Lecture 28
The First Atoms, Molecules and Stars

1. Reionization and the First Stars
2. The First Atoms and Molecules
3. Formation of the First Stars

References

Barkana & Loeb, Repts Prog Phys, 70 627 2007
Lepp, Stencil & Dalgarno, J Phys B 35 57 2002
Seager, Sasselov & Scott, ApJS 128 407 2000
Yoshida et al. ApJ 652 6 2006, ApJ 663 687 2007

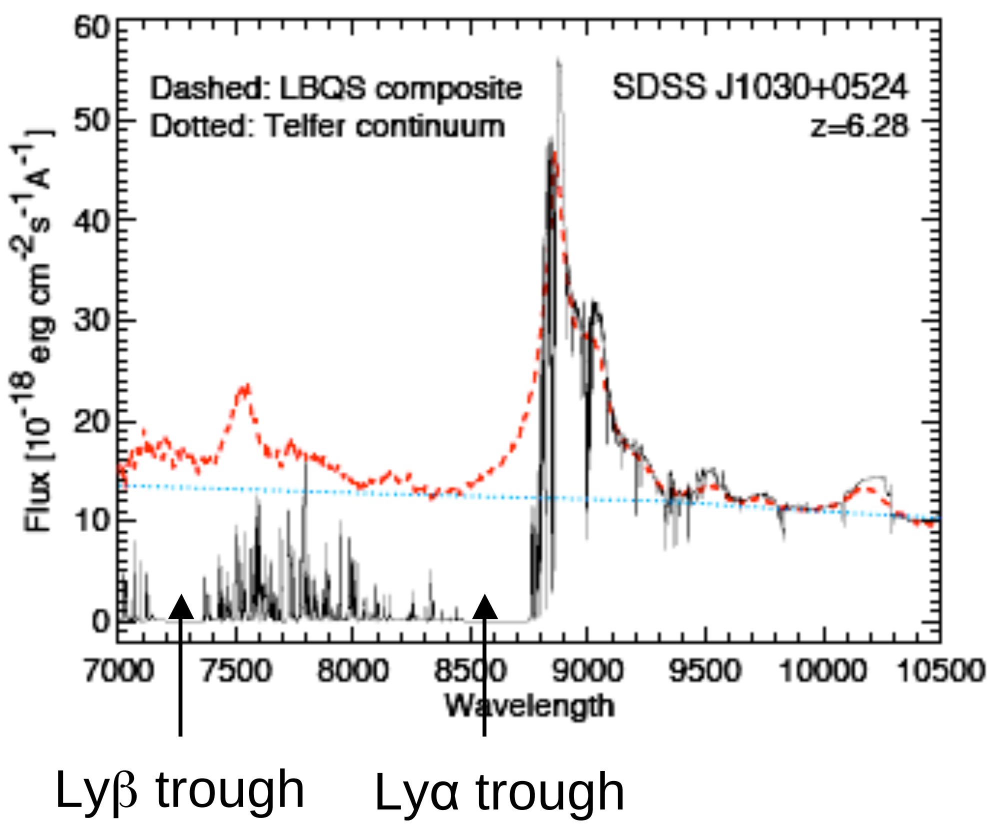
1. Reionization and the First Stars

Observations of the Lyα forest and especially the GP troughs for high-*z* quasars indicate that H I reionization occurred before *z* = 6 and for He II somewhat later.

White et al. AJ 126 1 2003

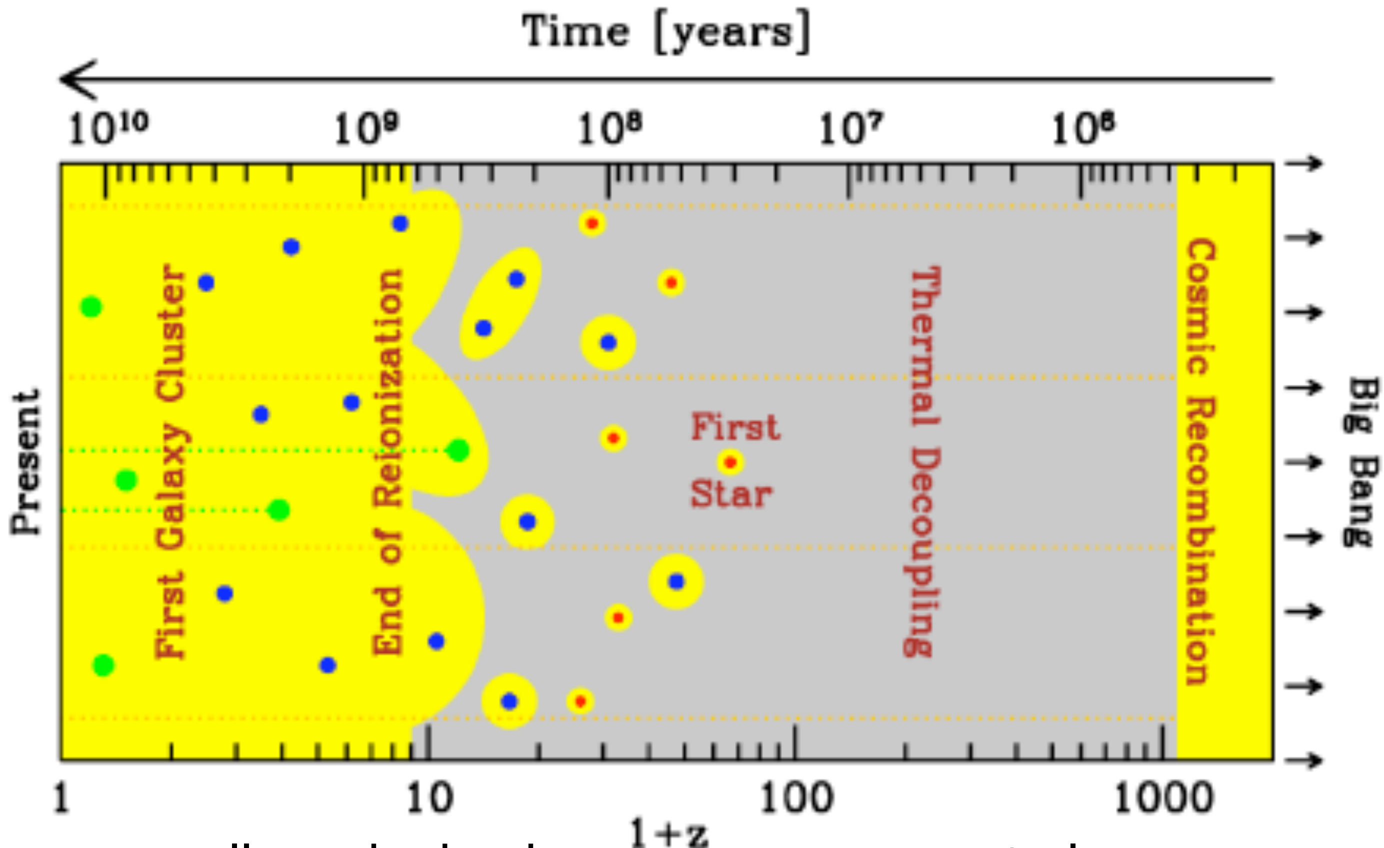
2nd highest Q redshift
black - observed spectrum
red - expected continuum
bars - Lyα and Lyβ GP
absorption troughs

Observations of other high-z Lyα absorption indicate that the degree of reionization varies for z = 5-6



Cartoon of Reionization by the First Stars

Barkana & Loeb (2007)



