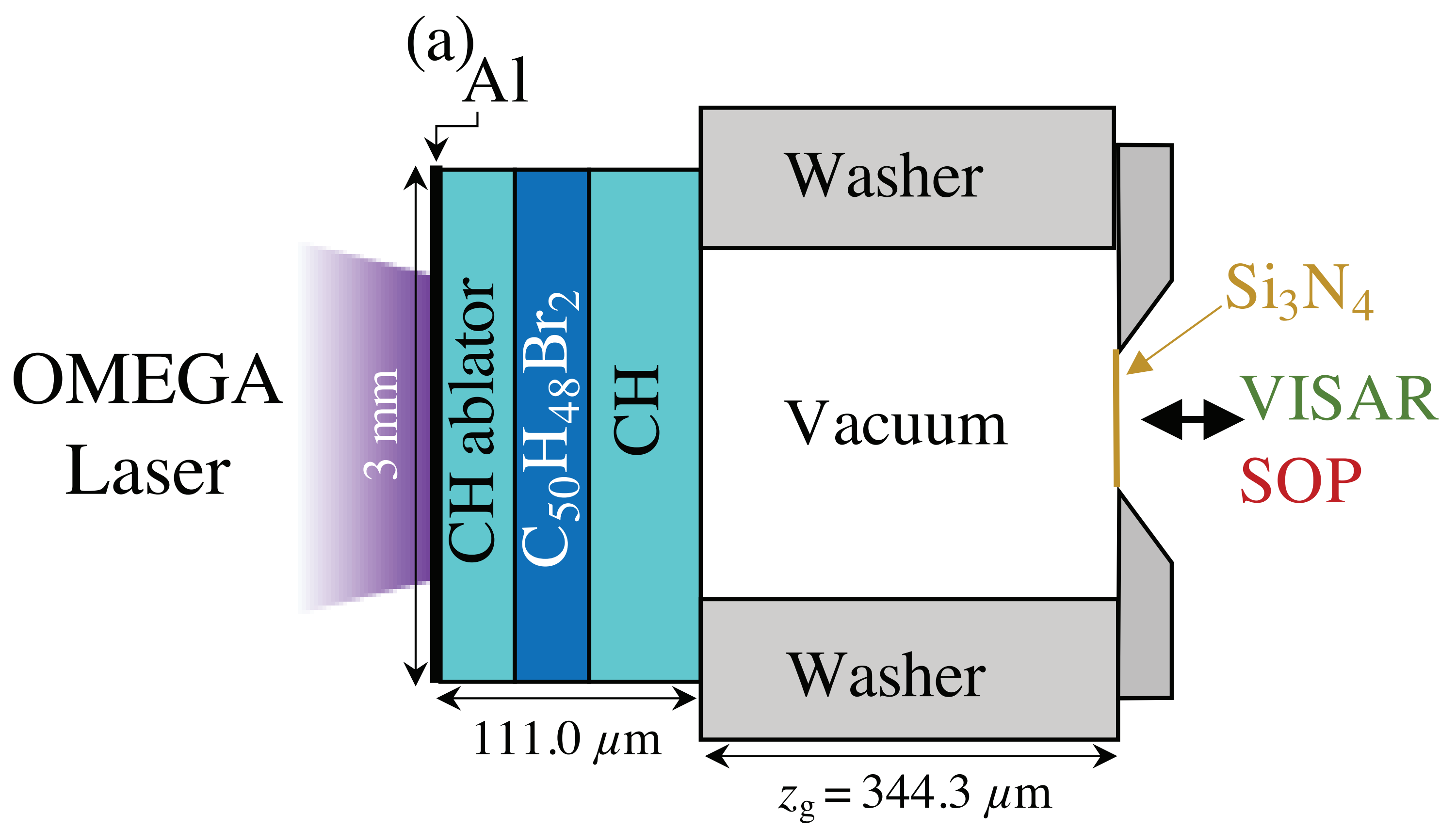
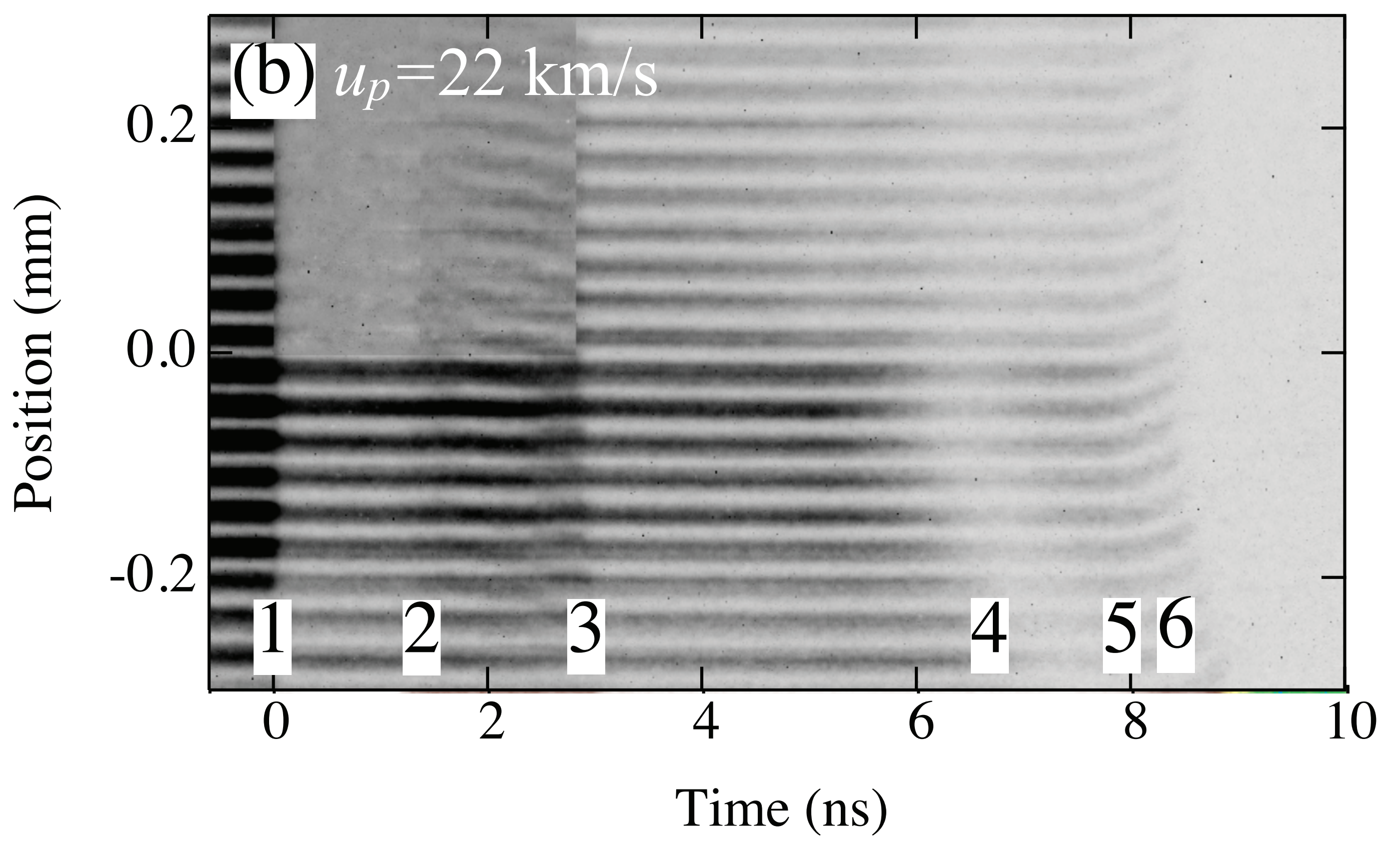
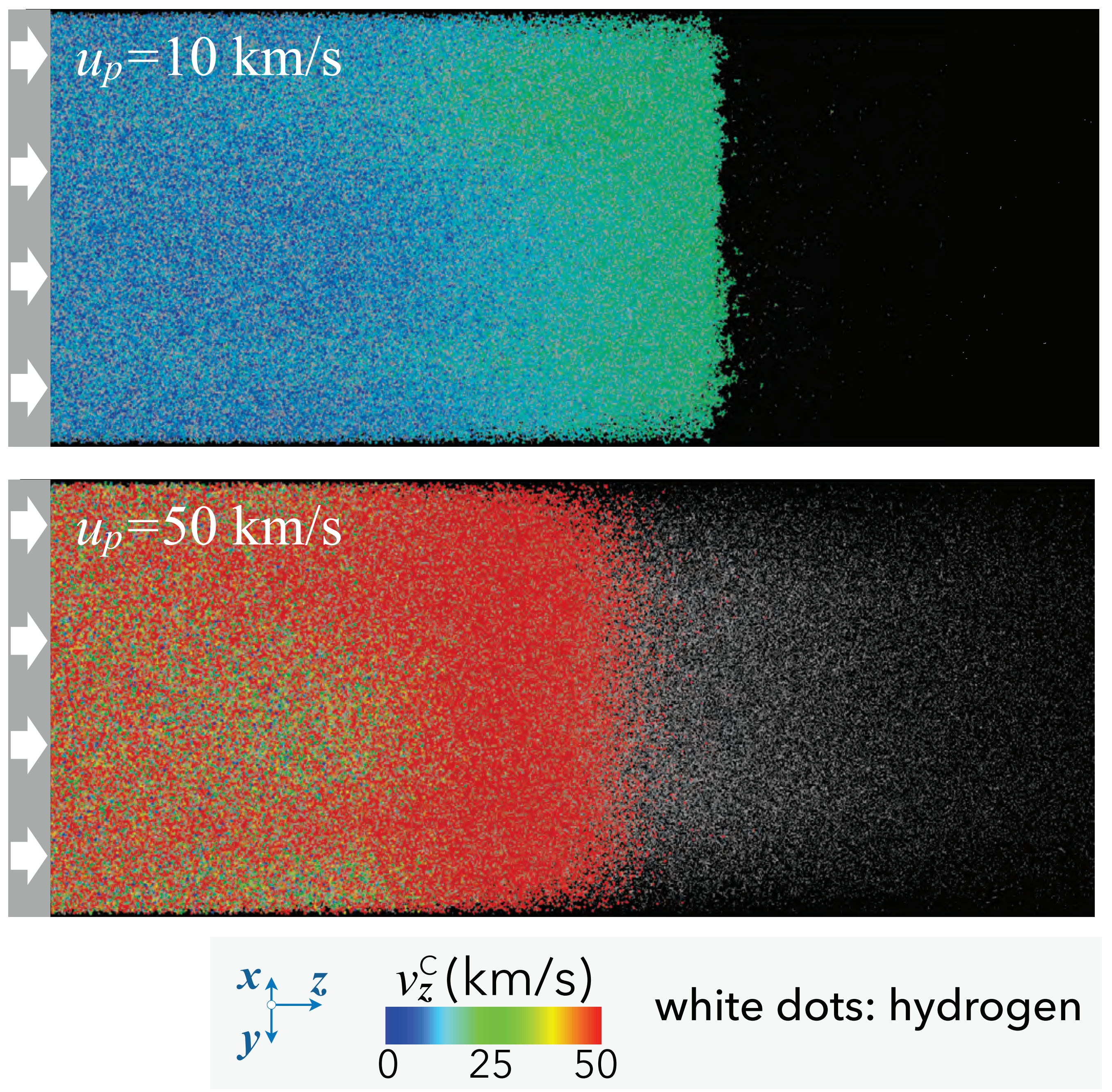
Species separation in polystyrene shock release evidenced by molecular dynamics simulations and laser drive experiments

Laser-drive experiment





CMD simulation



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APS DPP Meeting
Pittsburgh, PA
Nov. 11, 2021

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SUMMARY

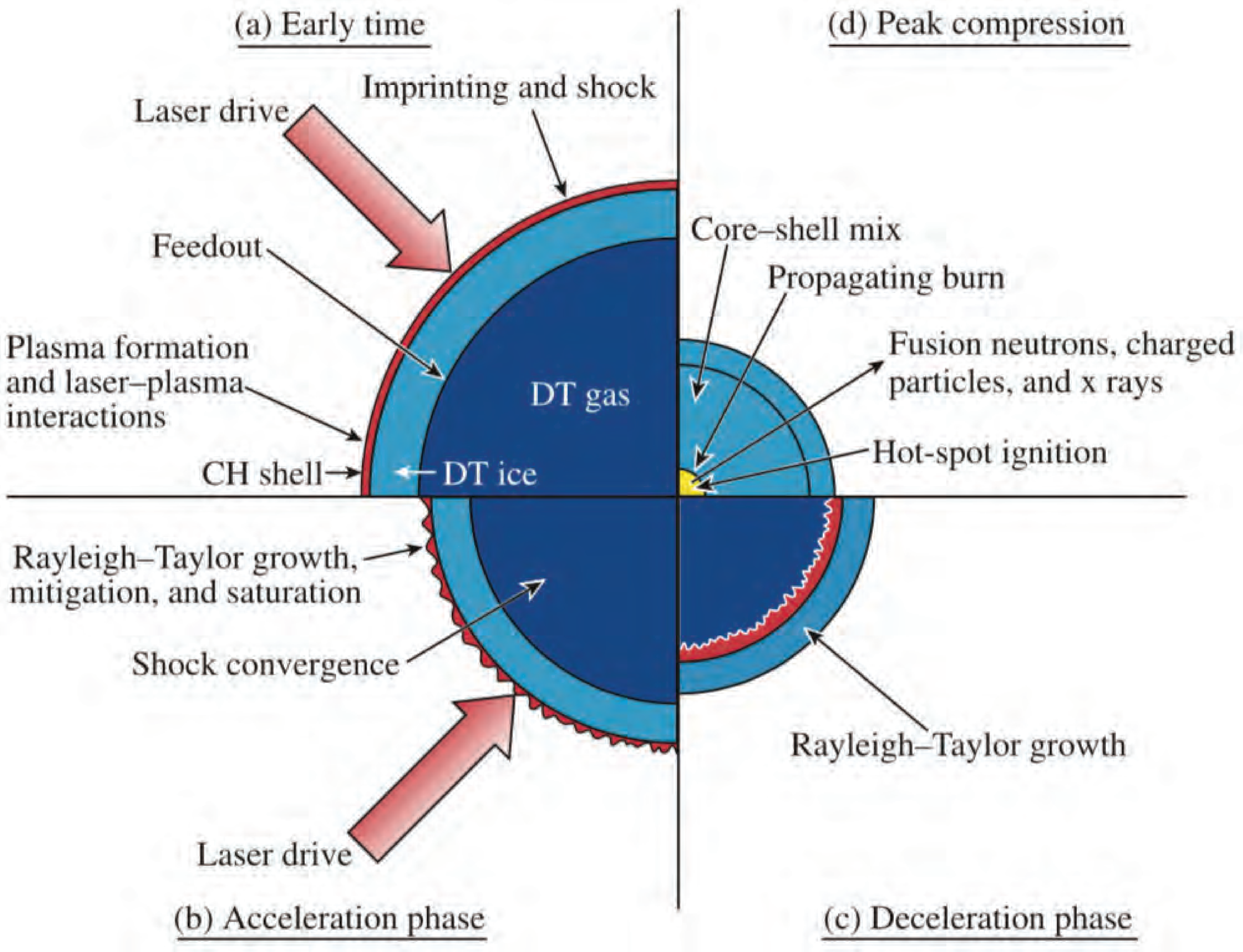
Species separation in polystyrene (CH) shock release evidenced by molecular-dynamics (CMD) simulations and laser-drive experiments

