Molecule formation in the early Universe

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The Low Metallicity ISM

Göttingen, 8-12 October 2012

A. Loeb (2006)

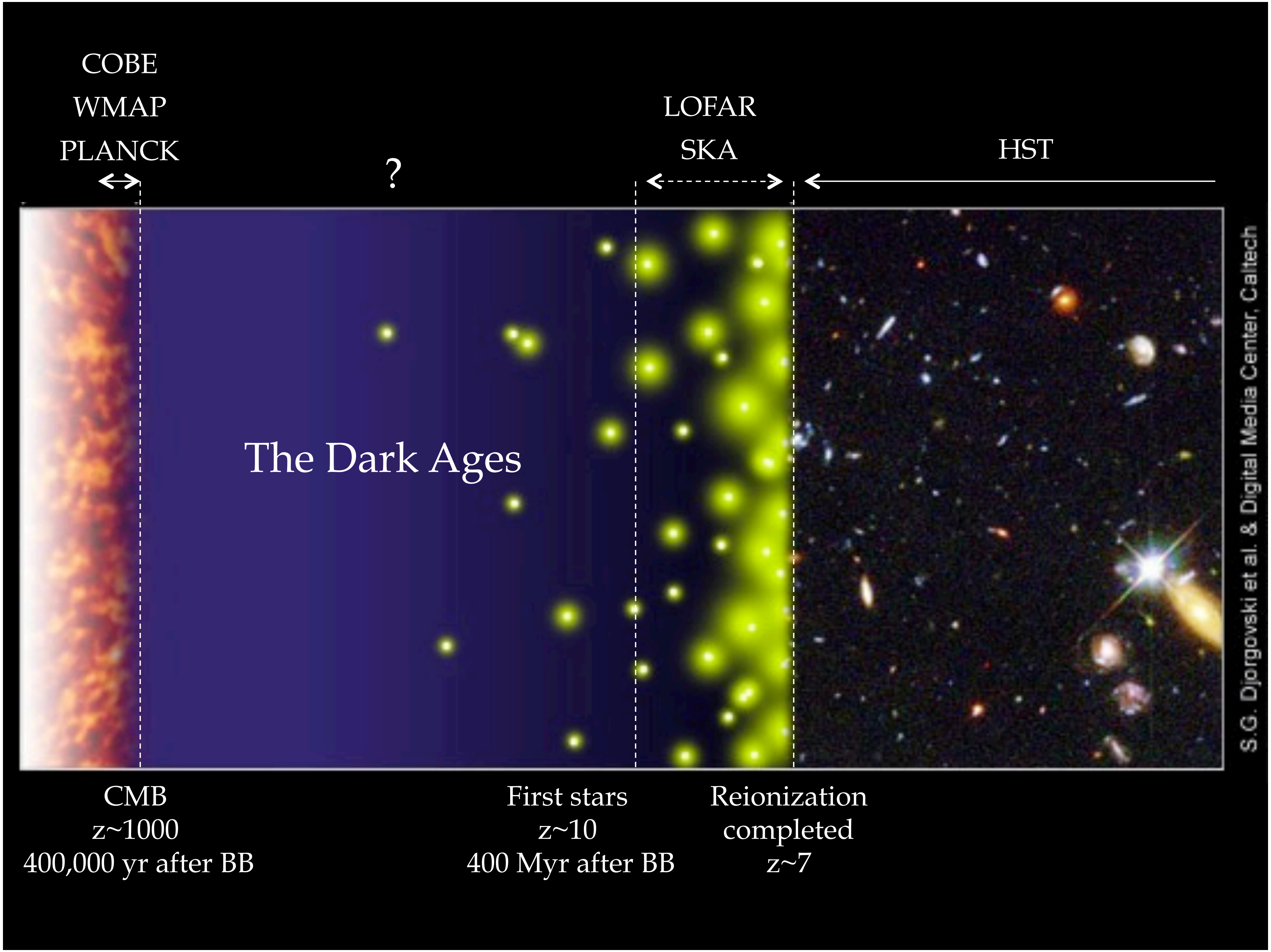
Outline

- The first molecules are formed from gas-phase reactions after H and He recombination (z=1000 to z=10, t=400,000 yr to t=400 Myr after BB).

Why are primordial molecules important?

- Control the thermodynamics of metal-free gas determining the mass of the first stars.

- Produce spectral/spatial signatures in the CMB that may allow to observationally probe the Dark Ages.


COBE
WMAP
PLANCK
?
LOFAR
SKA
HST
The Dark Ages
S.G. Djorgovski et al. & Digital Media Center, Caltech
CMB
z~1000
400,000 yr after BB
First stars
z~10
400 Myr after BB
Reionization
completed
z~7

Chemistry in the Dark Ages

Unfavorable environment for chemical enrichment:

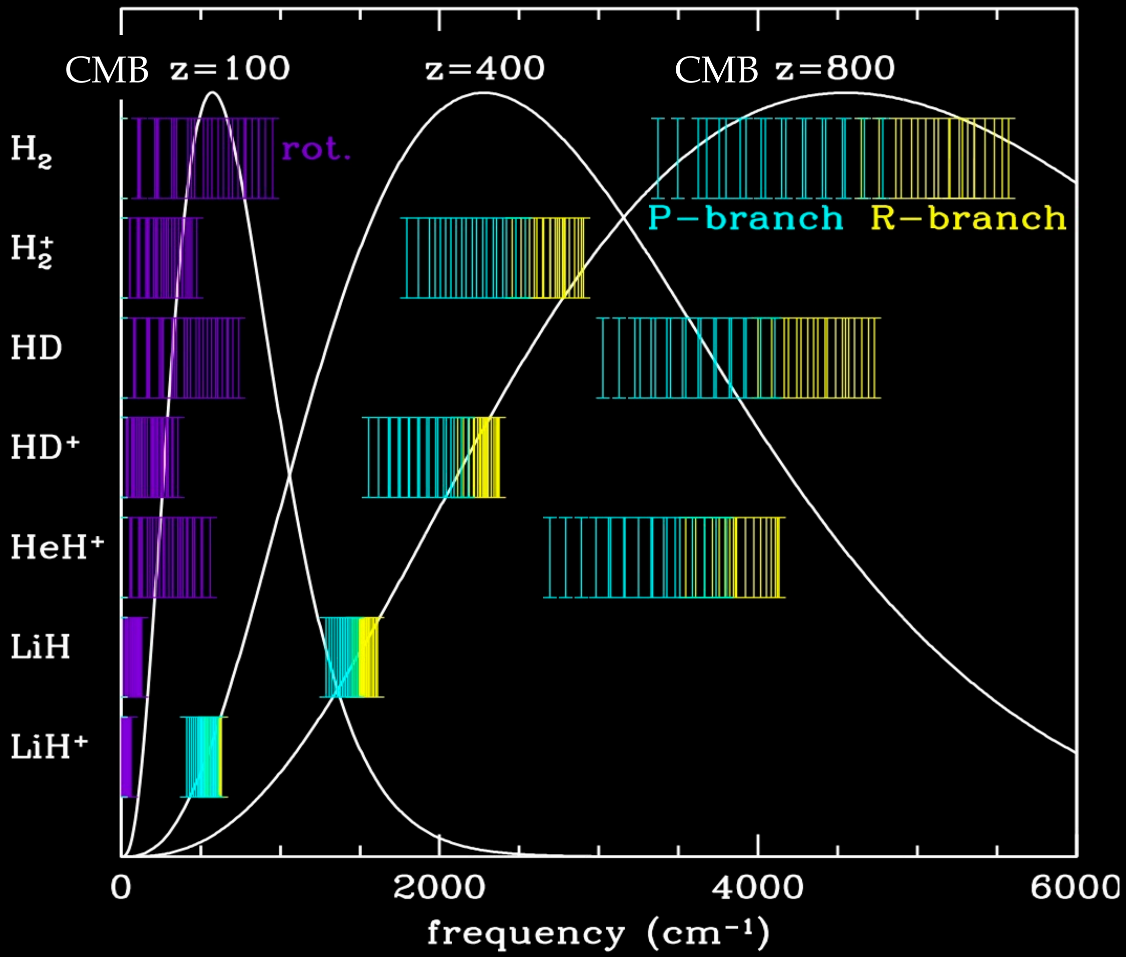
- rapid expansion (low density and temperature)
- strong radiation field (CMB)
- gas chemically inert (H=0.924, He=0.076, D=$2x10^{-5}$, Li=$4x10^{-10}$)
- no solid particles (catalyzers)

→ low molecular abundances

Main molecules and molecular ions formed after recombination (z<1000):

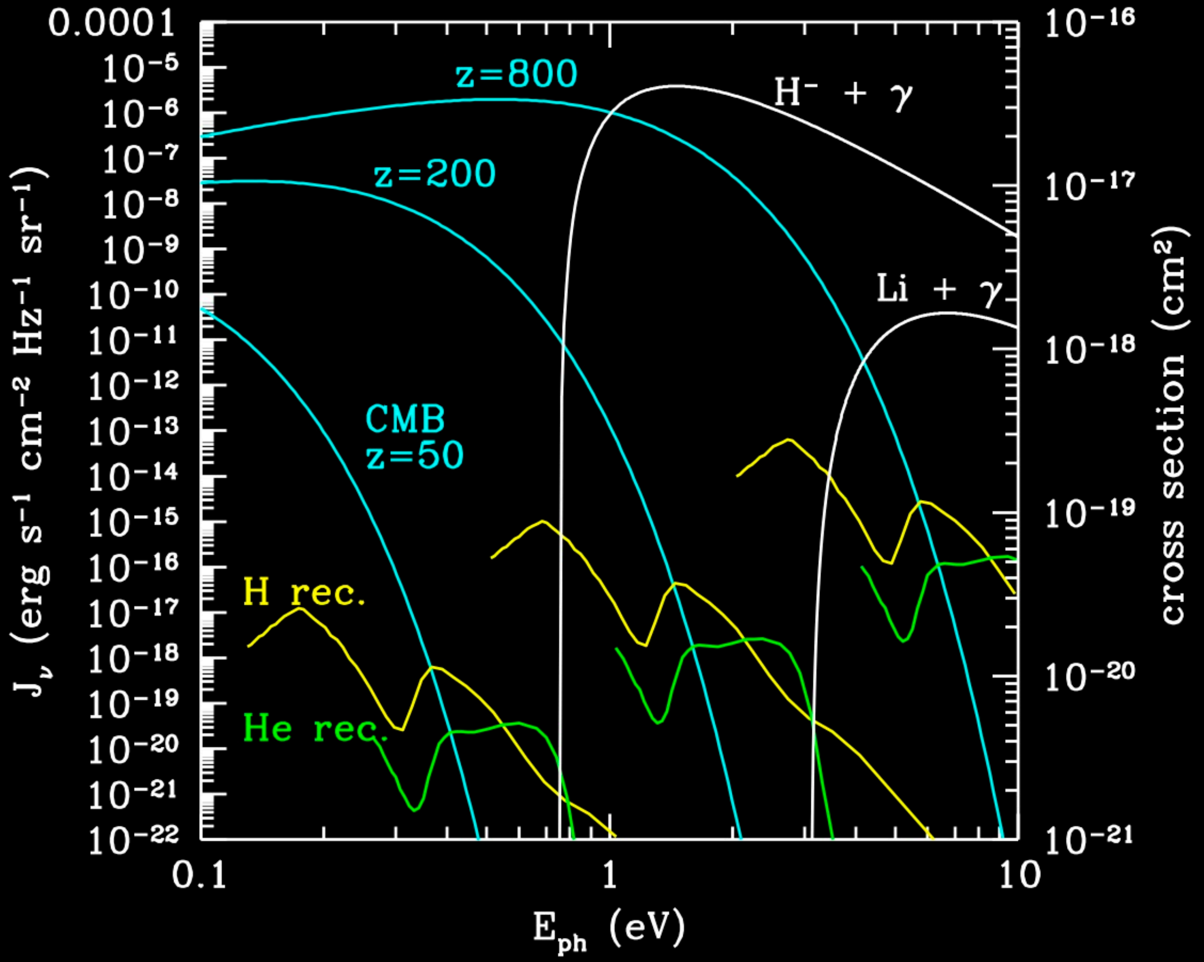
- Hydrogen subsystem: H_2, H_2^+, H_3^+, H^-
- Deuterium " ": HD, HD^+, H_2D^+
- Helium " ": He_2^+, HeH^+
- Lithium " ": LiH, LiH^+, $LiHe^+$