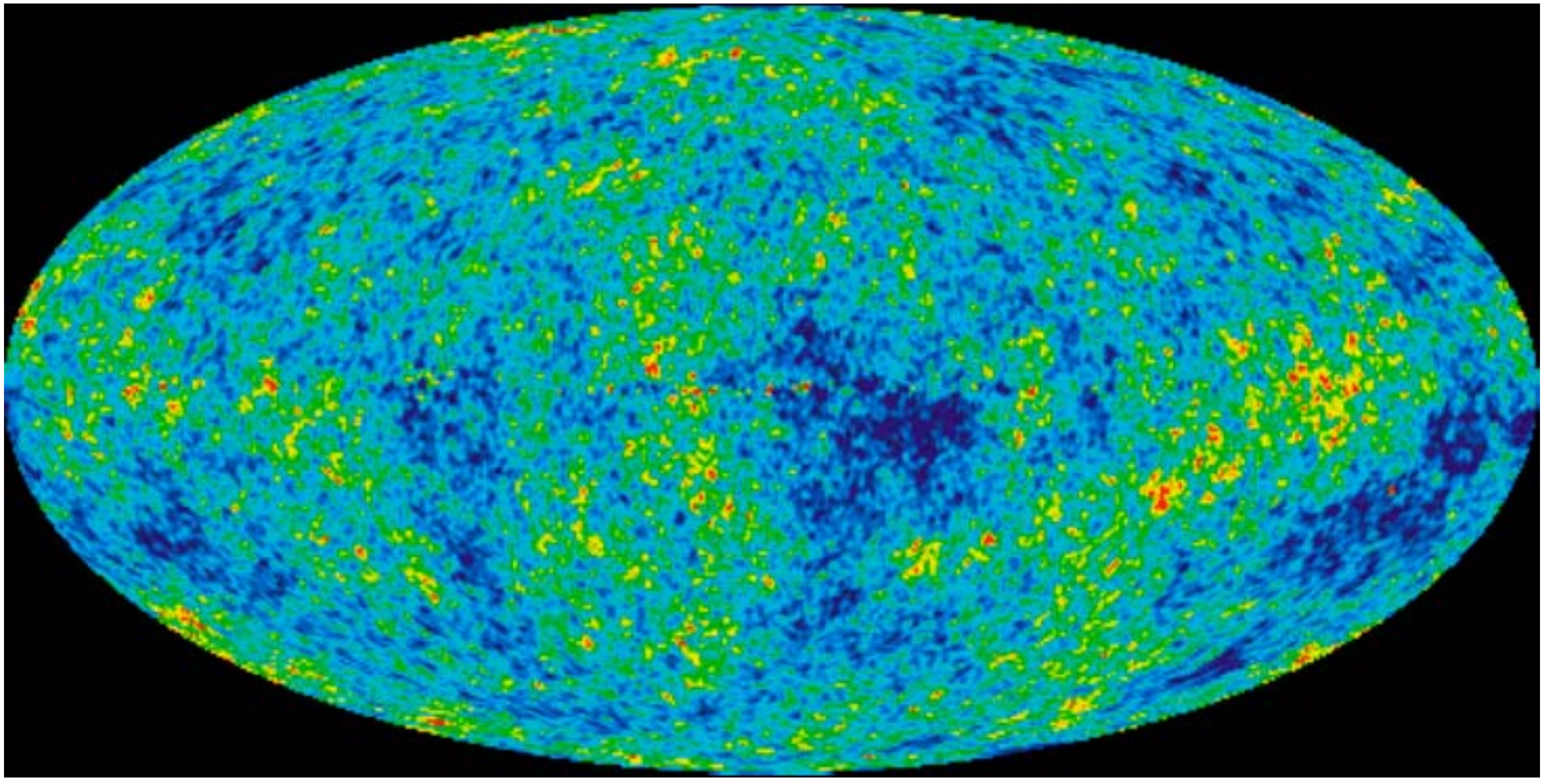
yellow - ionized grey - neutral

DM halo masses (solar masses):

red - 10^5 blue 10^8 green 10^{12}

Observations of high-z quasars (Lec27) suggests that reionization was complete just above z ~ 7

Origins of Structure

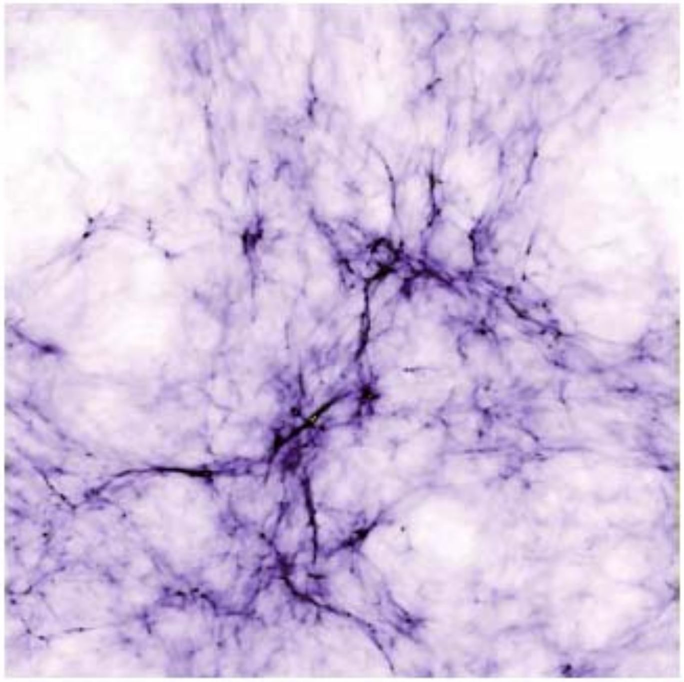


2008 WMAP image of the CMB fluctuations

<T> = 2.725 K red $+2\times10^{-4}$K blue - 2×10^{-4}K

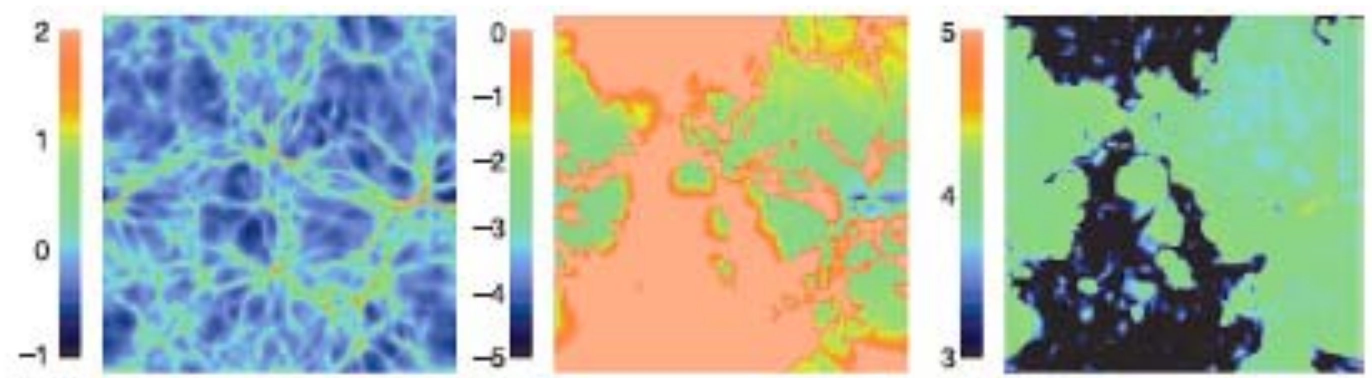
These fluctuations, seen above at z ~ 1200 (330,000 yr), grow until, somewhere between z ~ 10 -100 (13.5 Myr - 375 Myr), they produce the first stars.

Star Formation and ΛCDM Simulations



Stars are presumed to form in high-density knots shown in this ΛCDM simulation at $z = 17$.
Yoshida et al. ApJ 592 645 2003

Massive new stars ionize and heat the gas.
Miralda-Escude,
Science 300 1907 2003



neutral fraction (blue) | atomic fraction (orange) | temperature (green ~ 10^4 K)

2. The First Atoms and Molecules

The physical conditions close to recombination are given by the mean cosmological hydrogen density and the CMB temperature:

$$n_{\rm H} = (1-Y)\frac{\rho_{cr}}{m_{\rm H}}\Omega_B(1+z)^3 \cong 1.6\times10^{-7}\,{\rm cm}^{-3}(1+z)^3$$

$$T_{\rm rad} = 2.728(1+z)$$

For z = 1200 (~ 330,000) years ago, these are:

$$n_{\rm H} \cong 275\ {\rm cm}^{-3} \qquad\qquad T = 3000\ {\rm K}$$

These are fairly mild conditions, e.g., thermal collisional ionization of H and He is suppressed, so recombination can occur.
But going back to z = 3000 (84,000 yrs), $n_{\rm H}$~ 4000 cm^{-3} and T ~ 8000 K, which allows for collisional ionization.

