# Stuff other than H I in the Early Universe

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# Summary

- Making the First Molecules
- Cooling & First Stars
- Metal Scattering Lines

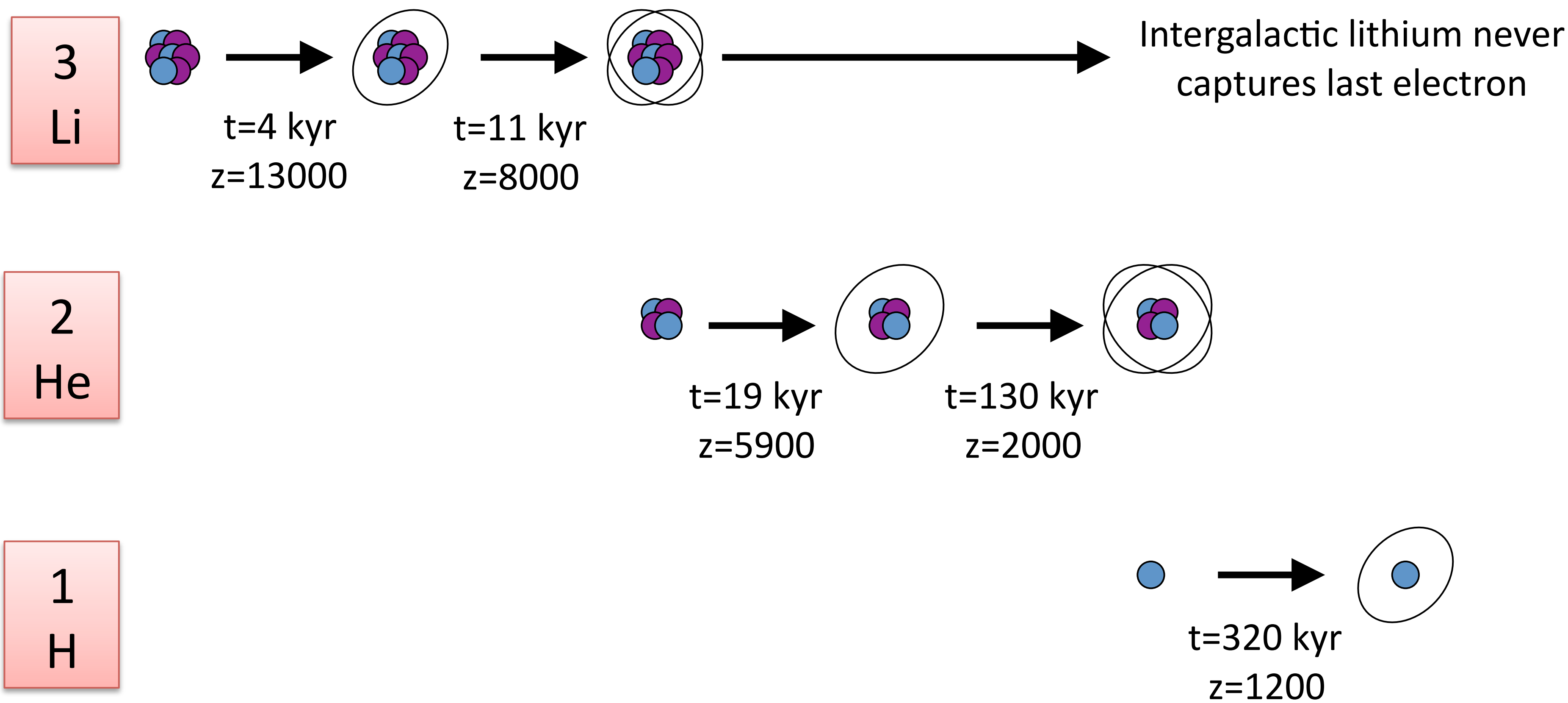
*Everything I will talk about will be hard (and maybe impossible?) to detect … if it weren't, we wouldn't need a KISS workshop!*

# Theoretical Approaches to the (End of) the Dark Ages

- Forward calculation:
  - ➔ Evolve baryons + CDM + CMB forward in time
  - ✓ Works well for CMB anisotropies
  - ✓ "First principles" calculation
  - ✗ Uncertainties multiply at each stage, at some point become intractable ... hard to know (yet) if we're missing something.

- Astrophysical approach:
  - ➔ "Best guess" or extrapolated behavior of baryons
  - ✓ Some of this is calibrated to $z \leq 6$ observations (galaxies, IGM)
  - ✗ No fundamental basis for extrapolating X-rays, escape fractions, metal yields ...

