Connecting Small Scale and Large Scale with CoDa III : Inhomogeneous Reionization and Chemical Enrichment with Observational Signatures

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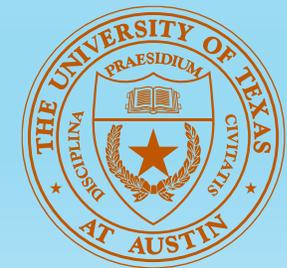
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https://coda-simulation.github.io/

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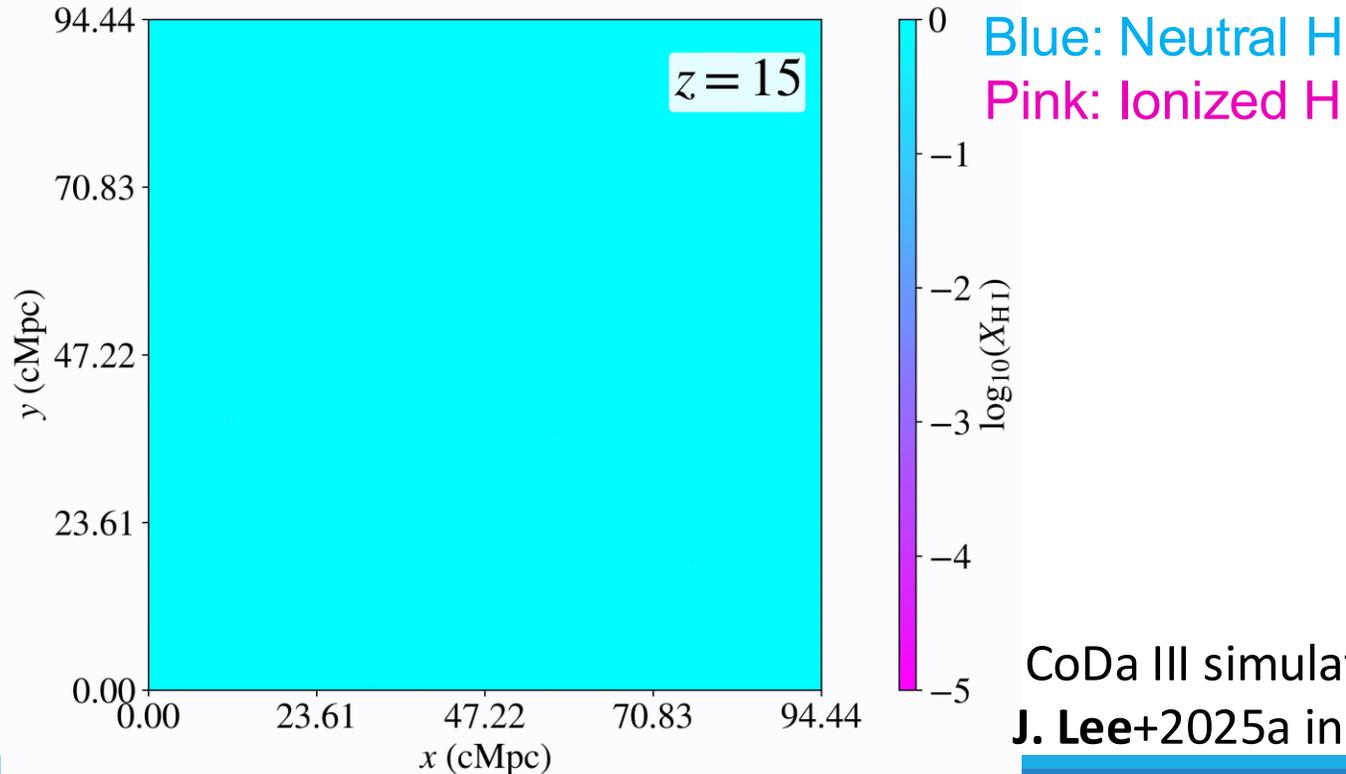
Cosmic Dawn: Epoch of Reionization (EoR)

- The second phase transition: neutral → ionized (cf. recombination: ionized → neutral)

- At $z{\sim}20-30$, first stars and galaxies start to form in DM (mini-)halos that collapsed early

- Ultraviolet (UV) photons emitted from **massive stars** in galaxies ionized surrounding intergalactic medium (IGM)
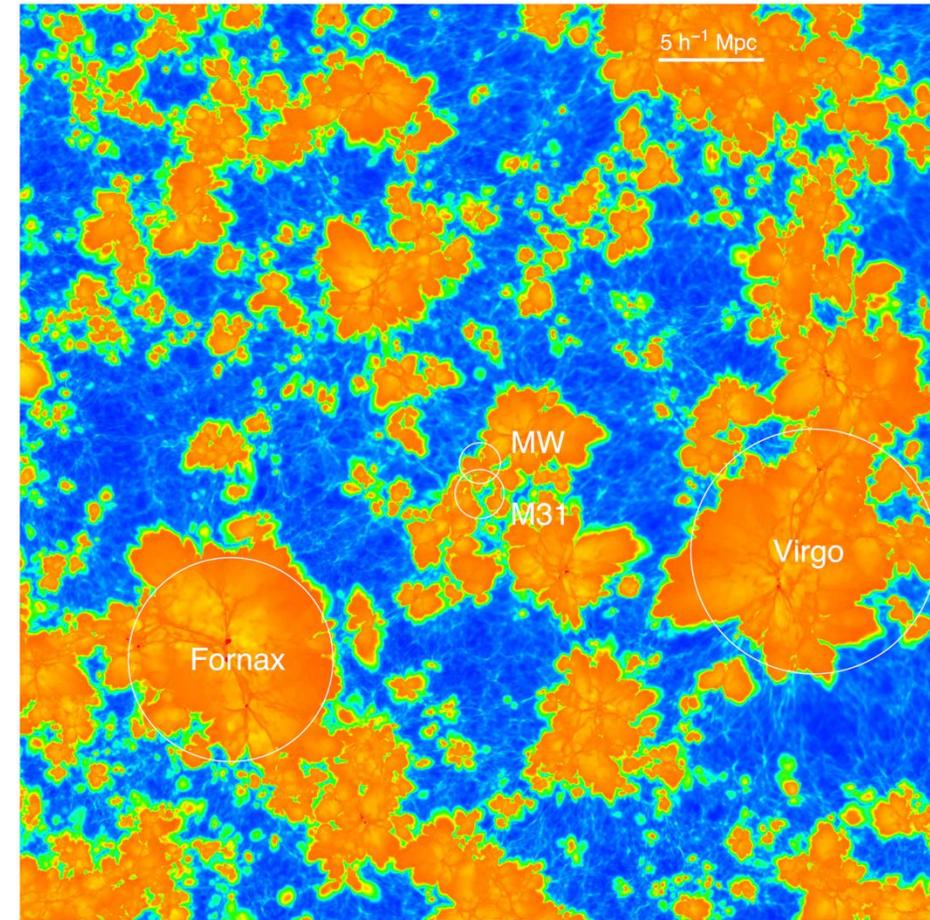

Robertson 2022

Inhomogeneous Reionization: Imprint of Large-scale Structure

- Cosmic HII regions (Shapiro & Giroux 97) or **ionized (hydrogen or HII) bubbles**

- **Inhomogeneity** arises from clustering of matter → traces underlying large-scale structure

Blue: Neutral H
Pink: Ionized H

$z = 15$

$\log_{10}(X_{HI})$

CoDa III simulation;
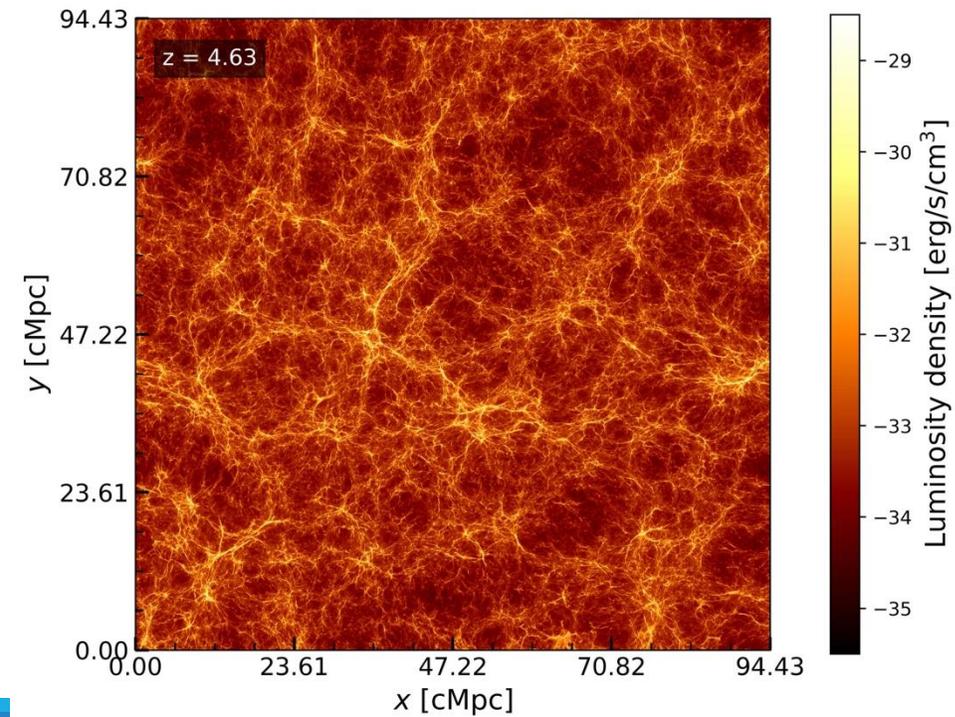**J. Lee**+2025a in prep

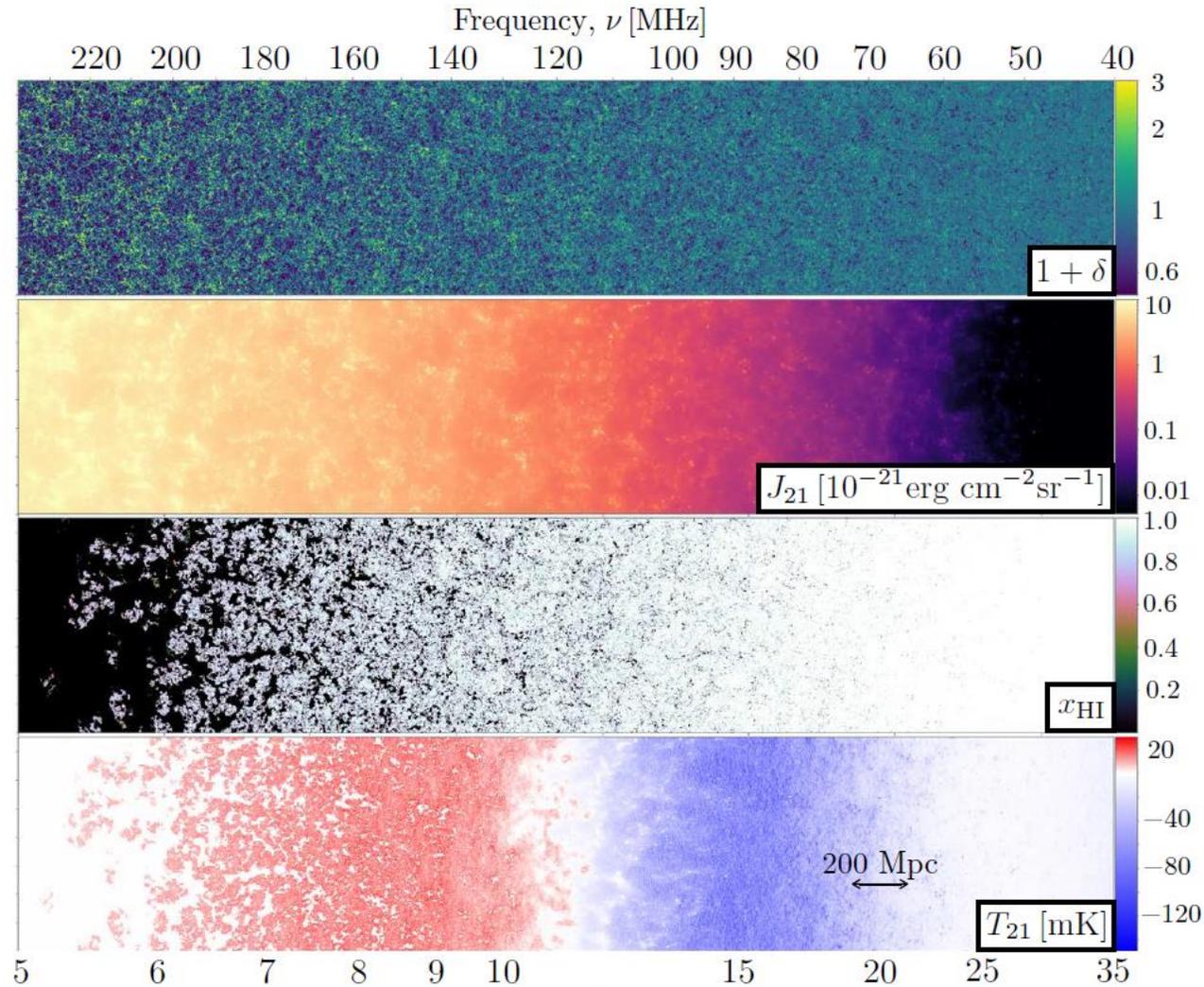

Blue: Neutral H
Orange: Ionized H

CoDa I simulation; Ocvirk+2016

Inhomogeneous Reionization: Imprint of Large-scale Structure

- Line-intensity mapping (LIM) observe reionization & clustering of matter directly: 21-cm (SKA, HERA, LOFAR, CHIME, etc.), Hydrogen lines, Lyα, Hα, Hβ (SPHEREx), molecular lines, CO (COMAP; Jianrong's talk)
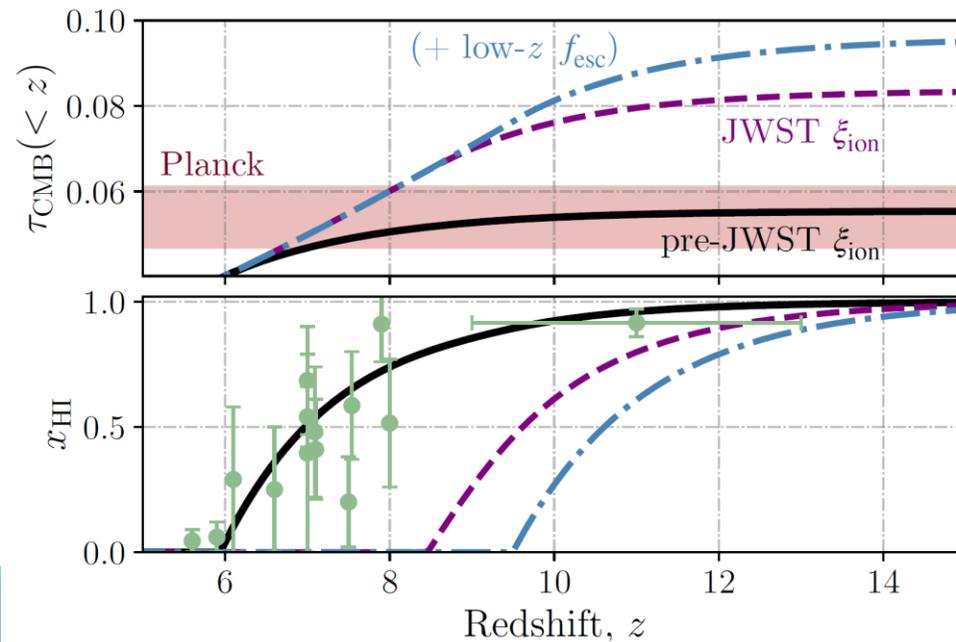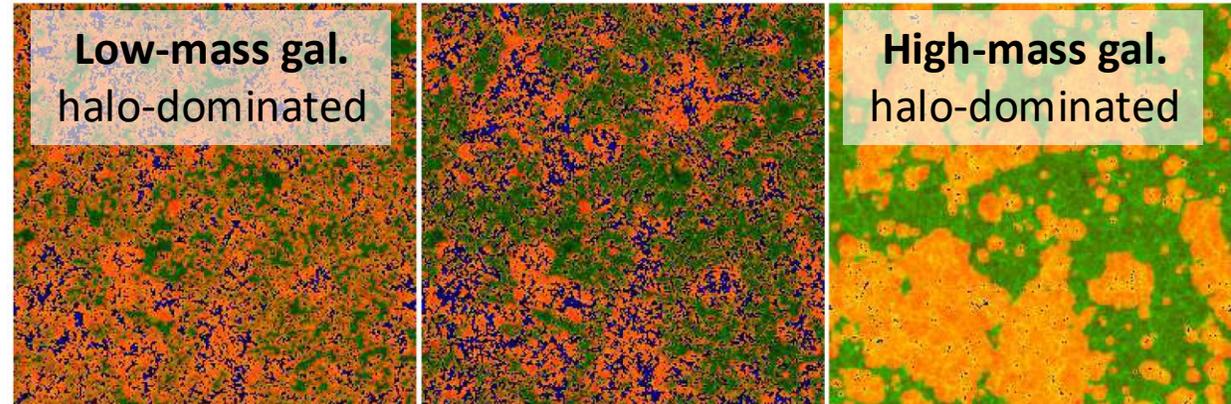
Hα map from CoDa III sim; H. Lee+2025

Semi-numerical prediction of 21-cm map; Muñoz+2022

Drivers of Reionization: Stars in Galaxies

- With same DM halos, galactic physics alter reionization topology & history

- Each galaxy has

1. Rate of ionizing radiation

   ($\dot{N}_\gamma$; cf., $\dot{N}_\gamma = L_{\mathrm{UV}}\xi_{\mathrm{ion}}$)