The First Elements and Atoms

(The beginning of chemistry)

Big Bang nucleosynthesis produced these stable nuclides:

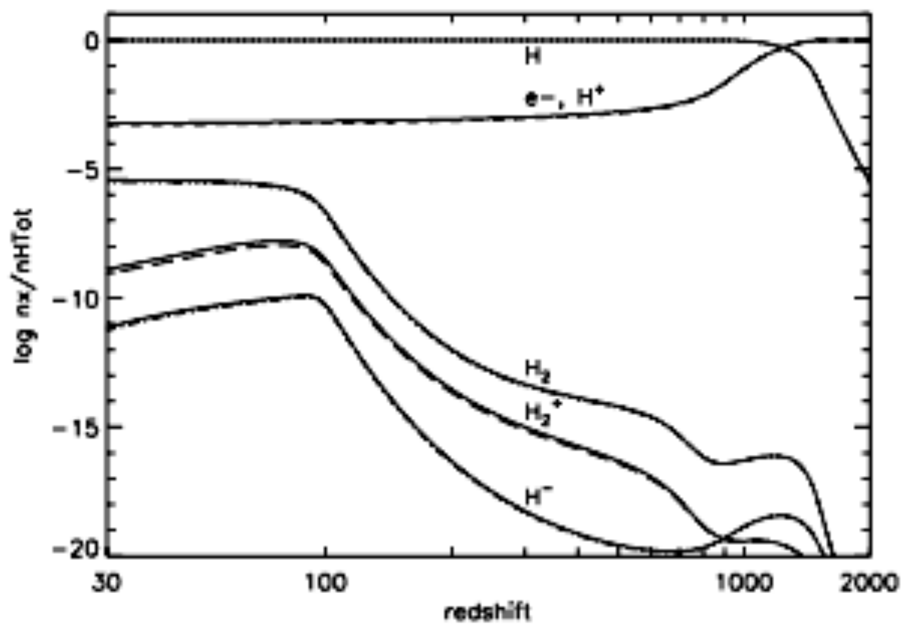
nuclide	abundance	IPs (eV)
H	1.0	13.60
D	$\sim 2\text{x}10^{-5}$	13.60
^{3}He	$\sim 10^{-5}$	13.60
He	0.06	24.59, 54.42
^{7}Li	$\sim 10^{-10}$	5.39, 75.64, 122.5

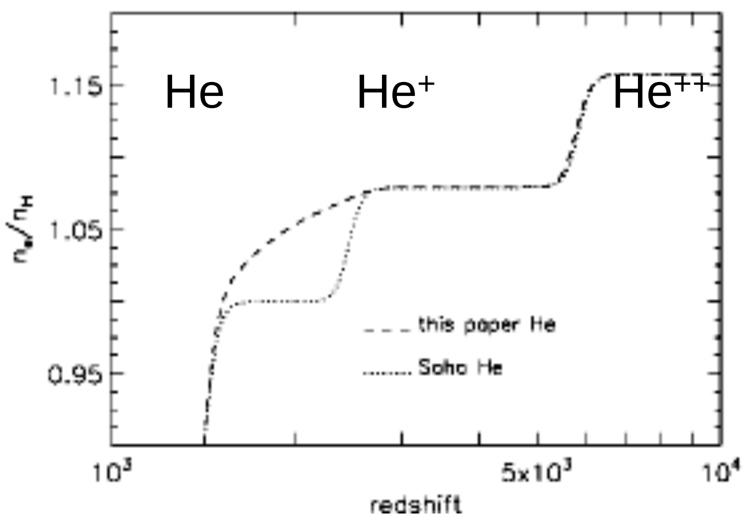
Starting with the Big Bang, the nuclei were stripped and the dominant ions were the ones with the highest charge: H^{+}, He^{2+} , and Li^{3+}. With time, the ions remained in chemical equilibrium, and those with the largest IPs were the first to disappear, starting with Li^{3+}, then Li^{2+}, He^{2+} and He^{+}. **He was the first atom to recombine.**

H and He Recombination

Seager et al. ApJ 523 L1 1999, ApJS 12 407 2000

- Detailed multi-level treatment of H and He atoms.
- Recombination of H occurs near z = 1300.
- H^+ freezes out at $x(H^+) \sim 10^{-3}$
- H_2 freezes out at $x(H_2) \sim 4 \times 10^{-6}$

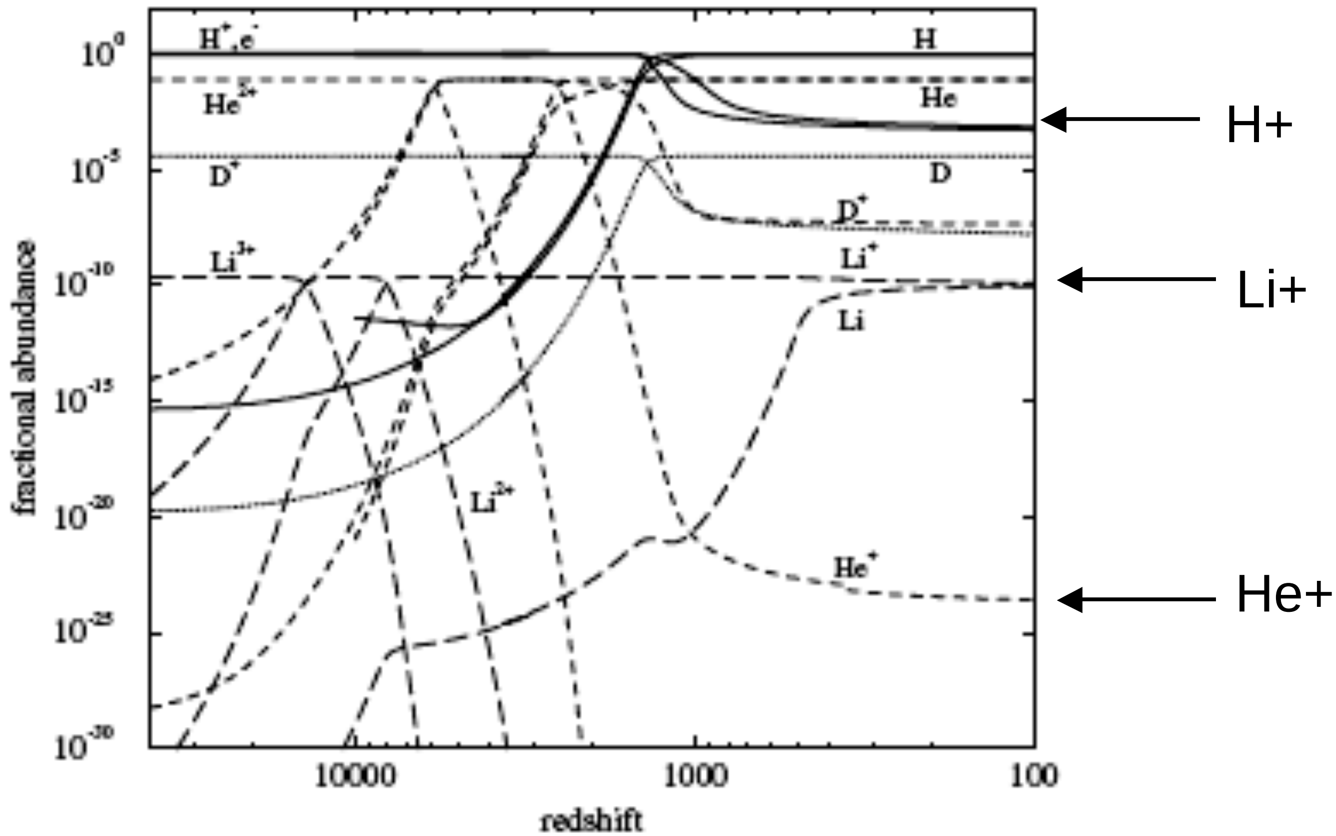




Blow-up just before recombination showing effect of He recombination on the electron abundance

Recombination Including D and Li

Lepp, Stancil & Dalgarno (2002)



Recombination timescales lengthen with decreasing z, and some H+, He+ and Li+ are frozen into the dark ages. The residual ionization level is ~ 10^{-4}

Formation of H_2

Starting from warm (< 3000 K) and moderately dense (275 cm^{-3}) atomic hydrogen and helium gas *without dust grains*, molecules can form by weak radiative processes, some of which discussed in Sec. 3 of Lec15.