# Step I: Recombination




***Peebles; Zel’dovich et al (1960s) …***

# The Tail End of Recombination

- Second order reaction of residual electrons & protons:

$$\mathrm{H}^+ + e^- \rightarrow \mathrm{H}(1s) + n\gamma$$

$$\frac{dx_e}{d\ln a} = -\frac{\alpha_B^{eff} n_H}{H} x_e^2 .$$

- Freezes out at $x_e \sim 2\times10^{-4}$ @ $z \sim 300$, $n_H \sim 5\ \mathrm{cm}^{-3}$.
- Compare to photon density:
  - CMB (~1000 K): $n_\gamma \sim 10^{10}\ \mathrm{cm}^{-3}$
  - Recombination photons (~2 eV): $n_\gamma \sim 10\ \mathrm{cm}^{-3}$
  - UV photons (≤10.2 eV): $n_\gamma \sim 10^{-3}\ \mathrm{cm}^{-3}$

# Pre-Stellar Lines

- Atomic:
  - Hyperfine: H I 21 cm, D I 92 cm
  - Optical: H I residual recombination lines
  - "Wrong" ionization state: $^{3}$He II 3.3 cm, Li I 671 nm
- Molecular:
  - $H_2$, binding energy 4.48 eV
  - Cooling lines: $H_2$ rotation @ 16 & 28 μm
  - Low temperature: HD rotation @ 112 μm

# Routes to Forming $H_2$

1. Radiative? No dipole moment.

$$2\mathrm{H} \not\rightarrow \mathrm{H}_2 + \gamma$$

2. Inverse Solomon?

$$2\mathrm{H} + \gamma \leftrightarrow \mathrm{H}_2^*(B^1\Sigma_u, C^1\Pi_u) \leftrightarrow \mathrm{H}_2 + \gamma$$

Possible only during recombination epoch (need UV) and produces small abundances [e.g. Dalgarno & van der Loo 2006; Alizadeh et al in prep]

3. Positive catalytic channel – but inefficient due to non-equilibrium of $H_2^+$ levels [Saslaw & Zipoy 1967; Hirata & Padmanabhan 2006]

