6.3 \times 10^4 T_{\mathrm{dust}}^{-1.9}\ \mathrm{s}$$
$$\gamma = 9 \exp(-170.5/T_{\mathrm{dust}})$$

τ_{des} is the effective desorption time-scale (thermally-driven)

Given the typically low value of T_{dust}, $\gamma \approx 0$ (Bovino et al. 2017).

Where do CRs enter here?

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$$k_{op} = k_{ads}^{oH_2} \eta_{op},$$
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$$\eta_{op} = \frac{t_{des}}{t_{des} + \tau_{conv}} \frac{1}{1+\gamma},$$
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Where do CRs enter here?

Modelling the H_2 ortho- and para- evolution

CR-induced reactions are typically modelled assuming a constant ionisation rate, and exploring different values.

However, CRs are attenuated as they penetrate deeper into MCs and filaments, and a self-consistent modelling should account for this attenuation (see David Neufeld's talk).

In **Lupi, Bovino & Grassi (2021)**, we considered an approximate model with a column density-dependent CRIR (Padovani et al. 2018):

$$\zeta_{H_2} = \zeta_{H_2,p} + \zeta_{H_2,e},$$

$$\zeta_{H_2,p} = \begin{cases} 6.8\times10^{-16} N_{20}^{-0.423} & N_{\rm eff} < 10^{25}\,{\rm cm}^{-2} \\ 5.4\times10^{-18}\exp(-\Sigma_{\rm eff}/38) & \text{otherwise} \end{cases}$$

$$\zeta_{H_2,e} = \begin{cases} 1.4\times10^{-19} N_{20}^{-0.04} & N_{\rm eff} < 10^{25}\,{\rm cm}^{-2} \\ 3.3\times10^{-20}\exp(-\Sigma_{\rm eff}/71) & \text{otherwise} \end{cases}$$

$$N_{20} = N_{\rm eff}/(10^{20}\,{\rm cm}^{-2})$$

$$\Sigma_{\rm eff} = 2.36 m_{\rm H} N_{\rm eff}\,{\rm g\,cm}^{-2}$$

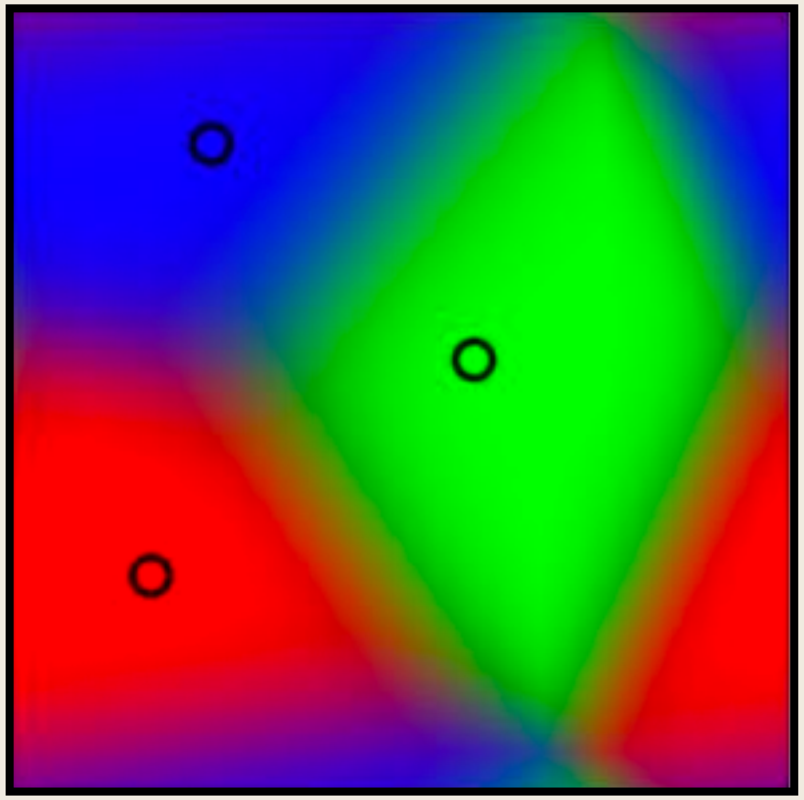
$$N_{\rm eff} \approx 1.87\times10^{21}\left(\frac{n_{\rm H_2}}{10^3}\right)^{2/3}{\rm cm}^{-2}$$

Towards a self-consistent model of the OPR evolution

(Lupi, Bovino, and Grassi 2021)

Modelling:

- **MHD + Gravity** (GIZMO; Hopkins 2015, 2016): intrinsic adaptivity and almost exact conservation of energy and angular momentum (as in SPH codes), excellent shock capturing and fluid mixing (as in grid codes)
- **Non-equilibrium chemistry and radiative cooling** (KROME, Grassi et al. 2014): reduced CO network suitable for MC studies including ortho and para H_2 states
- **Supersonic turbulence:** turbulence driving at large scales, triggering the formation of filaments (Federrath et al. 2010, Bauer & Springel 2012)



Initial conditions:

- 200 pc homogeneous box with $n_\mathrm{H} = 5\,\mathrm{cm}^{-3}$ and $T = 5000$ K (a patch of warm neutral medium filled with gas and dust), corresponding to a total mass $M_\mathrm{cloud} \sim 1.3 \times 10^6\,\mathrm{M}_\odot$.
- High mass ($m_\mathrm{gas} = 0.2\,\mathrm{M}_\odot$) and spatial (adaptive softening down to $\varepsilon = 60$ AU) resolution, to ensure that filaments can be resolved
- Initially constant magnetic field along the x axis $B_x = 3\mu$G

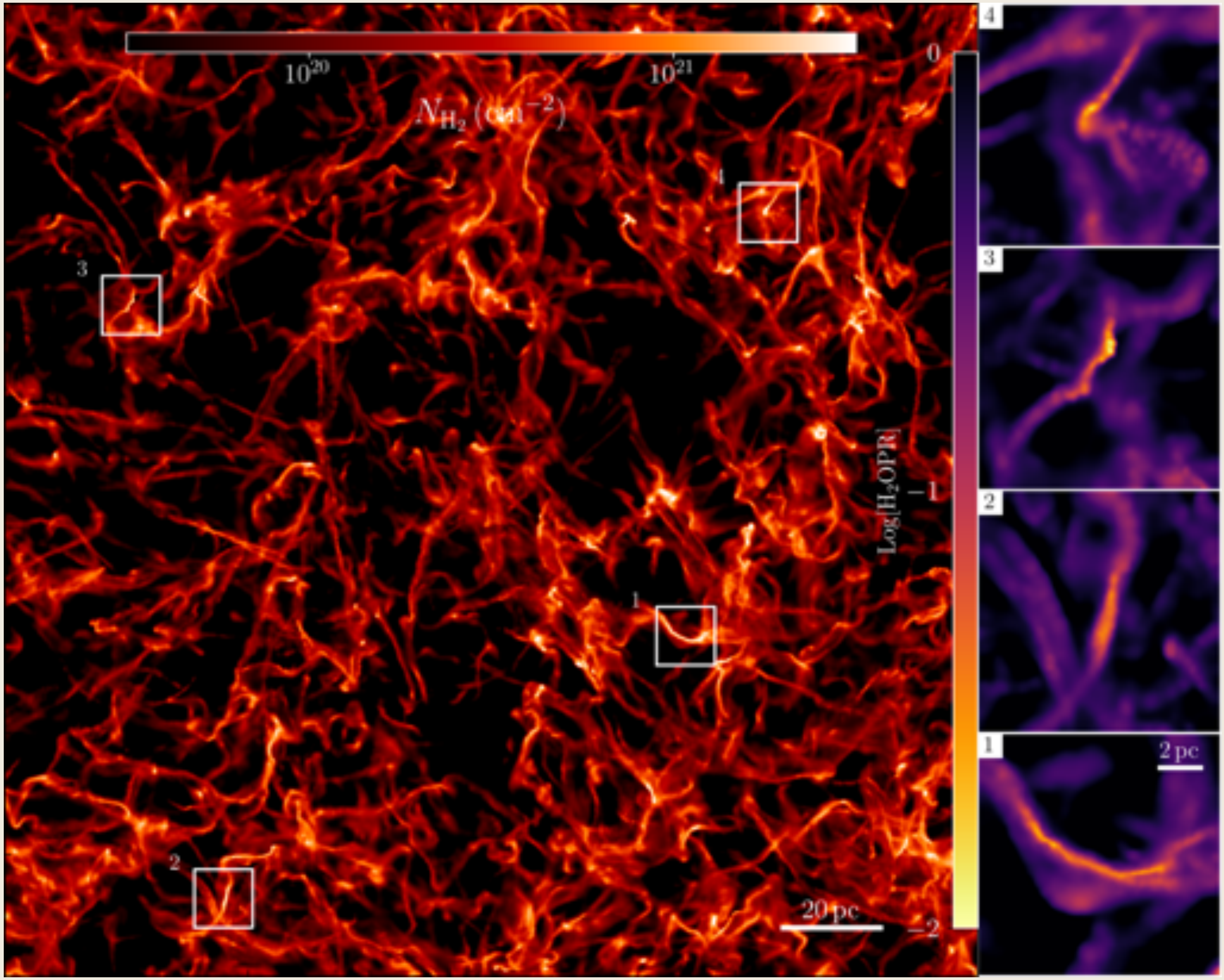
Towards a self-consistent modelling of the OPR