- New experiments and CMD simulations consistently suggest species separation and hydrogen running ahead of carbon in the release of strongly shocked CH
- Lighter species/isotopes can carry more mass and energy to larger depth than heavier ones
- Radiation preheat does not explain observations in CH shock release experiments, species separation does

S. Zhang & S. X. Hu, *Phys. Rev. Lett.* 125, 105001 (2020).
S. Zhang et al., *Phys. Rev. Research*, submitted.

Shock release is important to ICF but challenging to experiments and theory

- Shock release of ablator (e.g., CH) and fuel (e.g., DT) materials affect the performance of ICF experiments
- Design of the experiments often rely on single-fluid hydro simulations



S. Craxton et al., Phys. Plasmas 22, 110501 (2015)

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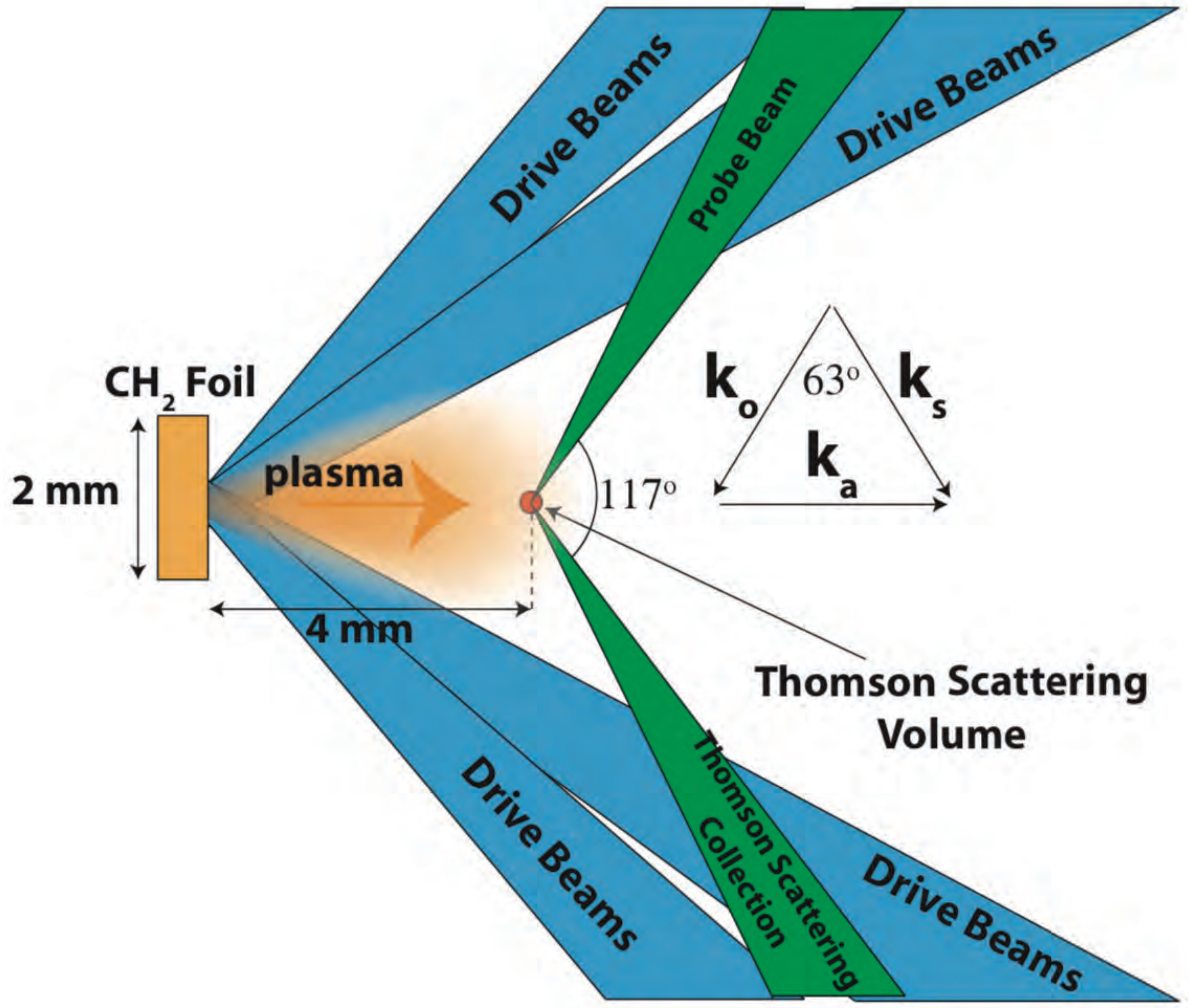
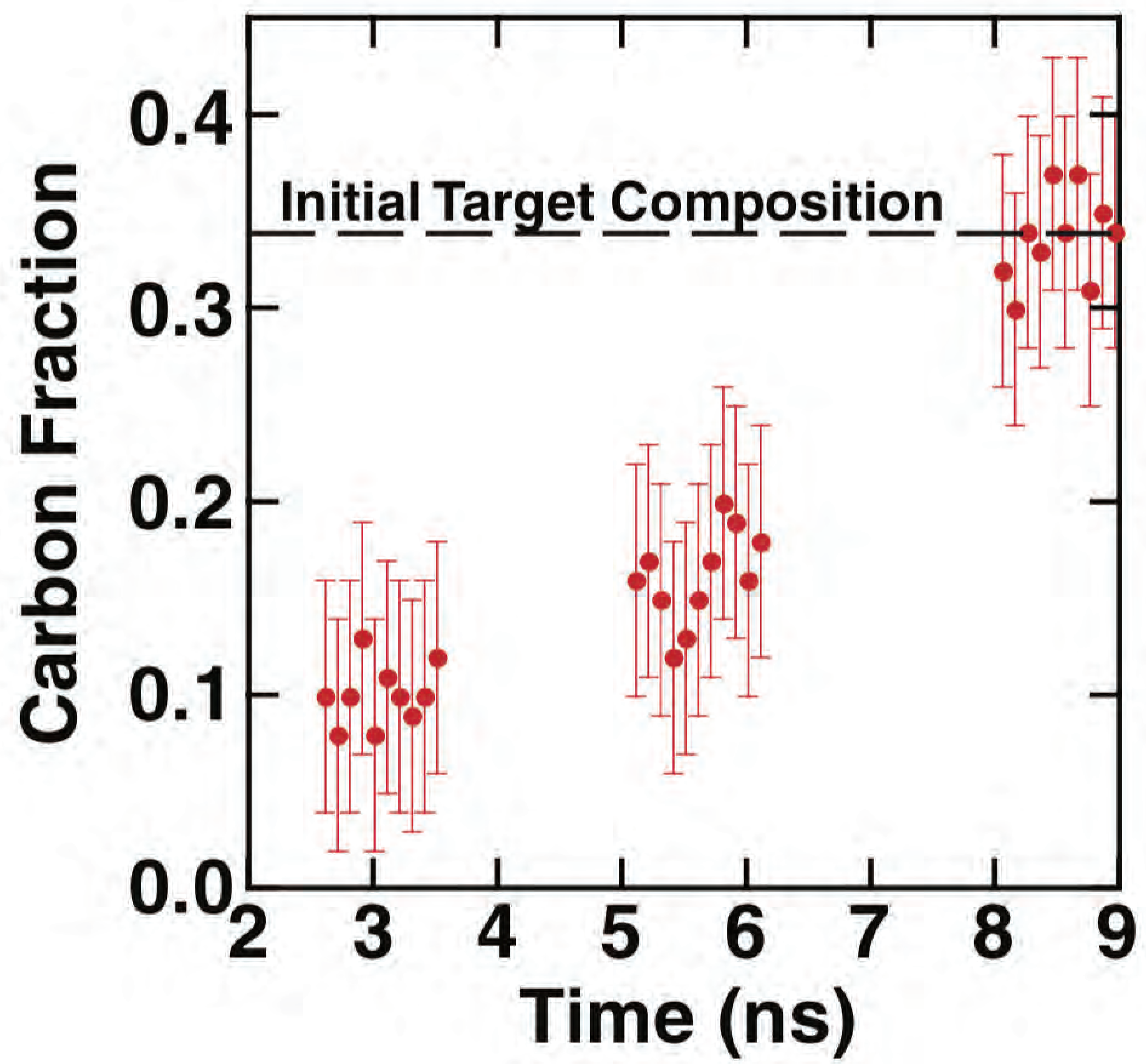
- Shock release of ablator (e.g., CH) and fuel (e.g., DT) materials affect the performance of ICF experiments
- Design of the experiments often rely on single-fluid hydro simulations
- Microscopic chemistry and physics could be important but missed by such simulations