Interaction of molecules with the CMB



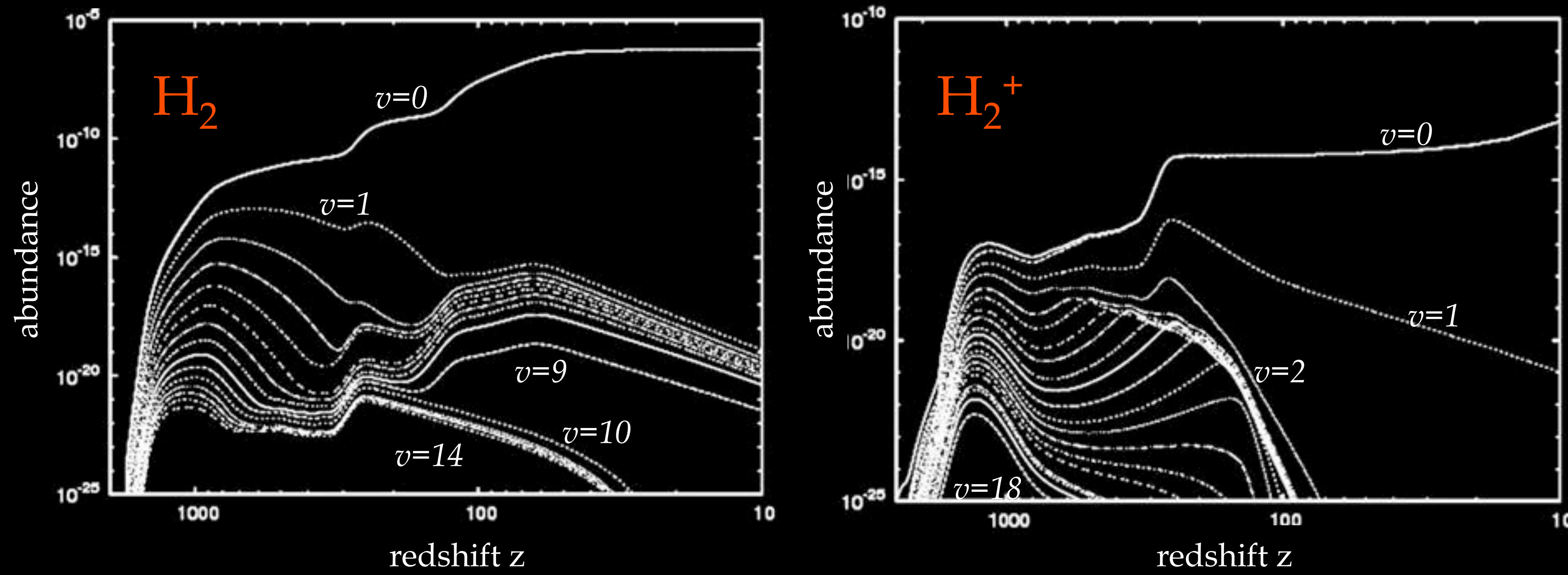
adapted from Maoli et al. (1996)

Importance of recombination photons



Switzer & Hirata (2005)
Hirata & Padmanabhan (2006)

Importance of state-resolved chemistry



Coppola et al. (2011) (see next talk)