(Lupi, Bovino, and Grassi 2021)

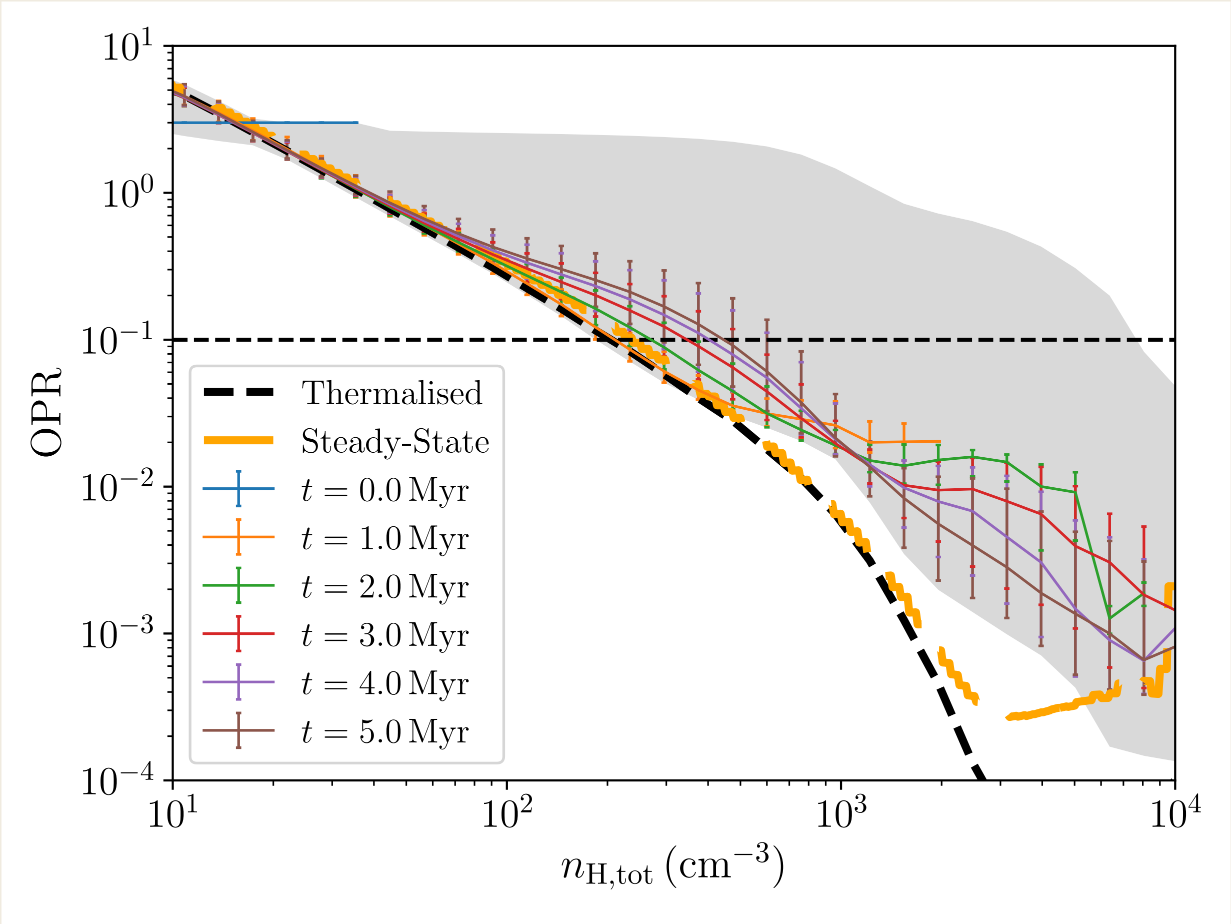
- Isothermal relaxation (50 Myr) to allow turbulence to fully develop