2. Escape fraction of radiation f_{esc}

- Decided by star formation history, initial mass function (IMF), interstellar medium (ISM) & dust, stellar spectrum models (e.g., inclusion of binary stars)
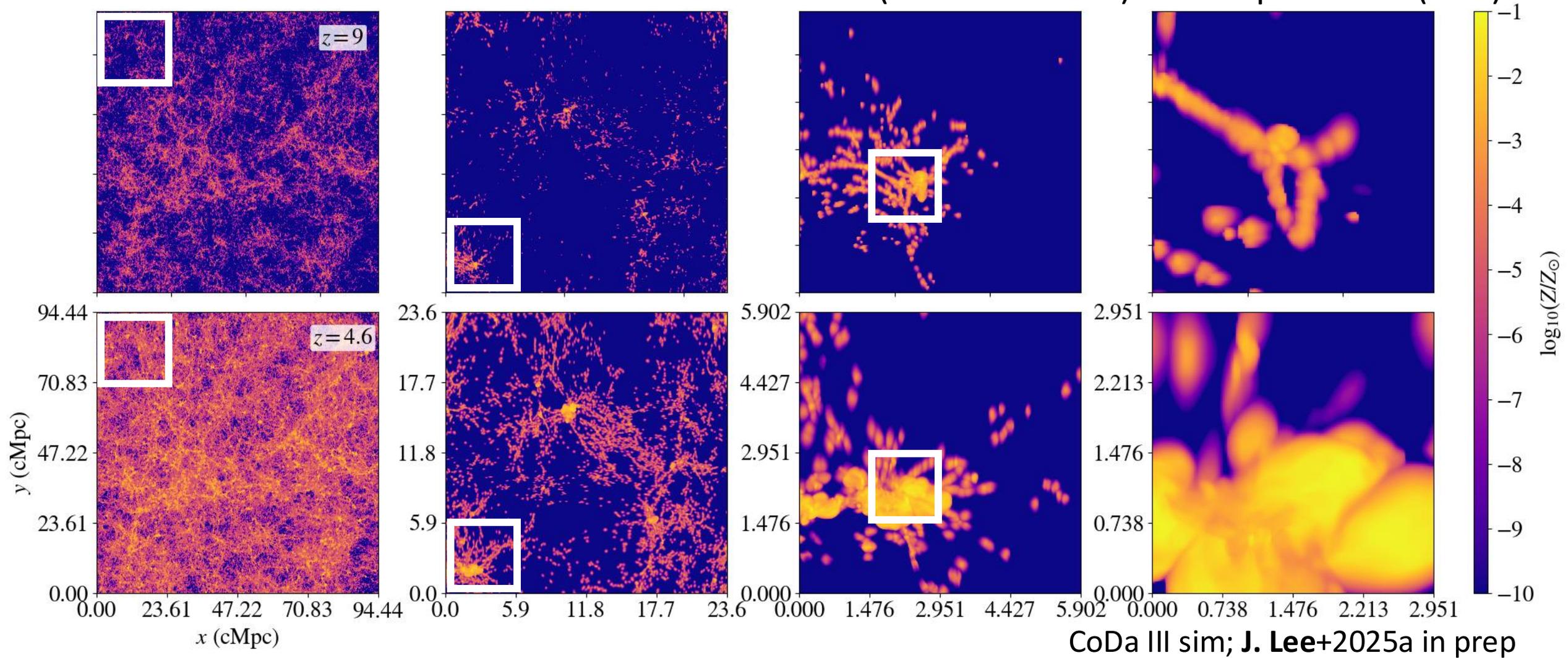
Green: Neutral H
Orange: Ionized H
Blue: Galaxies

Low-mass gal. halo-dominated

High-mass gal. halo-dominated

Reionization topology; Iliev+2012

Reionization history; Muñoz+2024
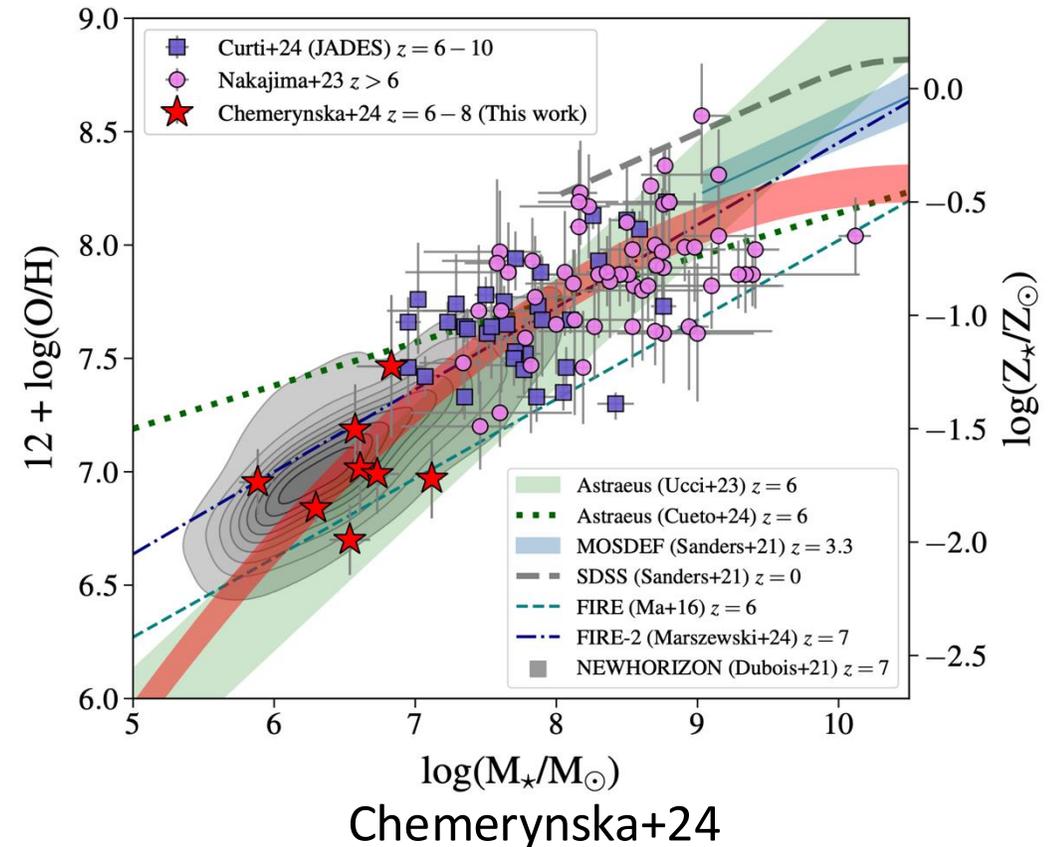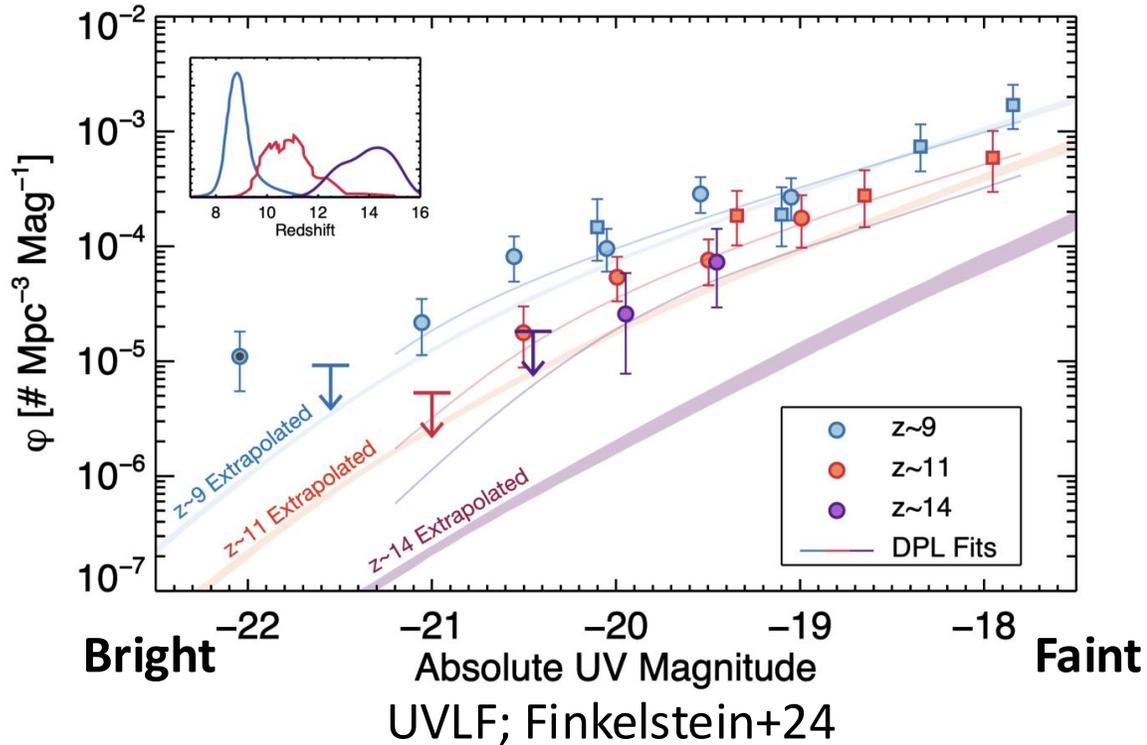
Metal Enrichment—Another Inhomogeneous Process

- Same **massive stars** reionized also metal-enriched (elements > He) with supernovae (SNe)

CoDa III sim; **J. Lee**+2025a in prep

Galaxies in EoR: Pushing the Limit with JWST

- UV Luminosity Function (UVLF) := Number density of galaxies with certain UV luminosity
  → Overabundance of UV-bright galaxies at high redshift, especially z > 10 (see Julian's talk)

- Mass-metallicity relation (MZR) := Stellar mass vs. metal abundance
  → Less metals & flatter slope than local relation
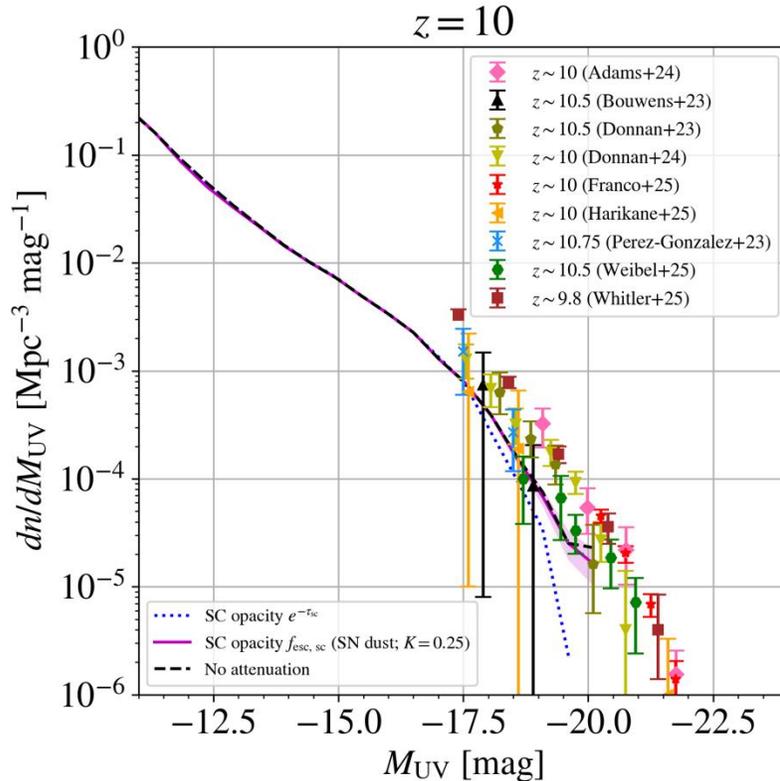
UVLF; Finkelstein+24

Chemerynska+24

Simulating EoR: Connecting Small-scale and Large-scale Physics
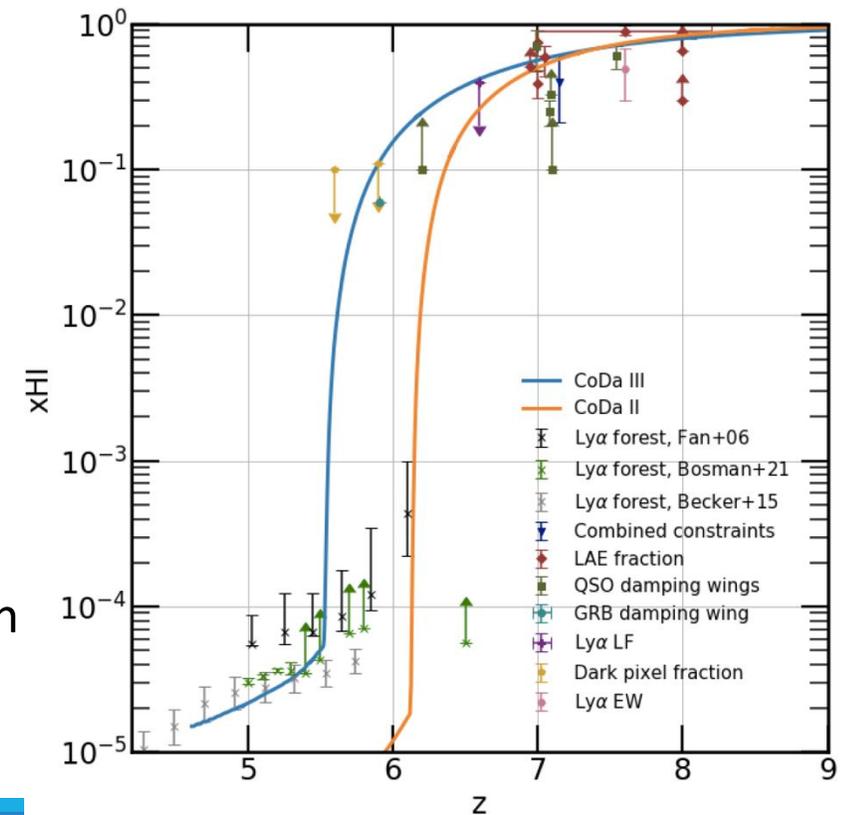
- Fully coupled radiation hydrodynamics simulation

1. Reproduces global reionzation history (large scale)

2. Matches observables (small scale): stellar mass function, UVLF, MZR, ionized H bubble size

Observable:
UVLF from CoDa III;
(**J. Lee**+2025b
in prep)

Reionization:
Neutral fraction
from CoDa III;
(Lewis+2022)

Cosmic Dawn (CoDa) III Simulation

- Evolution of metal & dust, with dust opacity in ionizing radiation

- 8192^3 particles + cells in $(94.4 \text{ Mpc})^3$, uni-grid rad-hydro simulation by RAMSES-CUDATON, GPU-accelerated code

  ➔ First **trillion-element** computer simulation of fully-coupled galaxy formation and reionization **(20 PB data!)**
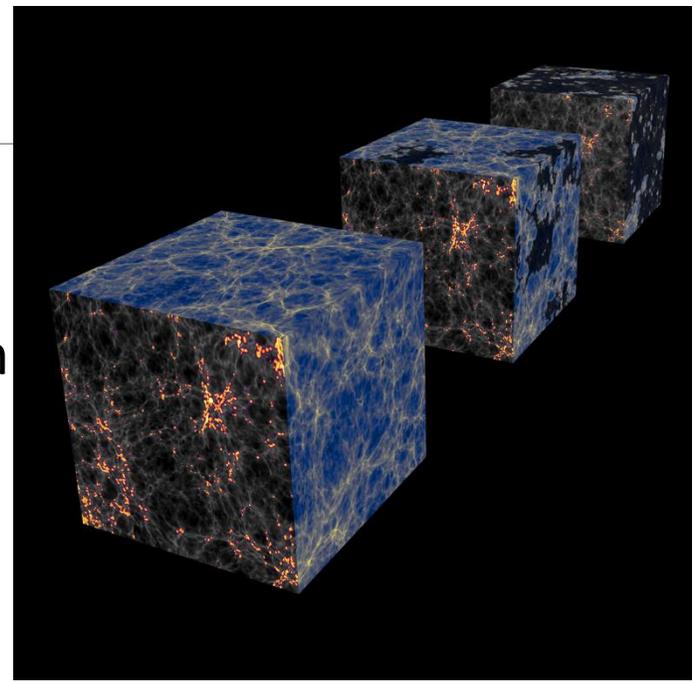
Advantages

1. **High mass resolution**: resolves all atomic cooling halos ($M_h \geq 10^8 M_\odot$) and IGM clumping

2. **Self-regulation of reionization**: ionizing radiation feedback suppresses star formation in low-mass halos

3. **Large volume**: tracks patchiness of reionization and full dynamic range of halo mass with good statistics