The first molecule produced at the onset of cosmic recombination was the molecular ion HeH^+, soon followed by H_2^+

$$He^+ + H \rightarrow HeH^+ + h\nu \qquad k \cong 2\text{x}10^{-16}\ \text{cm}^3\text{s}^{-1} \quad (\text{at } 3000\ \text{K})$$

$$He + H^+ \rightarrow HeH^+ + h\nu \qquad k \cong 4\text{x}10^{-17}\ \text{cm}^3\text{s}^{-1}$$

$$H^+ + H \rightarrow H_2^+ \qquad k \cong 2\text{x}10^{-16}\ \text{cm}^3\text{s}^{-1}$$

These ions are destroyed by dissociative recombination, photodissociation and by reaction with H to form H_2^+:

H_2^+ /HeH$^+$ and H$^-$ Formation of H_2

$$HeH^+ + H \rightarrow H_2^+ + He \qquad k \cong 1.3x10^{-9}\ cm^3s^{-1}\ \ (at\ \ 3000K)$$

$$H_2^+ + H \rightarrow H^+ + H_2 \qquad k \cong 6x10^{-10}\ cm^3s^{-1}$$

Just as important as this HeH$^+$/H_2^+ route is formation of H_2 from H$^-$:

$$e^- + H \rightarrow H^- + h\nu \qquad k \cong 2x10^{-15}\ cm^3s^{-1} \quad (at\ 3000\ K)$$

$$H^- + H \rightarrow H_2 + e \qquad k \cong 1.2x10^{-9}\ cm^3s^{-1}$$

Lastly, HD can be formed by similar sets of reactions, but unlike the highly forbidden reaction, H + H $\rightarrow$ $H_2 + h\nu$, the direct radiative association of H and D is allowed but weak:

$$H + D \rightarrow HD + h\nu \qquad k \cong 8x10^{-26}\ cm^3s^{-1}$$

Destruction of H_2^+, HeH^+, and H^-

These ions are all formed by weak radiative association with H and then H_2 is formed by a fast reaction with another H

$$
\begin{array}{l}
\begin{array}{lcl}
H^+ & & H_2^+ \\
H_2^+ \;\; + \;\; H & \rightarrow & HeH+ \;\; + H \;\; \rightarrow \;\; H_2 \\
e & & H^-
\end{array} \\
\qquad\qquad\qquad \rightarrow \text{destruction by } h\nu \text{ in all cases} \\
\qquad\qquad\qquad\quad \text{by e for } H_2^+ \text{ and HeH+ and by H+ for } H^-
\end{array}
$$

The thresholds for photo-destruction are:

$D(H_2^+)$	$= 2.65$ eV	4680 Å
D(HeH+)	$= 2.03$ eV	6110 Å
$B(H^-)$	$= 0.754$ eV	16400 Å

CMB radiation destroys H^- at recombination, so the H^- route to H_2 is relatively weak until smaller z ~ 500.

Three-Body Formation

In Lecture 15 three-body formation was mentioned as a way of synthesizing H_2 in dense regions like cool stellar atmospheres and the disk of YSOs:

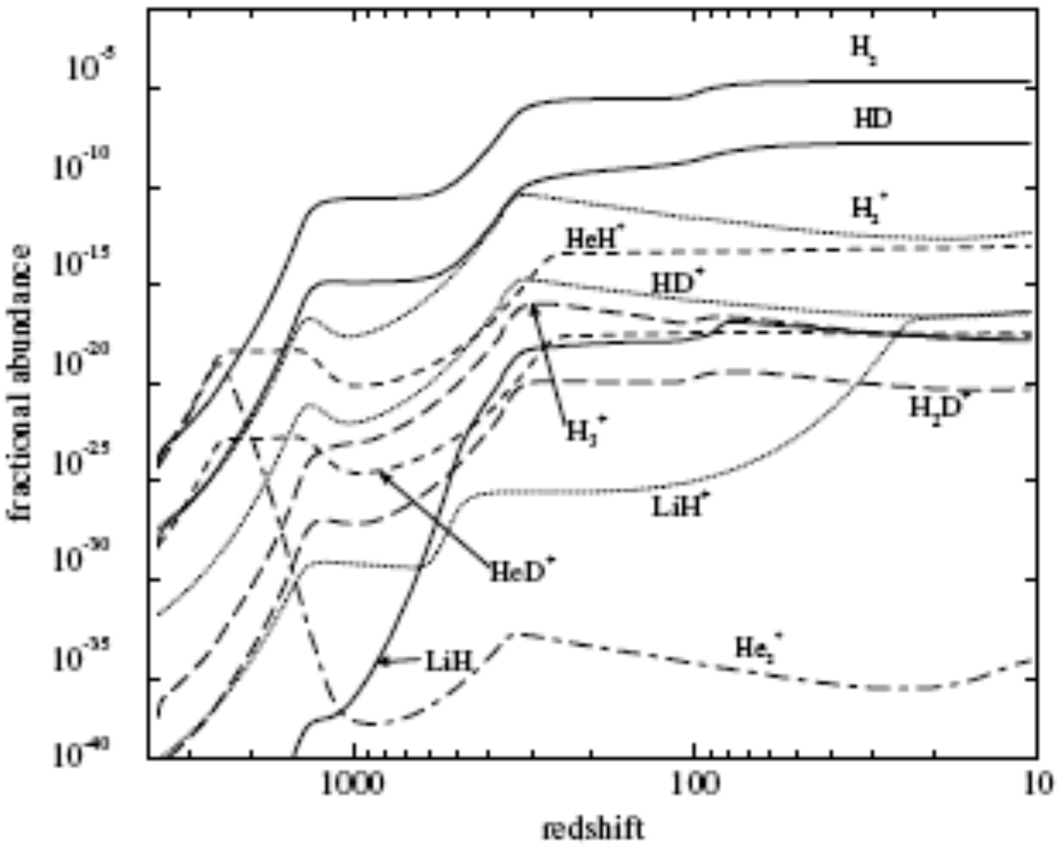
$$3H \rightarrow H_2 + H \qquad\qquad 2H + H_2 \rightarrow 2\,H_2$$

These reactions also play a role when gas inside DM halos becomes dense. Cooling by H_2 then regulates the temperature in these cores. The inverses of these three-body reactions may also destroy H_2 by collisional dissociation.

Similarly, evaluations of the role of reactions based on the mean density after recombination will not hold once star formation has started. For example, the first stars will generate UV radiation that will destroy H_2^+ and HeH+ (as well as H_2) and photoionize H from excited levels.

Molecule Production in the Recombination Era

Lepp, Stancil & Dalgarno (2002)



These results go together with the figure in slide 9 for atoms.
The most abundant species in decreasing order are:

$$
\begin{array}{ccccccccccccc}
H & : & He & : & H+ & : & D & : & H_2 & : & HD & = \\
1 & : & 0.08 & : & 4\times10^{-4} & : & 4\times10^{-5} & : & 10^{-5} & : & 2\times10^{-8} &
\end{array}
$$

Milky May and Cosmic Molecule Formation

The key distinctions between contemporary and primeval molecule formation are the presence in the former case of (1) “metals” and (2) ionizing radiation in the form of stellar UV and cosmic rays.

The metals permit the formation of H_2 on grains. They also provide for the presence of O and other heavy atoms, so that OH and other hydrides form (with the help of H^+ and H_3^+), which then leads to molecules like CO and H_2O.

Cosmic molecule formation is a much slower process because it relies on weak radiative-association reactions to form H_2^+, HeH+ and H^-, which have very small abundances in local gas. On the other hand, cosmic star formation takes a long until the fluctuations grow big enough.

Significance of Molecular Abundances

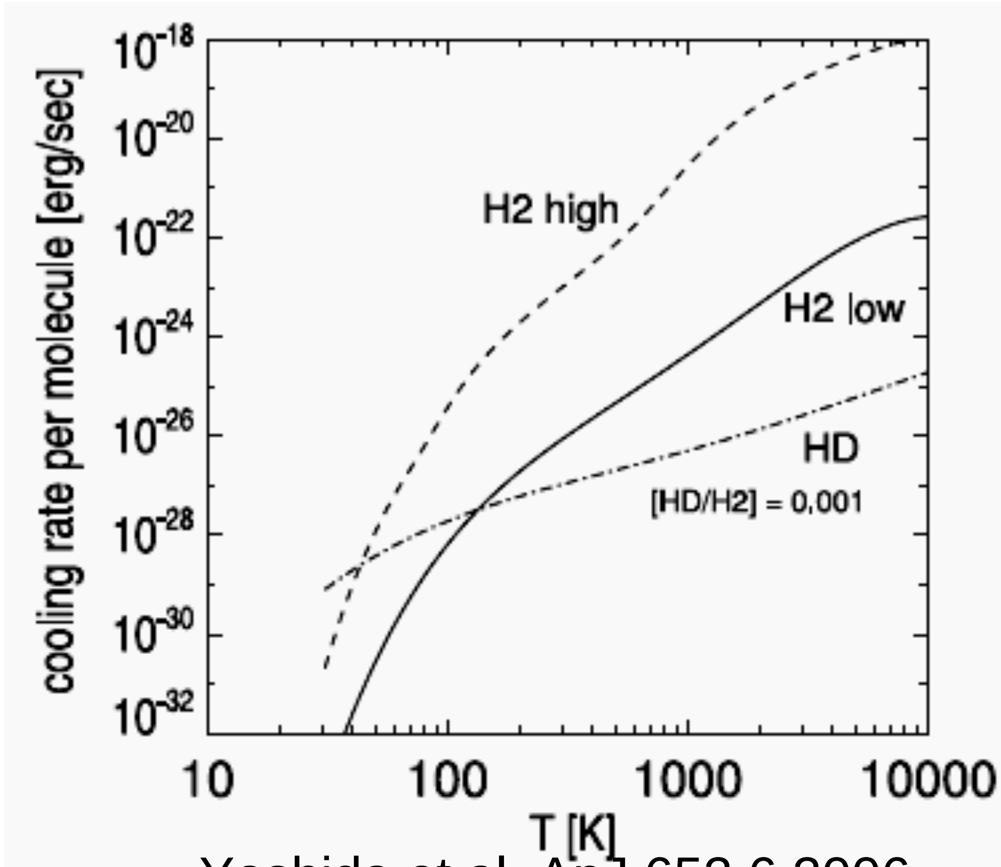
- **The central role of molecules is to cool the gas**.
- The temperature is critical for the growth of fluctuations.
- If we assume that the Jeans criterion is a valid one for the early universe, it would predict that the first stars (or clusters of stars) would have been very massive.