Species separation in laser-ablated CH_2



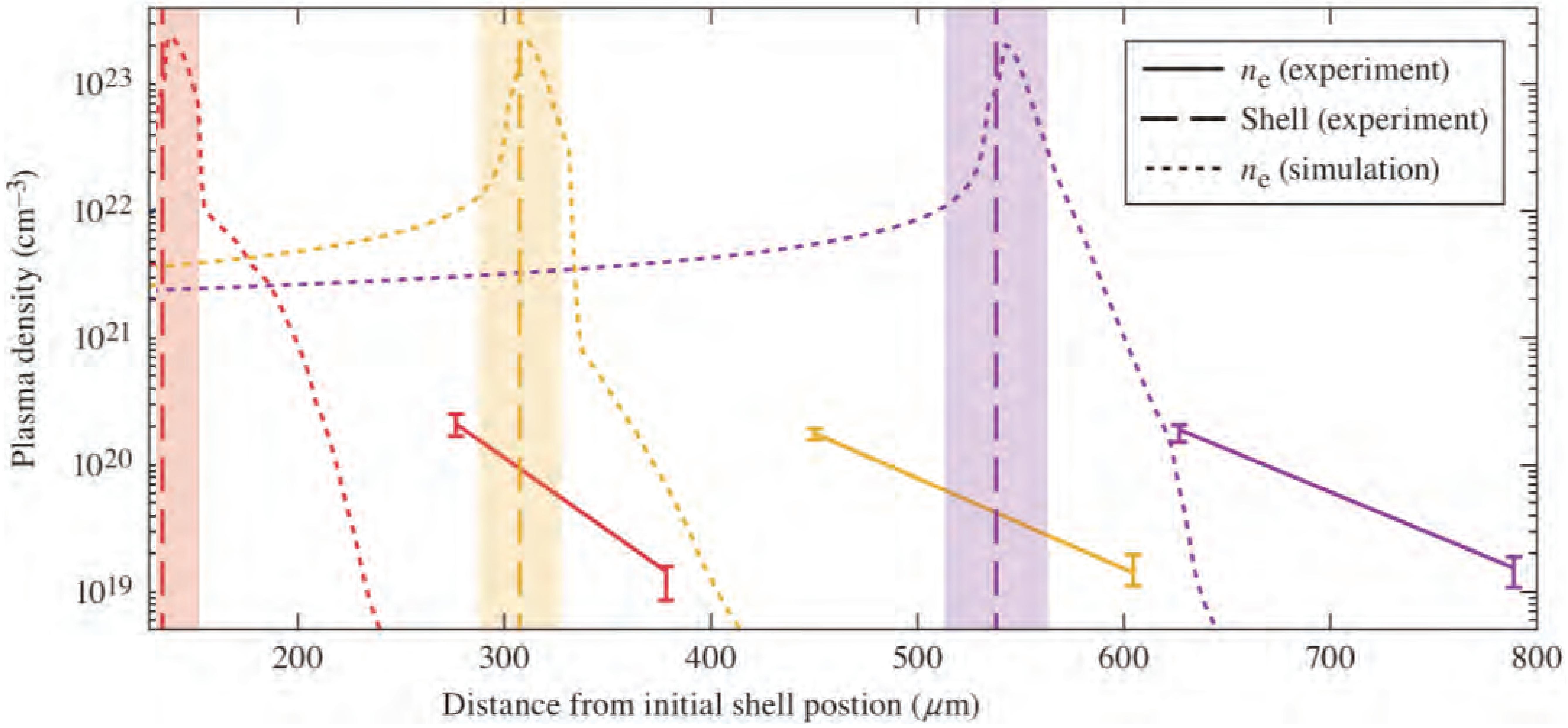


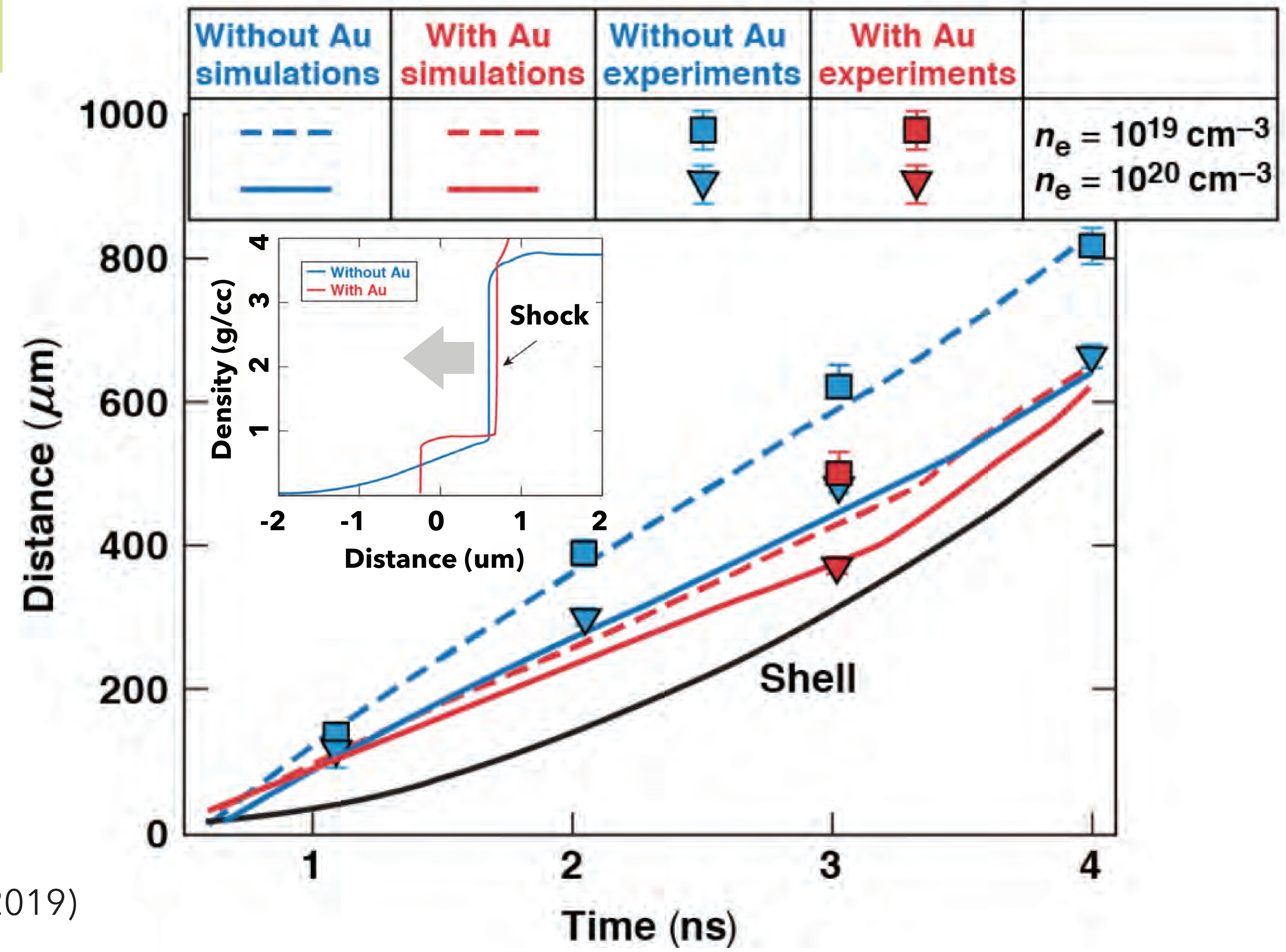
J. S. Ross et al., Rev. Sci. Instrum. 83, 10E323 (2012)

Low-density plasmas from shock released CH run ahead of hydro predictions

- Improved agreements with experiments can be reached when considering radiation transport and pre-expansion at the rear surface of CH before shock arrival
- **Inconsistency remains** between simulations and experiments with gold shield

Optical interferometry measurement of CH shock release

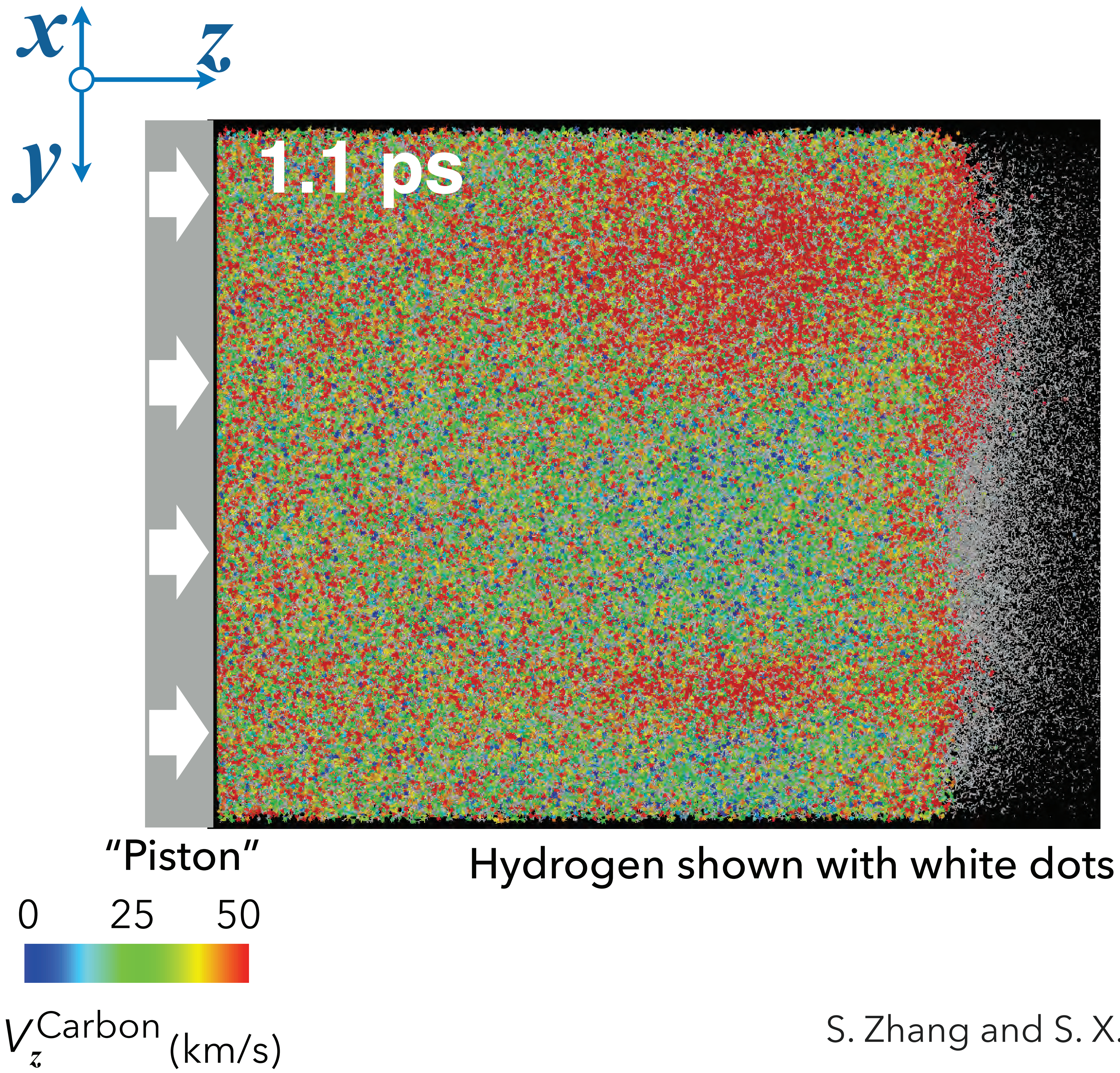


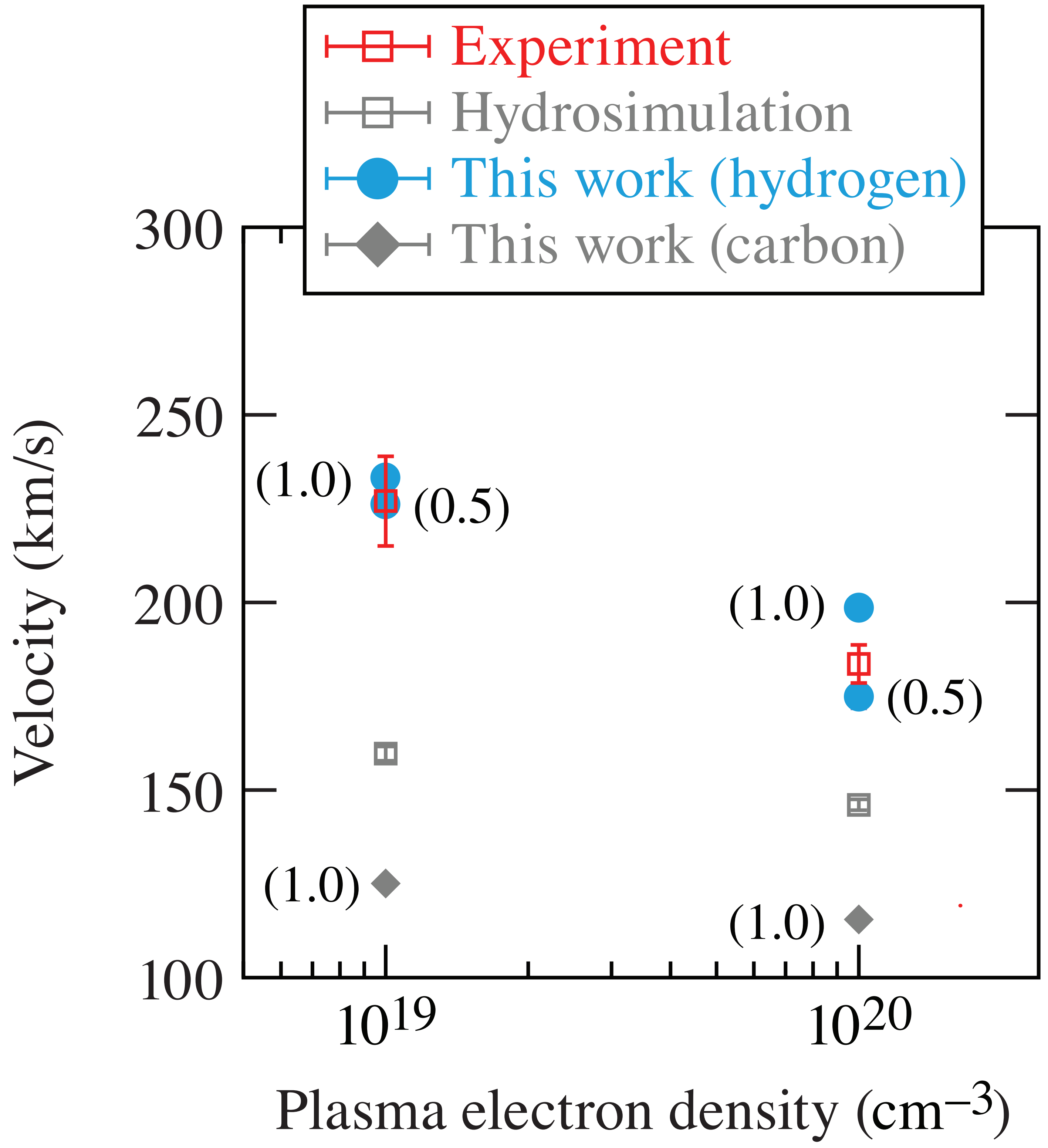


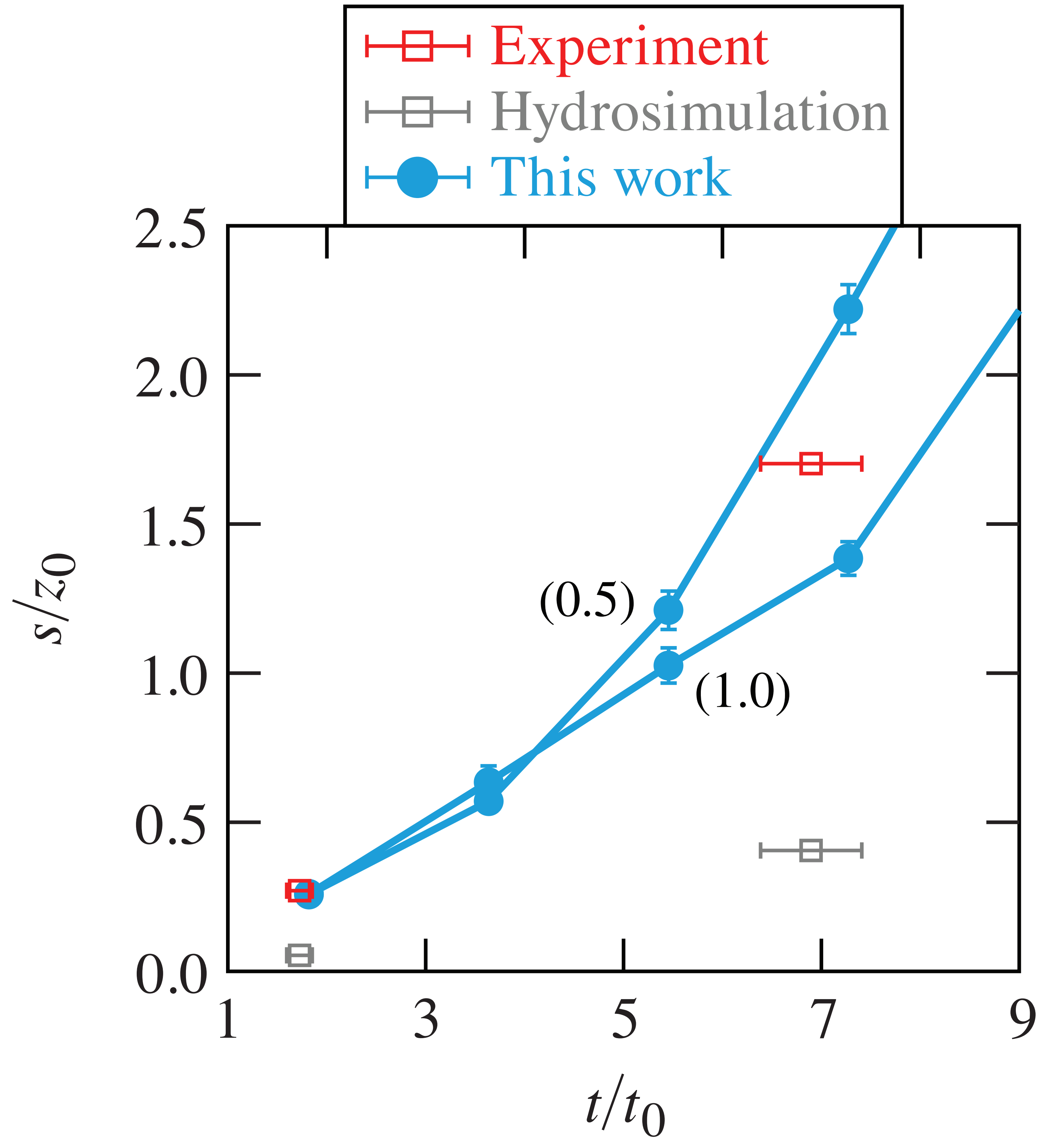
D. Haberberger et al, Phys. Rev. Lett. 123, 235001 (2019)
A. Shvydky et al., Phys. Plasmas 28, 092703 (2021)