The Cosmic Dawn ("CoDa") Project Website
https://coda-simulation.github.io/
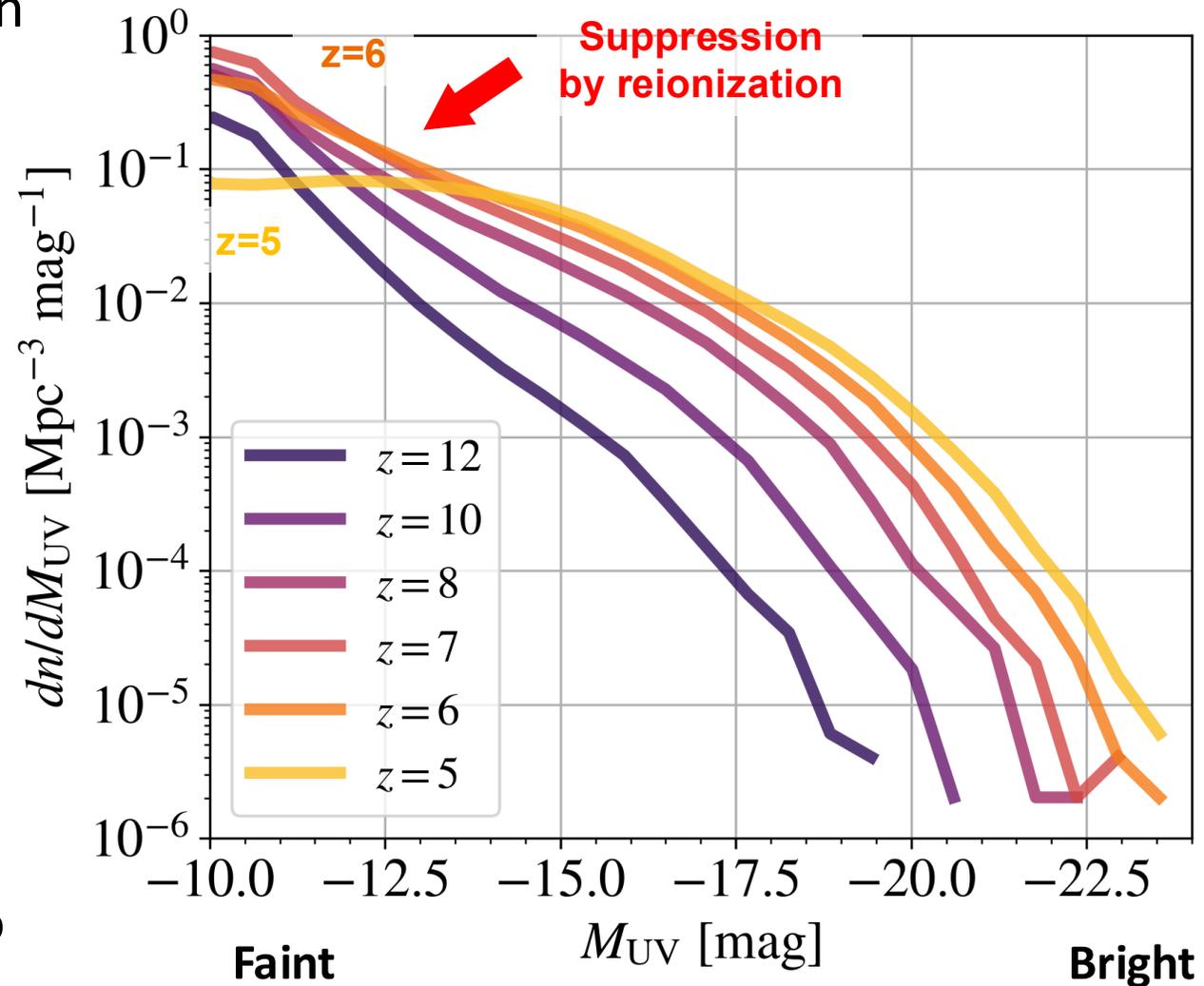

Lewis+2022

Blue: Ionized H
Black: Neutral H
Pink: High-T gas

Redshift Evolution of UVLF: Roll-over in UV-faint Galaxies

- Suppression of star formation by reionization in galaxies $M_{\mathrm{UV}} > -14$
  → **Signature of reionization!**
  (may be observable using lensed field with enough # of galaxies…)

- In reionized regions, Jeans-mass filtering prevents gas supplied to low-mass halos
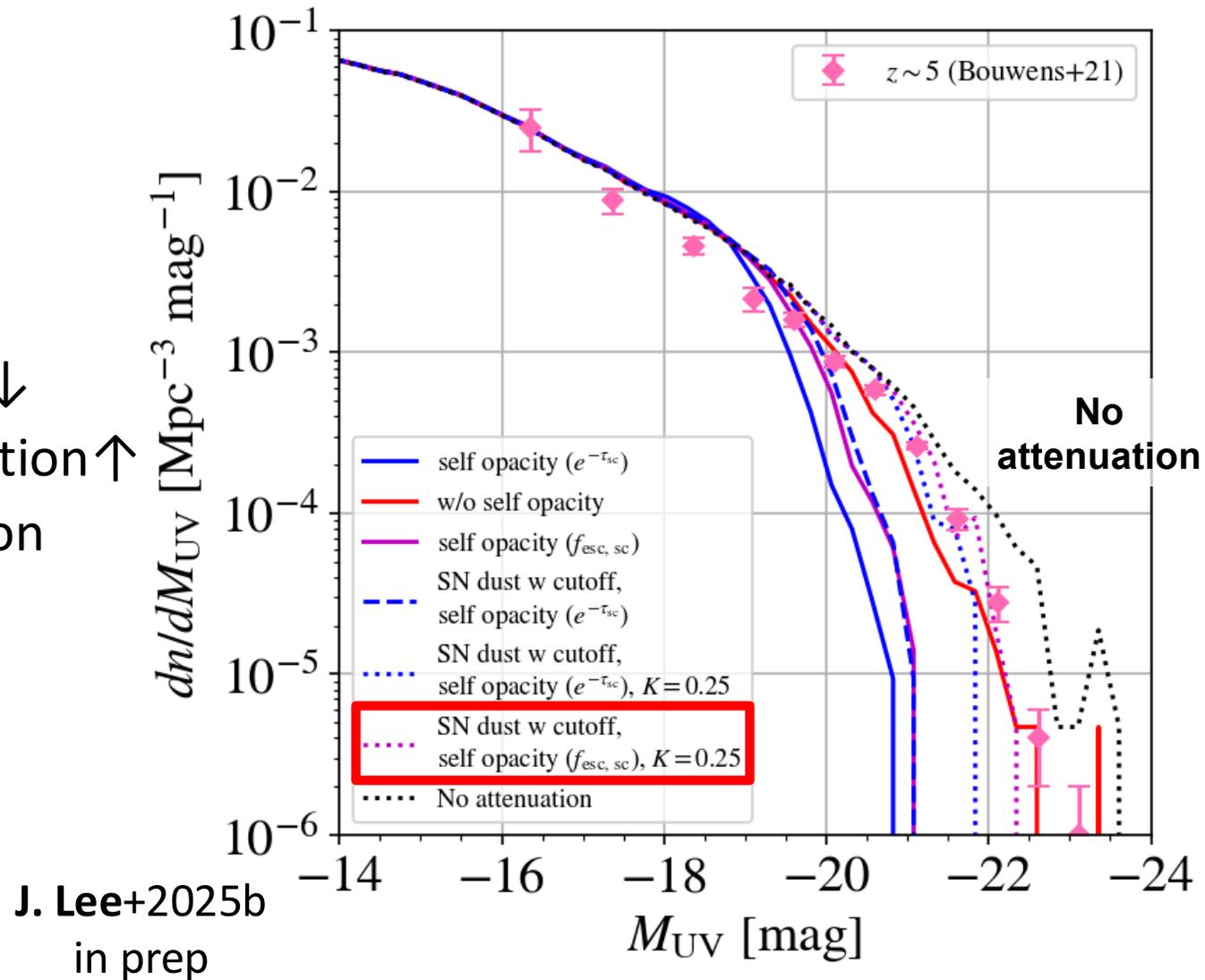 → Reduces UV luminosity in low-mass halos

J. Lee+2025b
in prep

Effect of Dust Attenuation Modeling on UV Luminosity Function

- With fixed dust mass, we can vary

1. Dust grain size distribution:

   Larger size → less UV attenuation

2. Sub-grid star-dust geometry:

   Evenly distributed stars → attenuation↓

   Centrally concentrated stars → attenuation↑
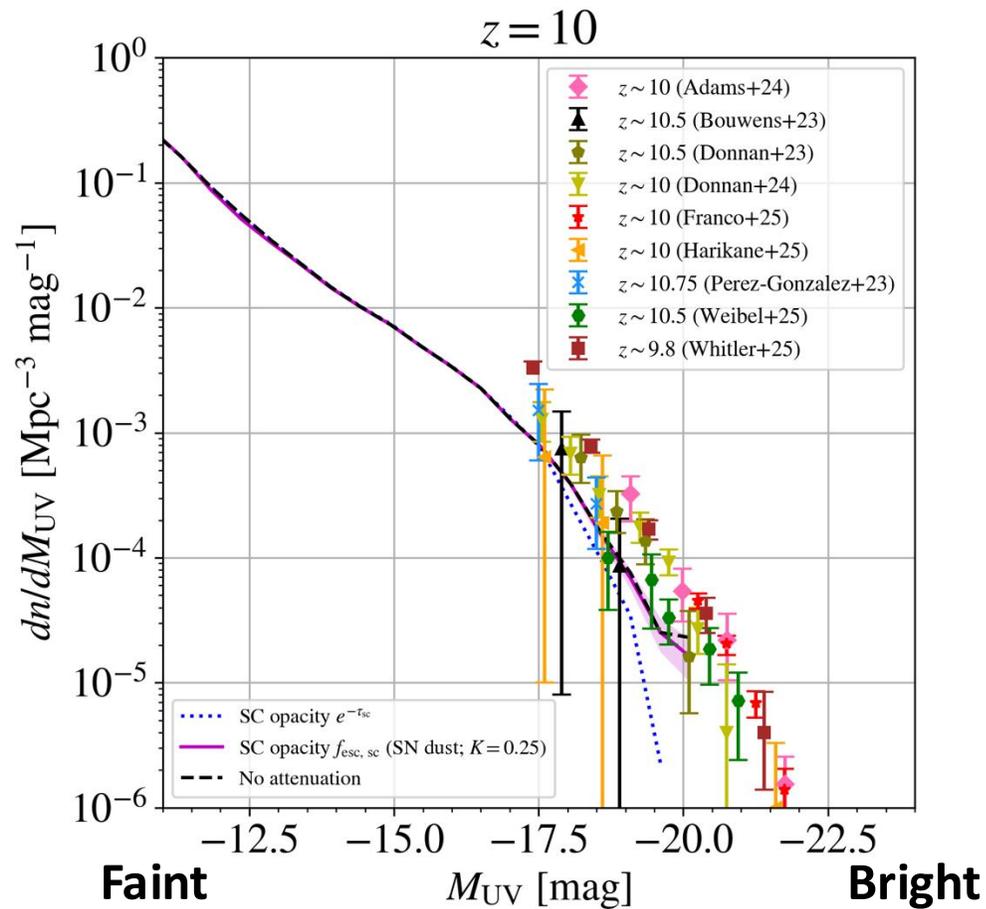
   Stars are in foreground → no attenuation

- Best match (z = 5):

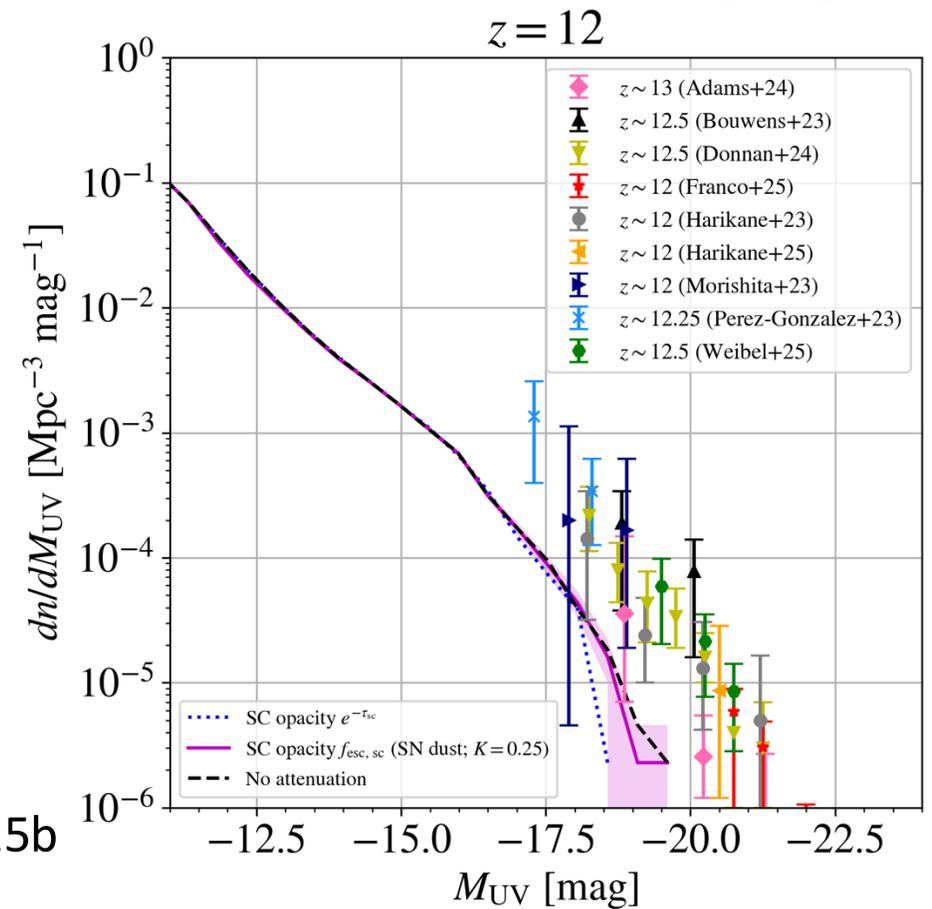 dust mass reduced by ¼

  + evenly distributed stars in a cell

J. Lee+2025b
in prep

UV Luminosity Function at z > 10: Success…?

- CoDa III matches z = 10 observations

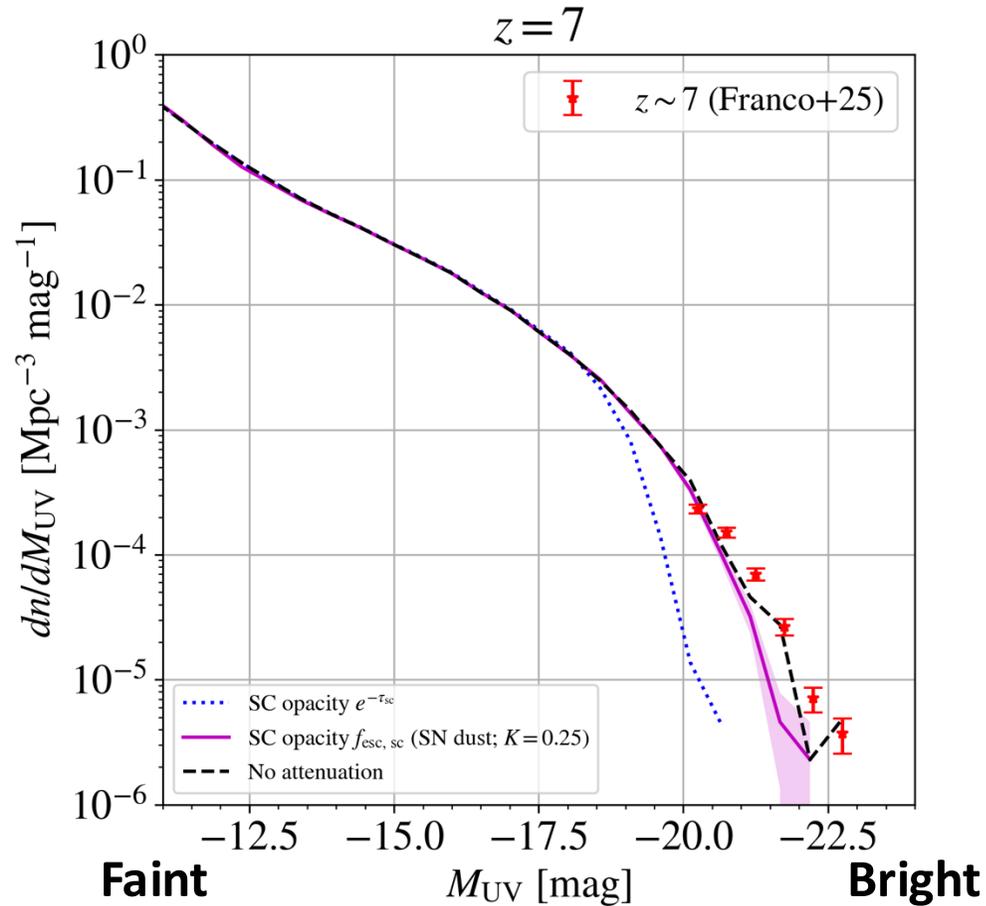- Compared to simulated UVLF, z = 12 observations found **overabundance of bright galaxies**
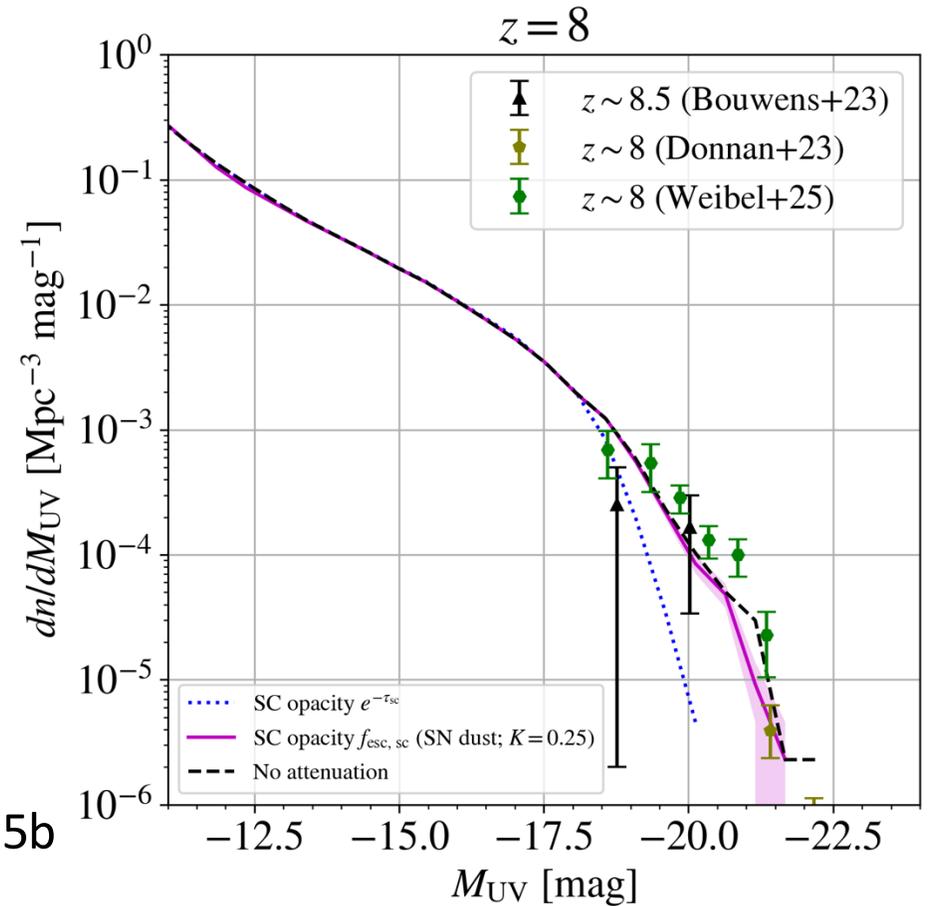

J. Lee+2025b
in prep

UV Luminosity Function at z = 7, 8: Success!