$$\mathrm{H} + \mathrm{H}^+ \leftrightarrow \mathrm{H}_2^+ + \gamma$$

$$\mathrm{H}_2^+ + \mathrm{H} \rightarrow \mathrm{H}_2 + \mathrm{H}^+$$

# Routes to Forming $H_2$

4. Negative catalytic channel [Peebles & Dicke 1968]

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

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

5. Three-body association (only at high densities)

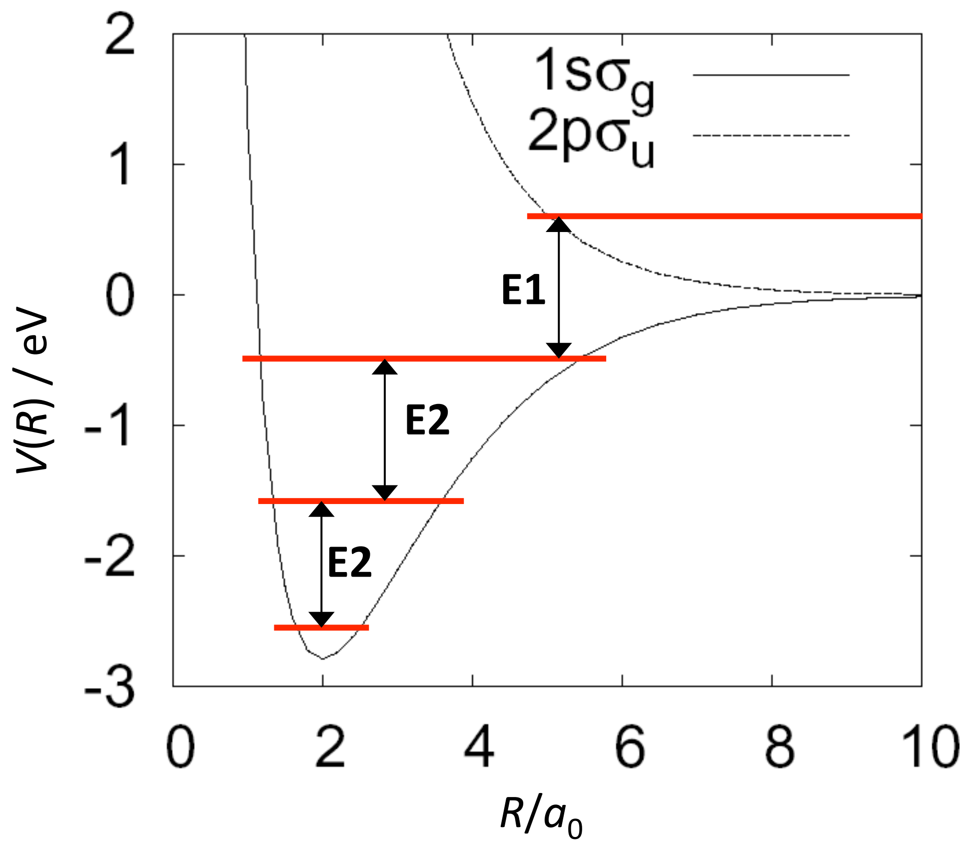
$$2H + X \rightarrow H_2 + X$$

# $H_2^+$: A Cautionary Tale

[Hirata & Padmanabhan 2006]

- $H_2^+$ is formed by decay from $2p\sigma_u$ continuum state ($H+H^+$) to $1s\sigma_g$ bound state ($H_2^+$).
- Wave function overlap implies excited $H_2^+$ states are preferred.
- Ground state populated by E2 decays ($A \sim 10^{-6}\ s^{-1}$).
- This results in non-equilibrium $H_2^+$ level populations; $H_2^+$ photodissociation is faster than implied by principle of detailed balance.
- Thus less $H_2$ is produced.

$H_2^+$ potential energy curves



# $H_2^+$: A Cautionary Tale

[Hirata & Padmanabhan 2006]

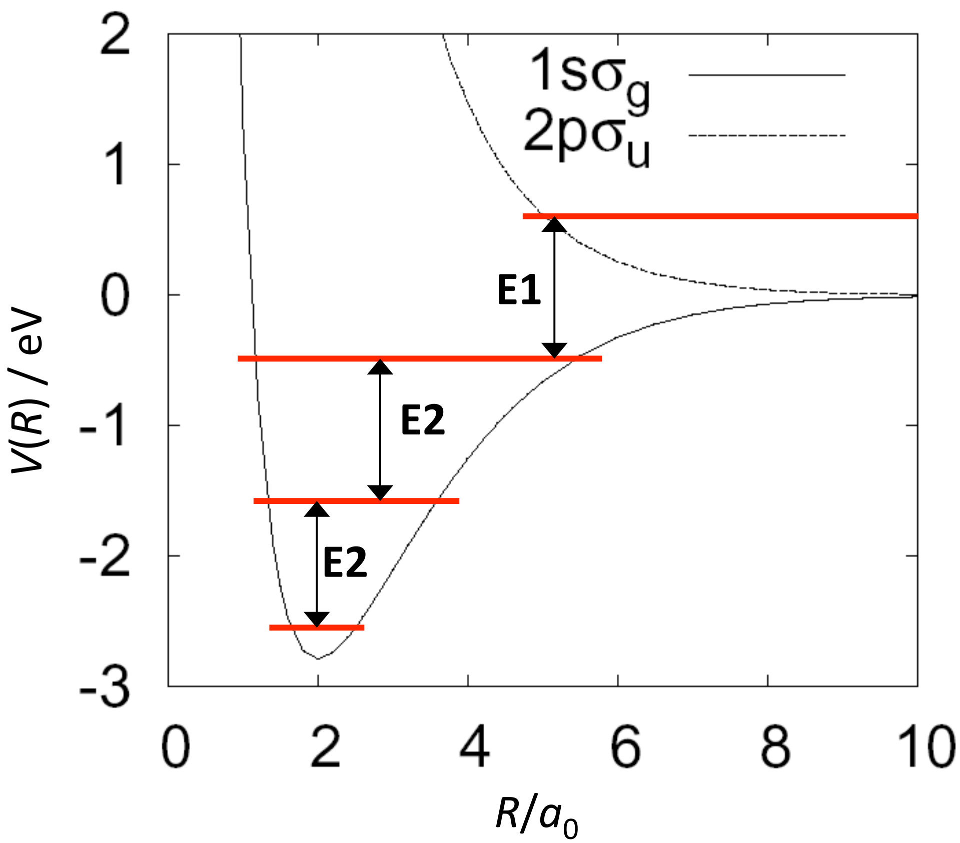
- … in fact at $z$<300, the main mode of producing $H_2^+$ is indirect:

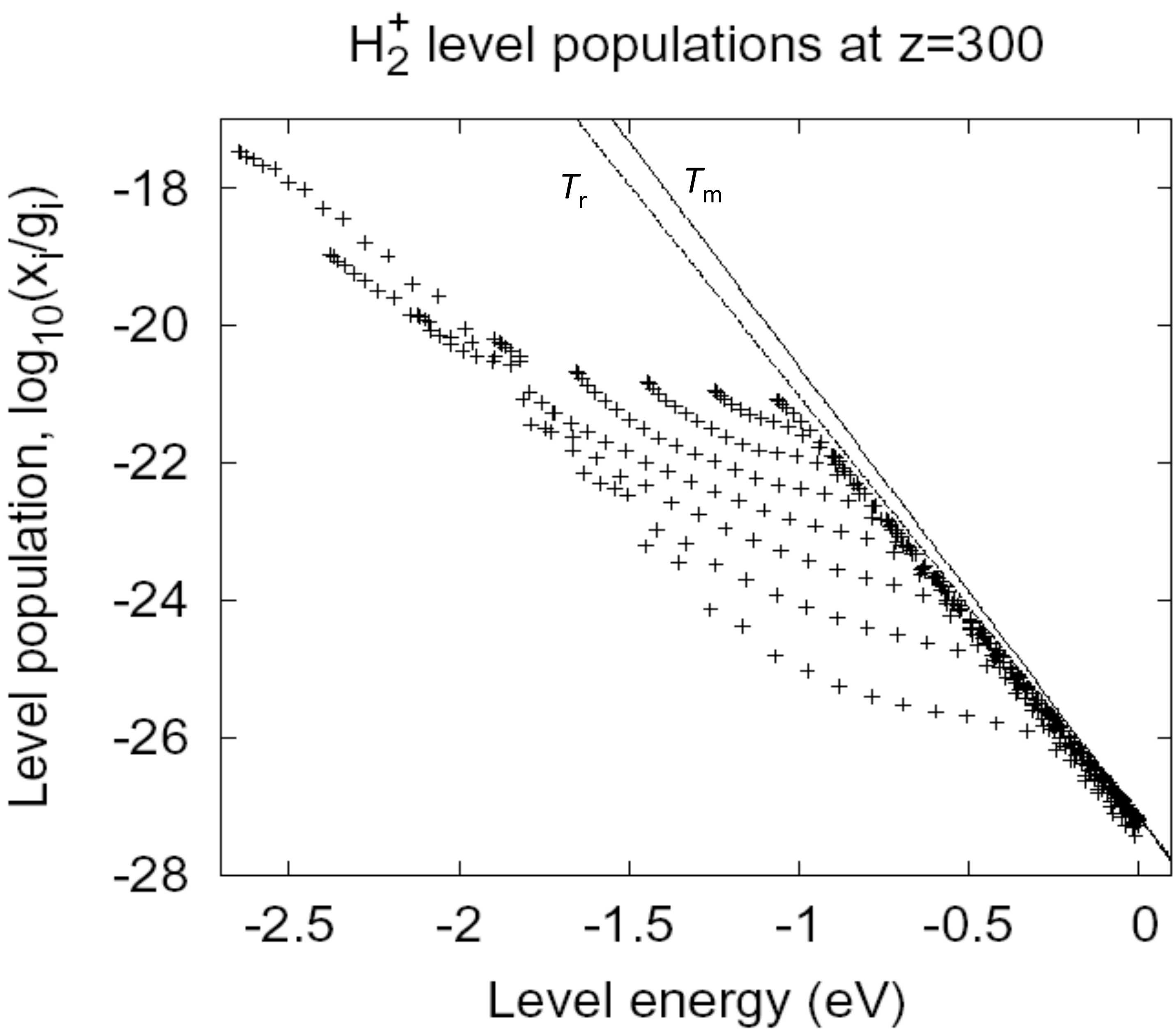
  $H^+ + He \leftrightarrow HeH^+ + \gamma$
  $HeH^+ + H \leftrightarrow H_2^+ + He$
  $H_2^+ + H \rightarrow H_2 + H^+$

- $HeH^+$ has a dipole moment and decays rapidly to the ro-vibrational ground state.

- This directly produces $H_2^+$ in a low-lying state and avoids photodissociation by CMB.