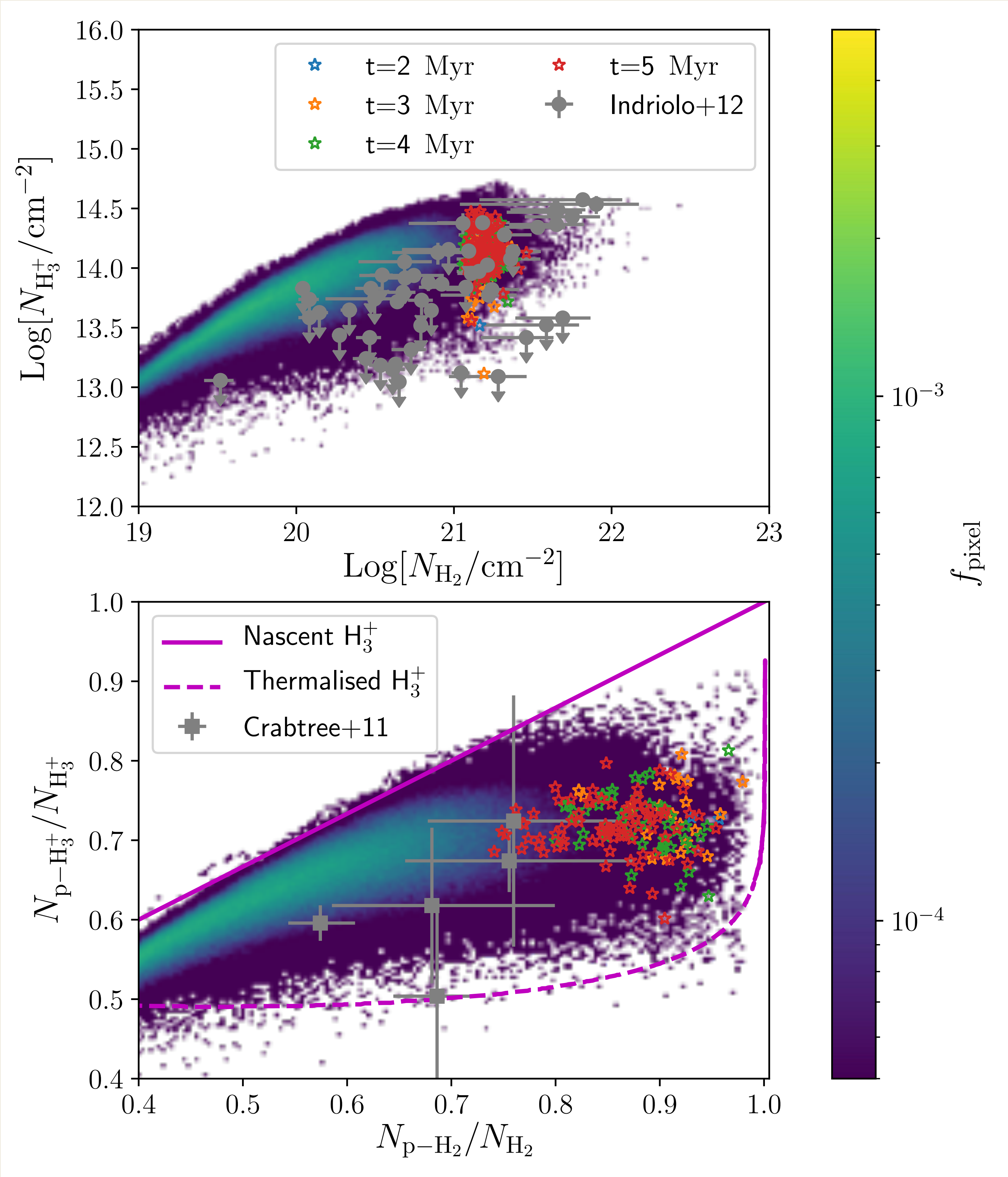
- Inclusion of self-gravity and chemistry for about 5 Myr

- Proto-filament analysis: dendrograms with minimum $N_{H_2} = 10^{21}\,\mathrm{cm}^{-2}$