- Matches well!

- More dust attenuation on the bright end

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in prep
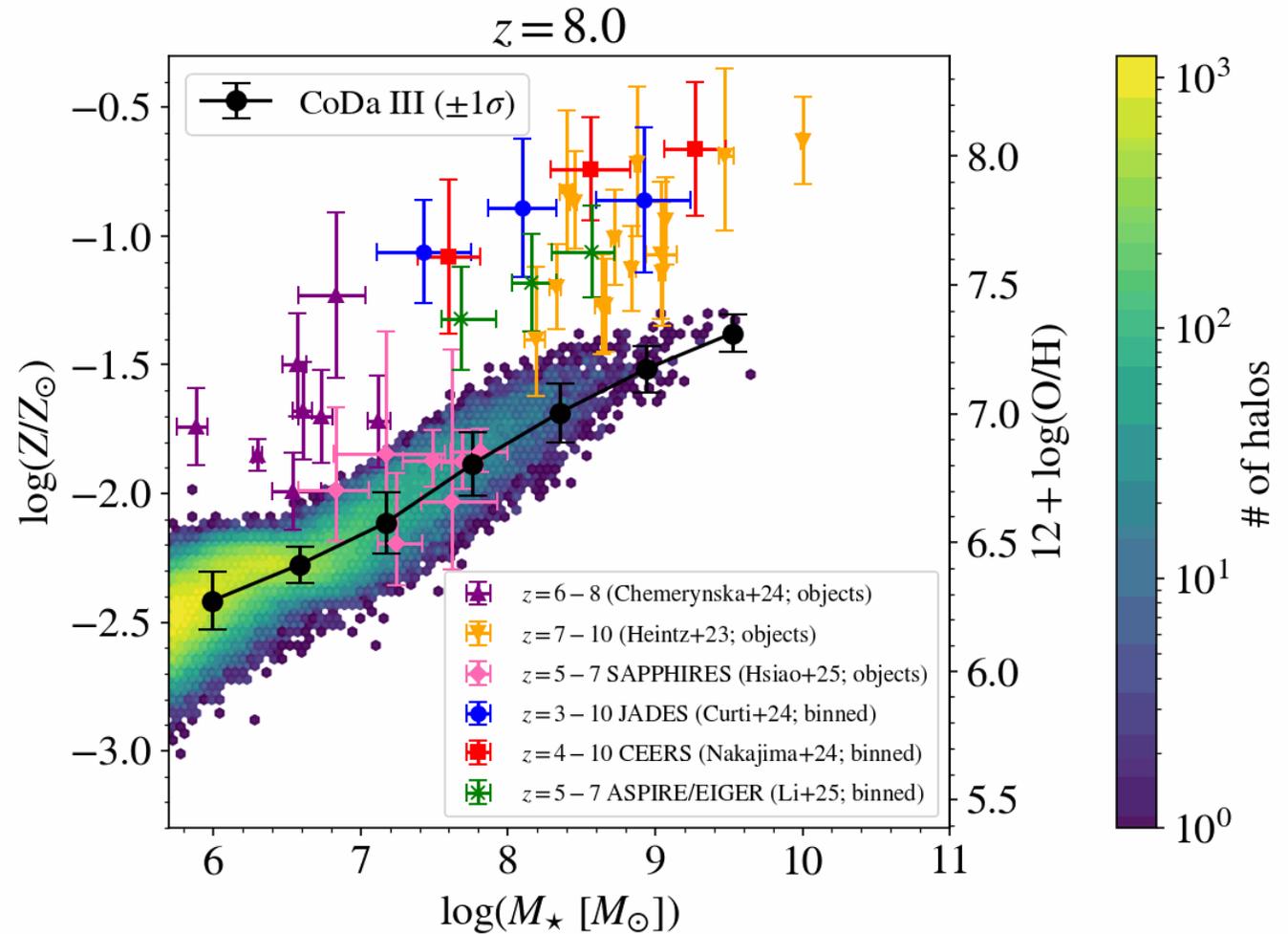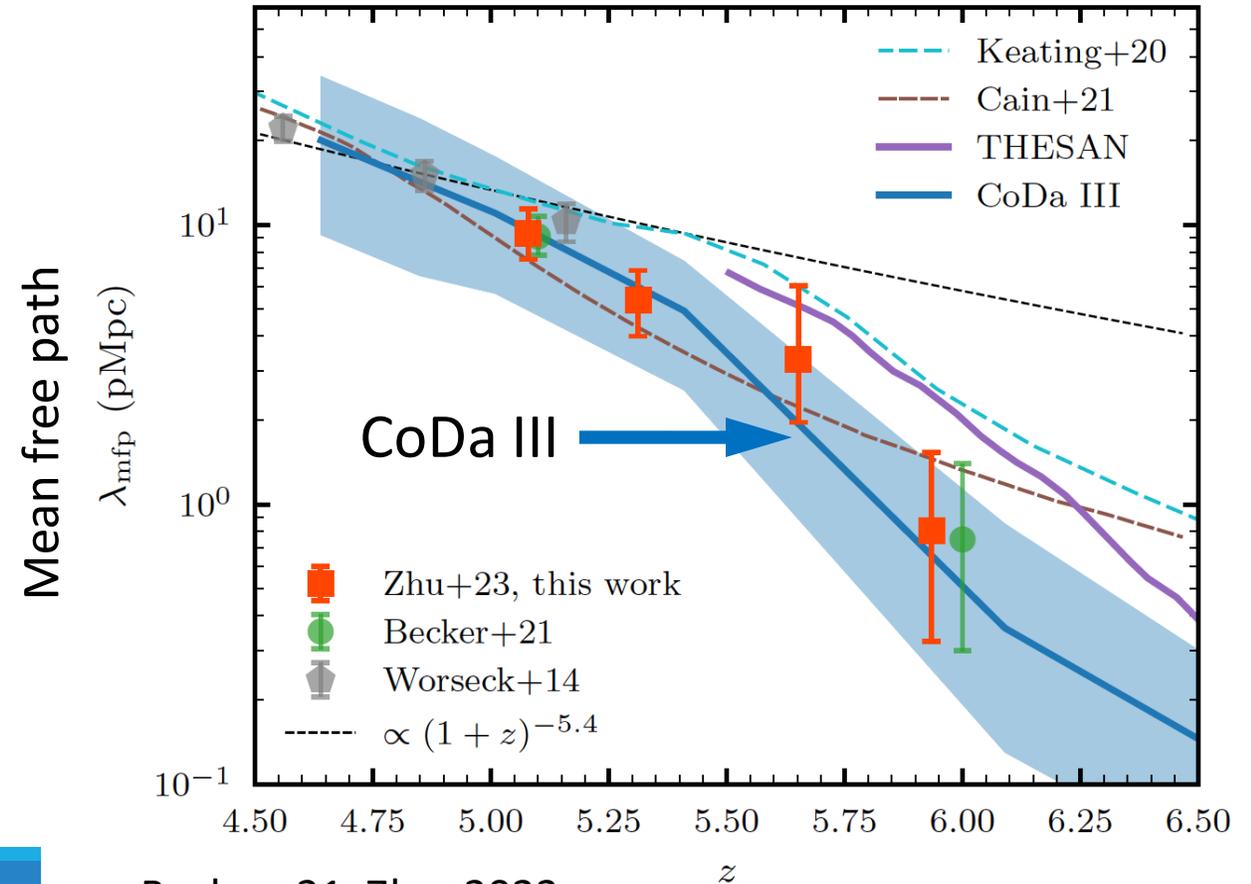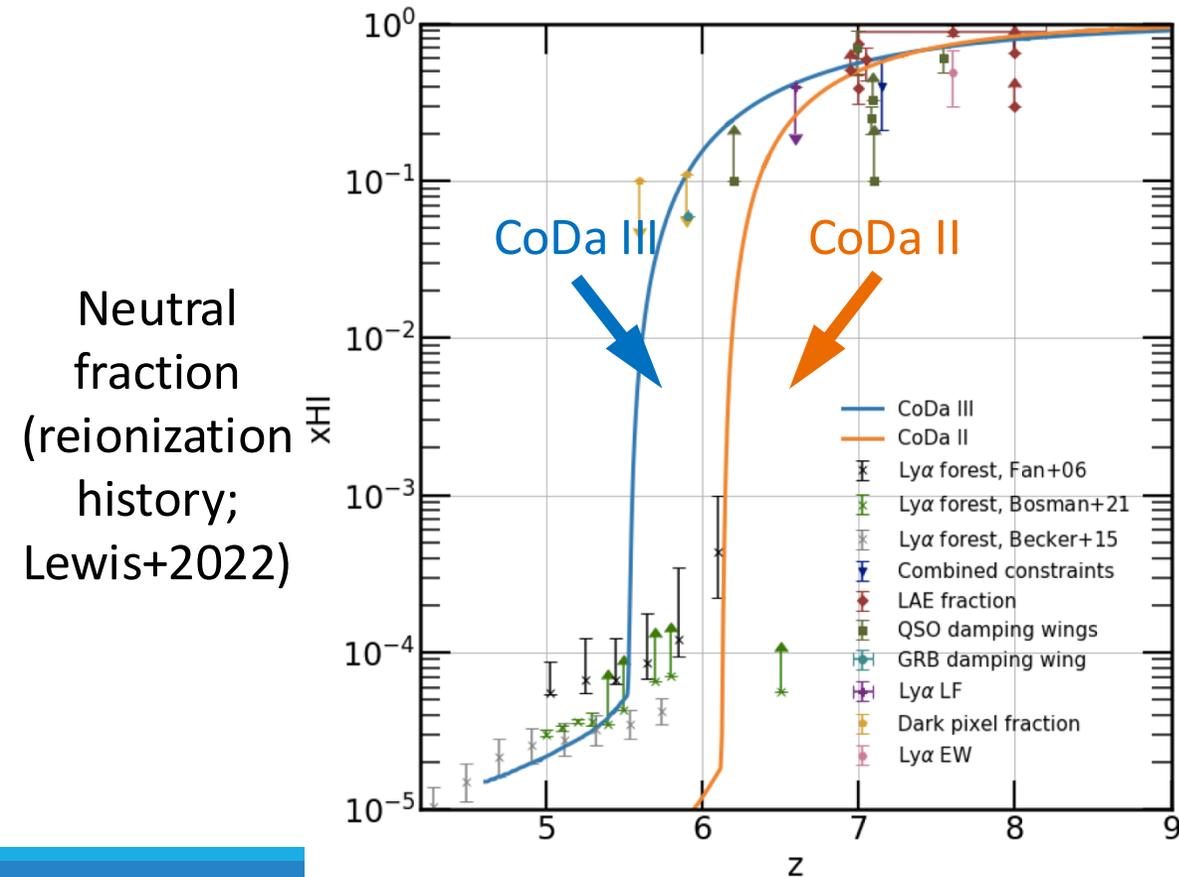
Galaxy Mass-Metallicity Relation (MZR)

- Little evolution at $z \sim 5 - 8$ for $M_\star \geq 10^7 M_\odot$; steepens over time for $M_\star \leq 10^7 M_\odot$

- A little lower than observations but within the scatter

- Slightly shallower slope ($M_\star \approx 10^7 M_\odot$) $\rightarrow$ shallower slope at low-mass end is hinted in observation (e.g., Curti+24)

J. Lee+2025a
in prep

Reionization History: Huge Success!

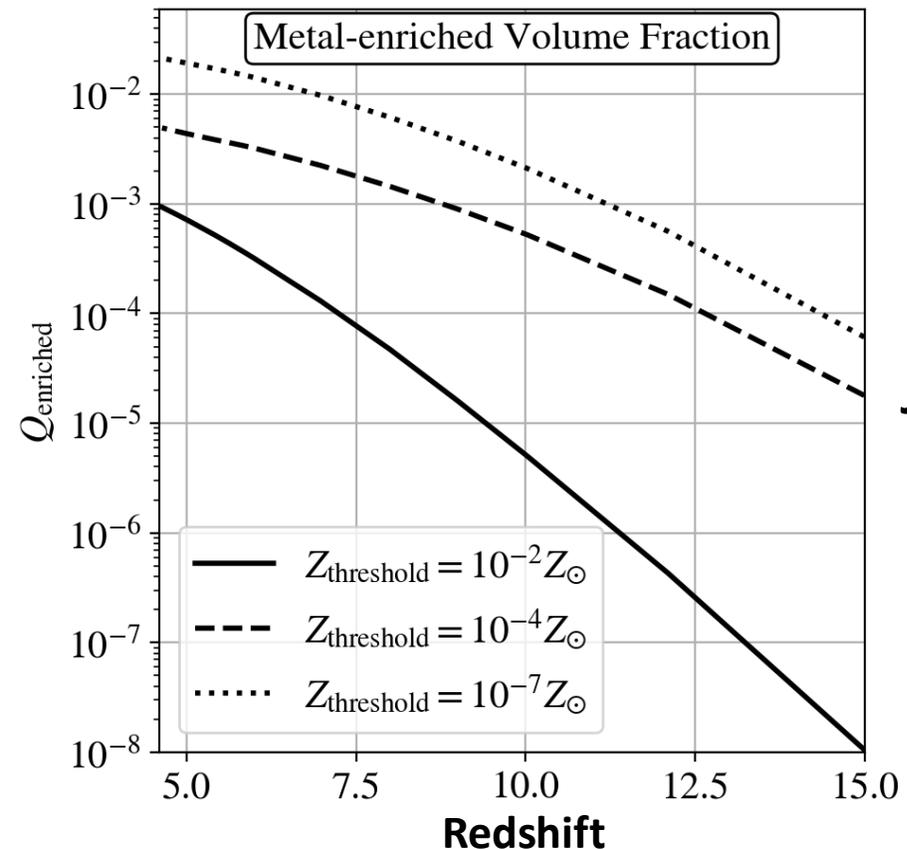- CoDa III matches both global reionization history & mean free path evolution at z < 6 while reproducing galaxy properties, UVLF and MZR

- (Remark: z > 12 overabundant galaxies do not affect reionization history)

Neutral fraction (reionization history; Lewis+2022)

CoDa III

CoDa II

Becker+21, Zhu+2023

Global Reionization vs. Metal Enrichment

- Reionization ionization-fronts (I-fronts) travel farther, faster than metal enrichment ("Z-fronts"; i.e., SN-driven galactic winds) ➜ Q = volume filling fractions, $Q_{\mathrm{H\,II}} > Q_Z$

- Even after EoR, most of IGM still metal-free: $Q_Z < 2\,\%\ (Z > Z_{\mathrm{threshold}} = 10^{-7}Z_{\odot})$

J. Lee+2025a
in prep

Global Metal Enrichment and Star Formation

- $Z_{\mathrm{baryon}}/Z_\odot \sim 1 \times 10^{-3}$ at $z_{\mathrm{reion}} = 5.53$ ($x_{\mathrm{H\,II}} = 99.99\%$)

- **Prediction from simple model correlating *reionization* and *metal enrichment* worked!**

- Pop III SF persists to z = 5.5

J. Lee+2025a
in prep

Reionization and Metal Enrichment in CoDa III

Ionized Fraction, $X_{\mathrm{H\,II}}$

Metallicity, Z

$z = 5.6$

J. Lee+2025a in prep

Hα Line-intensity Mapping: Probe of Star Formation and Reionization (?)

- Hα produced from ionized H can trace star-forming galaxies and ionized IGM

- Non-negligible contribution from IGM: SPHEREx might see with galaxy-Hα cross-correlation?