Species separation & H streaming can explain CH shock release expt

- **CMD**: promising for large-scale non-equilibrium (as in shock release) simulations
- **Atomic level kinetic effect** is explicitly included; **reactive force fields** available for high-pressure applications (error for CH Hugoniot: <20%)







z_0: initial sample thickness; t_0: duration of shock propagation through the sample

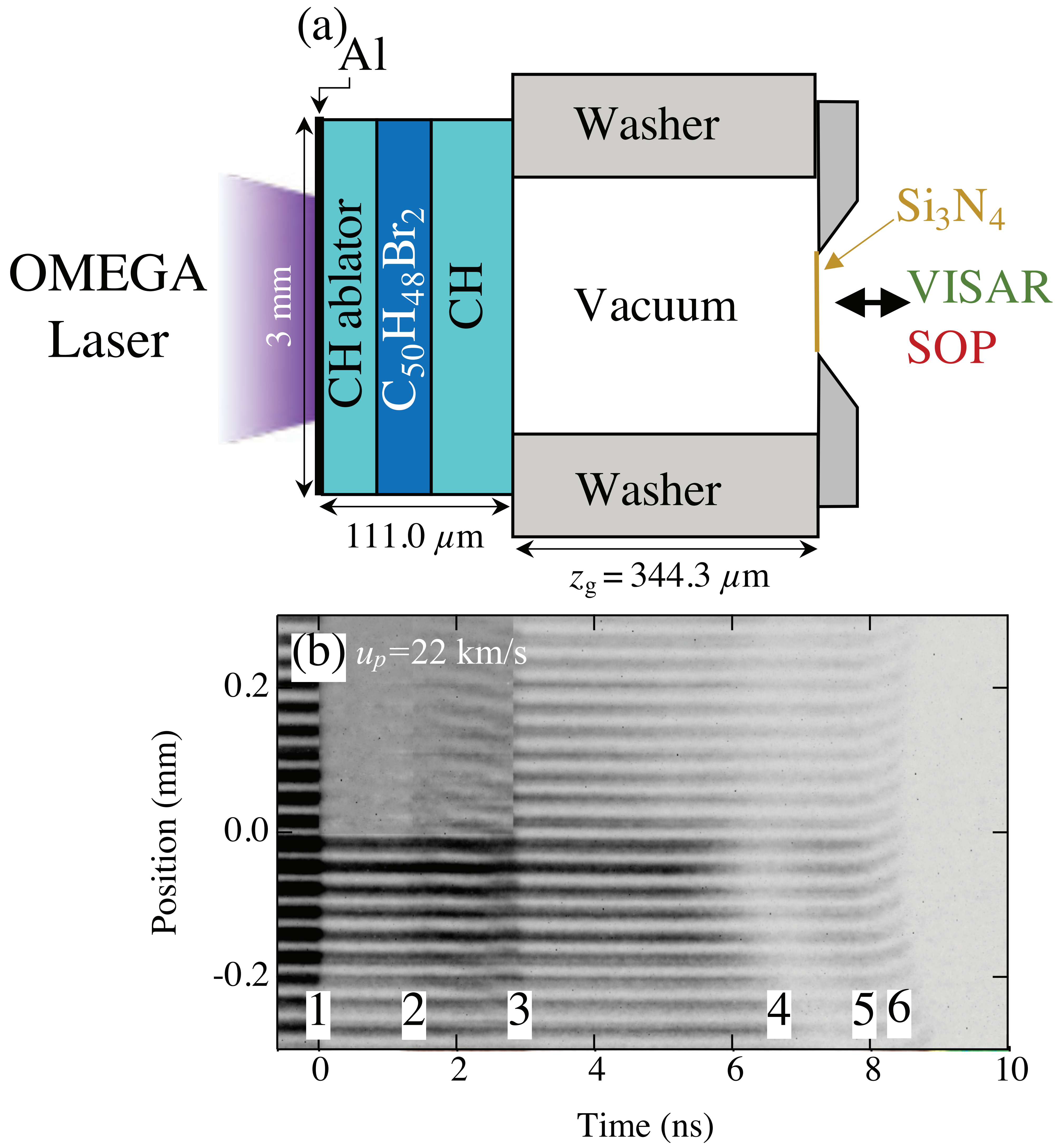
S. Zhang and S. X. Hu, Phys. Rev. Lett. 125, 105001 (2020)

New CMD calculations reveal shock strength dependence of CH release

- Species separation upon shock breakout and during release
- Significant for strong shocks ($P \geq 350$ GPa), absent for weak shocks ($P \leq 160$ GPa)

white dots: hydrogen

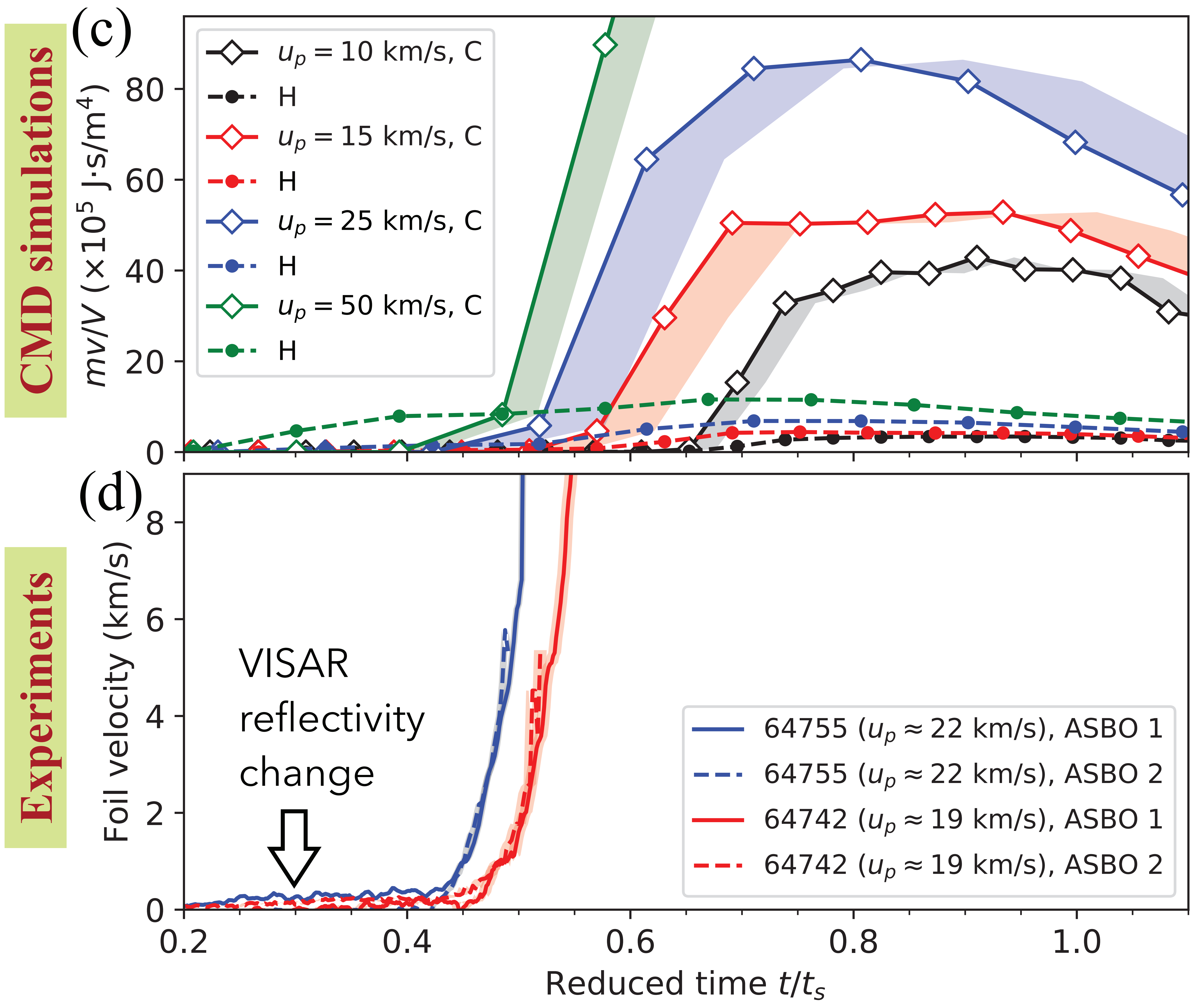
New experimental results on CH shock release support species separation



- **Our experimental design** prevents radiation preheat of the sample and employs a witness foil to investigate the release of shocked CH across a vacuum gap
- **We observe** VISAR reflectivity changes (4) before fringe shifts (5), similar changes observed in all GDP and CH experiments when shocked to above 550 GPa, but not in experiments of pure diamond or beryllium

These observations are all consistent with the CMD predicted species separation and hydrogen streaming!

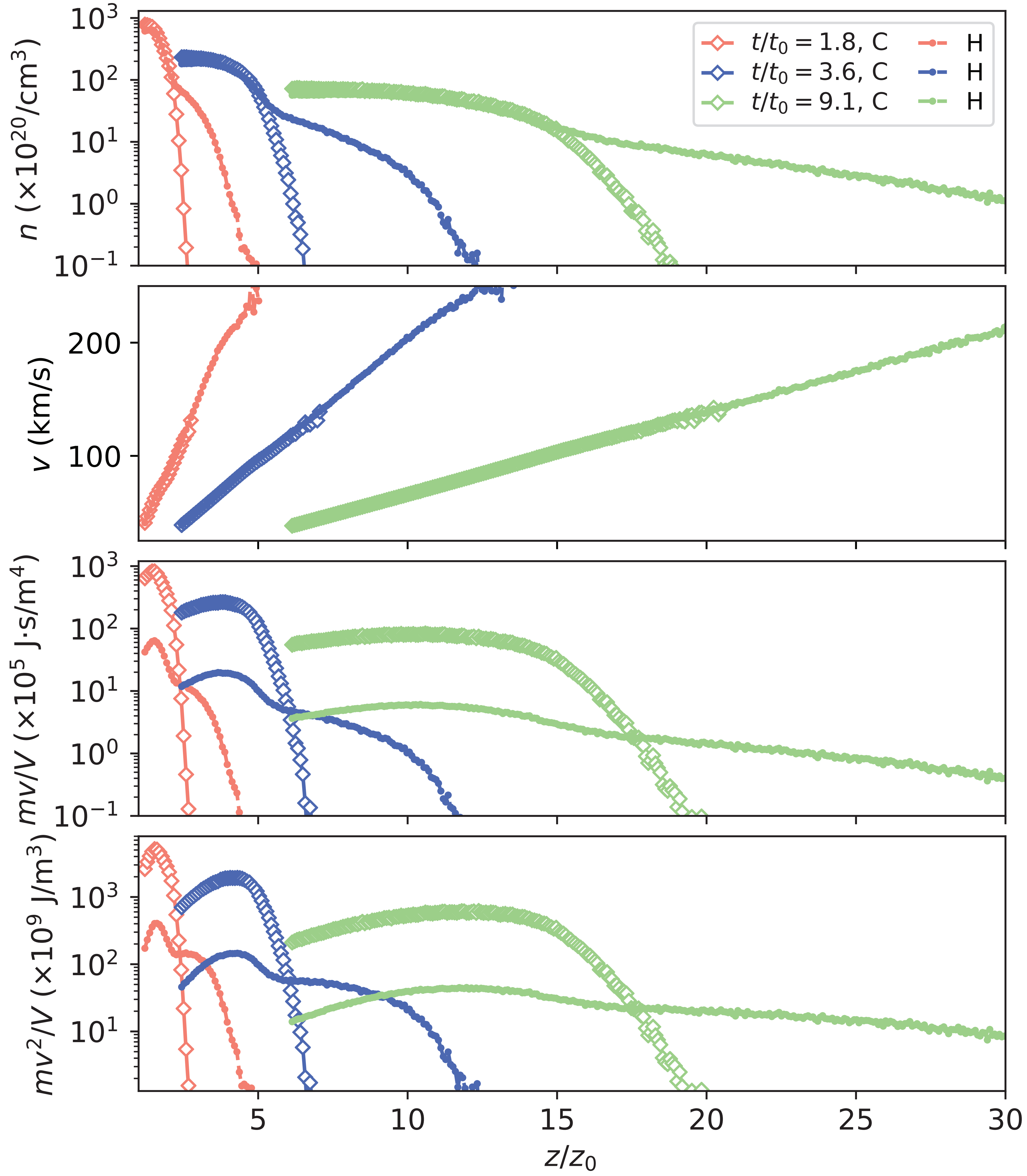
Experimental results agree with CMD predictions for the release



- **CMD**: species momentum ramps up before jumping up, earlier for higher u_p
- **Experiment**: foil velocity jumps up after VISAR reflectivity change, earlier in case of stronger shock

Time originates at shock breakout.
Scaling parameter $t_s = z_g / u_s$;
z_g: vacuum gap thickness;
u_s: shock velocity upon breakout.