Hydrogen chemistry

H_2^+ channel

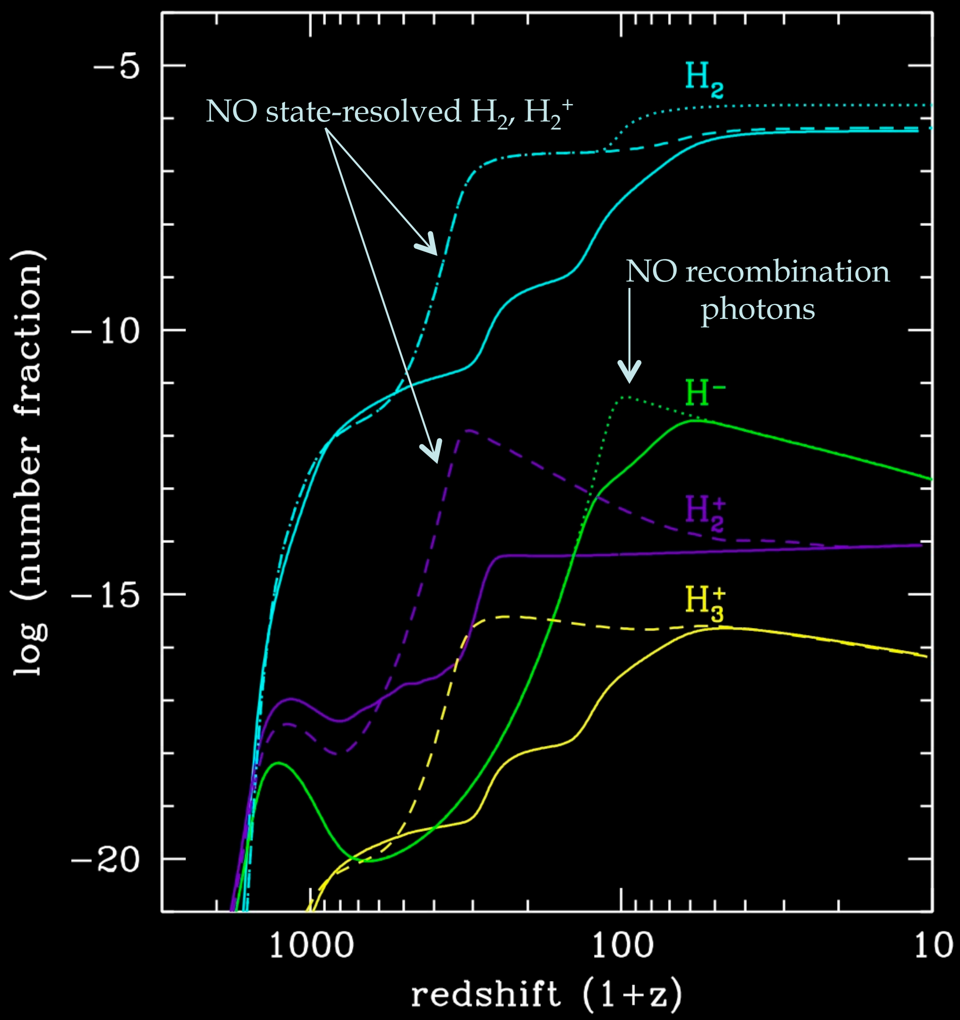
$H + H^+ \rightarrow H_2^+ + \gamma$

$H_2^+ + H \rightarrow H_2 + H^+$

H^- channel

$H + e^- \rightarrow H^- + \gamma$

$H^- + H \rightarrow H_2 + e^-$



Galli & Palla (1998), Coppola et al. (2011)

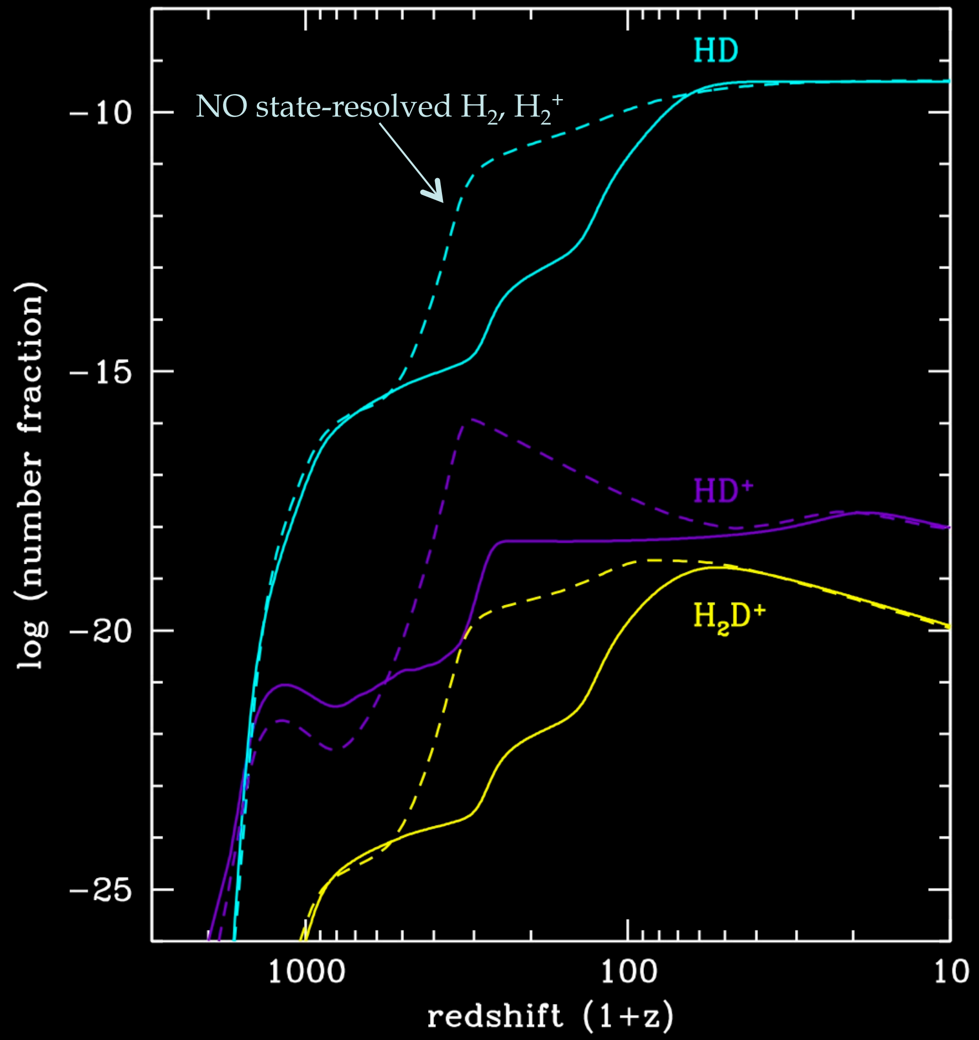
Deuterium chemistry

Formation of HD:

$H_2 + D^+ \rightarrow HD + H^+$

Destruction of HD:

$HD + H^+ \rightarrow D^+ + H_2$



Stancil et al. (1998), Galli & Palla (2002)

Helium chemistry

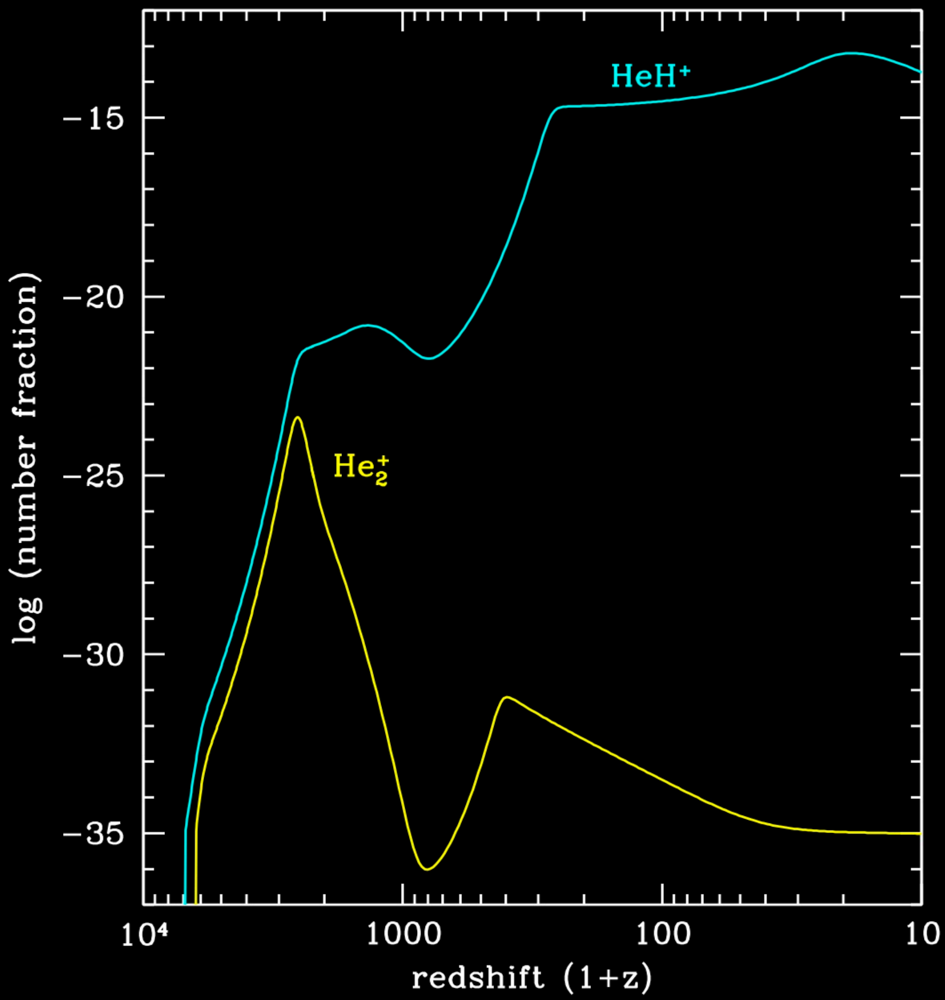
Formation:

$He + H^+ \rightarrow HeH^+ + \gamma$

Destruction:

$HeH^+ + H \rightarrow He + H_2^+$

$HeH^+ + \gamma \rightarrow He + H^+$



Galli & Palla (1998), Bovino et al. (2011)

Lithium chemistry

Formation of LiH:

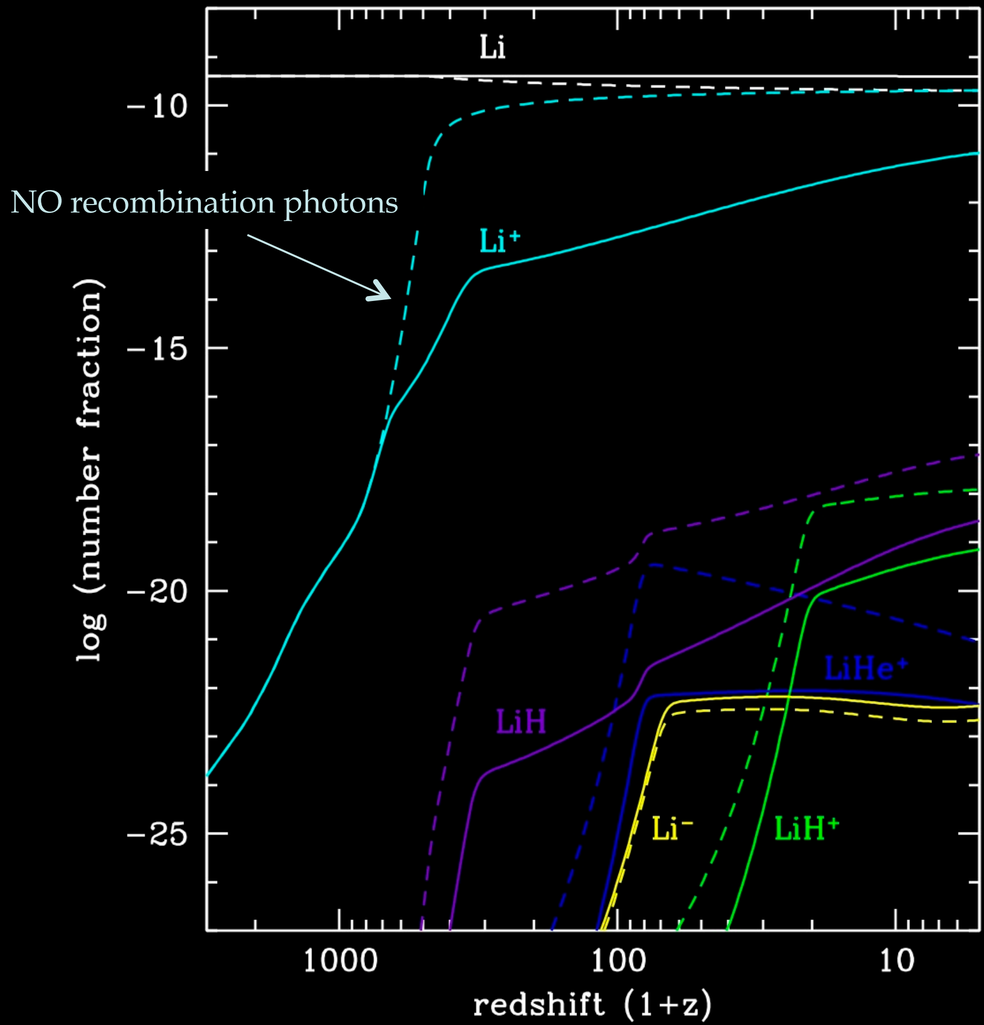
$Li + H \rightarrow LiH + \gamma$

$Li^- + H \rightarrow LiH + e^-$

Destruction of LiH:

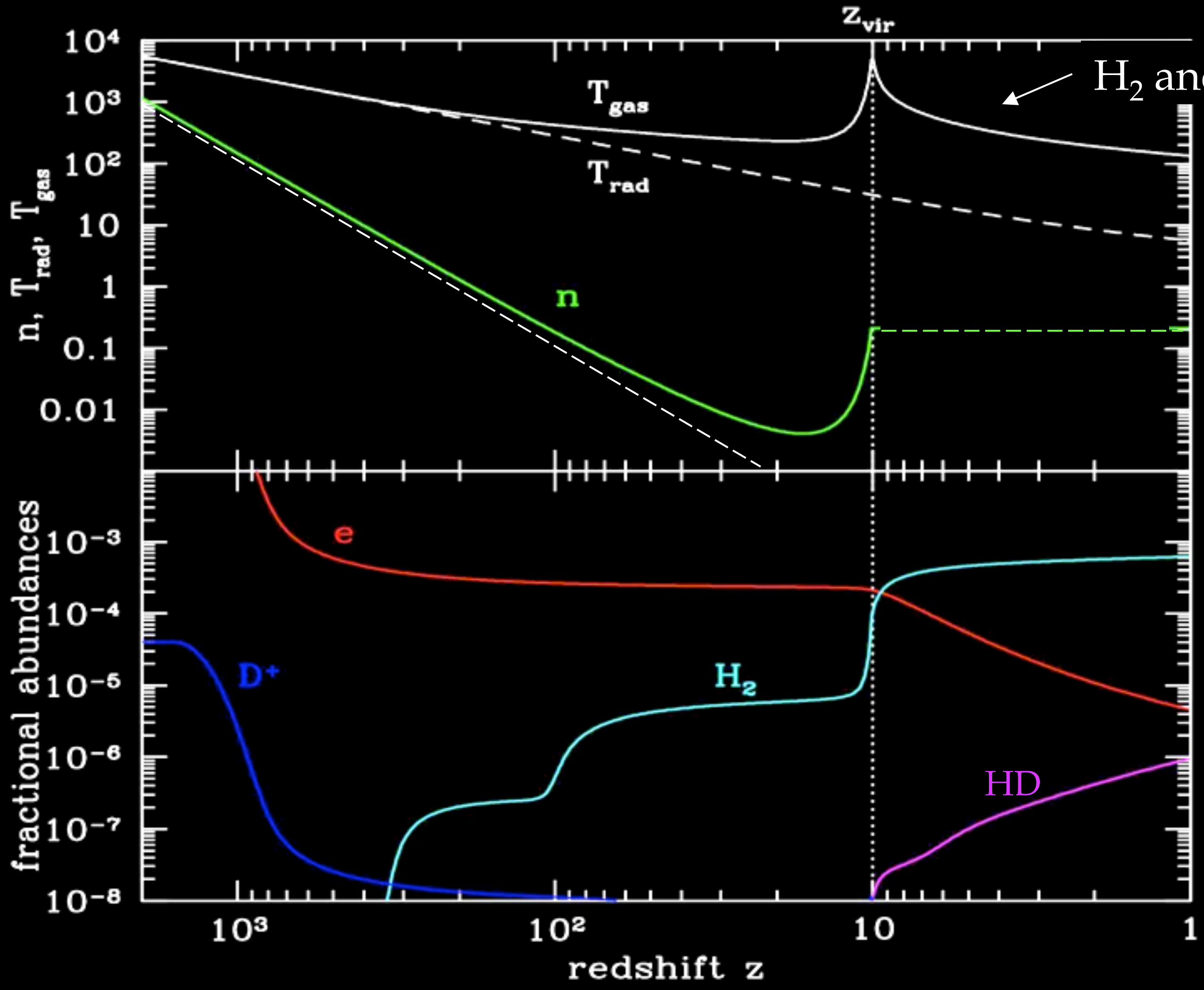
$LiH + \gamma \rightarrow Li + H$

$LiH + H \rightarrow Li + H_2$



Stancil et al. (1996), Bovino et al. (2011)