$$M_{\mathrm{J}} \approx 12 M_{\mathrm{sun}}\ T^{3/2} n_{\mathrm{H}}^{-1/2}$$

i.e., the Jeans mass is very sensitive to the temperature
Using the conditions just after recombination
(T = 3000 K, n_{H} = 200 cm^{-3}) leads to masses ~ 10^5 M_{sun}.

- On collapse, the density would increase and promote molecule formation and cooling.
  Fragmentation might occur as the Jeans mass decreases.
  - *These arguments are meant for illustration only: At recombination the CMB fluctuations are too small to collapse of gas clouds and form stars.*

Cooling of H_2 and HD



Yoshida et al. ApJ 652 6 2006

Unless T > 8,000 K, the main coolants are H_2 and HD. The greater cooling efficiency of HD (arising from its finite dipole moment) makes up for its low abundance.

Effect of HD Cooling

Yoshida et al. ApJ 652 6 2006

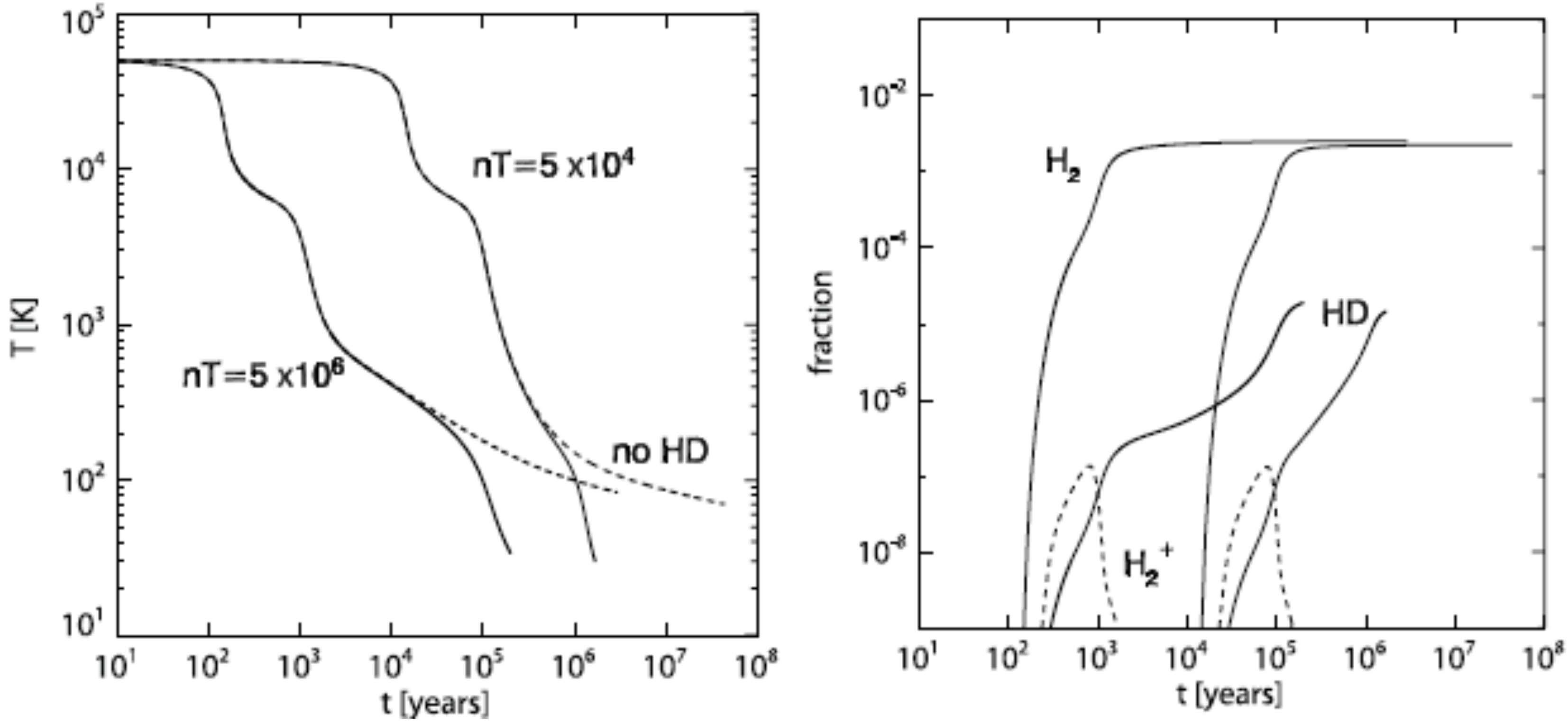


FIG. 2.— Evolution of the gas temperature (*top*) and molecular fractions (*bottom*) for an isobarically cooling gas. The gas is assumed to be fully ionized initially, with a temperature of $T = 50{,}000$ K. We run two cases with initial densities of $n_{\rm H} = 1$ and $100\ {\rm cm}^{-3}$. The dashed lines in the top panel are for runs without HD cooling. The effect of HD cooling can be seen in the temperature and chemical evolution at $t > 10^5$ yr. In the bottom panel, we also show the fraction of H_2^+ ionic molecules.

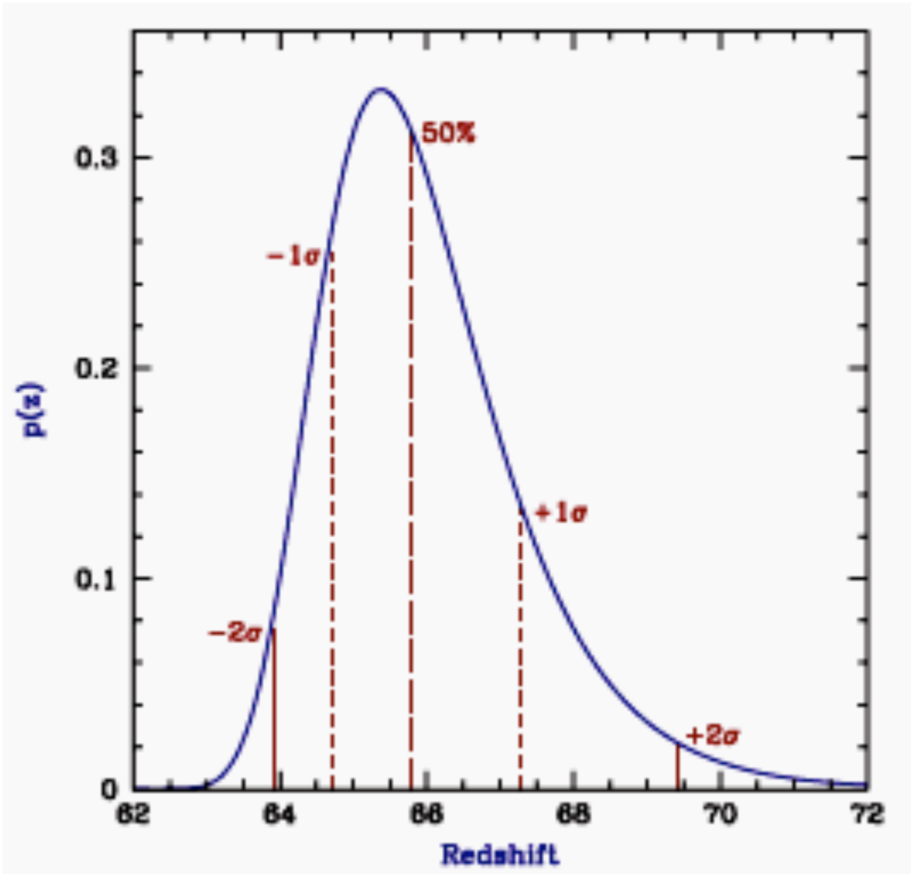
3. The Formation of the First Stars

- The seeds that eventually lead to stars and galaxies are the fluctuations imprinted in the CMB.
- The dynamics of both the dark matter (DM) and the baryons have to be considered.
- Dark matter halos are the sites of star formation.
- The baryon collapse inside halos is governed by the thermal-chemical properties of the gas, including shocks.
- An analog with local star formation: baryon core - DM halo, with molecule formation playing a key role.
- This model of star formation is developed by generalizing the ΛCDM simulations to include the necessary atomic and molecular physics required to treat the formation of molecules and their thermal consequences.
- Examples of these simulations from CfA follow:

When the First Stars Formed

The growth of fluctuations eventually becomes nonlinear, and this point can be used to date the first stars at z ~ 65, or 30 Myr after the Big Bang.