We further quantify the effect of hydrogen isotopes on CH shock release



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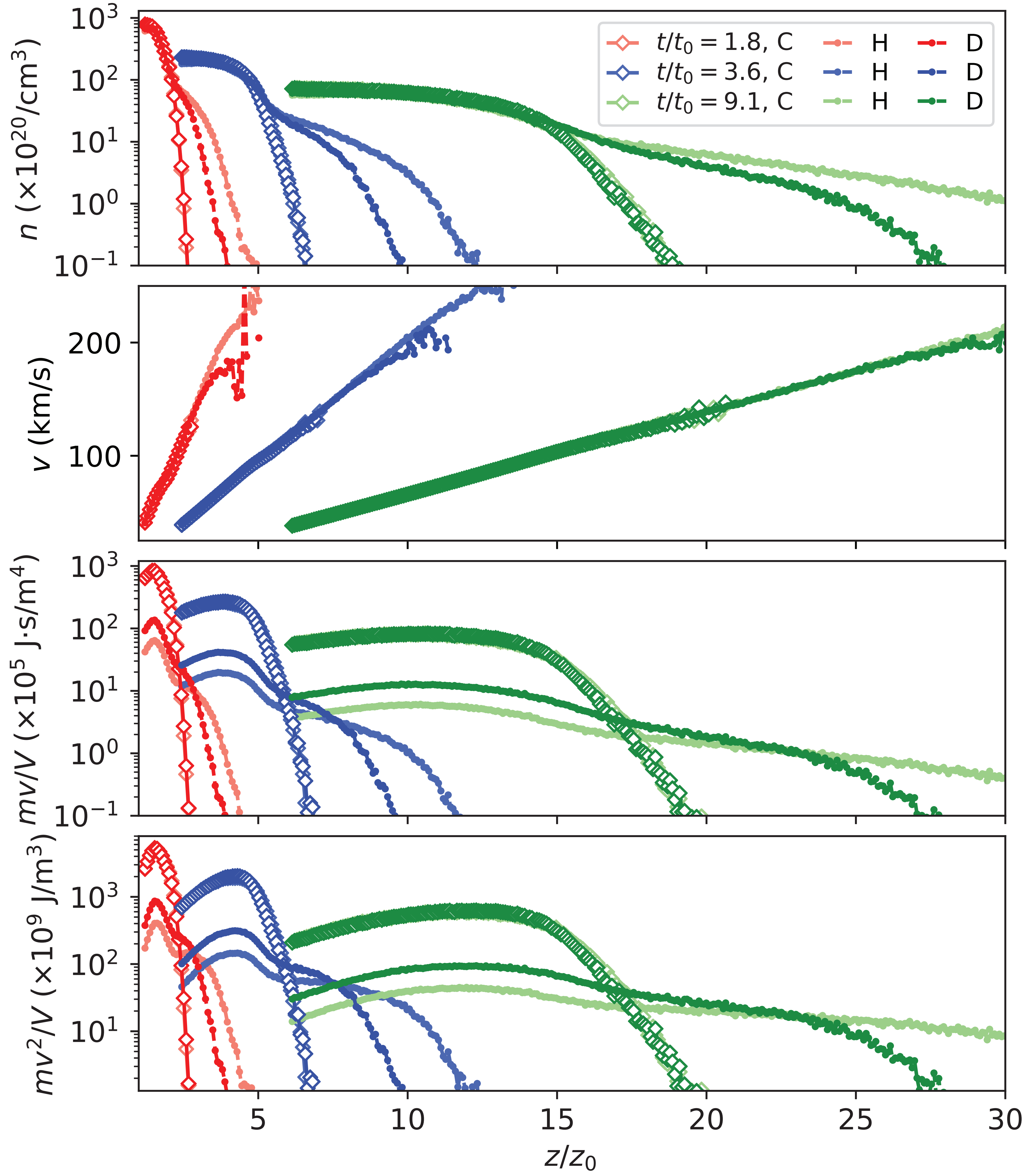

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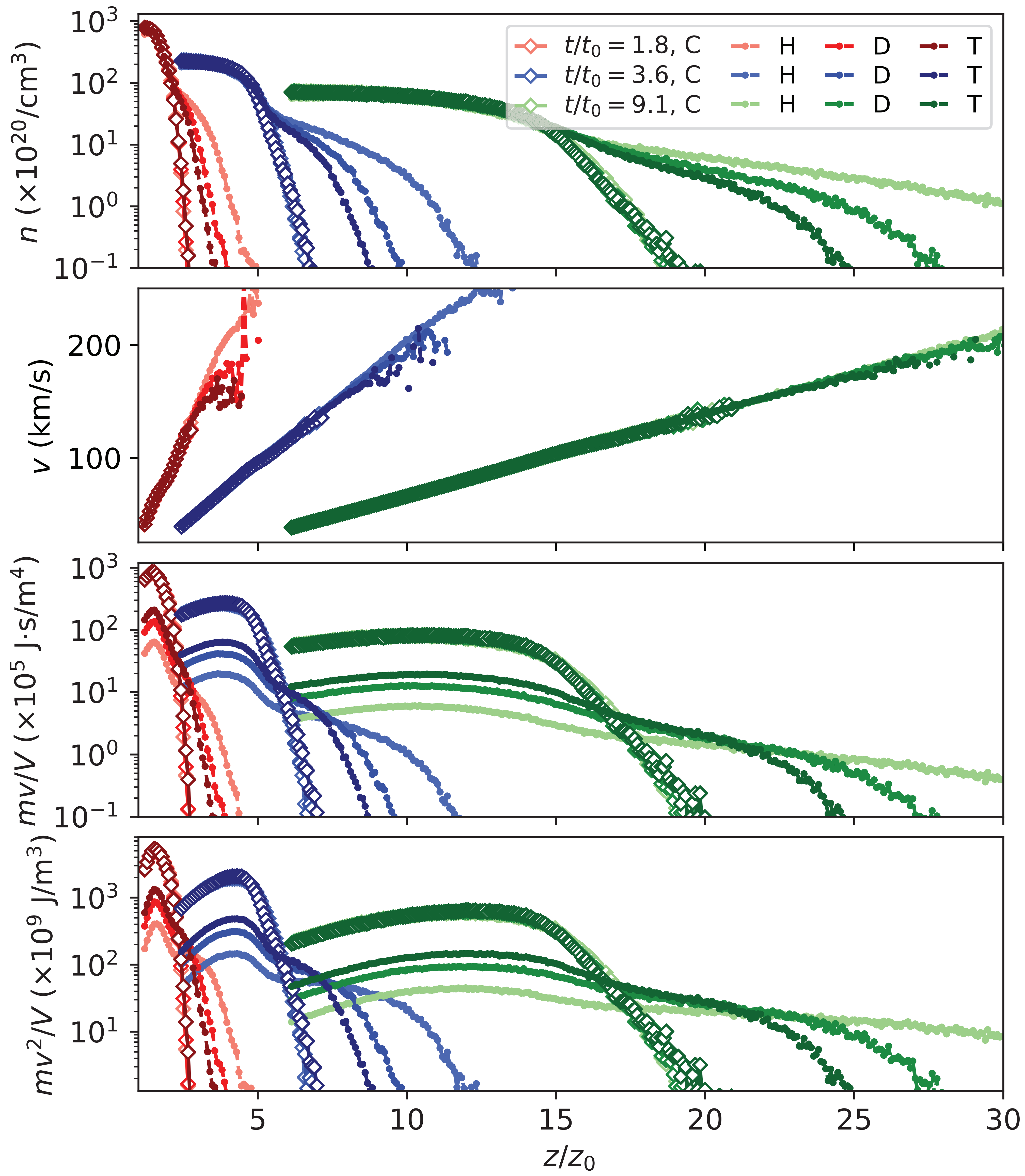

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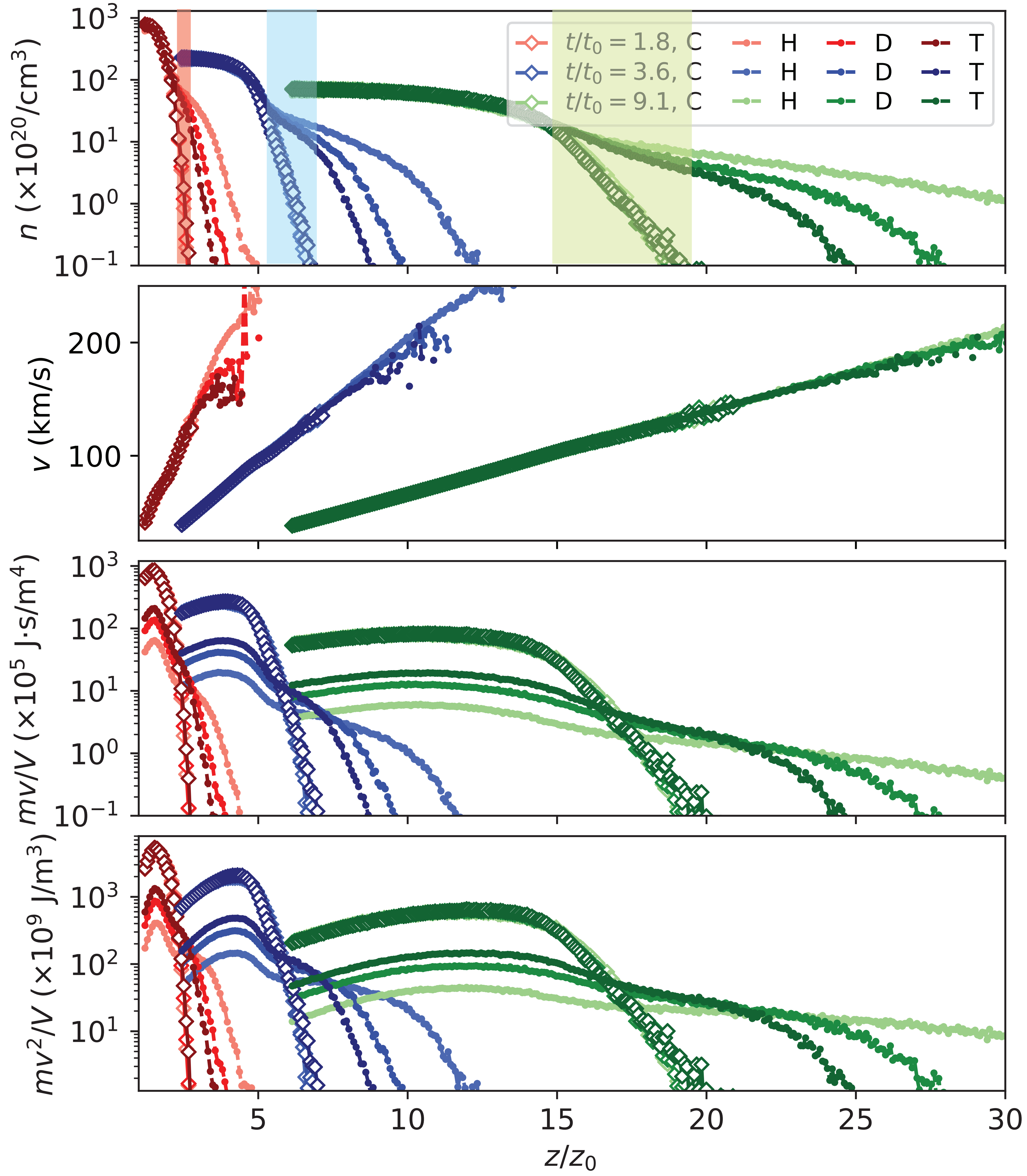