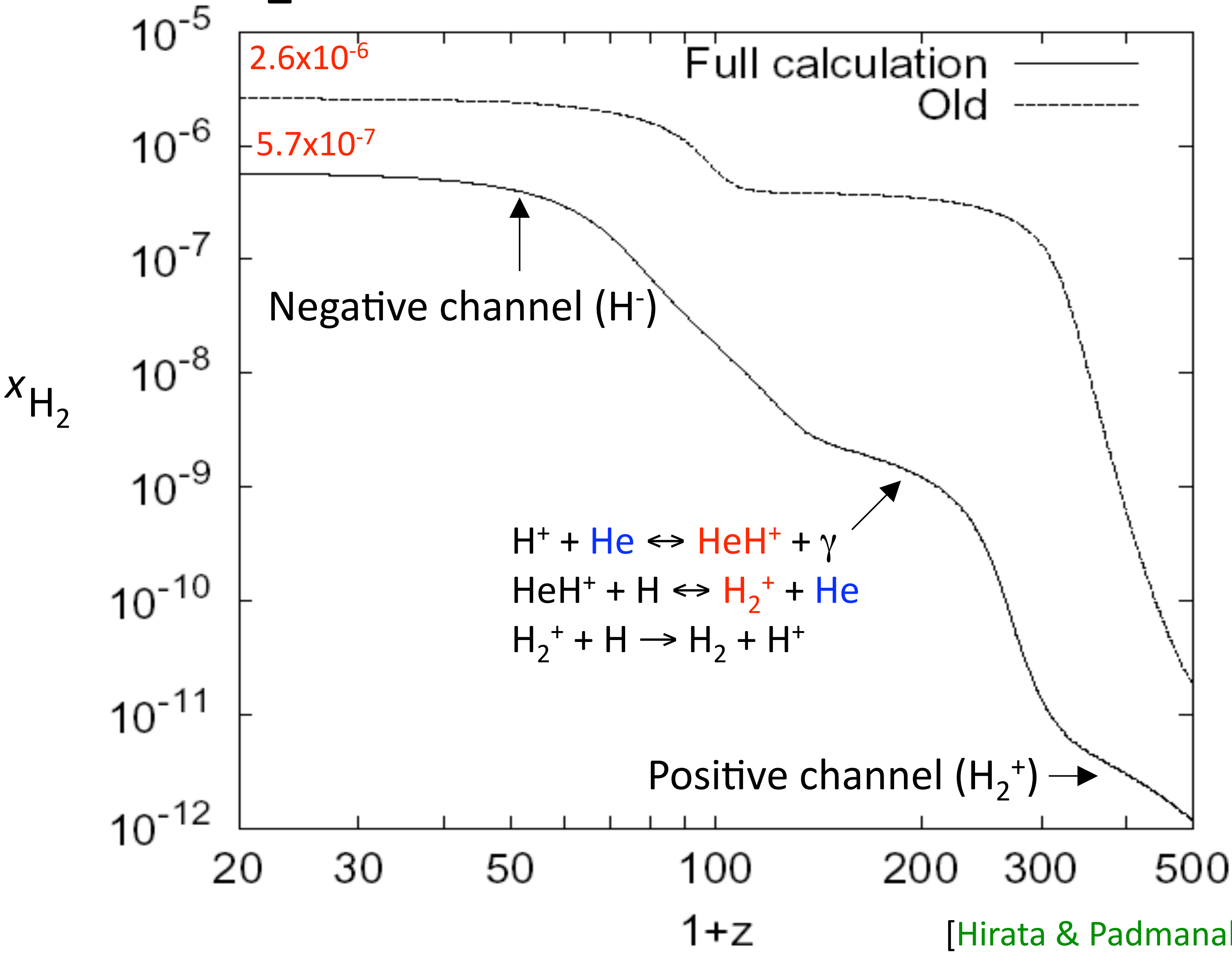
$H_2^+$ potential energy curves






[Hirata & Padmanabhan 2006]

# $H_2$ Abundance vs. redshift




[Hirata & Padmanabhan 2006]

# Cooling Radiation & First Stars I

- The negative catalytic channel speeds up and "re-starts" $H_2$ formation when early halos form.
- If the temperature is sufficiently high to excite $H_2$ rotation lines, these can radiate and allow gas to cool and form a molecular cloud, then a star(s).
  - Both analytics and simulations [e.g. Tegmark et al 1997; Abel, Bryan, Norman 2002]
- Should result in $H_2$ radiation @ z~30 ($\lambda \sim 800$ μm)

# Cooling Radiation & First Stars II

- Can we see the isotropic background of $H_2$ rotation lines from the formation of the very first stars? Unfortunately:
  - Energy release per baryon before switching to other lines is ≤1 eV or ~20 photons.
  - Fraction of baryons participating is <<<1 (depending on definition of "first").
  - Harder than primordial Hα line? (similar λ, Δλ/λ)
- Fluctuations? … but there are many more photons from mid-IR lines at lower z.

