GEORG-AUGUST-UNIVERSITÄT GÖTTINGEN

INSTITUT FÜR ASTROPHYSIK GÖTTINGEN

Out of equilibrium: the interesting case of early Universe chemistry

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OUTLINE:

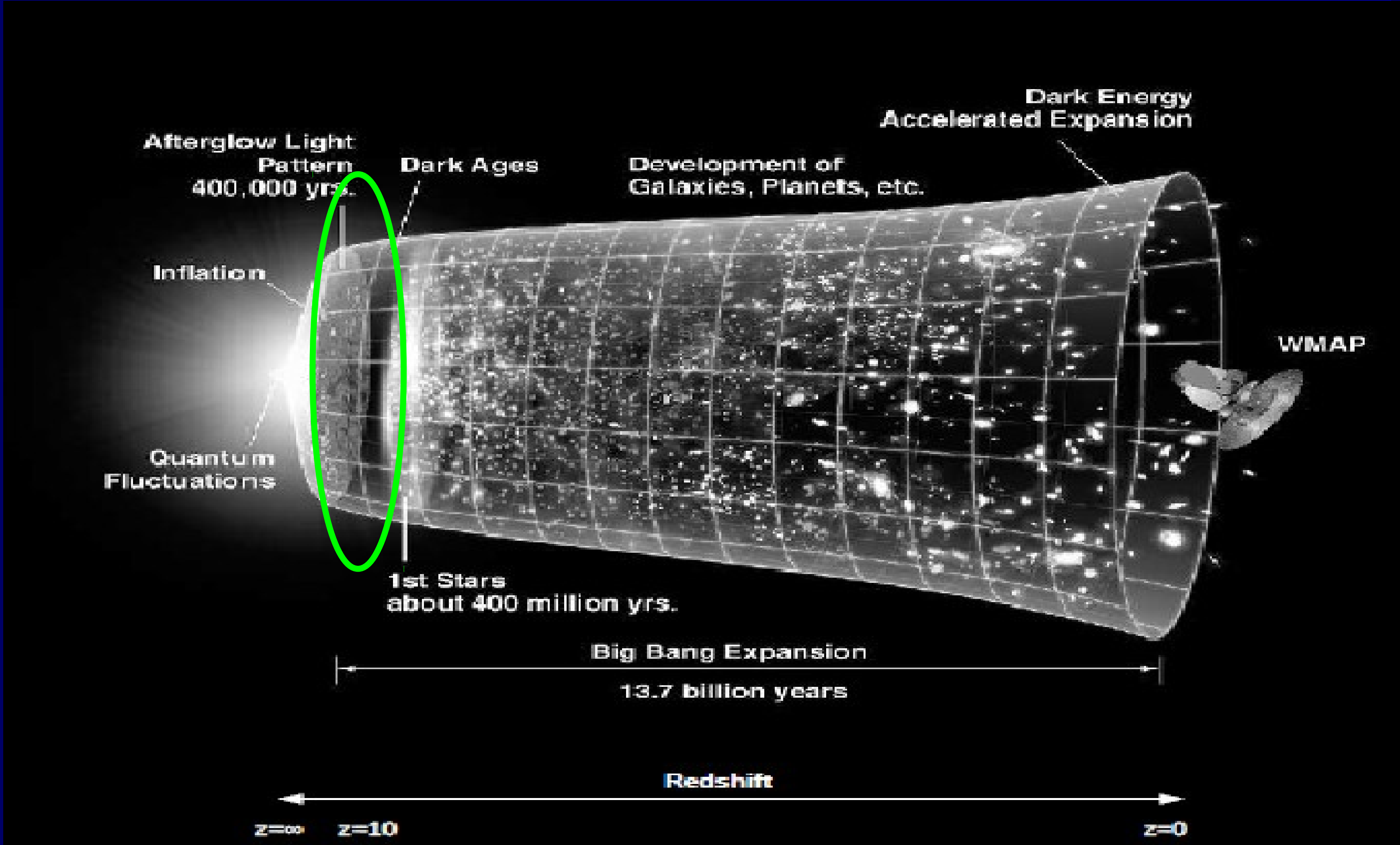
1. **early Universe: the “standard” chemistry**

2. **non-equilibrium distributions**

- molecular internal states resolution:
  - vibration;
- spectral distortions:
  - primordial atomic recombination;
  - molecular processes

3. **“modified” chemistry**

UNIVERSE HISTORY…



KINETIC MODELS: CHEMICAL SPECIES (I)

H^+ D^+

H D

H^- D^-

He^{++} He^+
He

Li Li^+

Li^-

e^- γ

HD^+

HD

H_3^+ H_2D^+

HeH^+

LiH LiH^+

H_2^+ H_2

KINETIC MODELS: A BRIEF OVERVIEW... (II)

'60s: studies on elementary processes useful in molecular hydrogen formation in the early Universe
(Saslaw & Zipoy (1967), Peebles & Dicke (1968))

Chemical kinetics in the early Universe (very few examples...):
Dalgarno & Lepp (1987)
Black (1990)
Shapiro (1992)
Puy et al. (1993,1996)
Dalgarno & Fox (1994)
Lepp, Stancil & Dalgarno (1996), Lepp & Stancil (1998)
Bougleux & Galli (1997)
Galli & Palla (1998, 2002)
Schleicher et al. (2008)
……......