The simulations support a "bottom-up" scenario, starting from tiny CMB fluctuations and ending with MIky-Way like galaxies at z ~ 11.

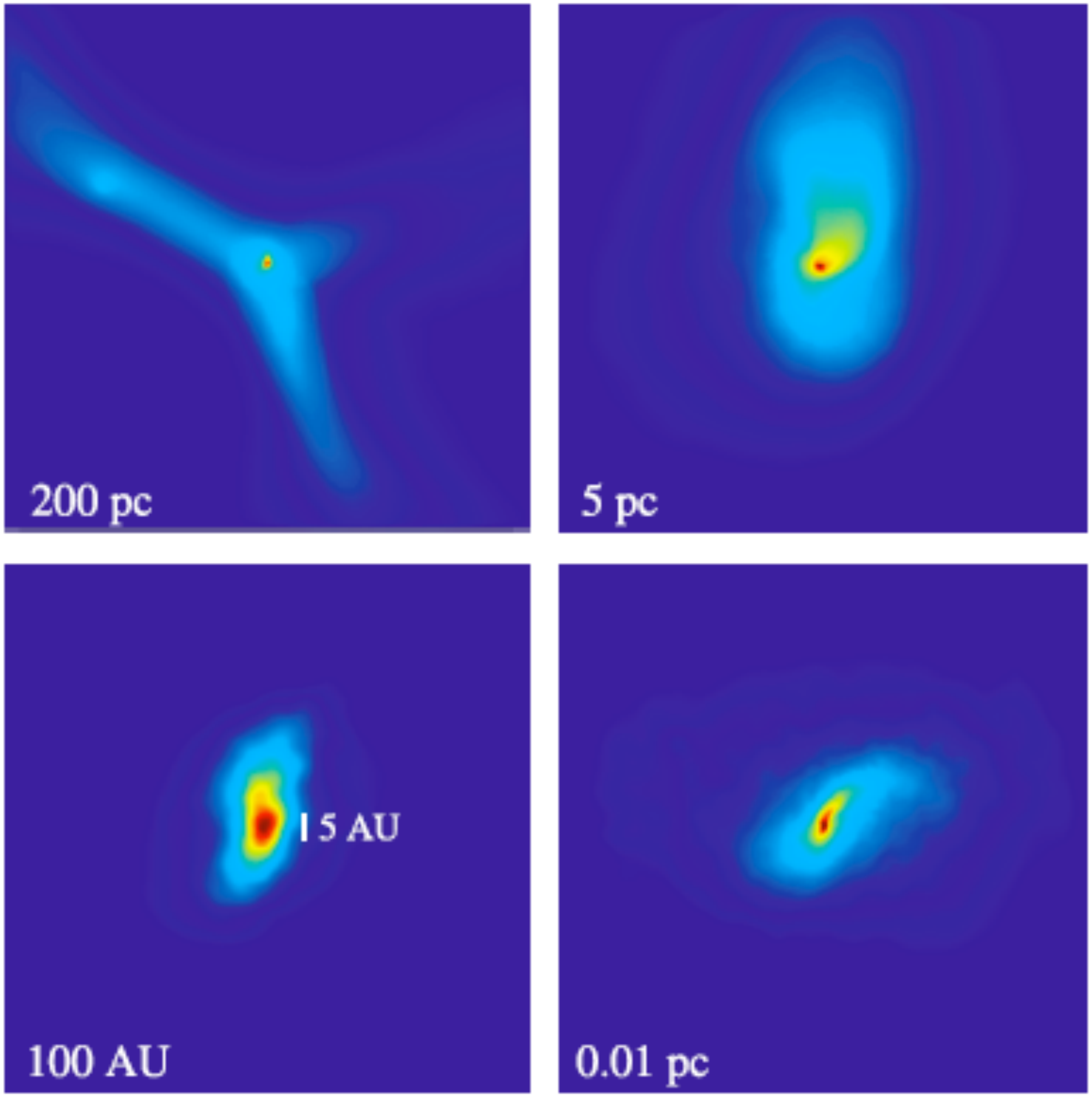


Naoz et al. MNRAS 373 L98 2006

High Resolution Simulation of One Halo

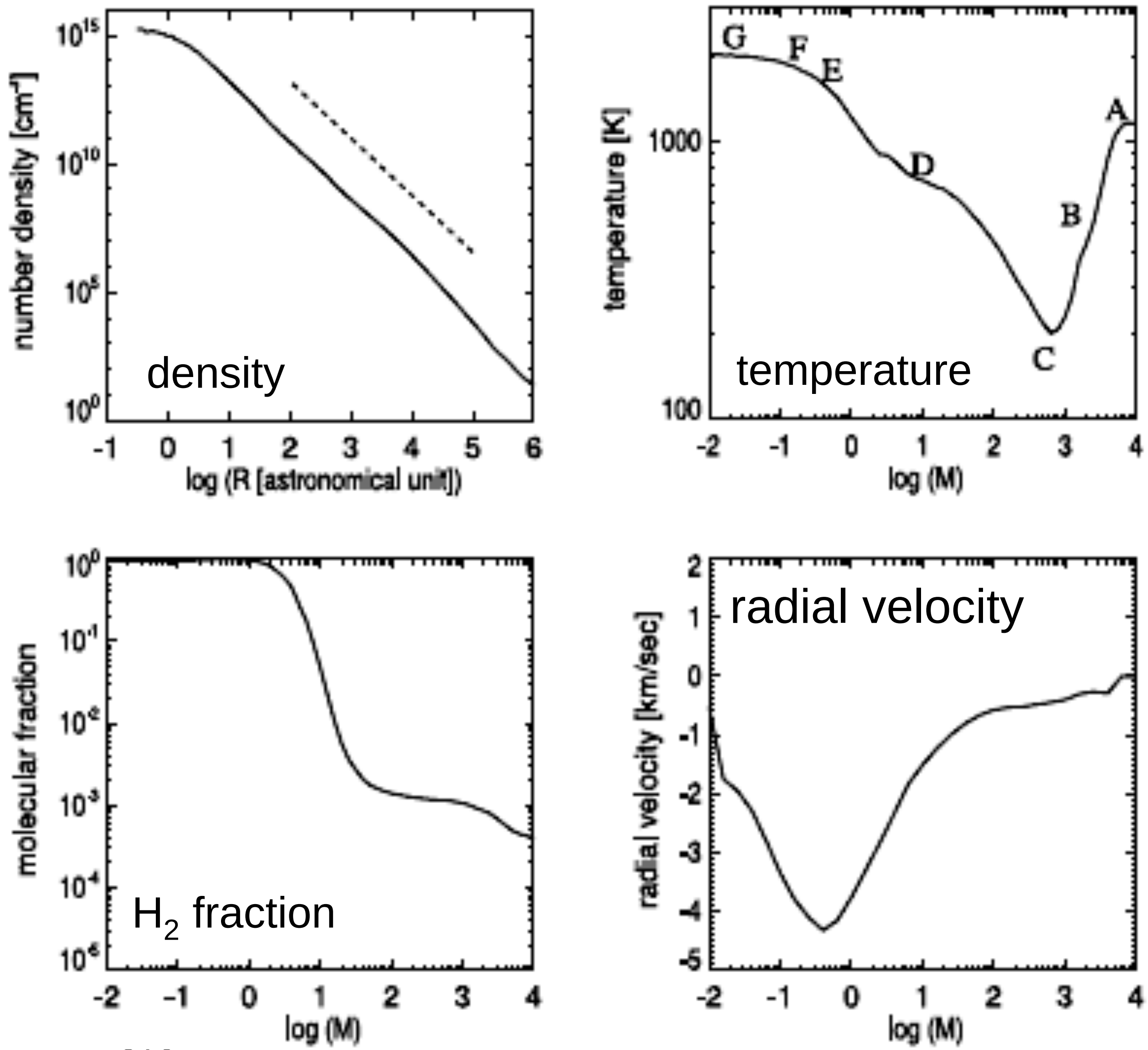
With Loads of Physics (Yoshida et al. 2006)