# Metal Fine Structure Lines

- Arise from coupling of unpaired electron spin & orbital angular momentum in $np^{1,2,4,5}$ atoms/ions.
- Magnetic dipole transition
- $np^1$: [C II] 158 μm; [N III] 57 μm; [O IV] 26 μm; [Si II] 35 μm; [S IV] 105 μm
- $np^2$: [C I] 370, 610 μm; [N II] 122, 205 μm; [O III] 52, 88 μm; [Si I] 68, 130 μm; [S III] 19, 33 μm
- $np^4$: [O I] 63, 146 μm; [S I] 25 μm

# Scattering of CMB by IGM Metal Lines

[Basu, Hernandez-Monteagudo, Sunyaev 2004]

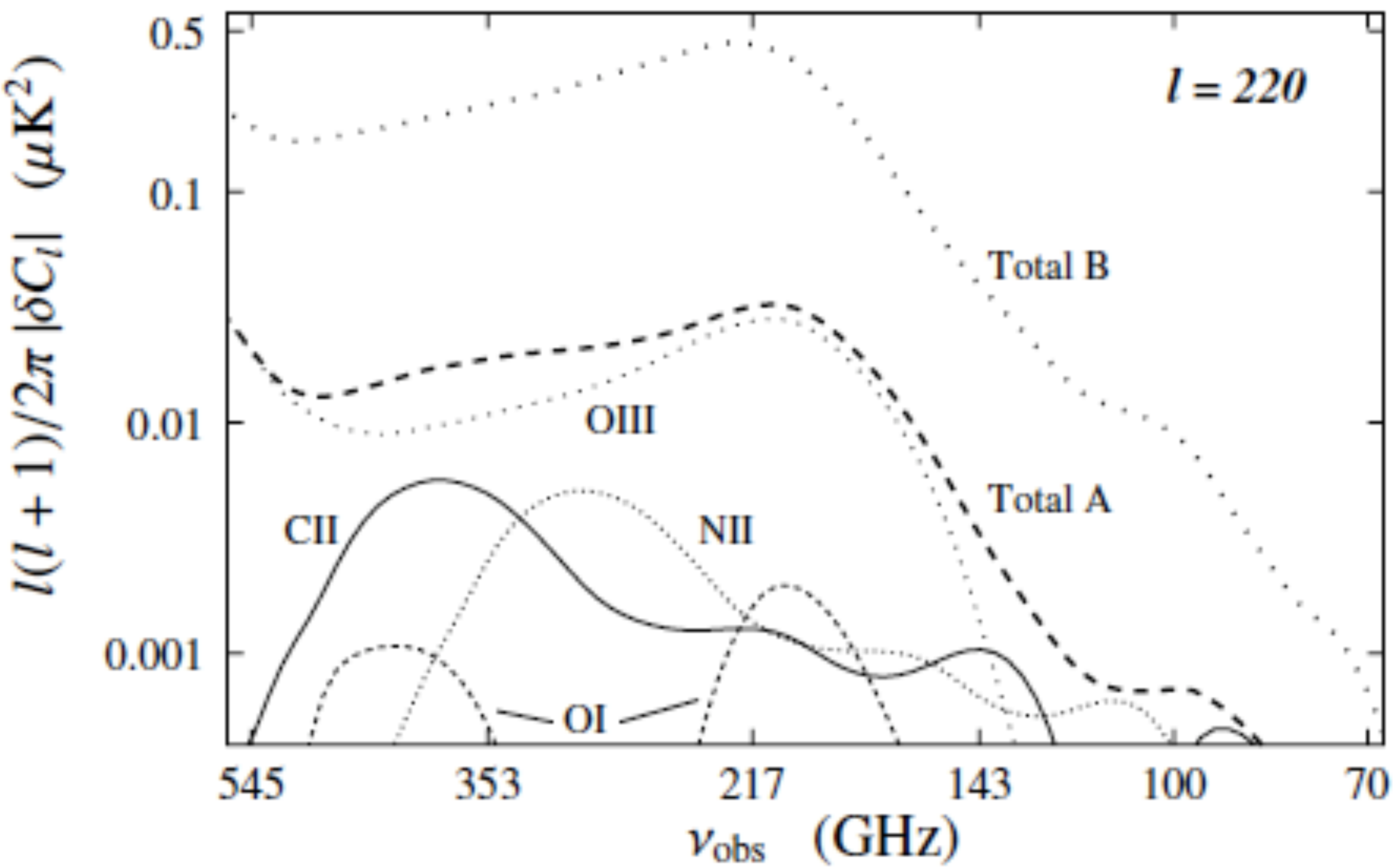
- Optical depth is small, down by a factor of $\alpha^2 x_M$ from Lyman-α:

$$\tau \sim 10^{-5}\left(\frac{1+z}{10}\right)^{1/2}\frac{x_M}{10^{-6}}B$$

  - $x_M$ = abundance of this metal/ionization state (by number)
  - B = fine structure level population factor (< ~ 1)
- Effects similar to reionzation (suppression of high-l CMB power & production of E-mode polarizaton) except frequency dependent.
  - Search for $C_l(\nu_1) - C_l(\nu_2)$.
  - No cosmic variance limit!
  - But: foregrounds, beam modeling, …

# Scattering of CMB by IGM Metal Lines

[Basu, Hernandez-Monteagudo, Sunyaev 2004]



# Ways to Search for Metal Scattering Feature

1. Correlation of frequency dependent anisotropy with primary CMB at any $l > l_{\rm reion} \sim 10$:

$$\left\langle T^*_{l'm'}(\nu_1)[T_{lm}(\nu_1) - T_{lm}(\nu_2)]\right\rangle = C_l^{T,\Delta T}(\nu_1,\nu_2)\delta_{ll'}\delta_{mm'} \propto \tau.$$

2. Scattering induced polarization @ low $l$: [Hernandez-Monteagudo et al 2007]

$$\left\langle T^*_{l'm'}(\nu_1)[E_{lm}(\nu_1) - E_{lm}(\nu_2)]\right\rangle = C_l^{T,\Delta E}(\nu_1,\nu_2)\delta_{ll'}\delta_{mm'} \propto \tau.$$

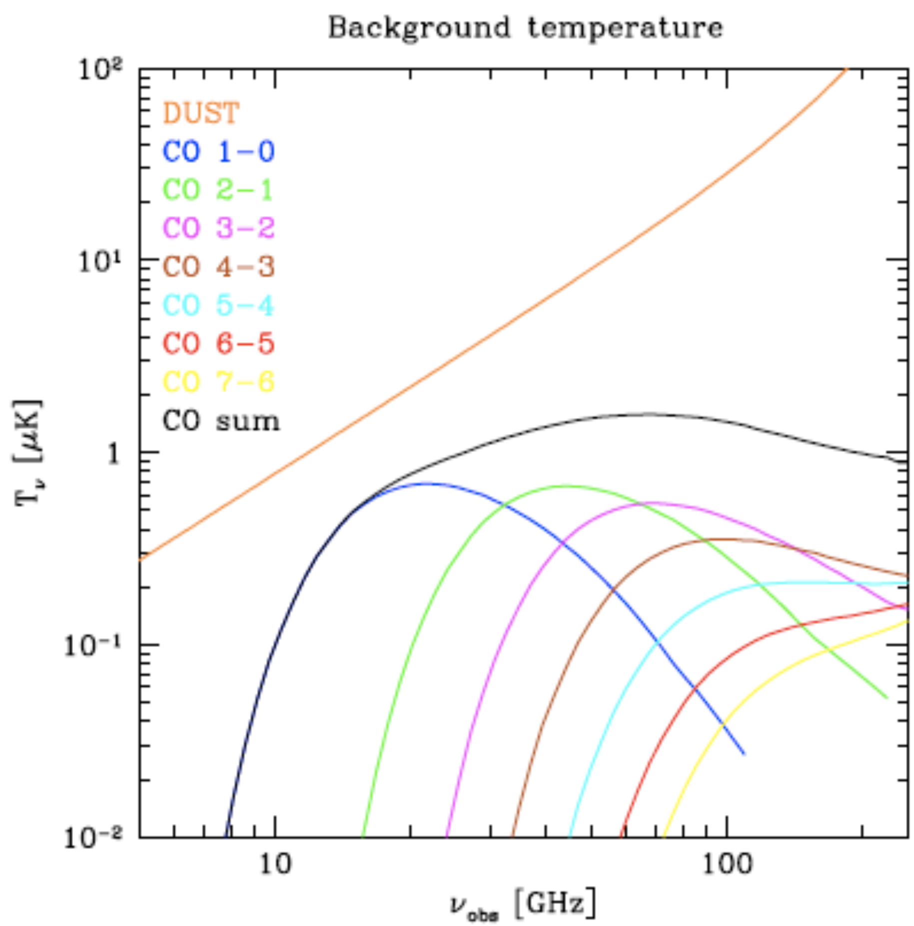
3. Inhomogeneities via 21 cm x-correlation:

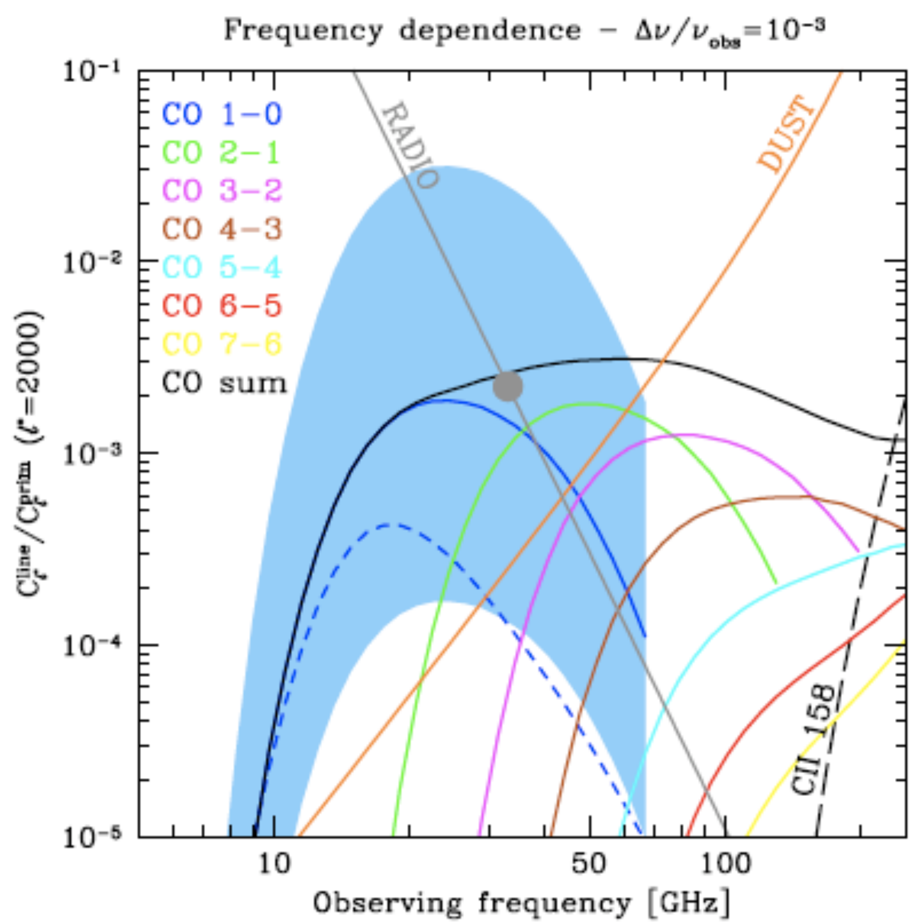
$$\Pi(\mathbf{n},z) = P_{\rm CMB}(\mathbf{n})\Delta T(21{\rm cm}(1+z))$$
$$\left\langle \Pi(\mathbf{n},z)\Delta P(\nu_1)\right\rangle \propto {\rm HI-metal\ x\text{-}corr}$$

# Diffuse Metal & Molecular Emission as a Foreground?

- The low-frequency sky ($\nu < 1.4$ GHz) contains a 3D map of the Universe in H I ($\nu \leftrightarrow z$)
- The high-frequency sky contains similar maps … from all the metal, CO rotation, etc lines … superposed!
  - Another way to do large scale structure if one could separate the lines, at least statistically (e.g. cross-correlations).
  - Provides frequency-dependent structure that is a foreground for metal scattering, very highest-z galaxy lines.

# Diffuse Metal & Molecular Emission as a Foreground?




Model by Righi et al 2008

# Summary

- There are lots of ways to make spectral signatures in the CMB and FIR background from $H_2$ & metal lines … but:
  - The signals are weak.
  - Some of the signals are correlated with the CMB so relative calibration & beam matching are big issues.
  - The foregrounds are bright.
  - Some of the foregrounds have frequency-dependent structure …
- Which, if any, approaches are possible?