H. Lee+2025, **J. Lee**+2026 in prep

Growth of Metal-enriched Bubbles—FoF

- Characteristic size ~100 ckpc

- Sharp reduction of smaller bubble number after reionization

→ **Signature of reionization end!!**

J. Lee+2025a
in prep

Metal-enriched bubble size

Growth of bubbles

Post-reionization flattening

Legend: $z = 15.0$, $z = 12.1$, $z = 9.0$, $z = 5.6$, $z = 5.4$, $z = 4.6$

x-axis: R [cMpc]
y-axis: dn/dR [(cMpc)$^{-4}$]

$z = 9$

$z = 4.6$

colorbar: $\log_{10}(Z/Z_\odot)$

Growth of Ionized Bubbles—Mean Free Path

- Bubble size is correlated with local reionization redshift (z_{re})

- CoDa III agrees with recent JWST observations using Lyα damping wing (if MFP bubble sizes traced from galaxies) **c.f., brighter galaxies are biased tracers of larger bubbles!**

All cells

$M_{\mathrm{UV}} < -20$

$M_{\mathrm{UV}} < -17$

Galaxy-biased

Local reionization redshift $z_{\mathrm{re,\,90\%}}$

MFP Bubble size $z = 15.0$, $\bar{x}_{\mathrm{HI}} = 0.999$

J. Lee+2025a

"Metallicity Gap"—Analog of Lyα "Dark Gap" on Quasar Sight Lines

- Ionized H II bubbles vs. (neutral) IGM patches optically thick to Lyα (or Lyβ)

  ←→ *"Dark gaps"* in Lyα (or Lyβ) forest, distances between ionized patches

"Metallicity Gap"—Analog of Lyα "Dark Gap" on Quasar Sight Lines

- Ionized H II bubbles vs. (neutral) IGM patches optically thick to Lyα (or Lyβ)
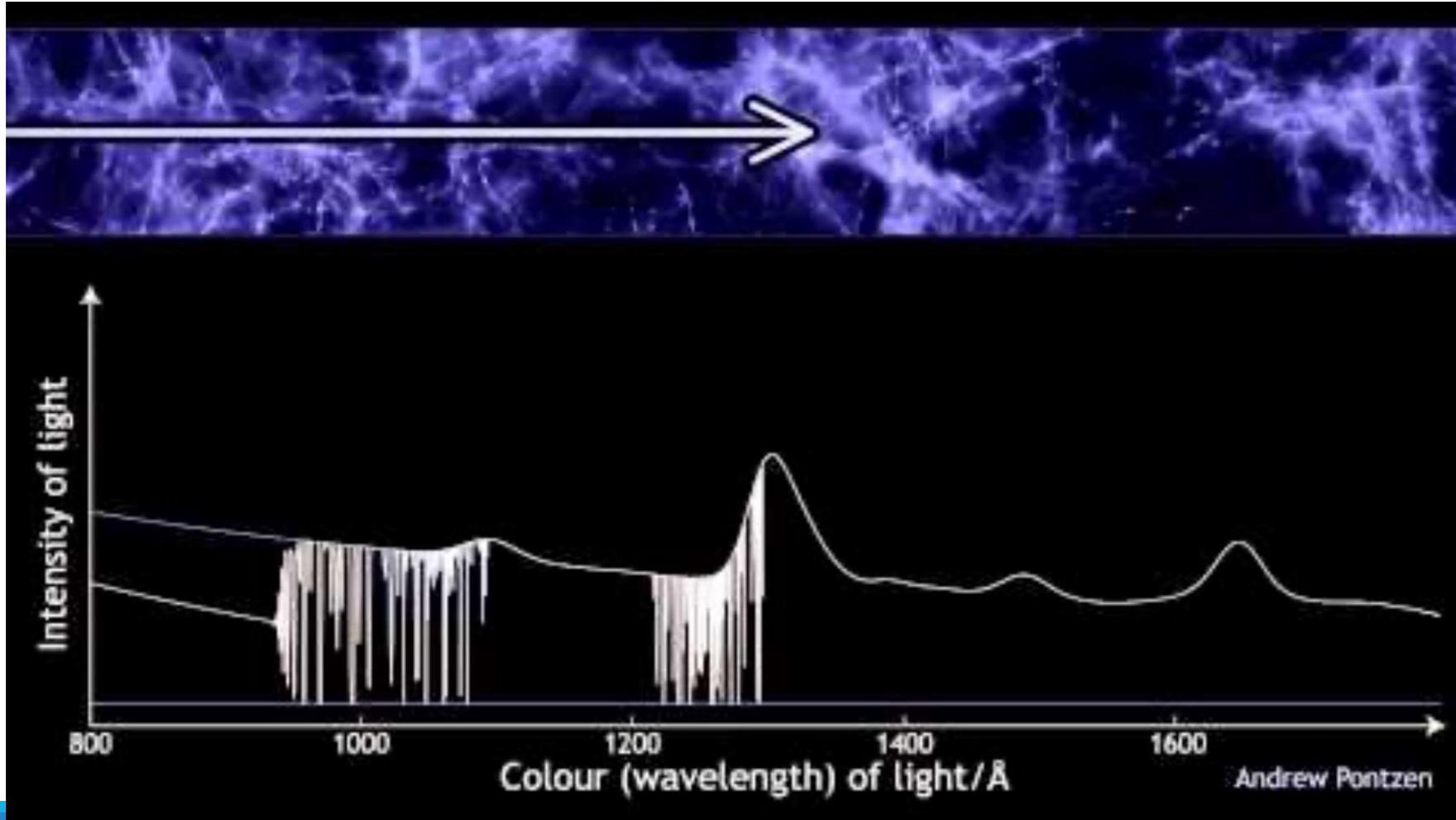
  ←→ *"Dark gaps"* in Lyα (or Lyβ) forest, distances between ionized patches

- Metal-enriched bubbles vs. Metal-free patches

  ←→ *"Metallicity gaps",* long distances between metal absorbers (e.g., C IV) in quasar spectra

Also see Fakhri's talk on CGM enrichment and metal absorbers

J. Lee+2025c in prep

Metallicity Gap Statistics

- Metallicity gap length decreases as the universe gets more enriched by metals

- Mean-free path of hitting metal-enriched regions (L_0) drops dramatically during EoR

Non-random clustering on small scales

J. Lee+2025c in prep

ρ_{gas}

$X_{\text{H I}}$

T_{gas}

Z

Metallicity gaps

Metallicity gap length decreases

Legend:
- $z = 10.02$, $L_0 = 52.4$
- $z = 8.00$, $L_0 = 25.6$
- $z = 5.99$, $L_0 = 15.0$
- $z = 4.64$, $L_0 = 12.8$
- Model Fit: $dN/d(\ln L) \propto L e^{-L/L0}$

$dN/d(\ln L_{Z,\,\text{gap}})$

$L_{Z,\,\text{gap}}$ [cMpc]

Summary

- **Small-scale—Galaxy**

  CoDa III galaxies match UV luminosity function (UVLF) & mass-metallicity relation (MZR) from JWST

- **Large-scale—Global**

1. CoDa III matches observed reionization history ($z_{\mathrm{re}} = 5.53$) & mean free path at the end of EoR

2. Same massive stars that reionized the universe enriched the universe to $\bar{Z}/Z_{\odot} = 10^{-3}$, with volume fraction $Q_Z < 2\%$ (when $Q_{\mathrm{HII}} = 100\%$), along with Pop III star formation down to $z = 5.5$

- **Large-scale—Inhomogeneous**

1. Hα line-intensity mapping (LIM) will detect both star-forming halos and reionization of IGM

2. Metal-enriched zones are characterized as "metal-enriched bubbles" along the cosmic web, and grow slower than ionized H bubbles, characterized and compared to observations

3. Metallicity gaps: a new observational diagnostic of inhomogeneous rise of metallicity & reionization

UVLF

- d

Massive Stars: Sources of Ionizing Photons & Metals

- *The same massive stars* **that released the ionizing photons also released the metals that enriched the universe by SNe** (Shapiro, Giroux & Babul 1994, Giroux & Shapiro 1996)

$$\Rightarrow \dot{n}_\gamma \propto \dot{\rho}_Z$$

- **Metals ejected in SNe per ionizing photon released over stellar lifetimes**

  For a Salpeter IMF, Shapiro and Giroux (1996) showed:

  η = **metal mass (in** $M_\odot$**) ejected per H ionizing photon (# of ph)** $\sim 10^{-62}$

- **# of ionizing photons per H atom required to finish reionization** ➔ **corresponding metallicity**

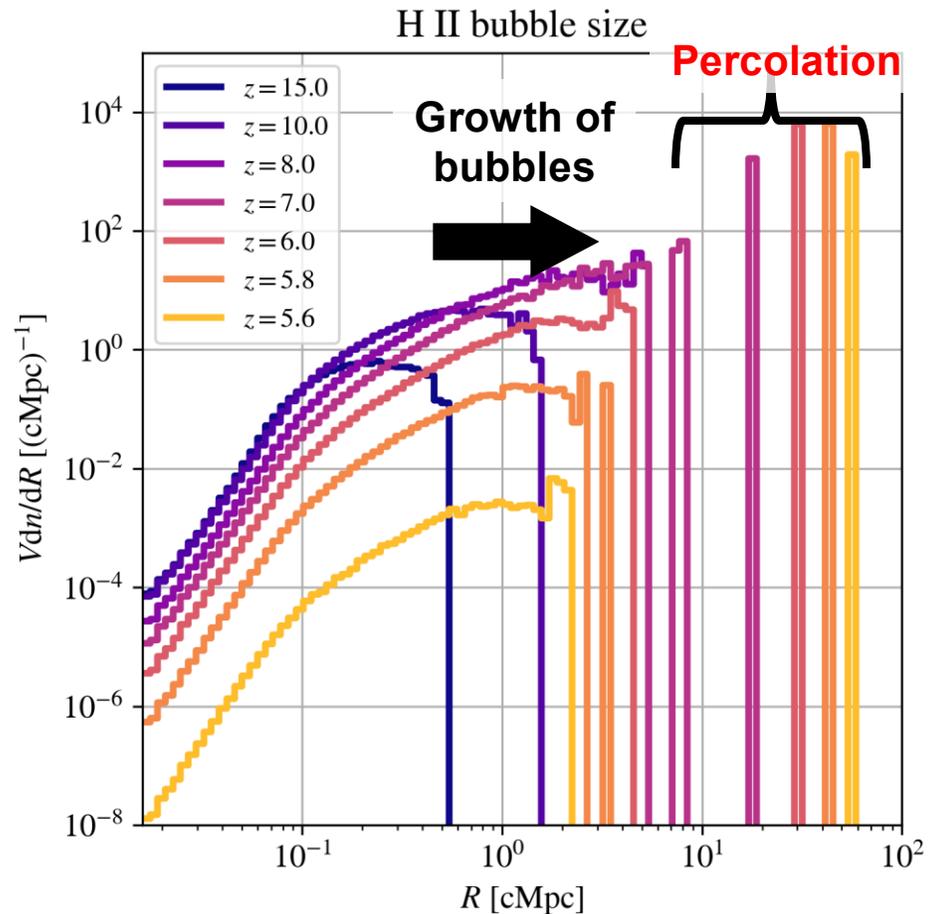 If $N_{\gamma,\mathrm{H}}$ = # of H-ionizing photons per H atom required to finish reionization,

  $$\left(Z/Z_\odot\right)_{\mathrm{reion}} \sim (\eta M_\odot N_{\gamma,\mathrm{H}})/(m_\mathrm{H} Z_\odot) = 5 \times 10^{-4} \times \left(\eta/10^{-62}\right) \times N_{\gamma,\mathrm{H}} \quad \text{(for } Z_\odot \sim 0.02\text{)}$$

  ➔ **For CoDa III (BPASS with Salpeter IMF),** $\eta = 0.25 \times 10^{-62}$**,** $N_{\gamma,\mathrm{H}} = 7.6$ **(from sim. Output)**
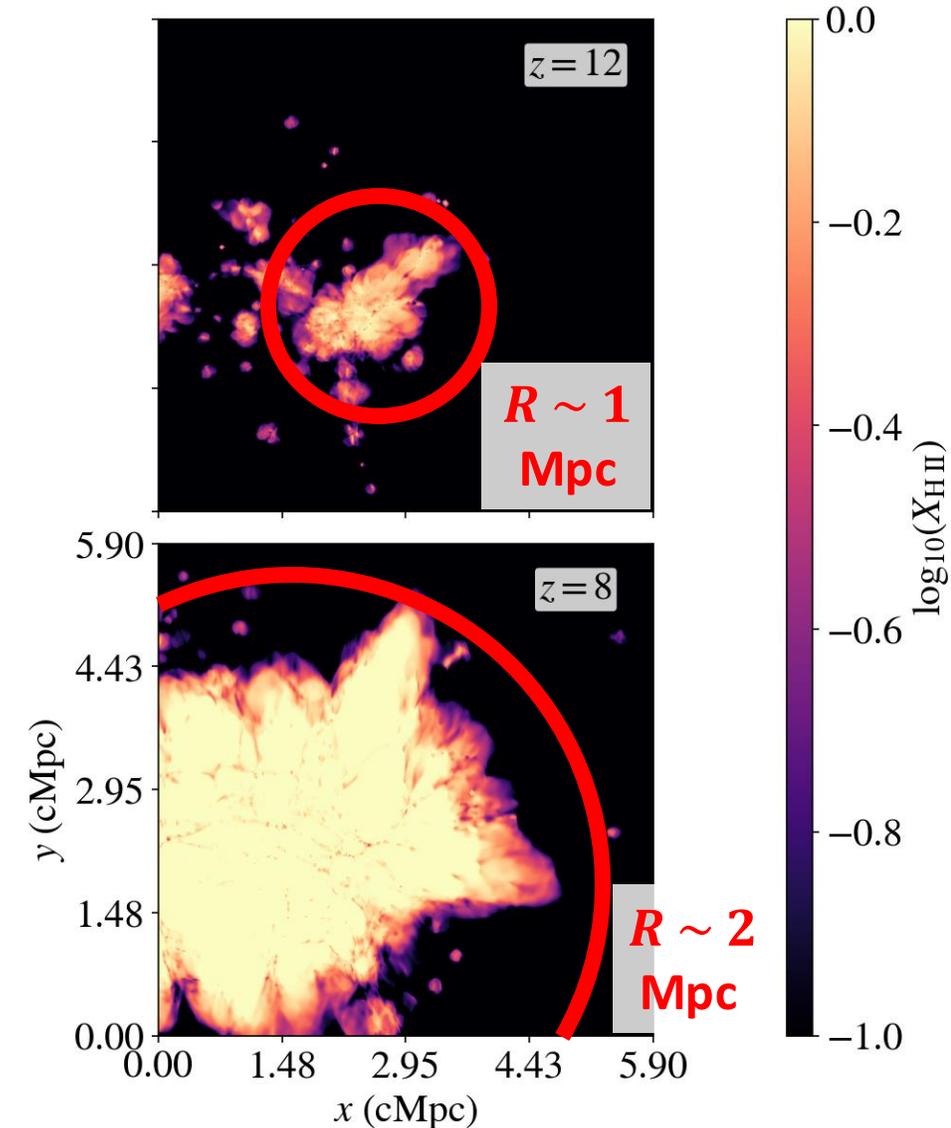
  $$\Rightarrow \left(Z/Z_\odot\right)_{\mathrm{reion}} = 10^{-3}$$

Growth of Ionized (H II) Bubbles—Friends-of-Friends (FoF)

- FoF algorithm (Einasto+1984, Iliev+2006)

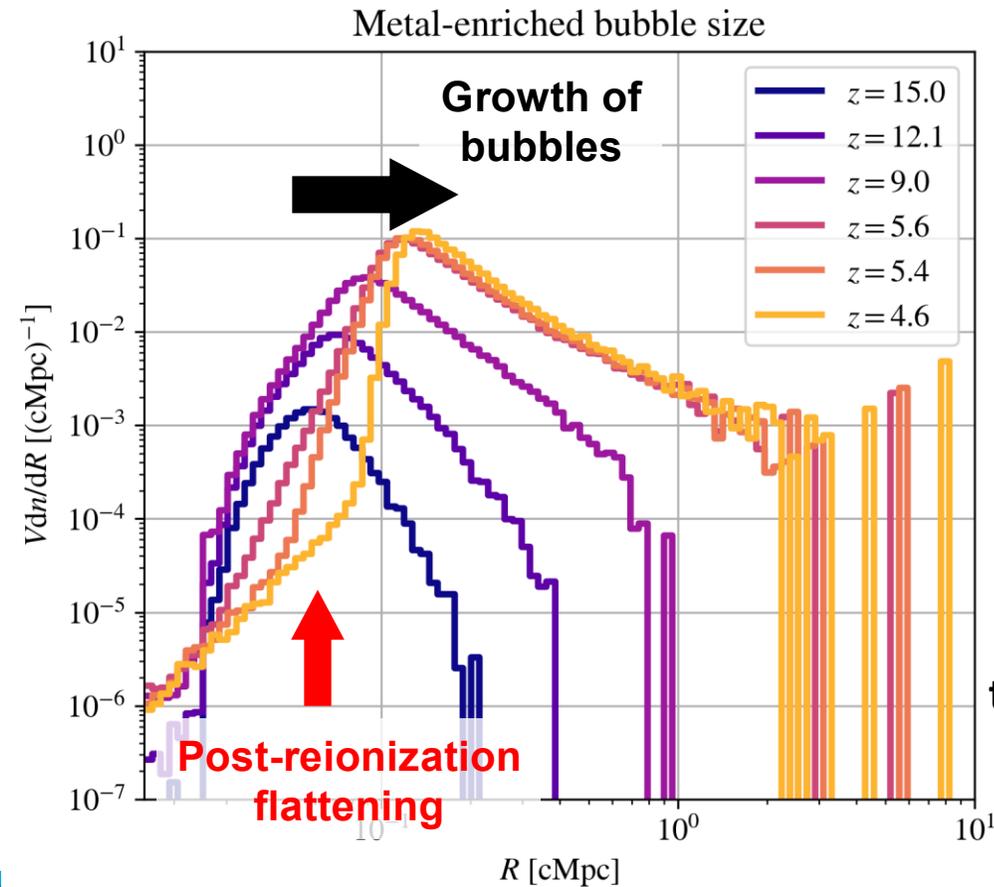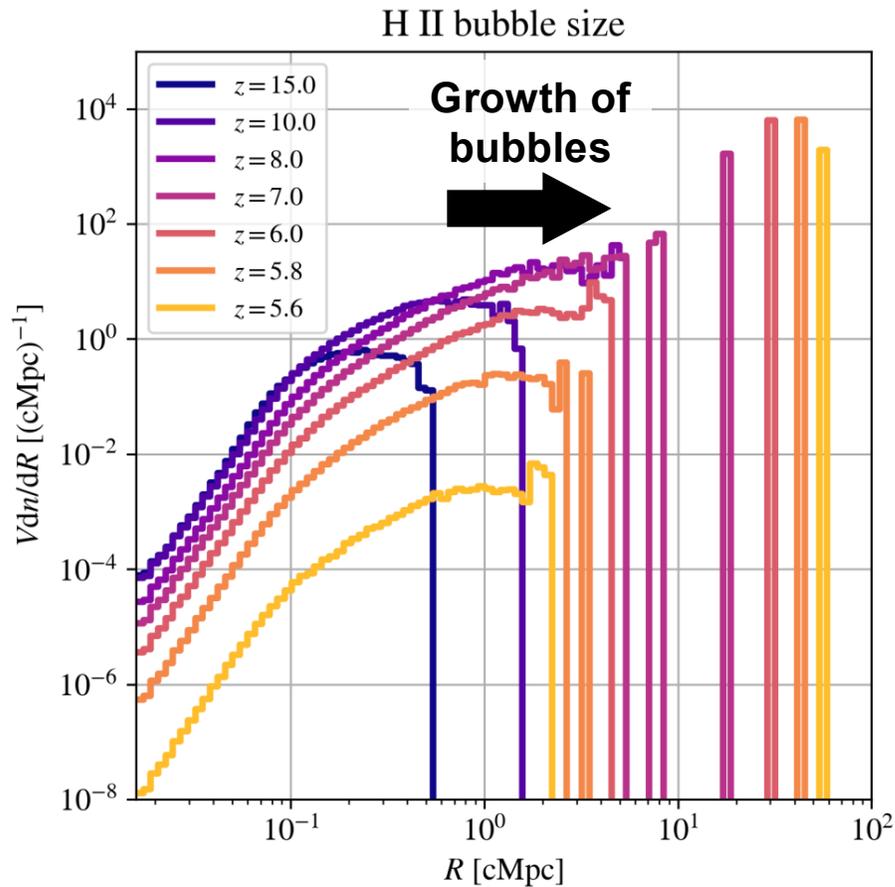- Size and number grow rapidly, until percolation at $z < 8$
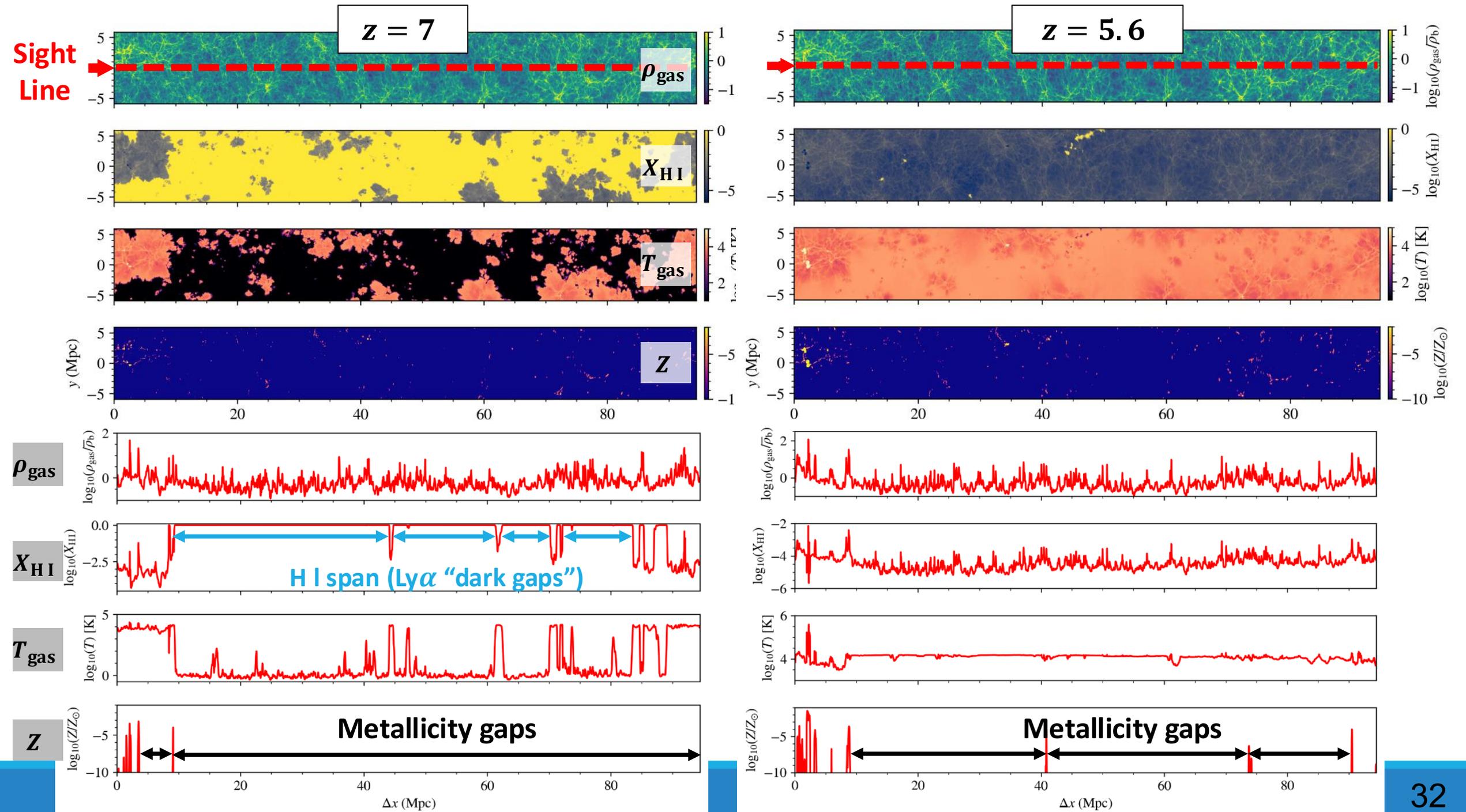
Lee+2025, to be submitted