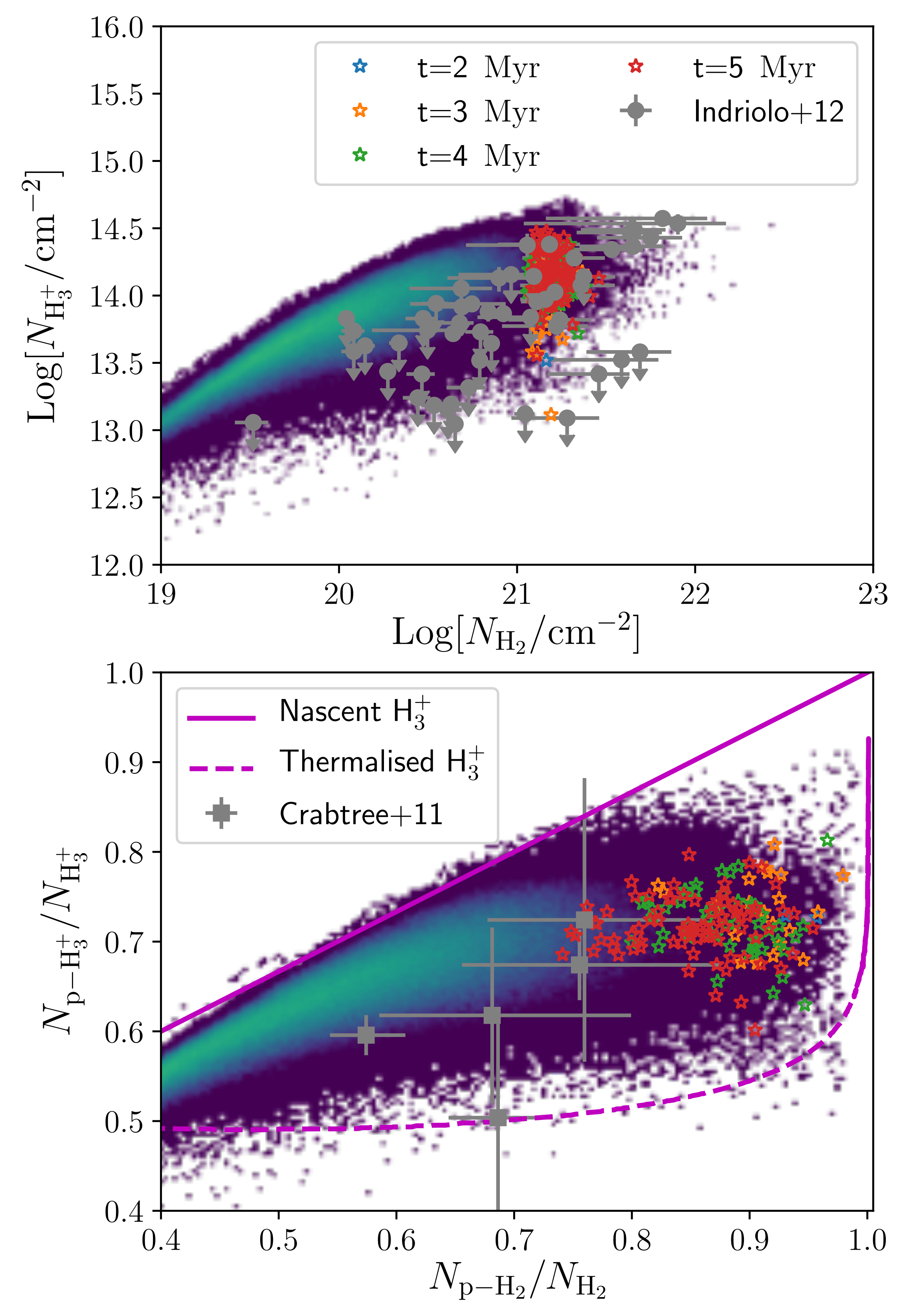


Towards a self-consistent modelling of the OPR

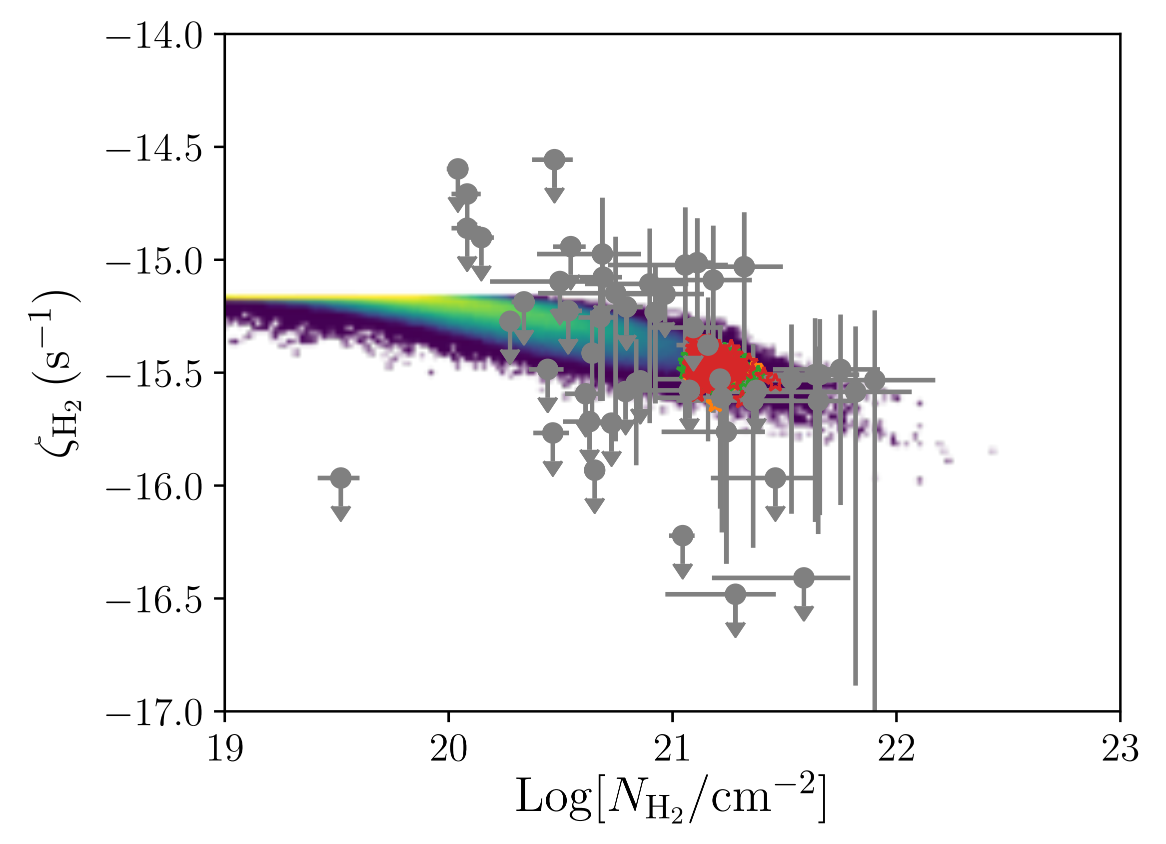