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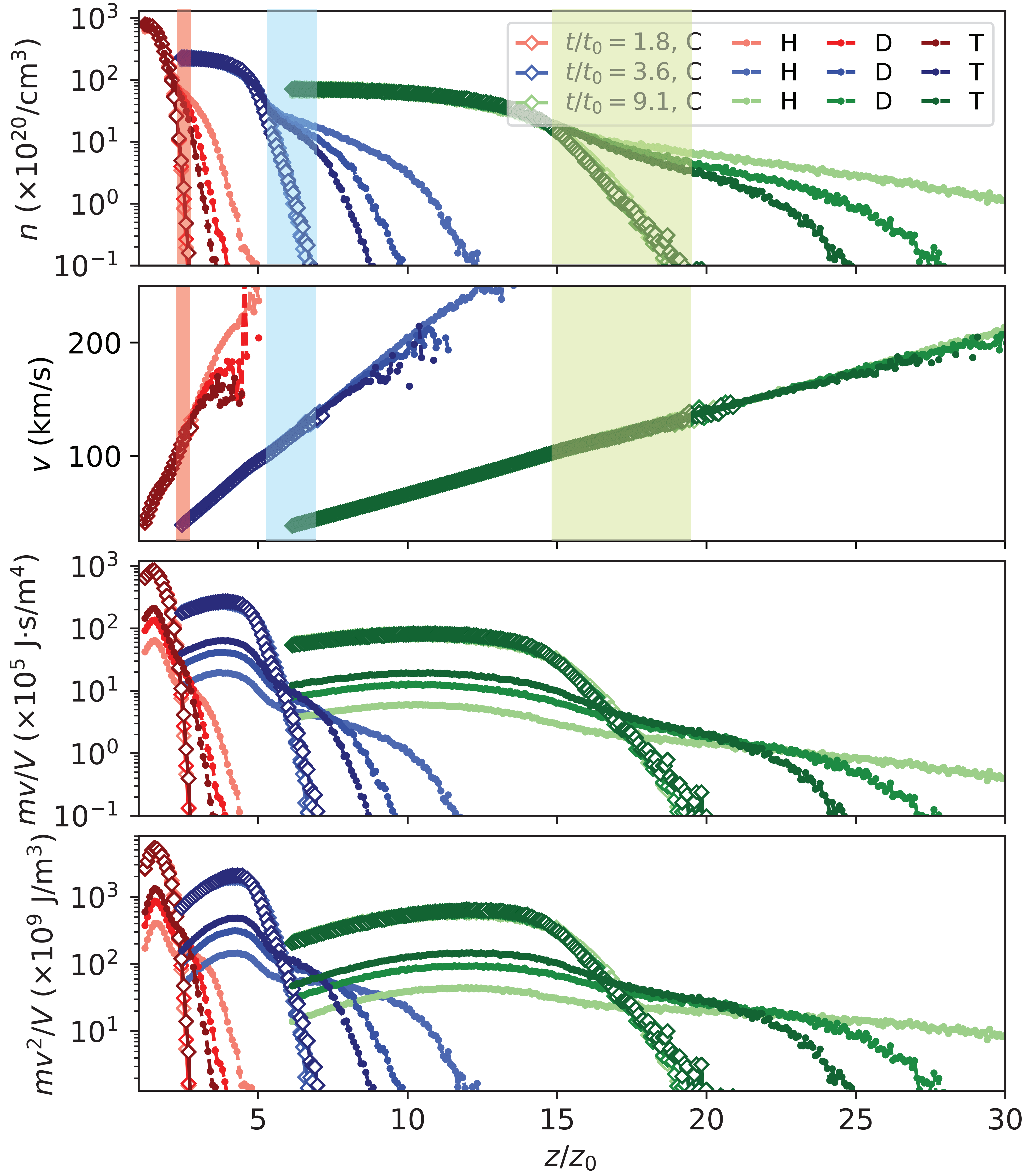

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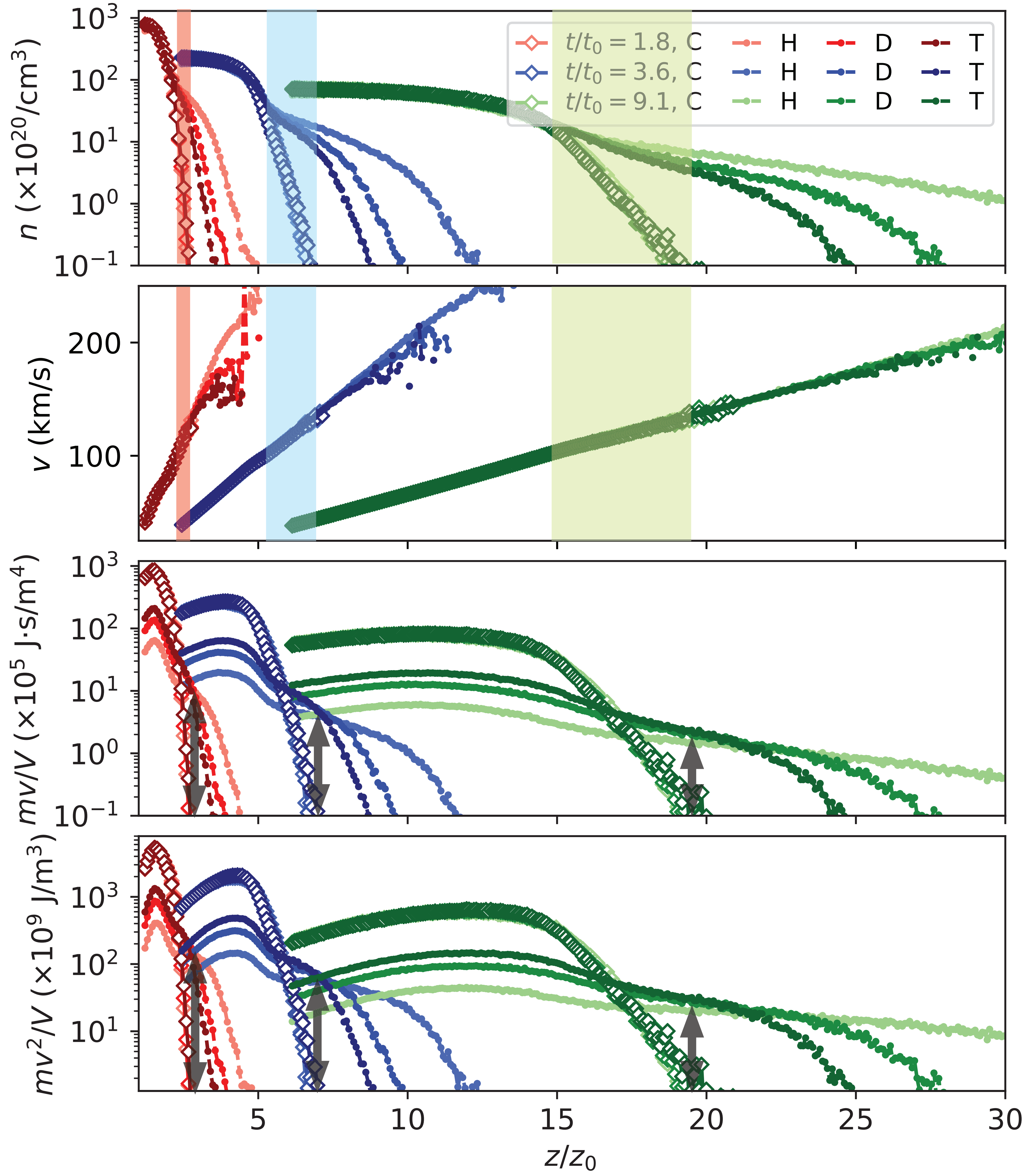

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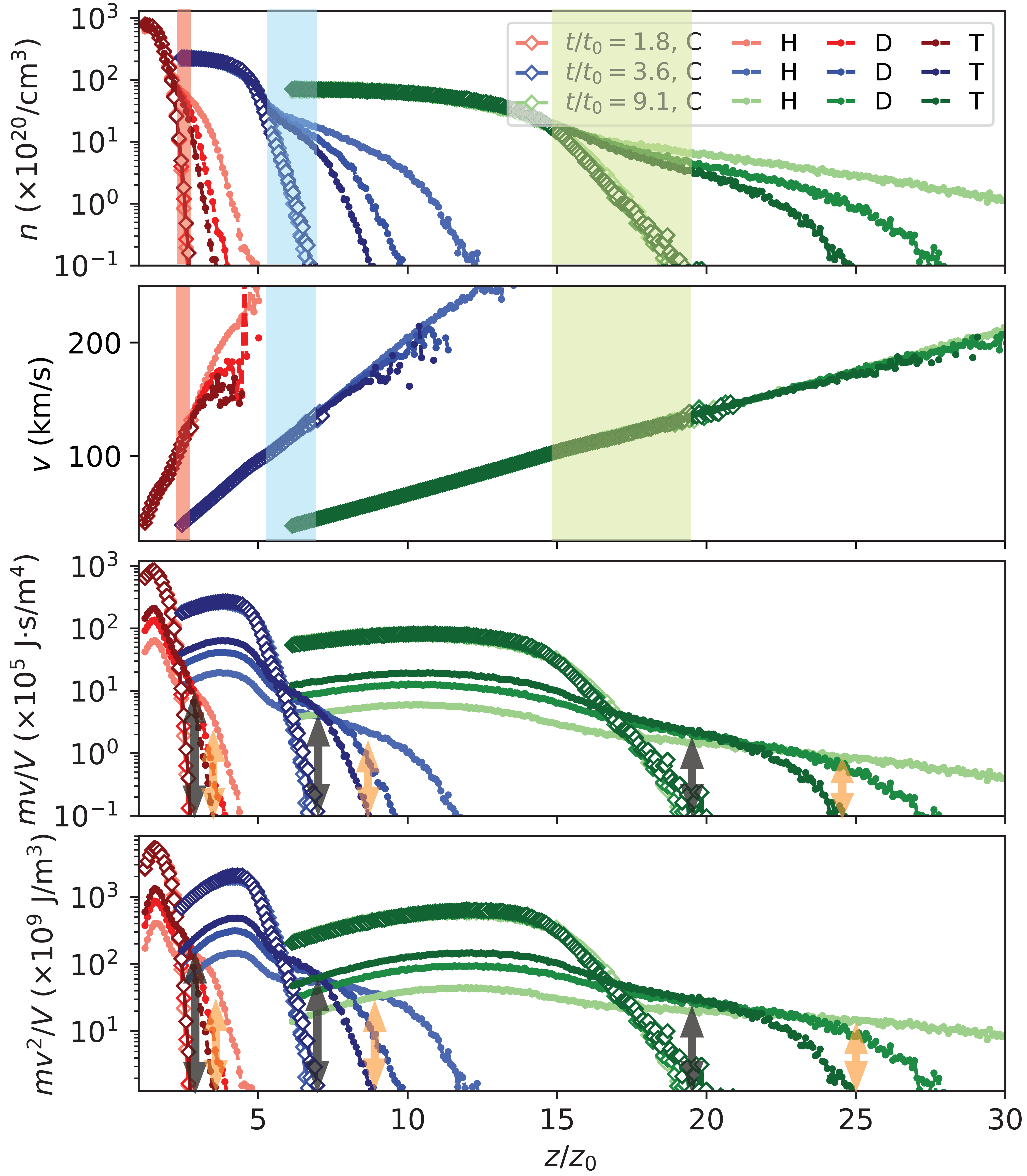

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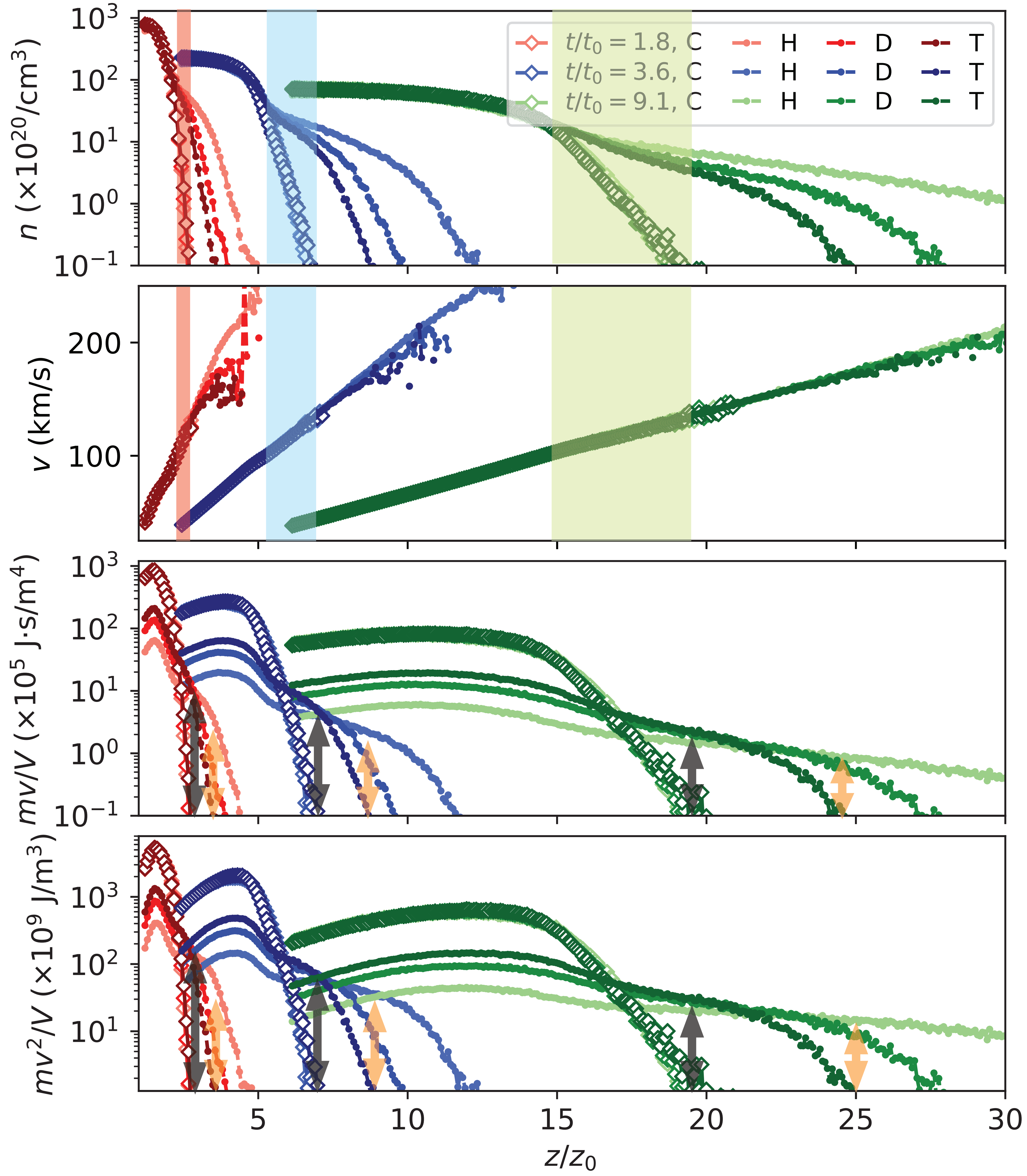