Growth of Metal-enriched Bubbles—Friends-of-Friends (FoF)

- Compared to ionized bubbles, metal-enriched bubbles
  - 1. grow much more slowly   2. percolate less
  - 3. show post-reionization flattening in slope on small radius end
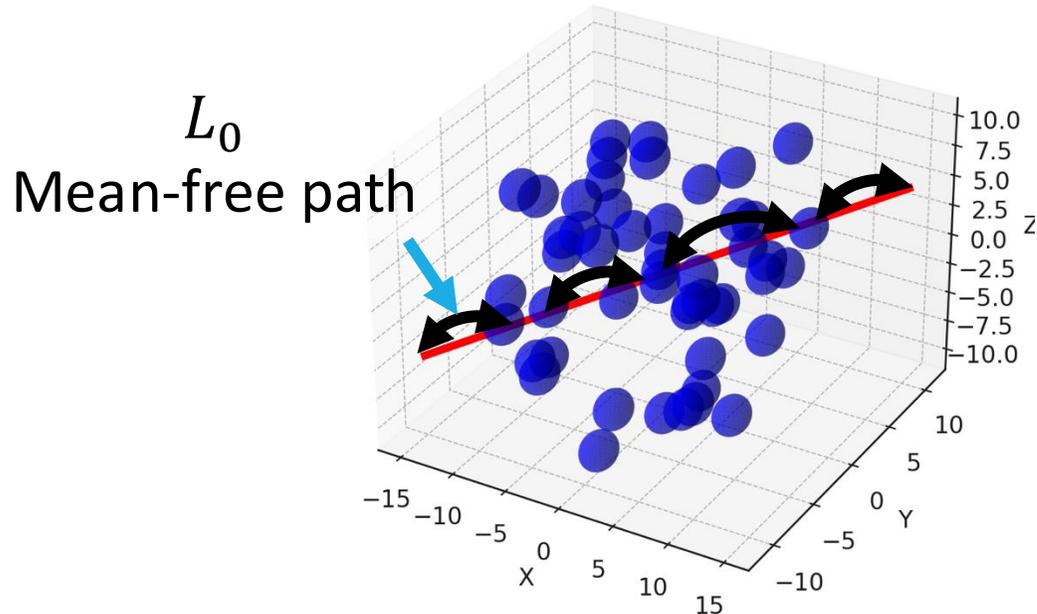

Lee+2025,
to be submitted

z = 7

z = 5.6

Sight Line

ρ_{gas}

$X_{\text{H I}}$

T_{gas}

Z

ρ_{gas}

$X_{\text{H I}}$

H I span (Lyα "dark gaps")

T_{gas}
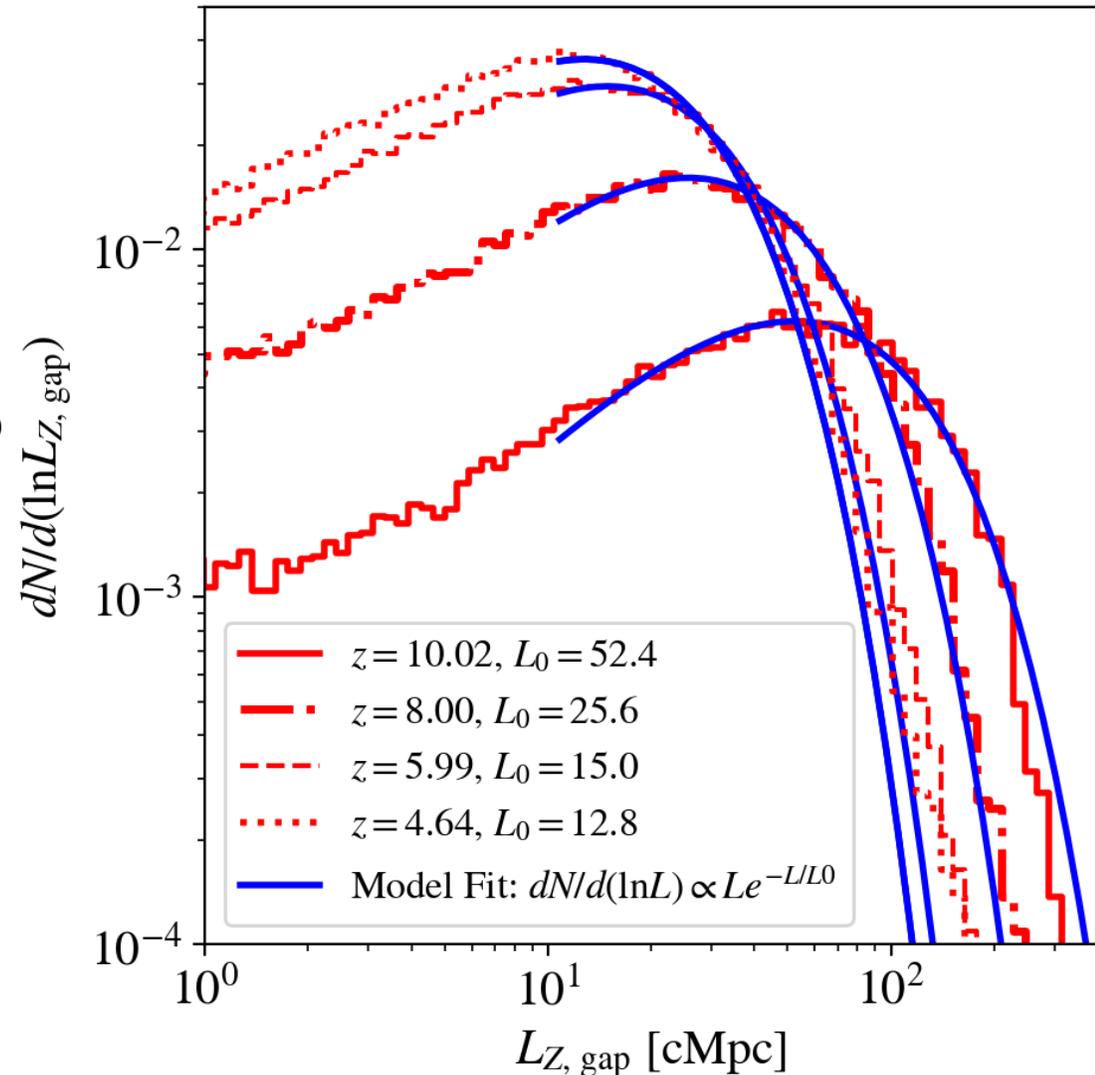
Z

Metallicity gaps

Metallicity gaps

Metallicity Gap Statistics

- A simple mathematical toy model:
  distribution of line-of-sight distances between
  spherical metal bubbles located randomly
  in empty space **fits the distribution well!**

$$dN/dL \propto e^{-L/L_0}, \ \text{where} \ L_0 = 1/(\pi R^2 n) = \lambda_{\text{mfp}}$$
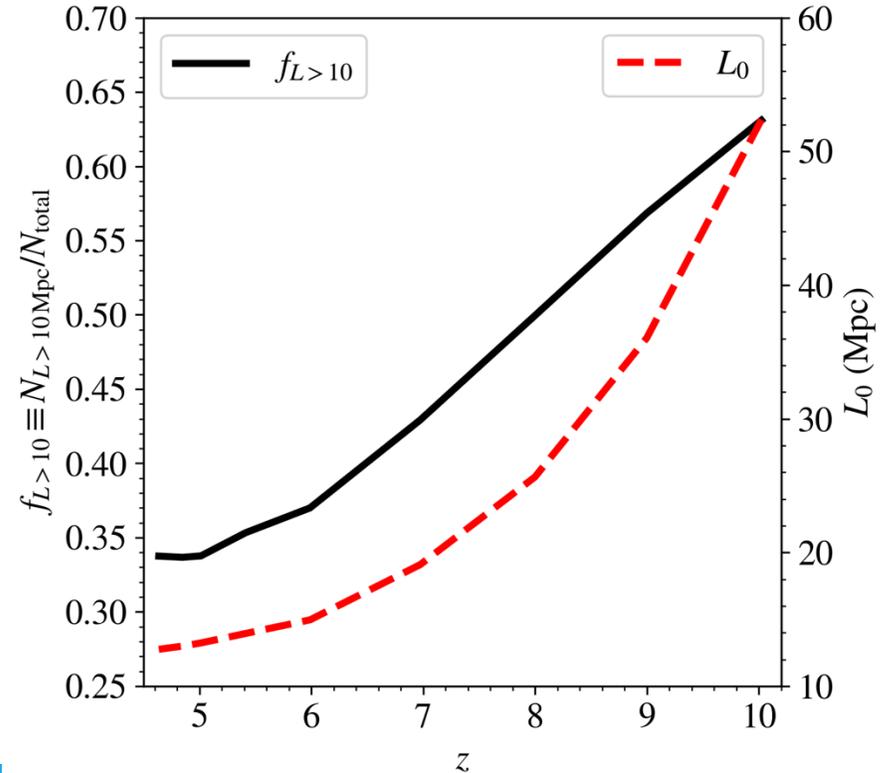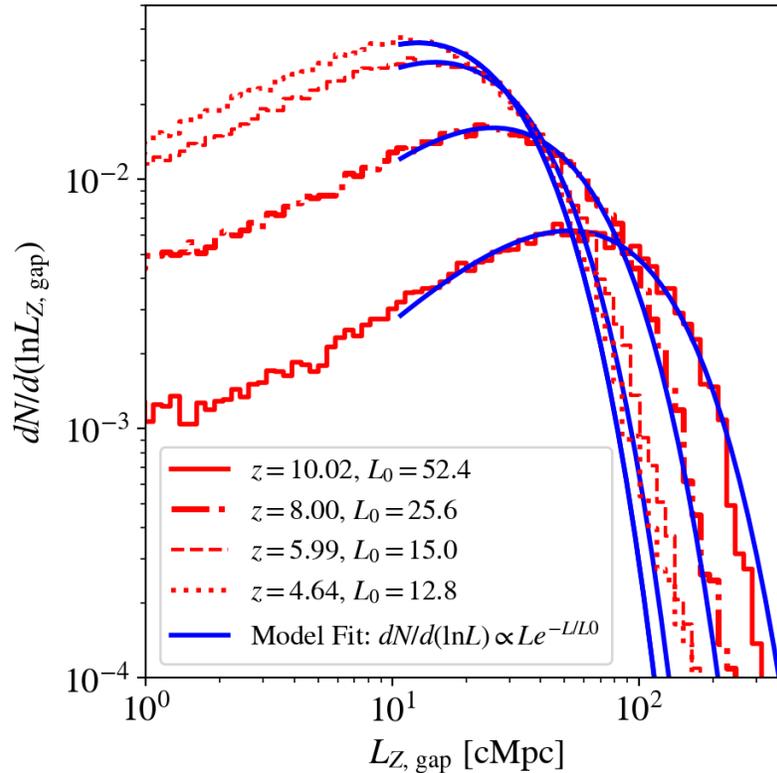
L_0
Mean-free path

Randomly distributed metal-filled spheres with radii R

Legend:
- $z = 10.02, L_0 = 52.4$
- $z = 8.00, L_0 = 25.6$
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- Model Fit: $dN/d(\ln L) \propto L e^{-L/L0}$

Axes: $dN/d(\ln L_{Z, \text{gap}})$ vs $L_{Z, \text{gap}}$ [cMpc]

Metallicity Gap Statistics

- The model fits long gap distribution well ($L \geq 10$ Mpc);
  but undershoots short gap distribution: "**non-random clustering**" on small scales

- MFP of hitting metal-enriched regions (L_0) drops dramatically during EoR:
  $@z = 10, \sim 50$ Mpc, $@z = 5, \sim 10$ Mpc

Lee+2025, to be submitted

Summary
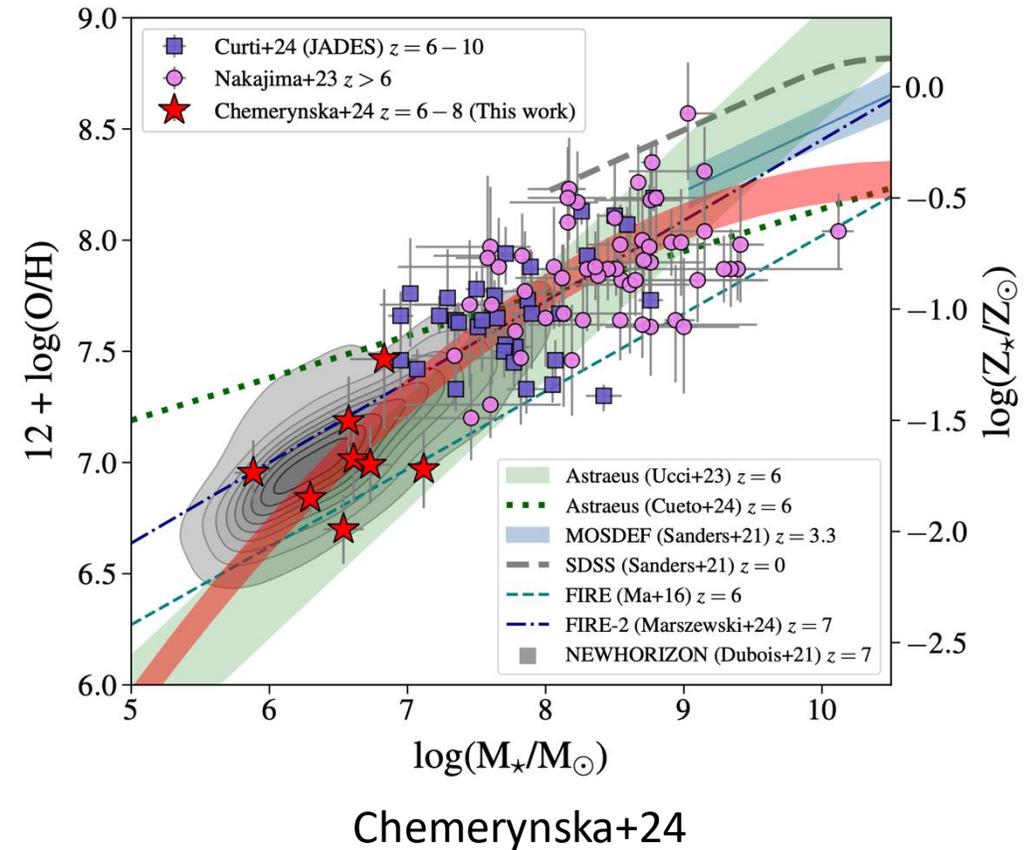
1. The same massive stars that reionized the universe enriched the universe to $\bar{Z}/Z_\odot = 10^{-3}$ by the end of the EoR, $z_{\rm re} = 5.53$ (99.99% ionized).