The impact of CR modelling



$$\zeta_{\mathrm{H}_2} = f(N_{\mathrm{eff}})$$



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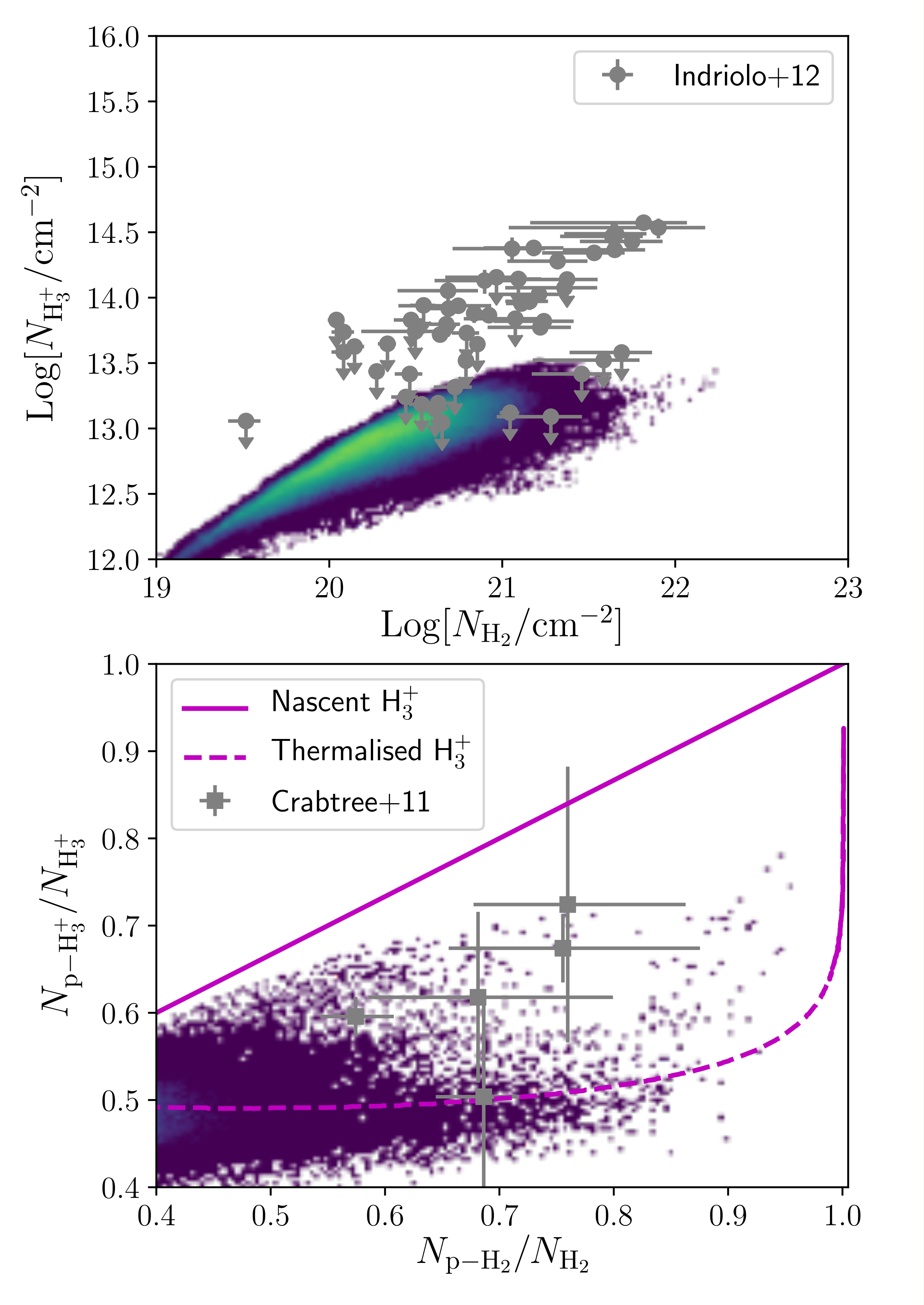
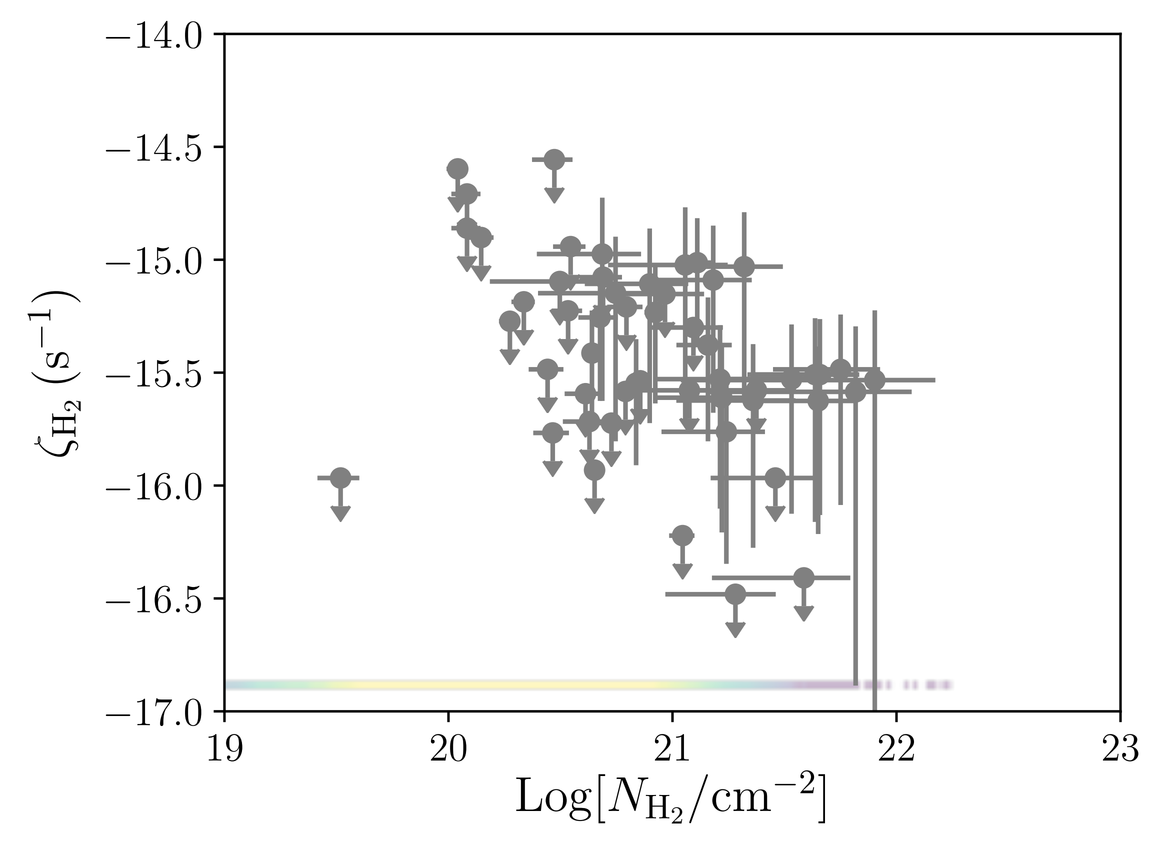