- Simulation at z = 15 in a 0.3 Mpc cube with 60 $M_{\oplus}$ resolution
- focus on a single DM halo of 600,000 M_{sun}
- central part of top right panel has 300 M_{sun} and diameter ~ 1 pc and is collapsing
- collapsing core does not fragment nor form a disk (low ang. mom.)
- estimated stellar mass ~ 300 M_{sun}



Evolution of Seed Physical Properties

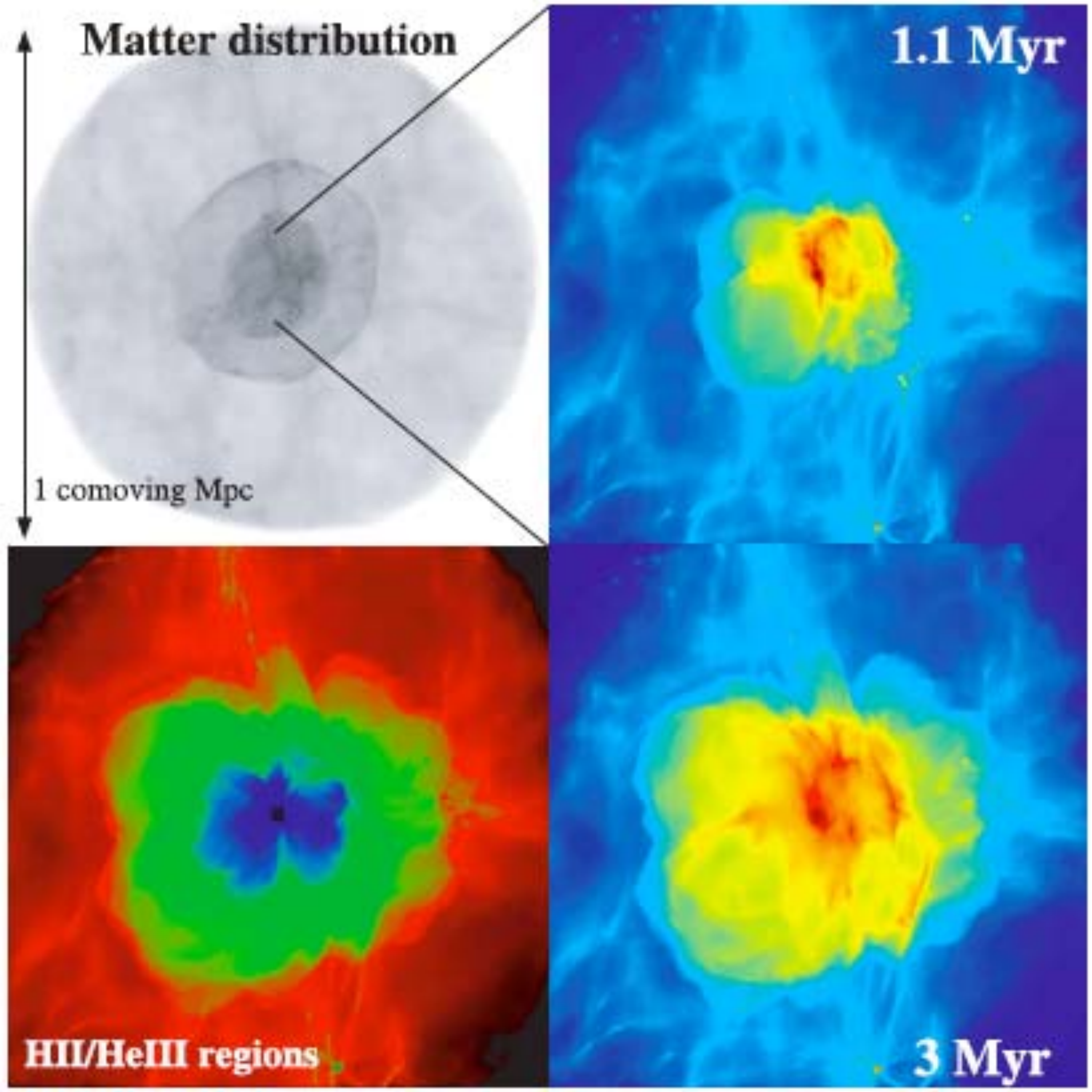
Yoshida et al. 2006



A-C low to high H_2 density cooling
D. 3-body formation; conversion to H_2 is complete
E. cooling iimited by trapping
F. collision-induced cooling
G. H_2 dissociation for $T < 2000$ K.