2. The metal-enriched volume fraction of the universe was tiny, during the EoR and well beyond it ($Q_Z < 2\%$ at $z_{\rm re} = 5.53$), accompanied by Pop III star formation.

3. CoDa III galaxy mass-metallicity relation (MZR) matches observed trend of MZR ($Z \propto M_\star$); CoDa III MZR is slightly lower than recent JWST observations within scatter.

4. Metal-enriched zones are well-characterized as "metal-enriched bubbles" arranged along the filaments and nodes of the cosmic web.

5. Metal bubble size distribution peaks at ~ 100 ckpc, with a slope becoming a plateau below the peak, a possible indicator of when reionization ended.

6. "Metallicity gaps" offer a new observational diagnostic of the inhomogeneous rise of metallicity and reionization, both!
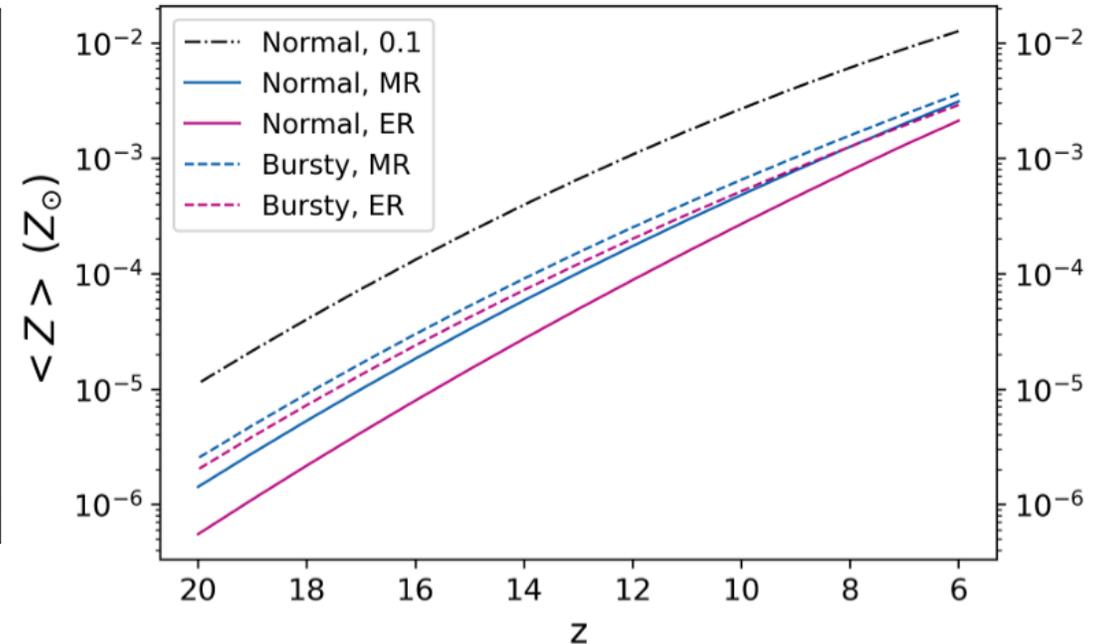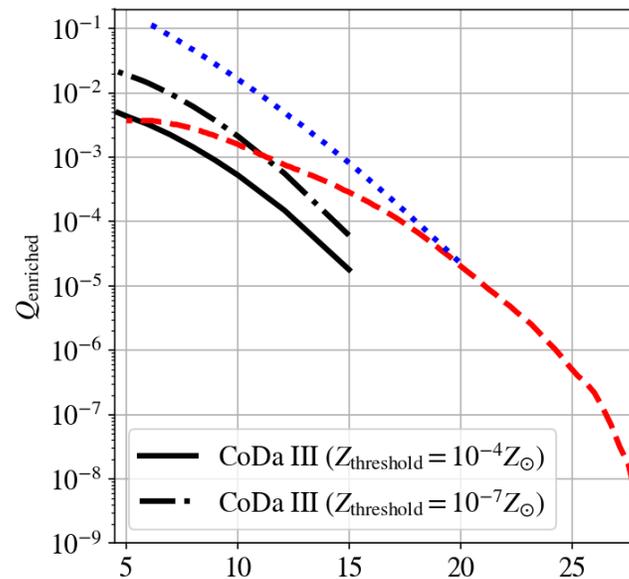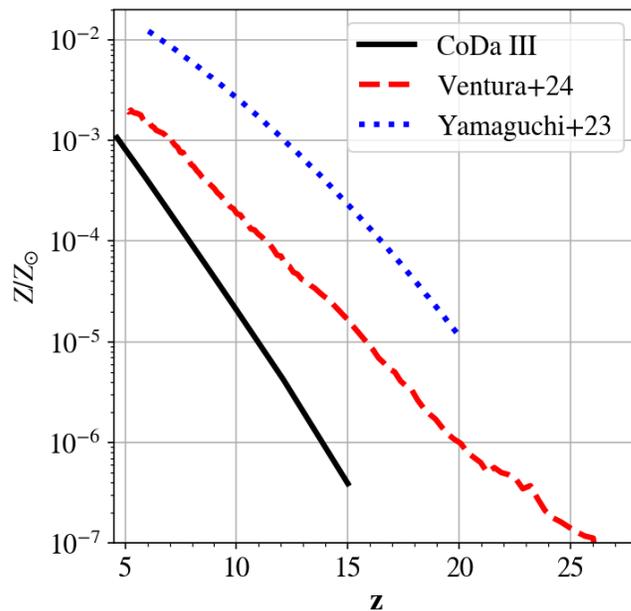
Metal Enrichment by The First Stars: Relevant Works

- Simulations:
  Wise+12, Finlator+18, Sarmento+18, Sarmento & Scannapieco 22, Jaacks+19, Venditti+23, Mead+25 (see Jeniffer's talk), …, etc.

- SAMs:
  Yamaguchi+23, Hegde & Furlanetto 23, Ventura+24, Hazlett+24, …, etc.

- Usually, simulations are small $\sim (1\ \mathrm{Mpc}/h)^3$ and SAMs cannot capture galaxy-scale physics (and inhomogeneous reionization) self-consistently → galaxy property predictions cannot be compared to observations
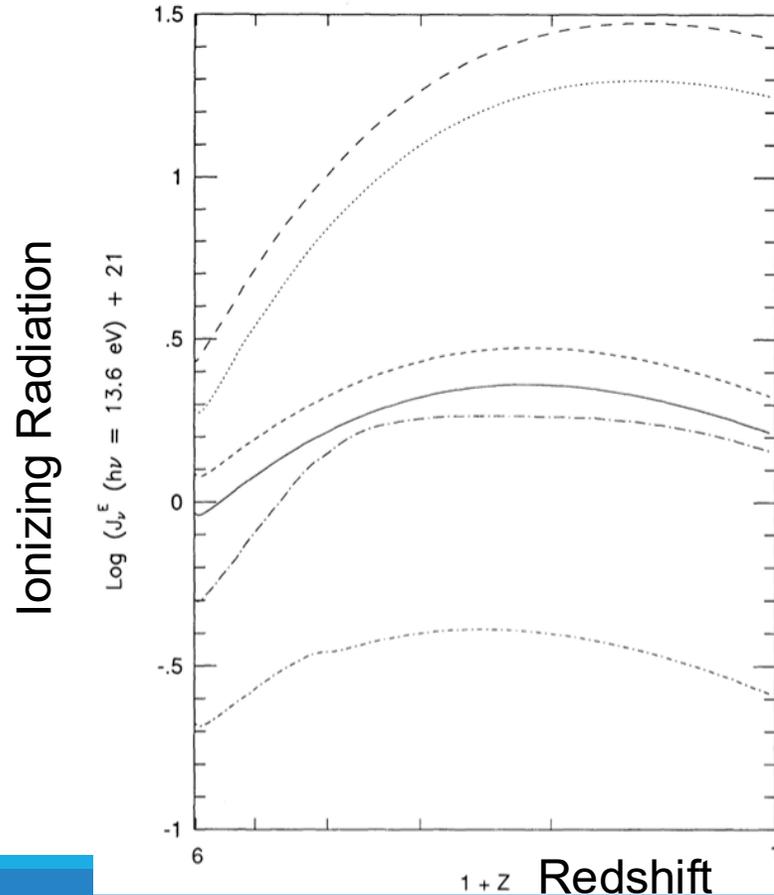

Chemerynska+24

Recent Related Works

- [Yamaguchi+2023](): analytic halo model + wind bubbles

- [Hennawi+2021](): paint metal-enriched spheres on Nyx N-body/hydro sim

- [Tie+2022](): paint metal-enriched spheres on Nyx N-body/hydro sim

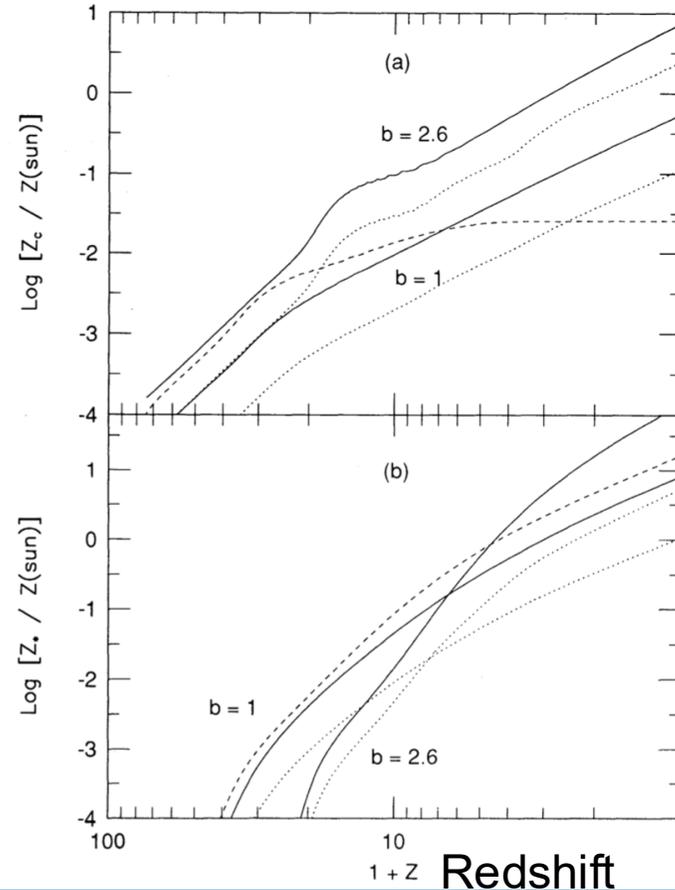- [Keating+2014](): assign metallicity as a function of overdensity

Massive Stars: Sources of Ionizing Photons & Metals

- *Reionization and metal enrichment are directly correlated!*

- *The same massive stars* that released the ionizing photons also released the metals that enriched the universe by SNe (Shapiro, Giroux & Babul 1994, Giroux & Shapiro 1996)
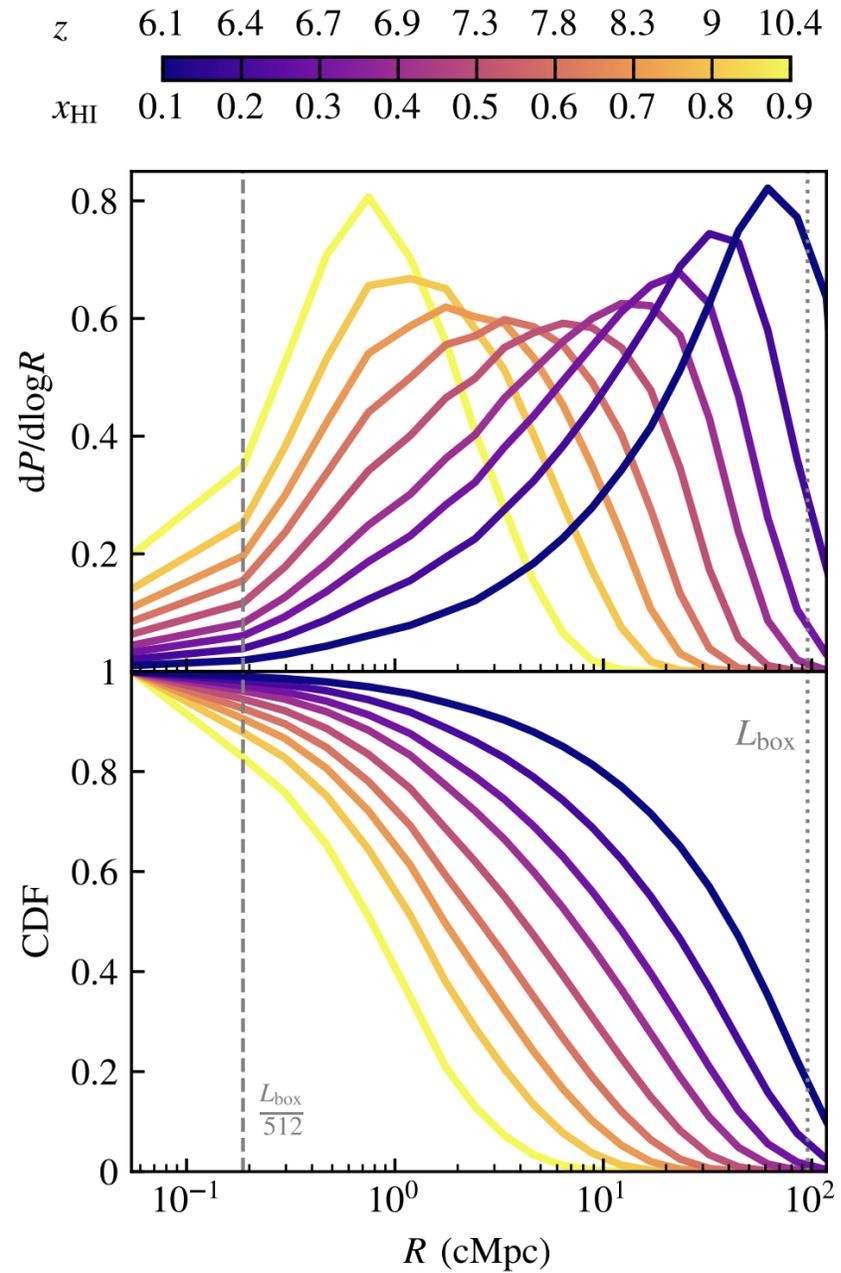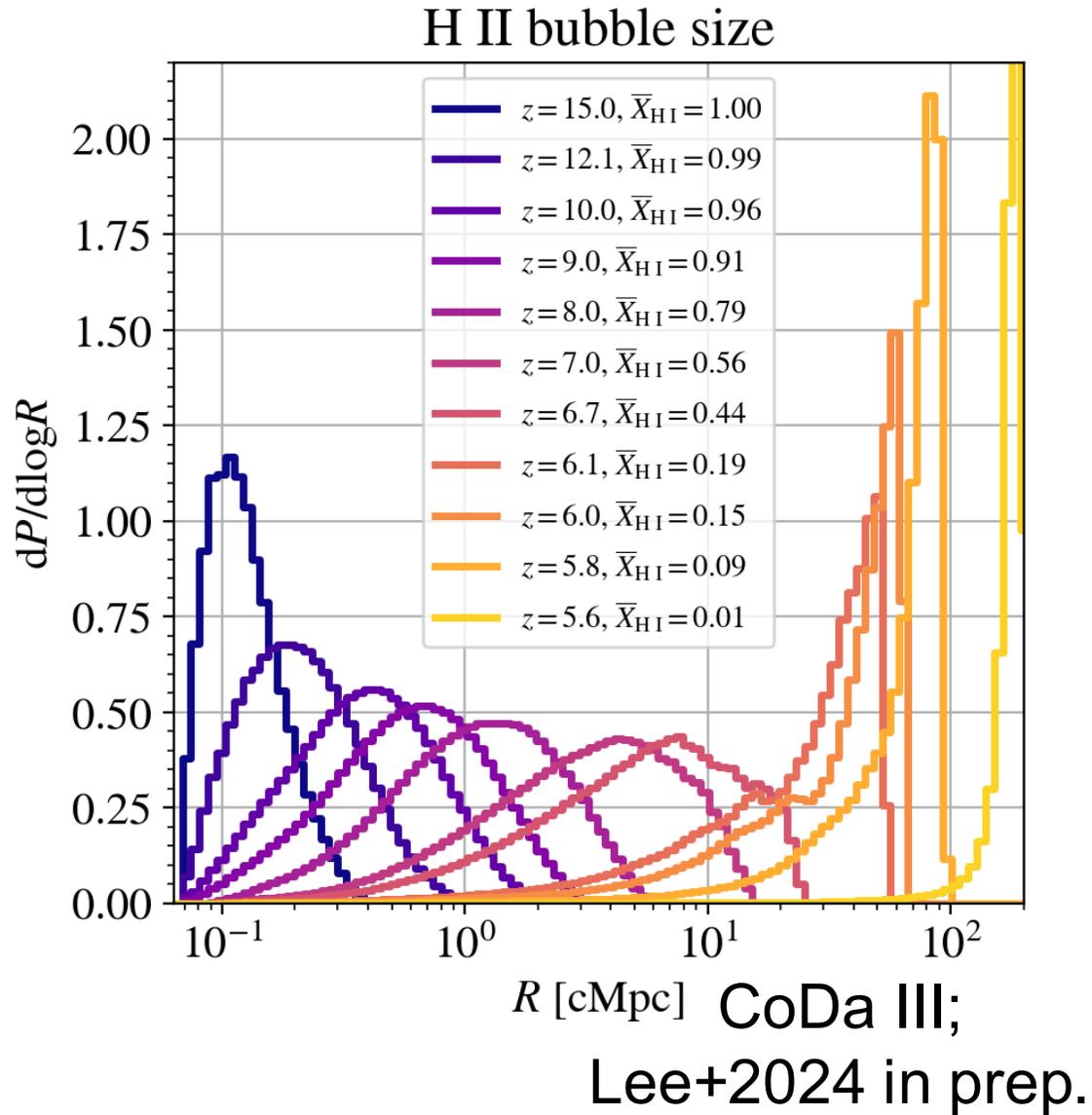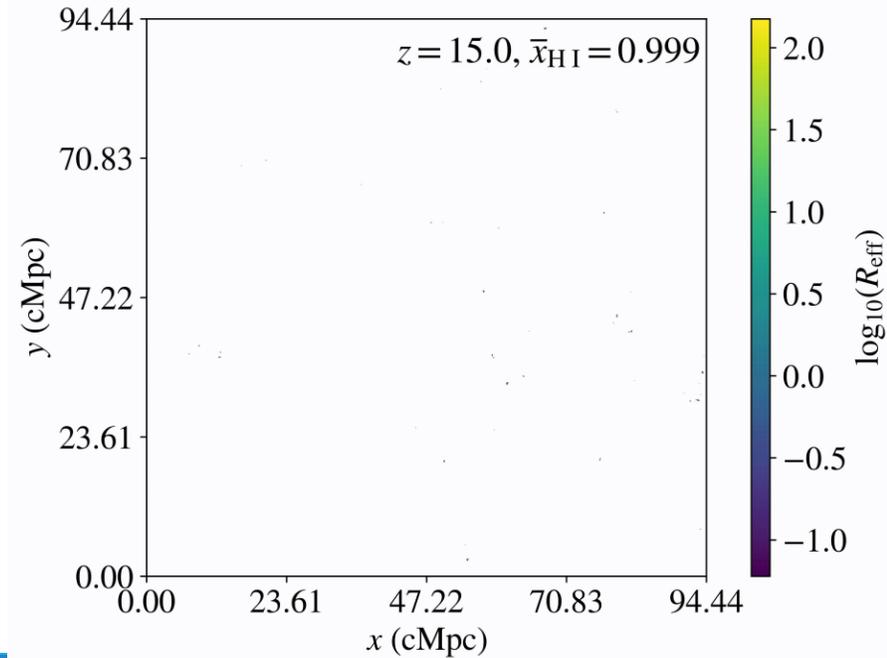