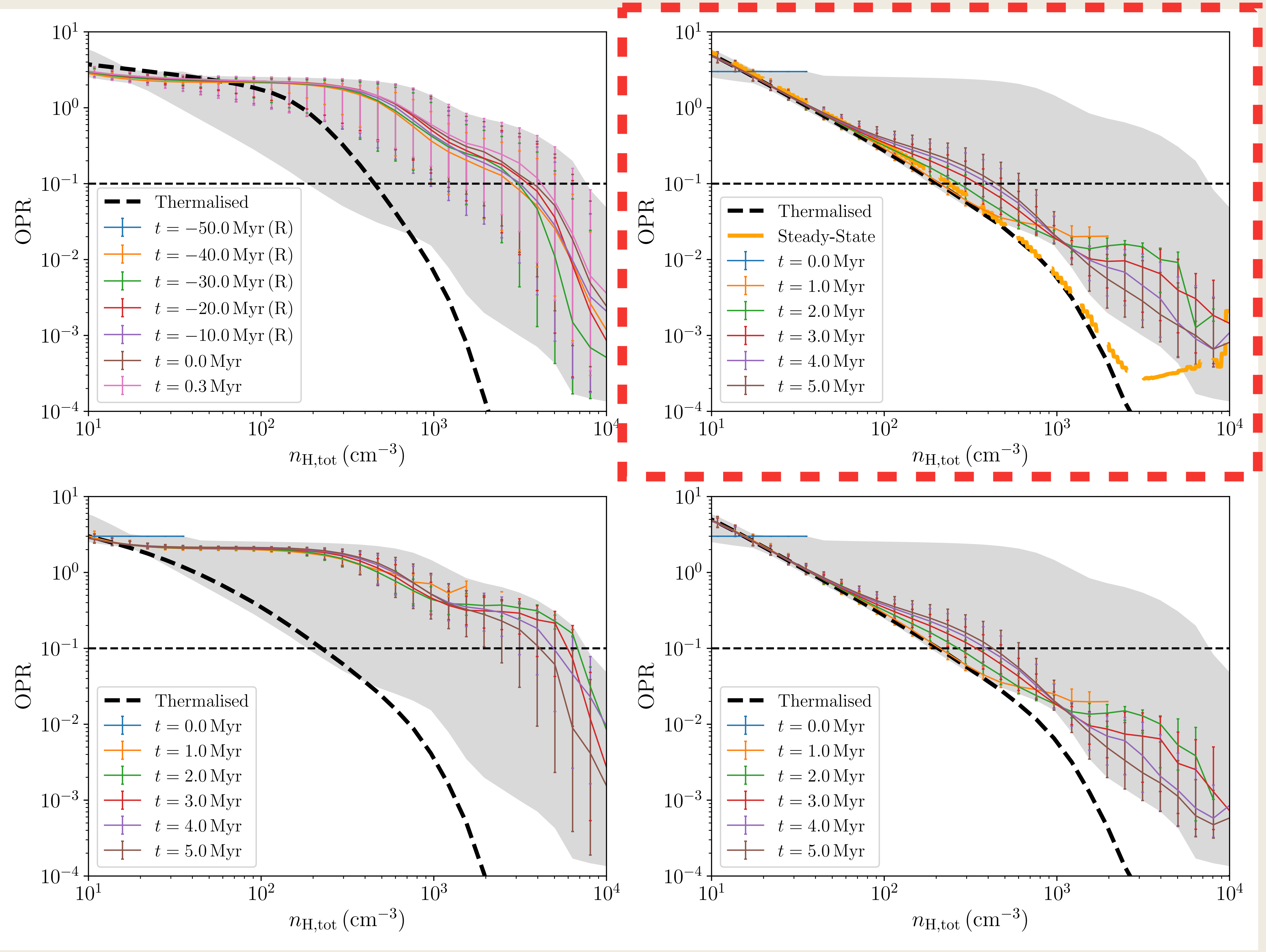


$$\zeta_{H_2} = 1.3 \times 10^{-17}\,\mathrm{s}^{-1}$$

The impact of CR modelling

$\zeta_{H_2} = 1.3 \times 10^{-17}\,s^{-1}$

$\zeta_{H_2} = f(N_{eff})$



CHEM
+
NOSG

FIDUCIAL

BASIC

FIDUCIAL
+
O/P on dust

Conclusions

We performed state-of-the-art 3D MHD simulations of molecular cloud formation, including on-the-fly non-equilibrium chemistry with self-consistent modelling of ortho- and para- H_2.

We also considered an effective model for CR attenuation, instead of a constant CRIR commonly employed.

- The H_2 OPR is mainly a function of gas density, not being significantly affected by time evolution
- The H_2 OPR reaches very low values (<< 0.01) already at moderate densities ($n_{\mathrm{H_{tot}}} \gtrsim 10^3\,\mathrm{cm}^{-3}$) typical of proto-filaments, and a more physically motivated CRIR model helps reducing the OPR below 0.1 already around $n_{\mathrm{H_{tot}}} \sim 10^2\,\mathrm{cm}^{-3}$
- The CRIR in proto-filaments must be high to match observations of diffuse clouds, consistently with observationally-inferred values
- Ortho-to-para and para-to-ortho conversion on dust grains has a moderate effect, and only at high densities

What next?

- Increasing resolution to probe higher column densities and start resolving fragmentation in filaments
- Adding a more physically motivated turbulence driving via supernovae (e.g. Padoan et al. 2016) and non-ideal MHD
- Adding stellar feedback during the proto-stellar and main sequence phase (radiation, jets, winds)