Simulation Including Ionizing Radiation:
HII Region of the First Star z = 26

Yoshida et al. ApJ 663 687 2007

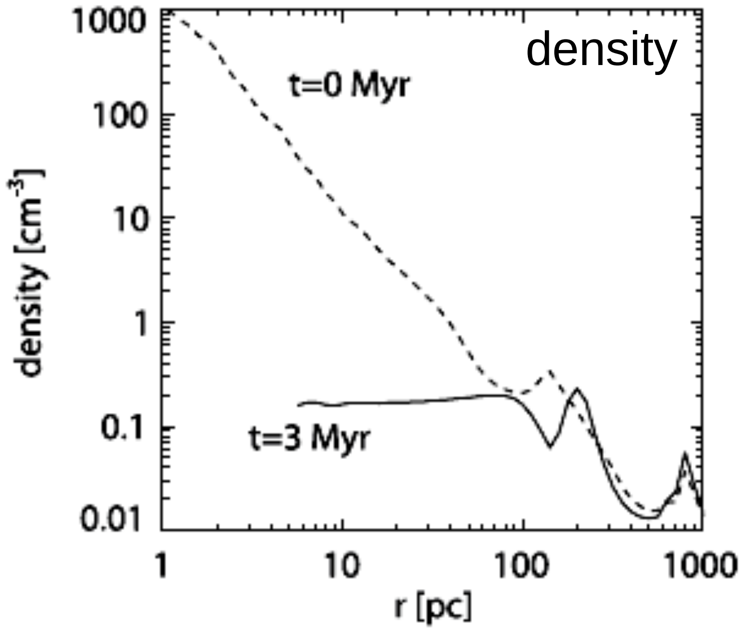


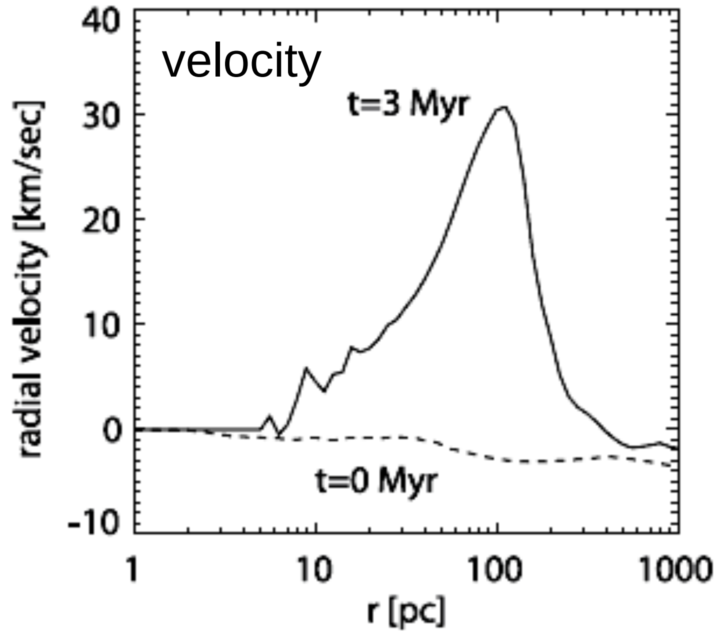
7 kpc

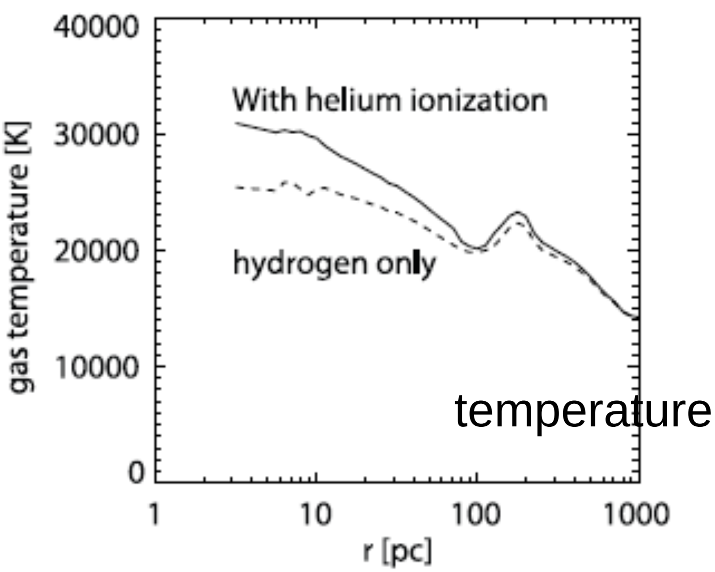
gas density weighted by ionization

Simulated Evolution of the First Star

Yoshida et al. 2007



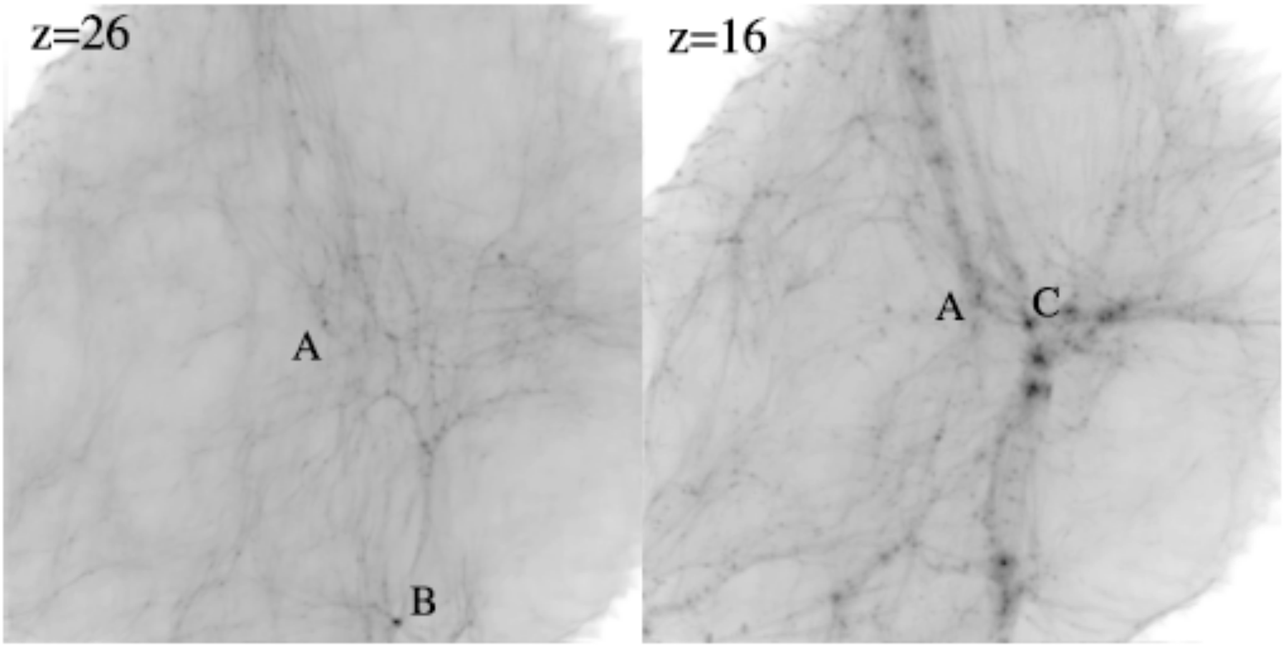




The estimated mass of the first star is now reduced to ~ 40 M_{sun} -- a massive rather than a very massive star

Protostars from Dark Matter Simulations

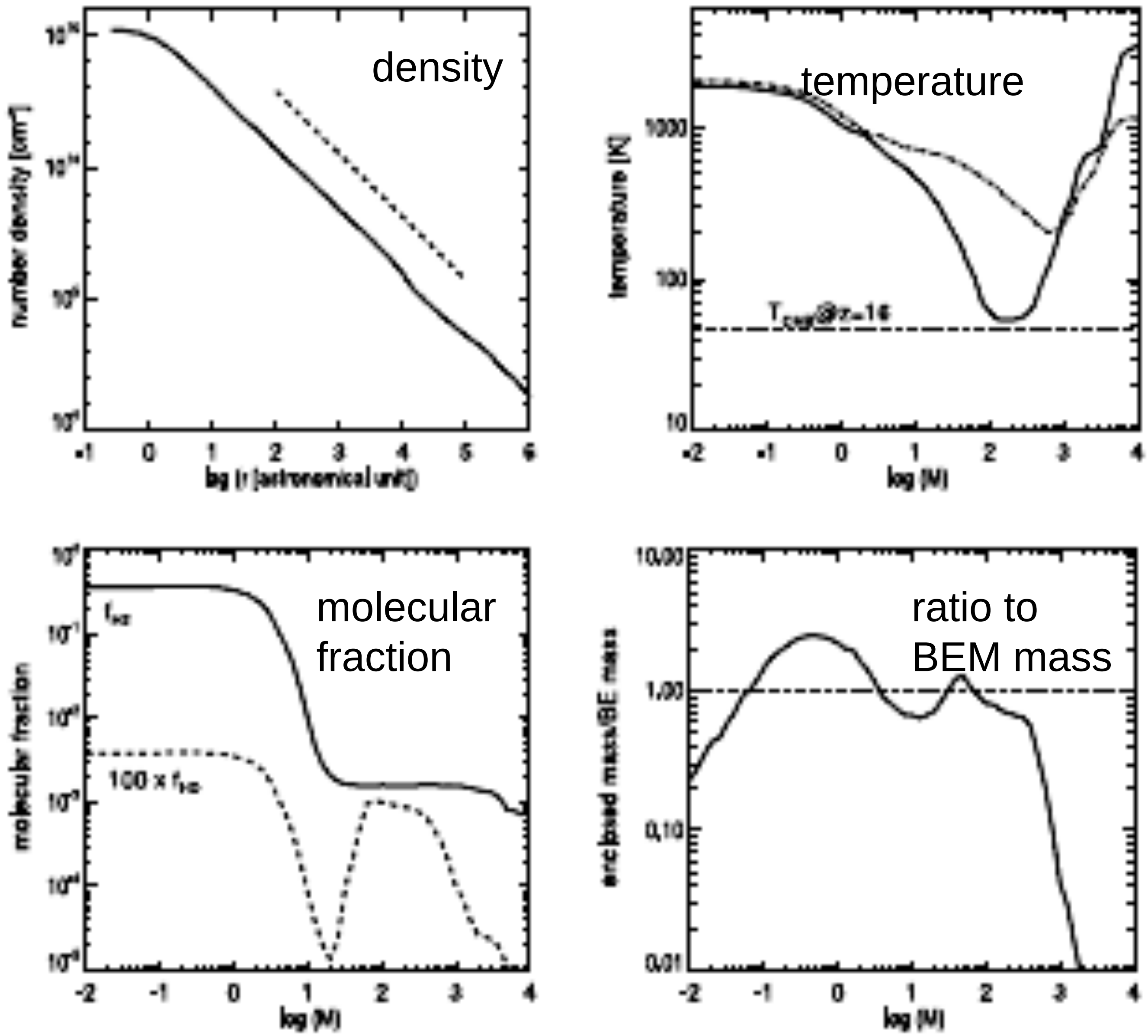
Yoshida et al. 2007



Change in DM evolution over 100 Myr, including effects of the ionizing radiation from the first star formed in halo A. A second generation star forms in nearby halo C under changed physical conditions. **More generally, the time from the first star to complete reionization is several hundred Myr.**

Evolution of the Second Generation Star

Yoshida et al. 2007



Summary

- The simulation of early star formation from baryonic cores inside dark matter halos involves the complicated atomic and molecular and radiation physics of a cooling and chemically active collapsing gas cloud.
- The results are incomplete, in part because present simulations can only treat small regions of the pre-IGM.
- Although the results are not yet definitive, they are convincing in indicating that stars (and presumably galaxies) can form at moderately-high redshifts.
- An important and obvious goal of the observations is to attempt to find quasars at $z > 6.3$.
- Other goals include using γ-ray bursts as light sources to probe the IGM and to detect the 21-cm emission from the dark ages and the epoch of recombination.