$$\Rightarrow \dot{n}_\gamma \propto \dot{\rho}_Z$$

Ionizing photon production

Metal production

Growth of Ionized Bubbles—MFP

H II bubble size

Legend:
- $z = 15.0, \overline{X}_{HI} = 1.00$
- $z = 12.1, \overline{X}_{HI} = 0.99$
- $z = 10.0, \overline{X}_{HI} = 0.96$
- $z = 9.0, \overline{X}_{HI} = 0.91$
- $z = 8.0, \overline{X}_{HI} = 0.79$
- $z = 7.0, \overline{X}_{HI} = 0.56$
- $z = 6.7, \overline{X}_{HI} = 0.44$
- $z = 6.1, \overline{X}_{HI} = 0.19$
- $z = 6.0, \overline{X}_{HI} = 0.15$
- $z = 5.8, \overline{X}_{HI} = 0.09$
- $z = 5.6, \overline{X}_{HI} = 0.01$

CoDa III;
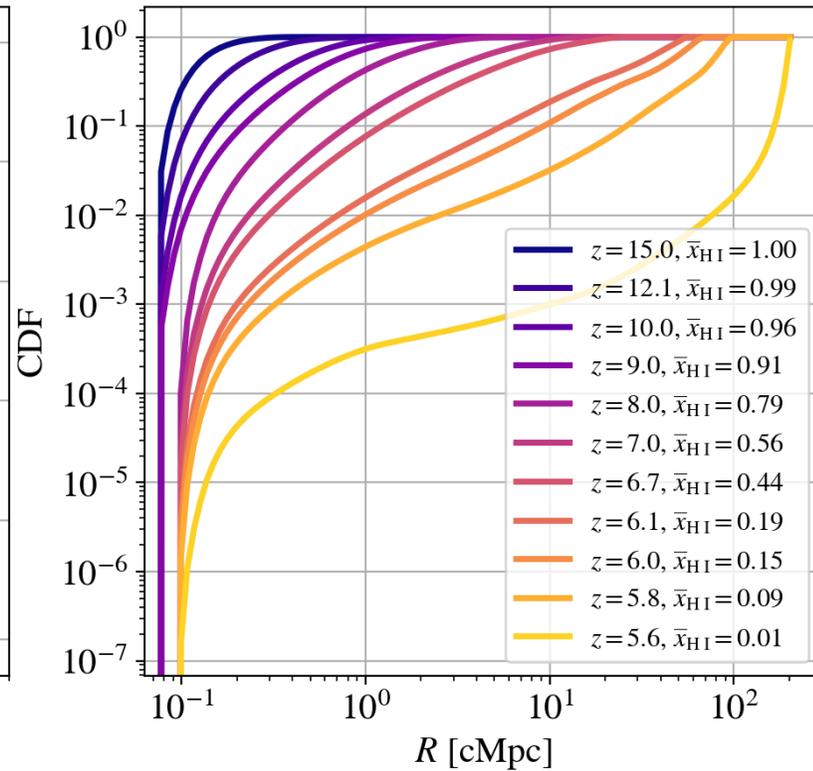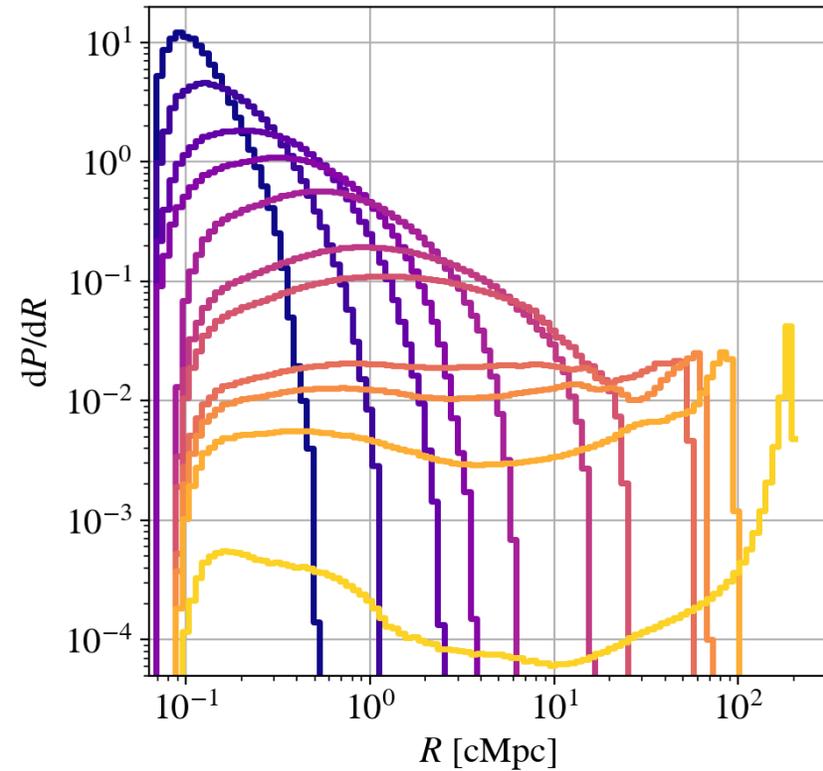Lee+2024 in prep.

THESAN;
Neyer+2023
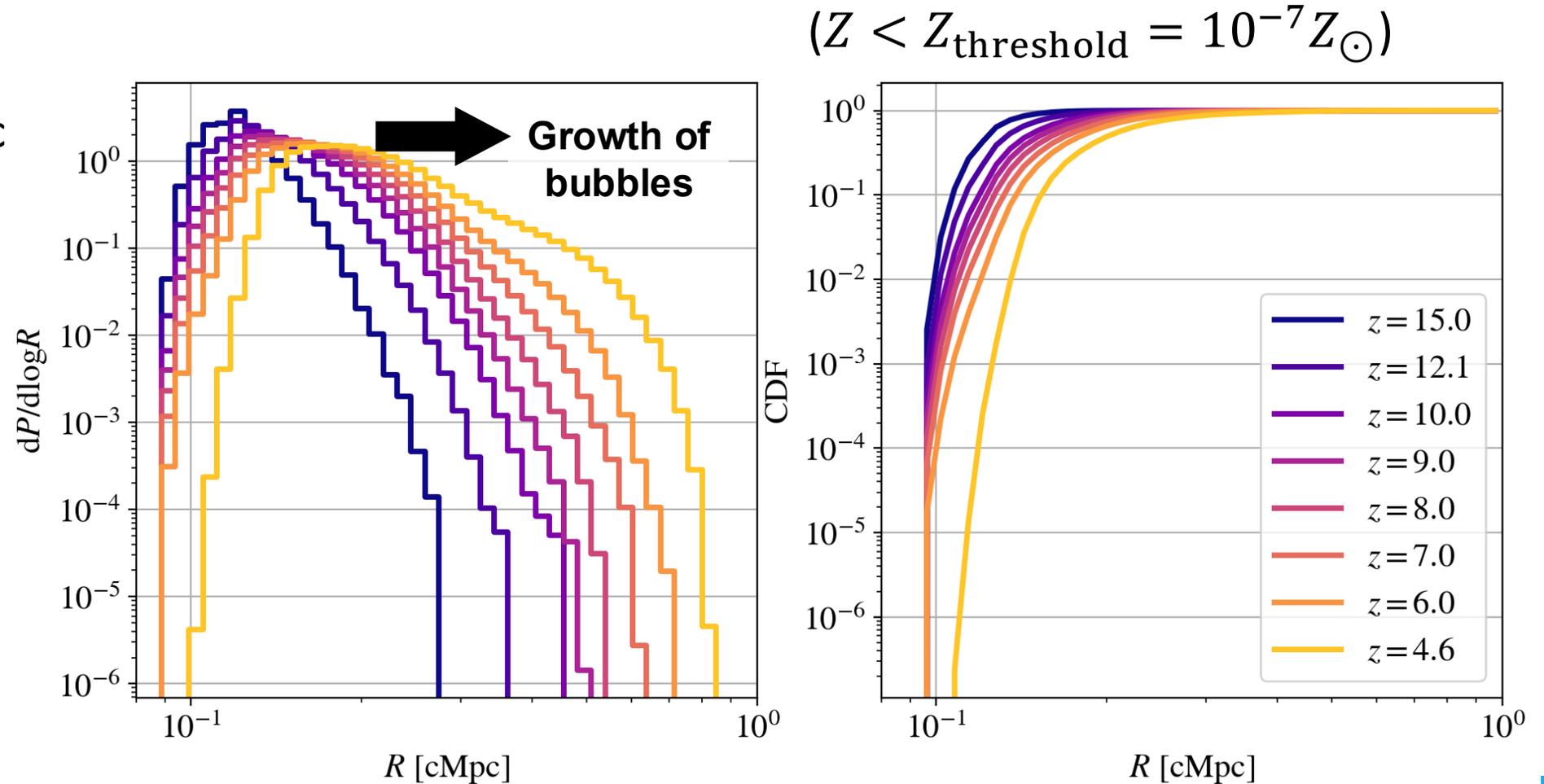
Growth of Ionized Bubbles—Mean Free Path

- Mean free path method (MFP; Mesinger & Furlanetto 2007)
  : measure "locally-defined" H II bubble sizes on 1024^3 grid
  = angle-averaged distance to nearest neutral cell

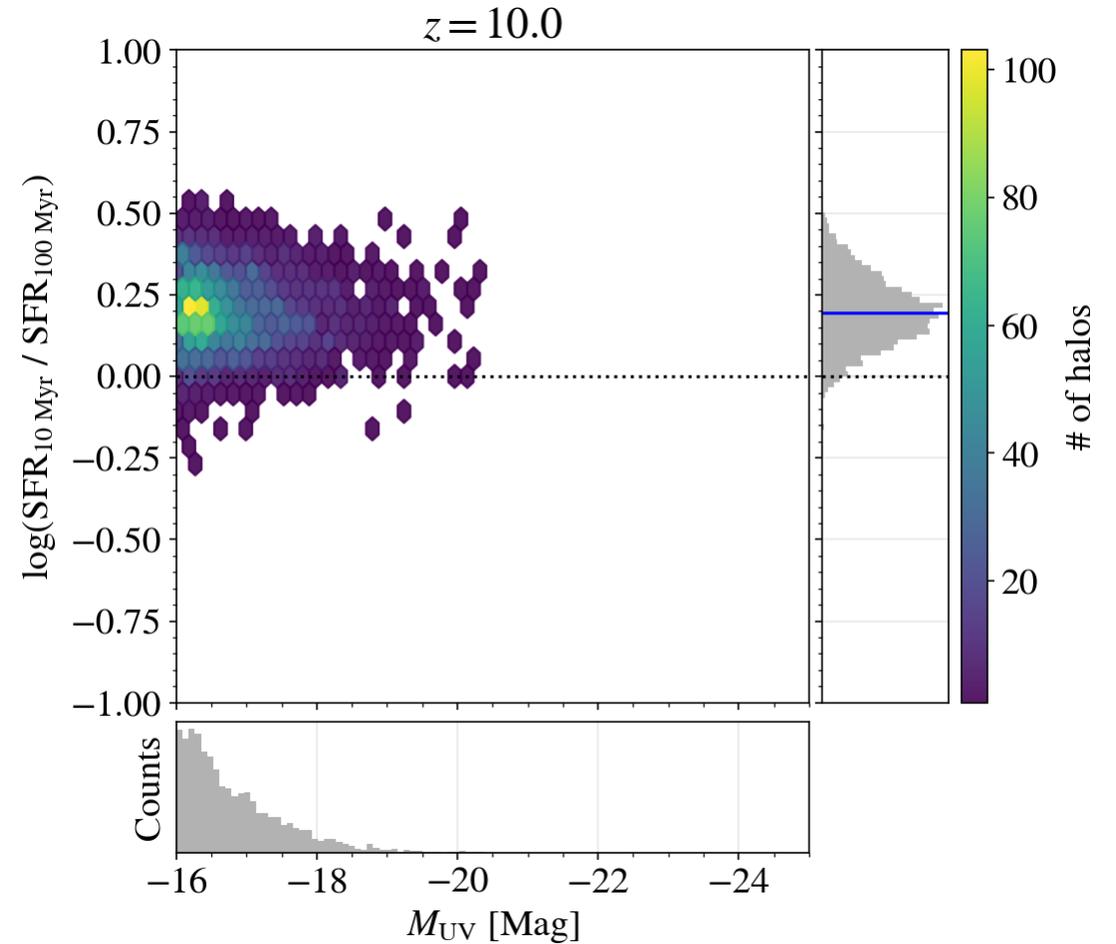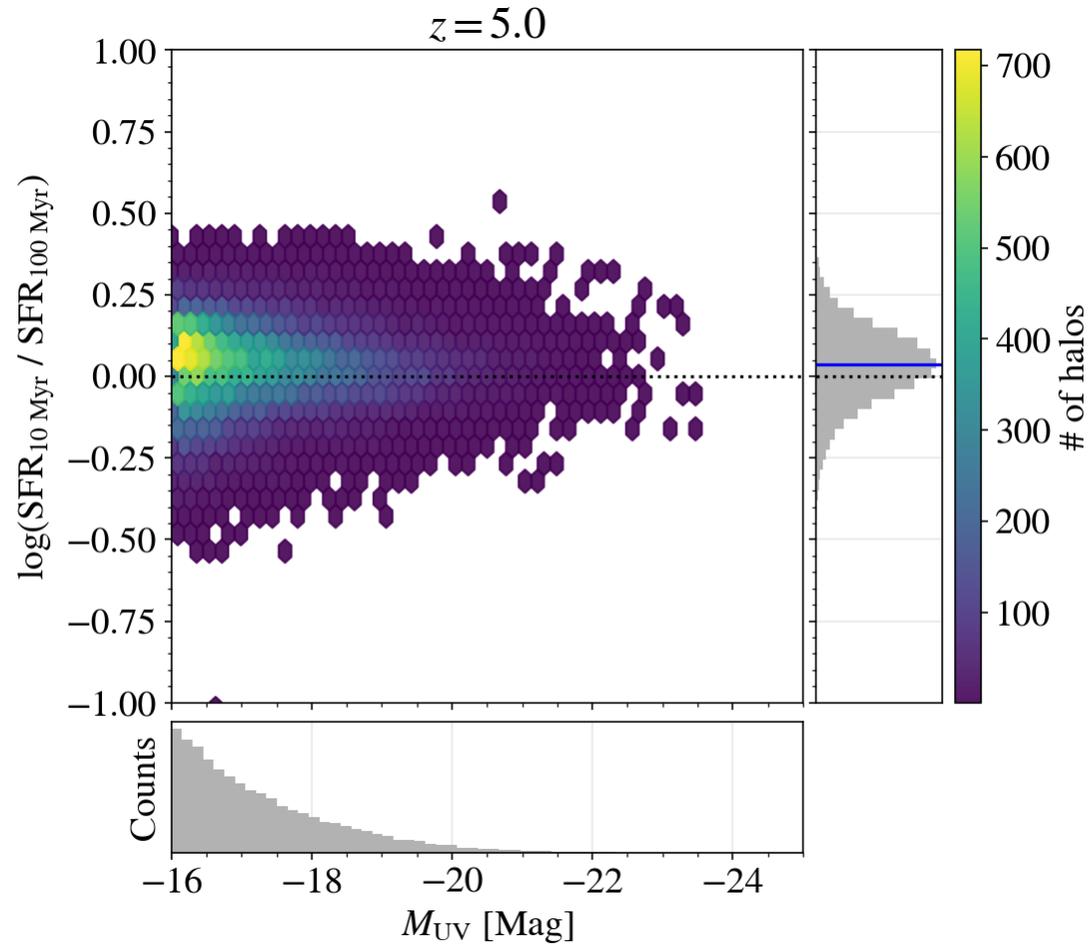# Growth of Metal-enriched Bubbles—Mean Free Path

- MFP method: "locally-defined" metal enriched bubble sizes

    = angle-averaged distance to nearest metal-free cell

$$(Z < Z_{\text{threshold}} = 10^{-7} Z_{\odot})$$

- Peaks at ~ 100 ckpc

Burstiness Increases at Higher Redshift

- Previous Works

Galaxy Star Formation Rate Main Sequence

- SFRMS