Evolution of an overdense region



H_2 and HD cooling

Tegmark et al. (1997), Galli & Palla (2002)

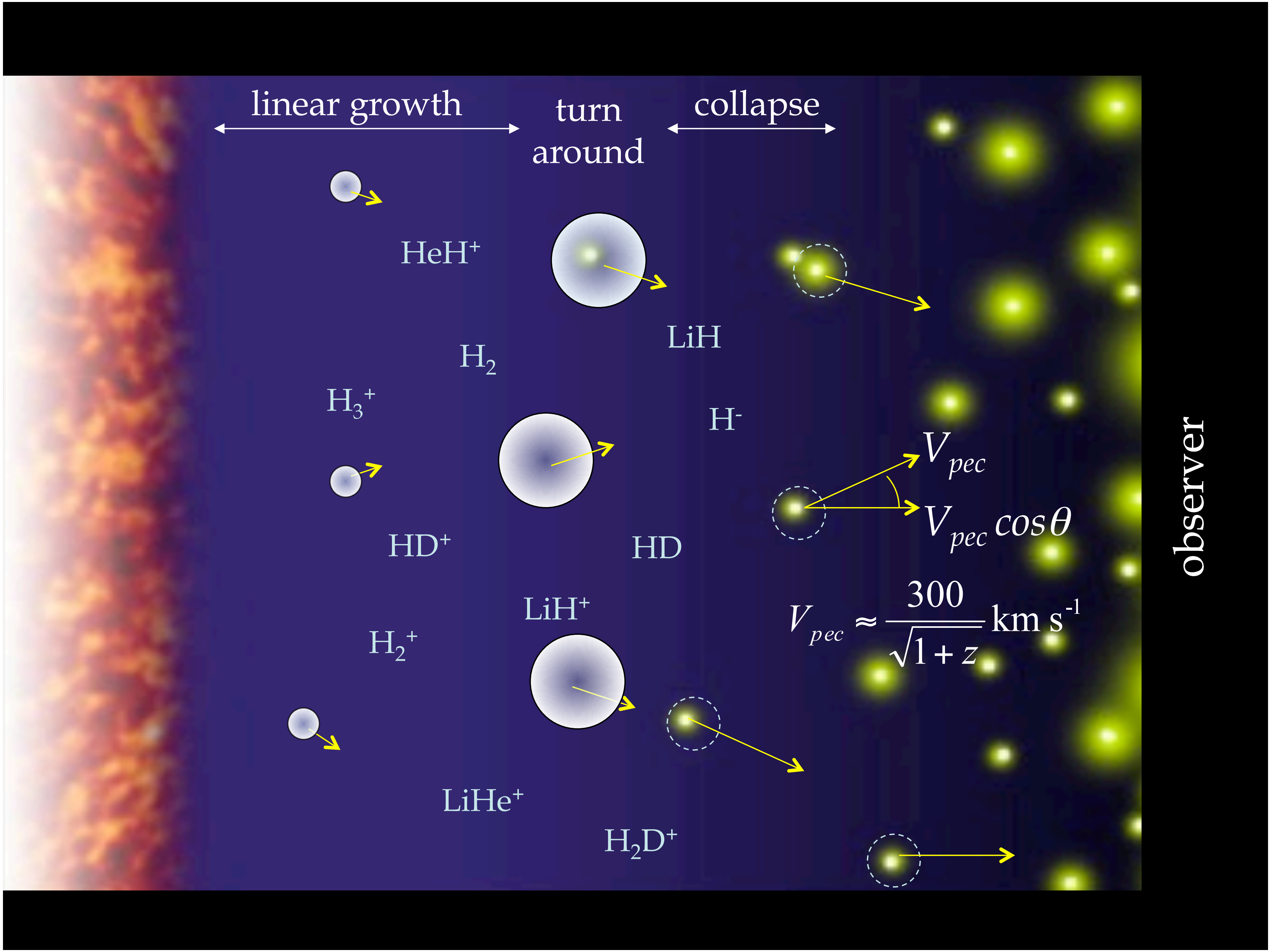
Molecular signals from the Dark Ages?