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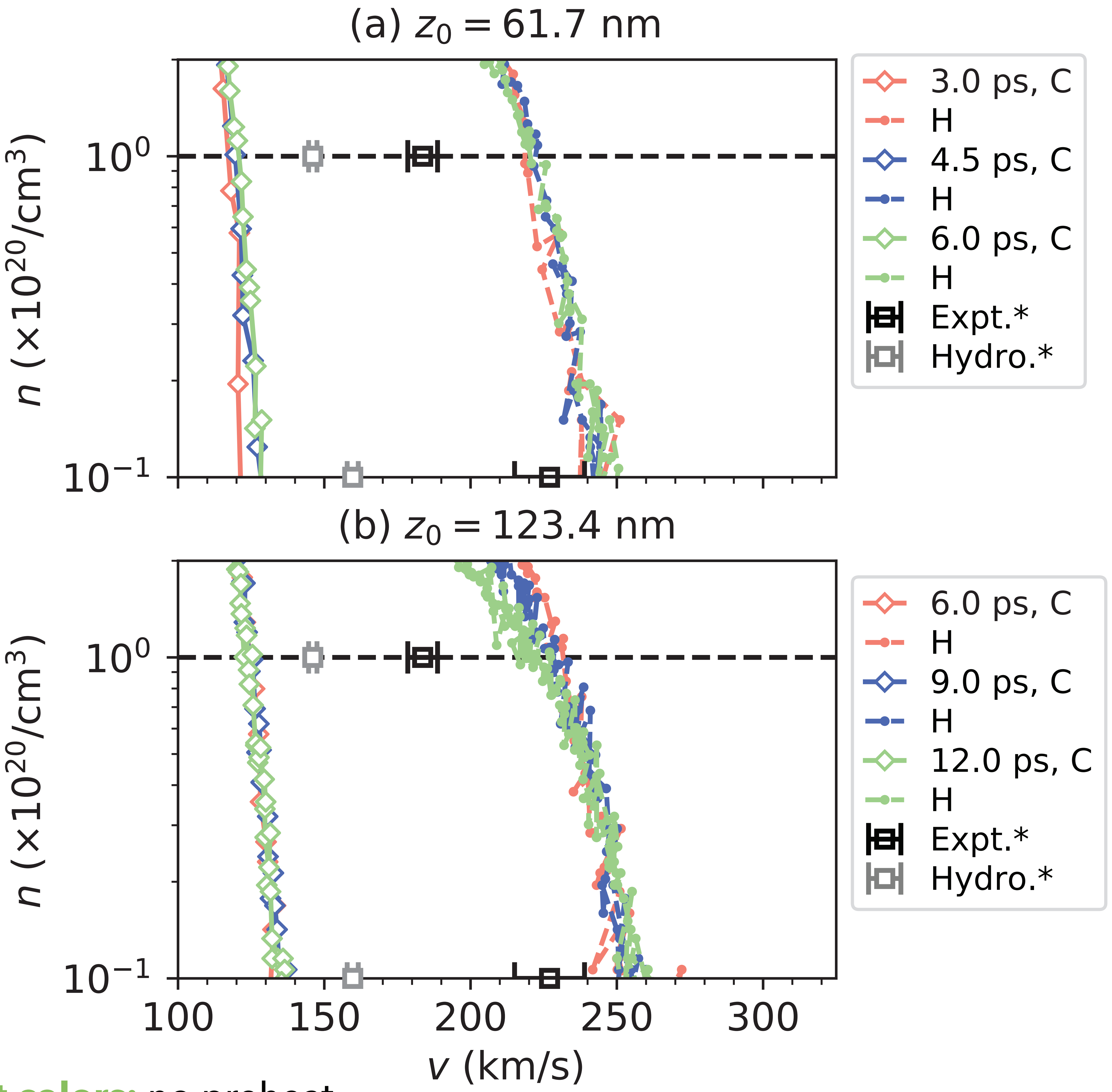
✦ **Compression degradation**

✦ **Discrepancies between hydro and expt.**

CMD results show radiation preheat cannot explain experimental observations



Light colors: no preheat

* D. Haberberger et al, Phys. Rev. Lett. 123, 235001 (2019)

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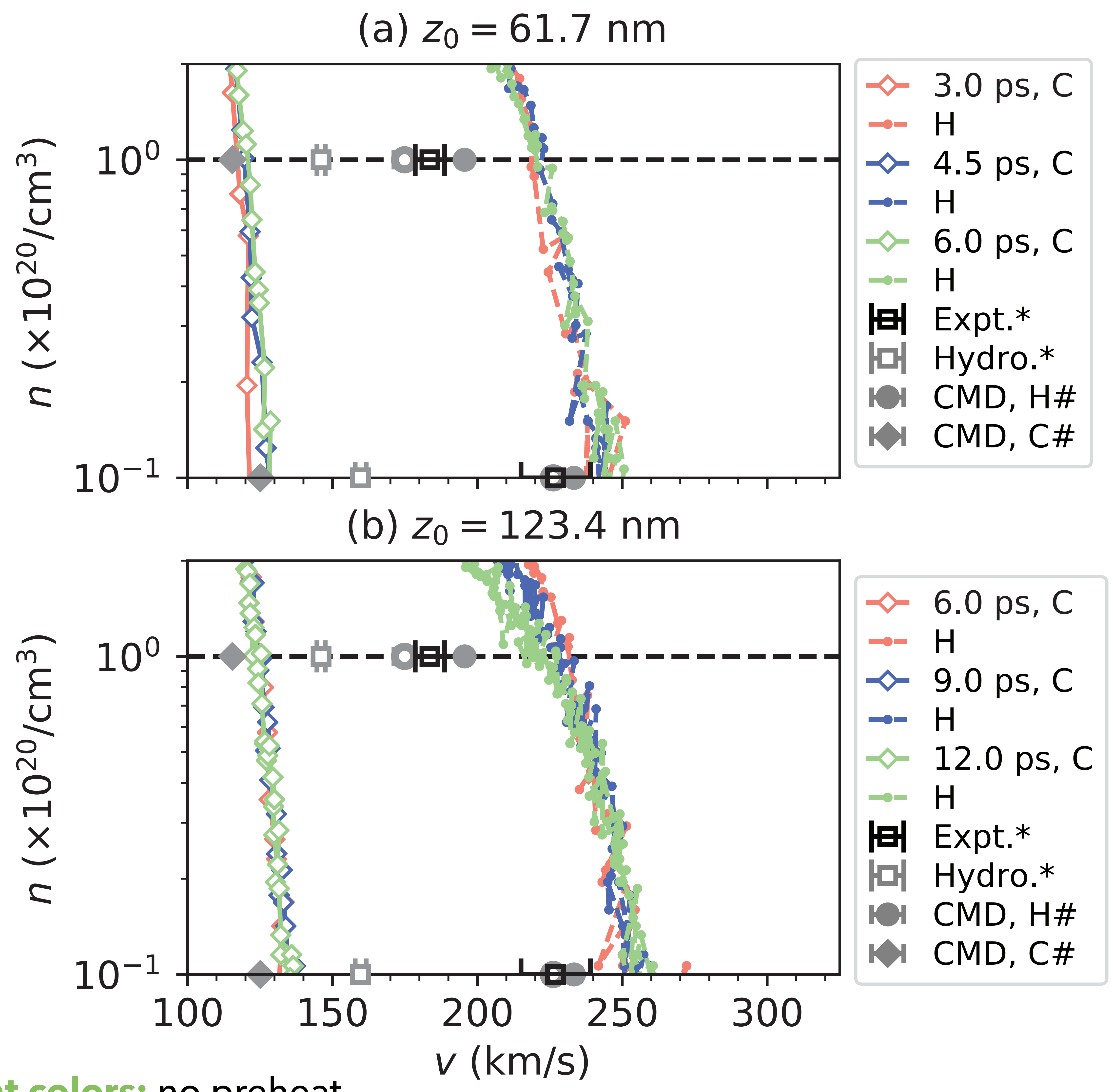

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\# S. Zhang & S. X. Hu, Phys. Rev. Lett. 125, 105001 (2020)

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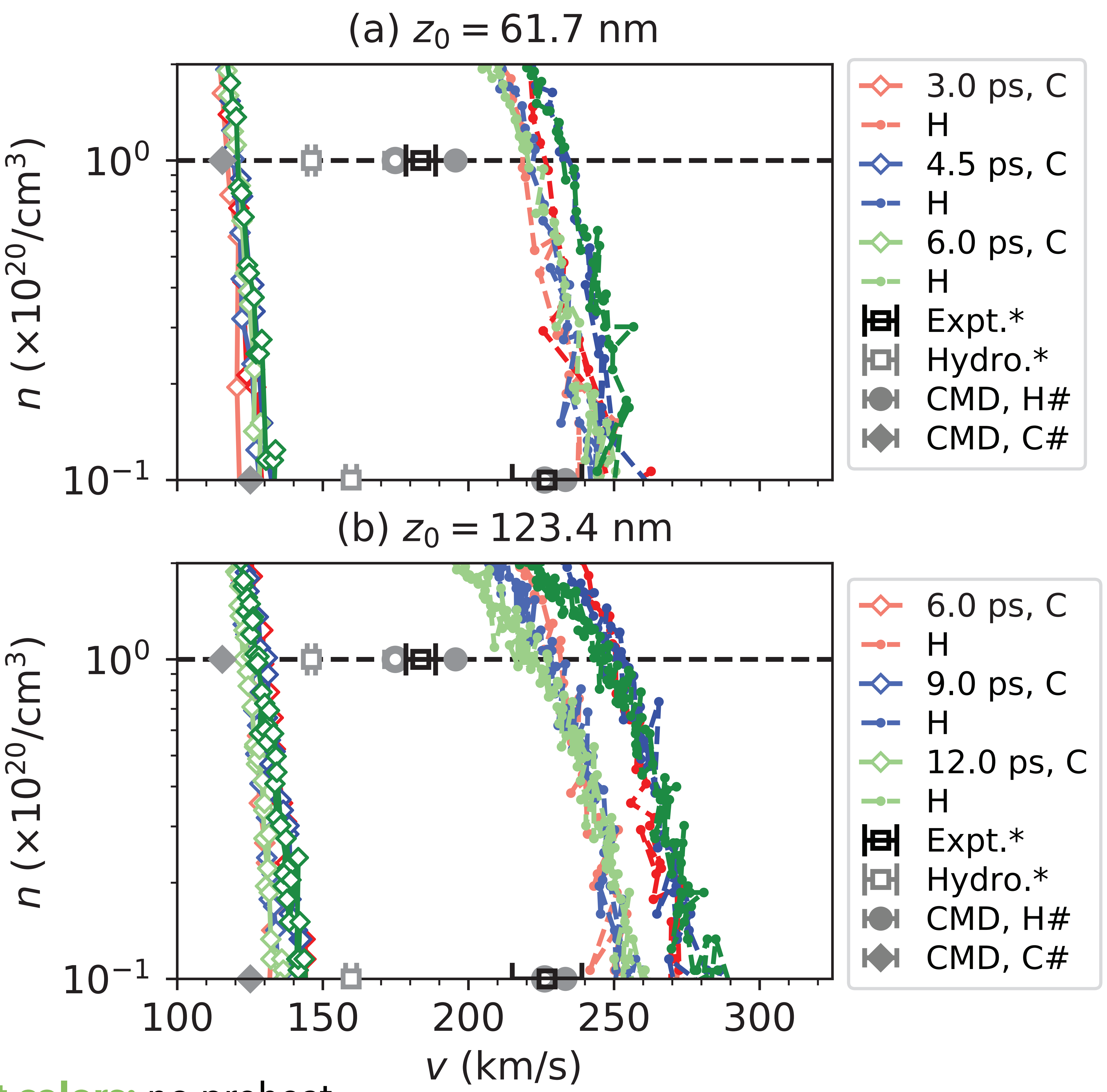

Light colors: no preheat

Intermediate colors: preheat at 5000 K for 5 ps (20% expansion)