- Problems: low abundances (low optical depth τ), absence of bright background sources

- Spectral features in absorption/emission against the CMB
  - <u>Phase of linear growth</u> ($n < n_{cr}$, $T_{ex} = T_{rad}$): resonant scattering
  - <u>Phase of gravitational collapse</u> ($n > n_{cr}$, $T_{ex} = T_{gas} >> T_{rad}$): line emission

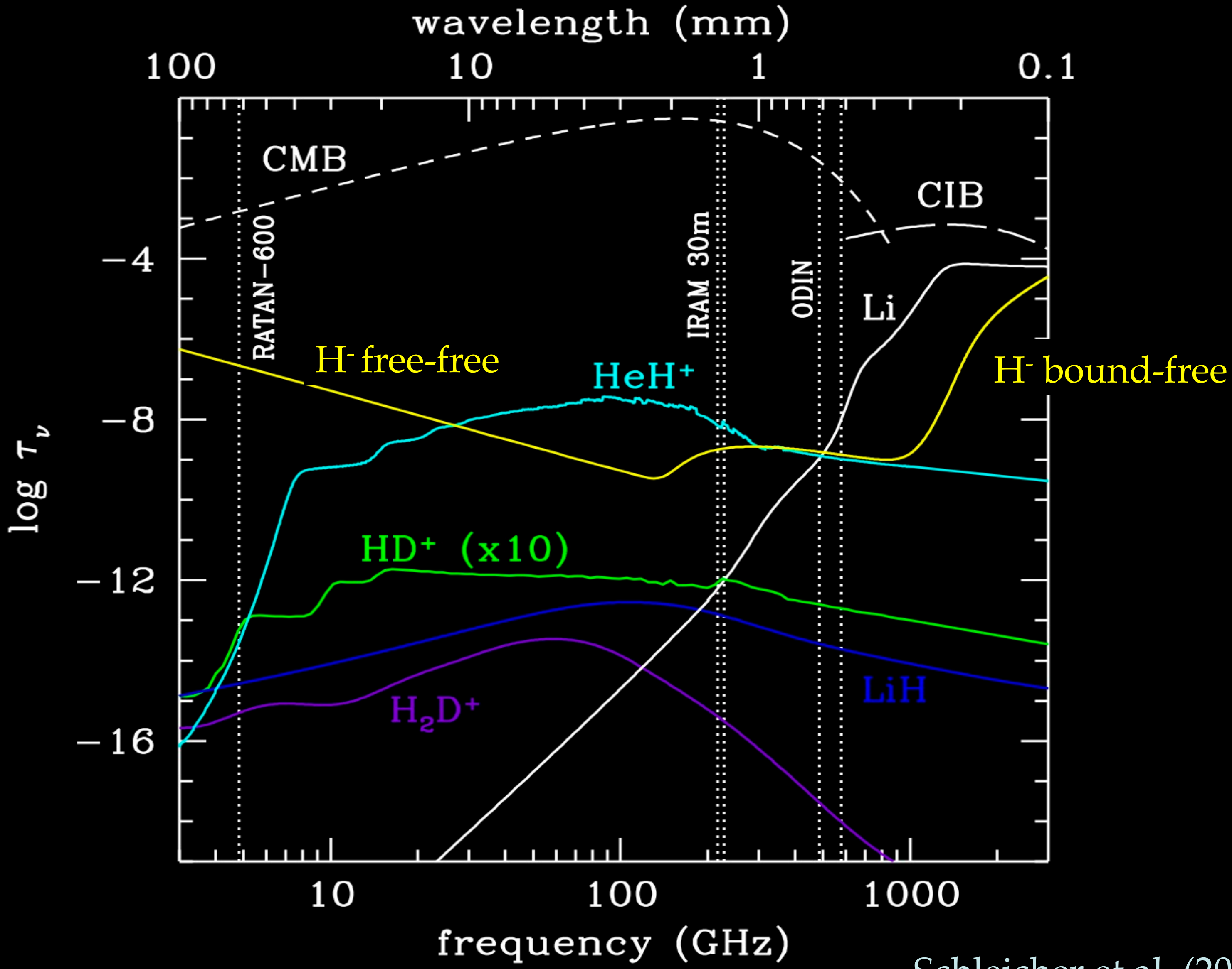
- Spatial anisotropies in the CMB

Dubrovich (1977), Zeldovich (1978), Maoli et al. (1994, 1996)



linear growth
turn around
collapse
HeH⁺
LiH
H_2
H_3^+
H^-
V_{pec}
$V_{pec}\cos\theta$
HD^+
HD
LiH^+
$V_{pec} \approx \frac{300}{\sqrt{1+z}}$ km s^{-1}
H_2^+
$LiHe^+$
H_2D^+
observer

Redshift-integrated optical depth



Schleicher et al. (2008)

1. Resonant scattering

- Absorption of a CMB photon followed by spontaneous emission
- Scattered photons are isotropically distributed in the rest frame of a cloud moving with $V_{\rm pec}$ but not in the observer's frame:

$$\frac{\Delta T(\nu)}{T_r} \approx -\frac{V_{pec}}{c}\cos\theta\,\tau_m(\nu)$$

- Analogous to kinematic SZ effect, but cross section for bound electrons >> Thomson cross section

2. Line emission

- Absorption of CMB photon followed by collisional de-excitation

$$\Delta T(\nu) = (T_{ex} - T_{rad})\,\tau_m(\nu)$$

- Largest τ for molecules with highest dipole moments: HeH^+, HD^+, LiH. But for high dipole moment, $T_{ex} \to T_{rad}$ if $n << n_{cr}$. $\to$ <u>no line</u> (only exception: 21cm HI line).

- For $n >> n_{cr}$ molecules couple to the gas $T_{ex} \to T_{gas} >> T_{rad}$ $\to$ <u>line emission</u>

3. Spatial anisotropies

- Primordial clouds “blur” primary anisotropies in the CMB:

$$\frac{\Delta T}{T} = \left.\frac{\Delta T}{T}\right|_{prim} e^{-\tau(\nu)}$$

- Effect on CMB angular power spectrum coefficients C_ℓ

$$\left.\frac{\Delta C_\ell}{C_\ell}\right|_{prim} \approx -2\tau(\nu) \qquad \text{at all } \ell$$