- w/o preheat: $v_{\text{hydro}} > v^{\text{C}}$
- w/ preheat:
  - v^{H} and v^{C} depend on cell sizes
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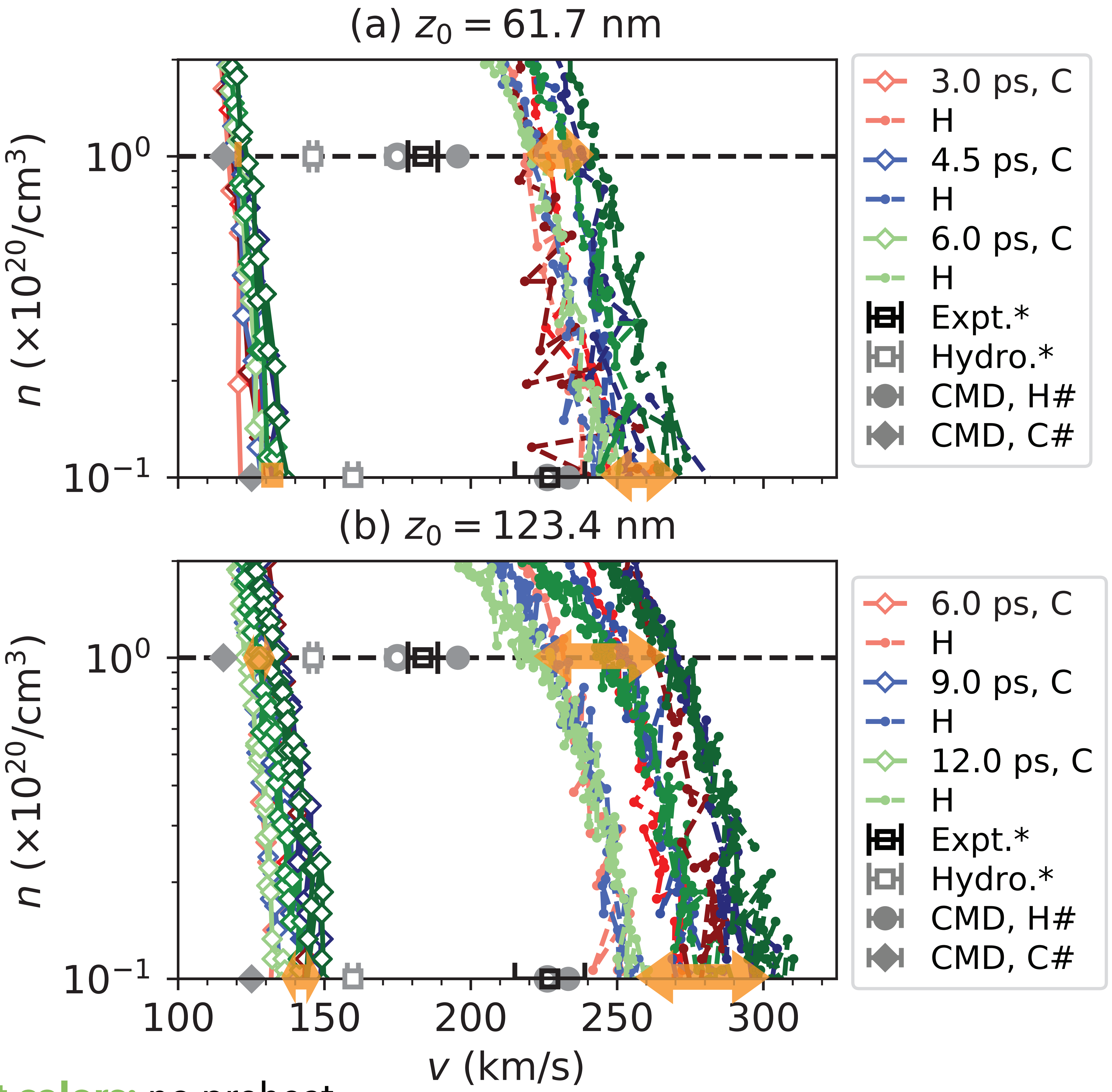

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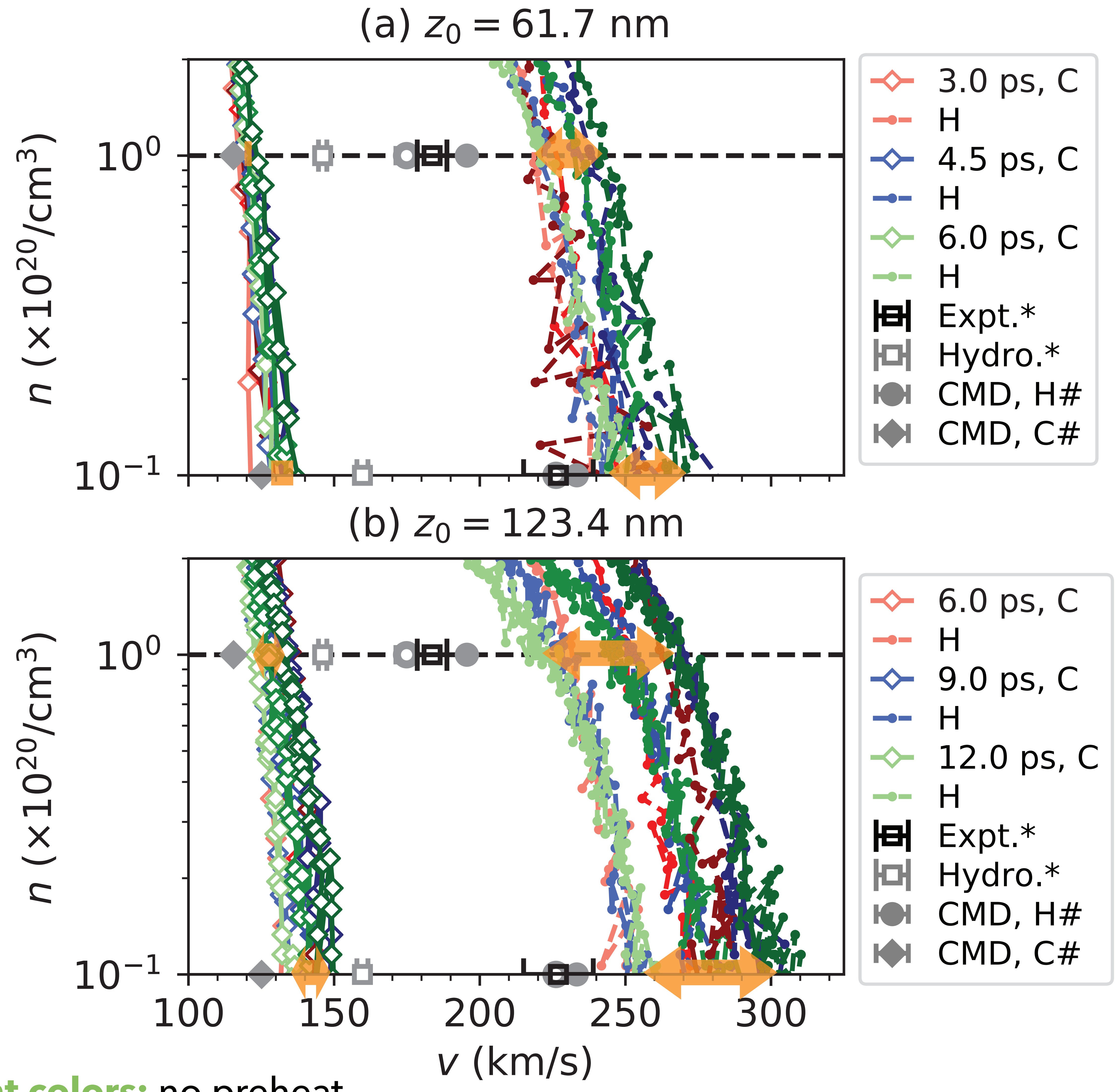

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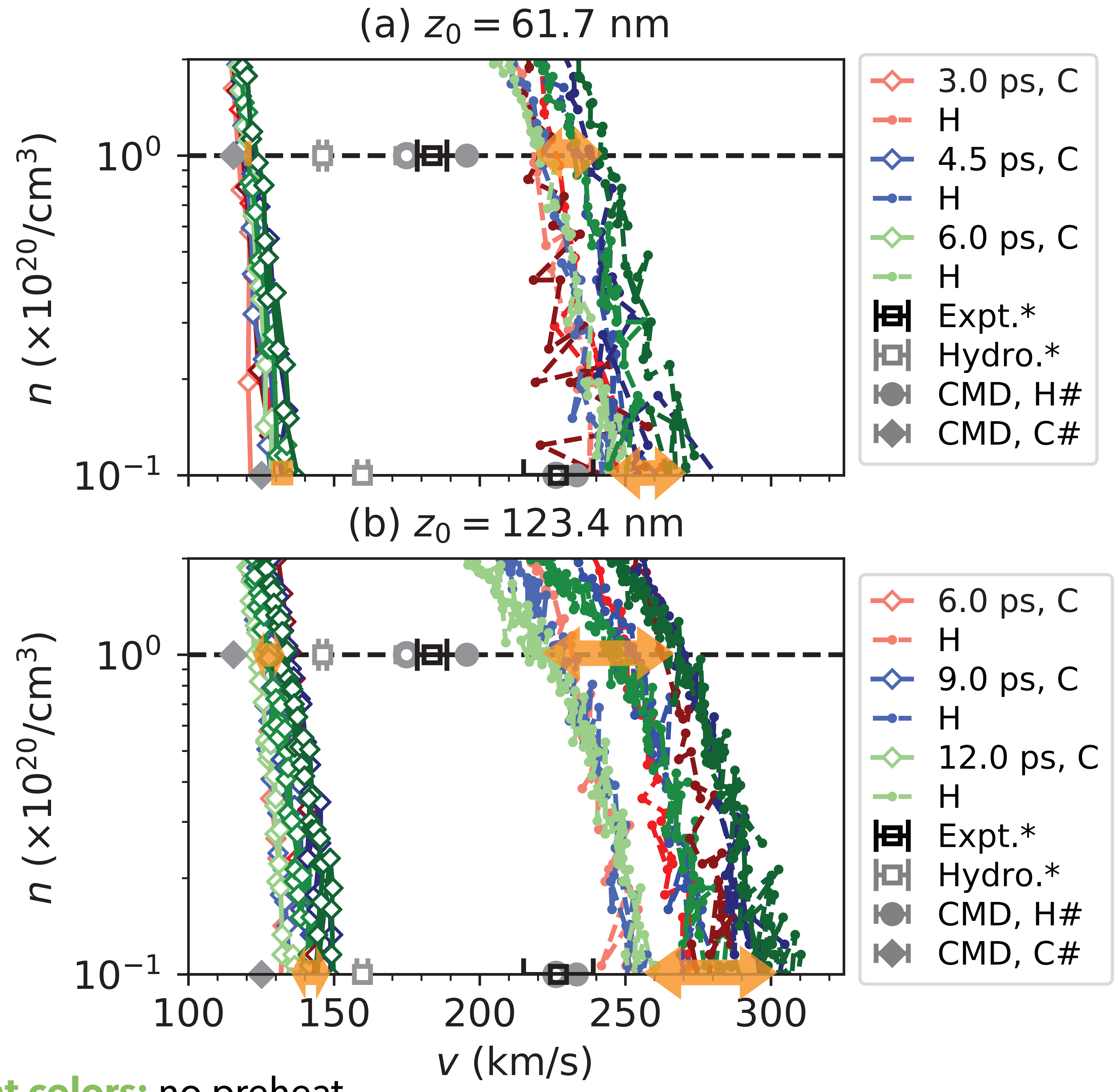

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Extrapolating to z_0=37 μm w/ 10% preexpansion

- v^C and s^C comparable to expt.
- H runs ahead w/ much higher v and s

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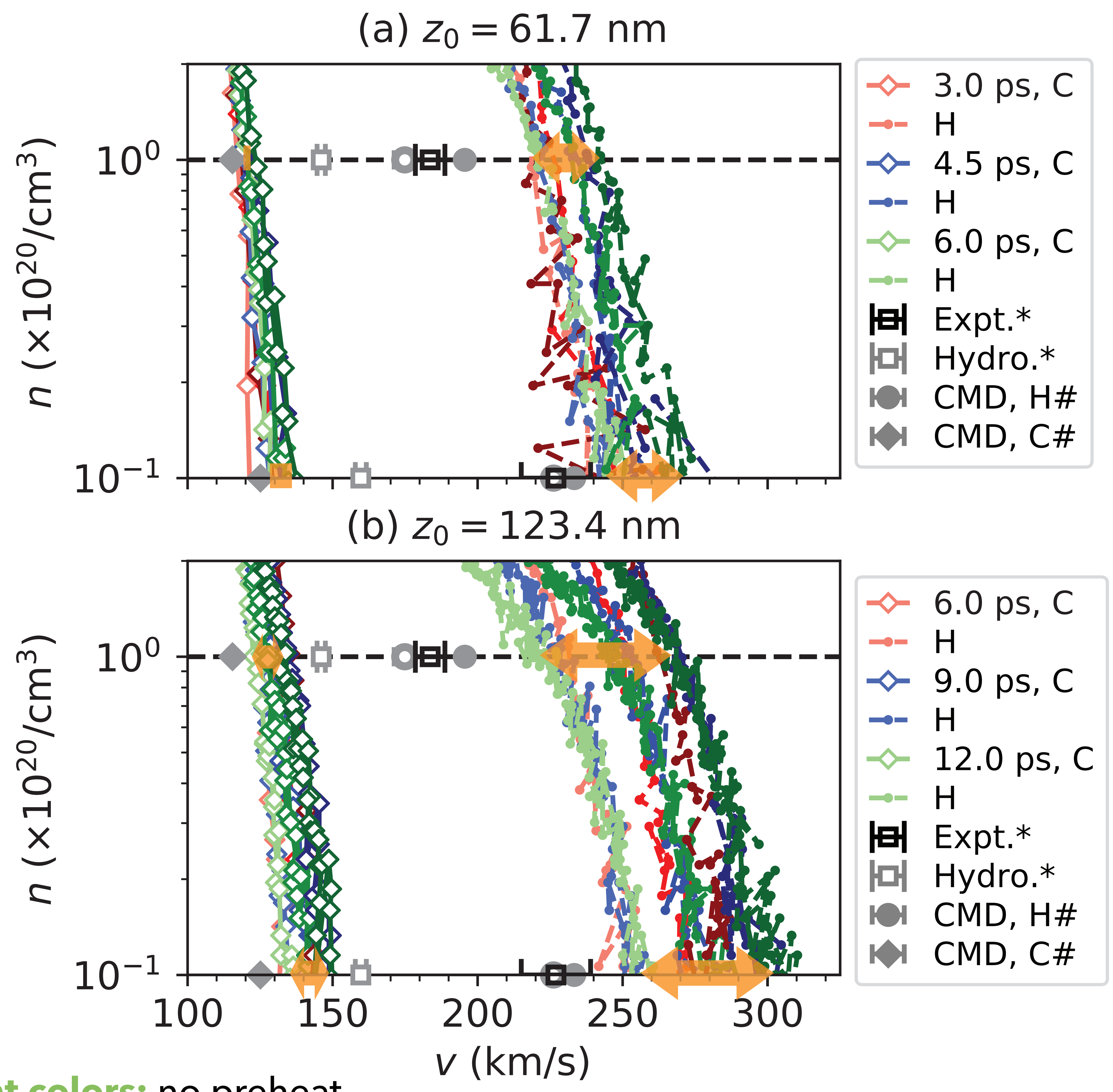

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Preexpansion, if happened in expt.*, shall be <<1 μm

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