KINETIC MODEL: ODEs SYSTEM (III)

$$\frac{dn_i}{dt} = k_{form} n_j n_k - k_{dest} n_i + \ldots$$

$$\frac{dn_i}{dz} = \frac{dt}{dz}\frac{dn_i}{dt}$$

$$n(z) = \Omega_{\rm b} n_{\rm cr} (1+z)^3$$

KINETIC MODEL: CHEMICAL PROCESSES (IV)

MASSIVE PARTICLES SCATTERING

$$k(T) = \left(\frac{2}{k_B T}\right)^{3/2} \frac{1}{\sqrt{\mu\pi}} \int_0^\infty dE\ E\ e^{-\frac{E}{k_B T}} \sigma(E)$$

$$n_b = 1.123 \times 10 \cdot (1 - Y_p) \Omega_b h^2 (1+z)^3 \quad [m^{-3}]$$

PHOTONIC PROCESSES

$$k_{rad}(\mathrm{T_{rad}}) = 4\pi \int_0^\infty \frac{\sigma(\nu)}{h\nu} J_\nu(\mathrm{T_{rad}}) d\nu$$

$$J_\nu(\mathrm{T_{rad}}) = \frac{2h\nu^3}{c^2} \frac{1}{\mathrm{e}^{\mathrm{h}\nu/\mathrm{kT_{rad}}} - 1}$$

KINETIC MODEL: MATTER AND RADIATION TEMPERATURE (V)

$$\frac{dT_m}{dt} = -2H(t)T_m + \frac{8\sigma_t a T_r^4 (T_r - T_m) x_e}{3 m_e c} + (\Gamma - \Lambda)_{\mathrm{mol}}$$

$$T_r = 2.7(1+z)$$

RECFAST

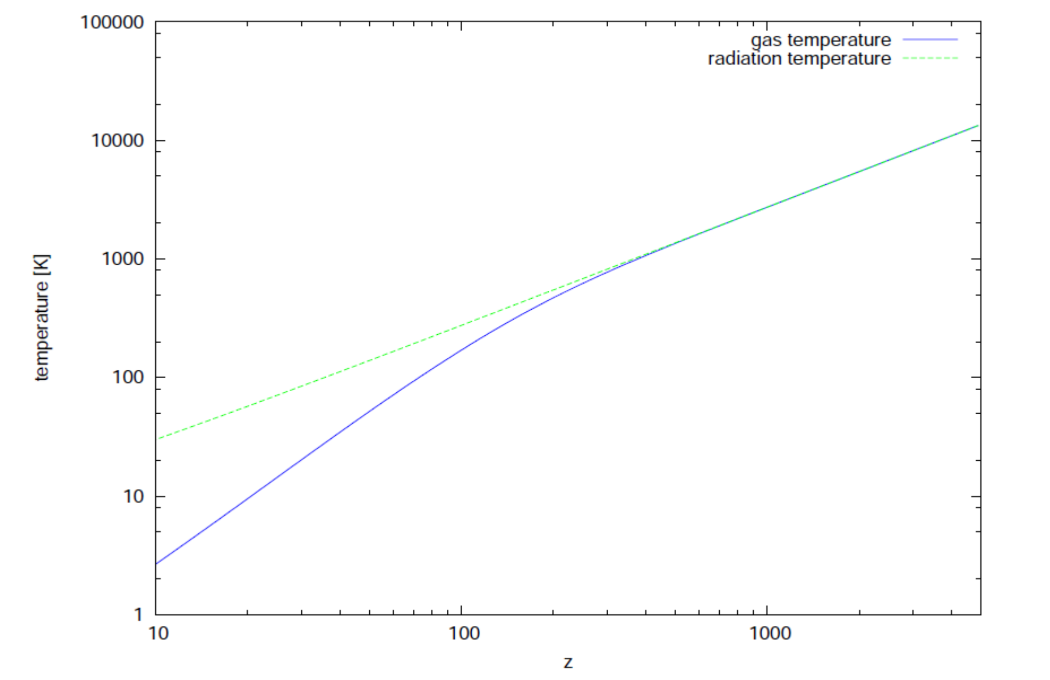
Wong et al.

2008, MNRAS, **386**, 1023-1028

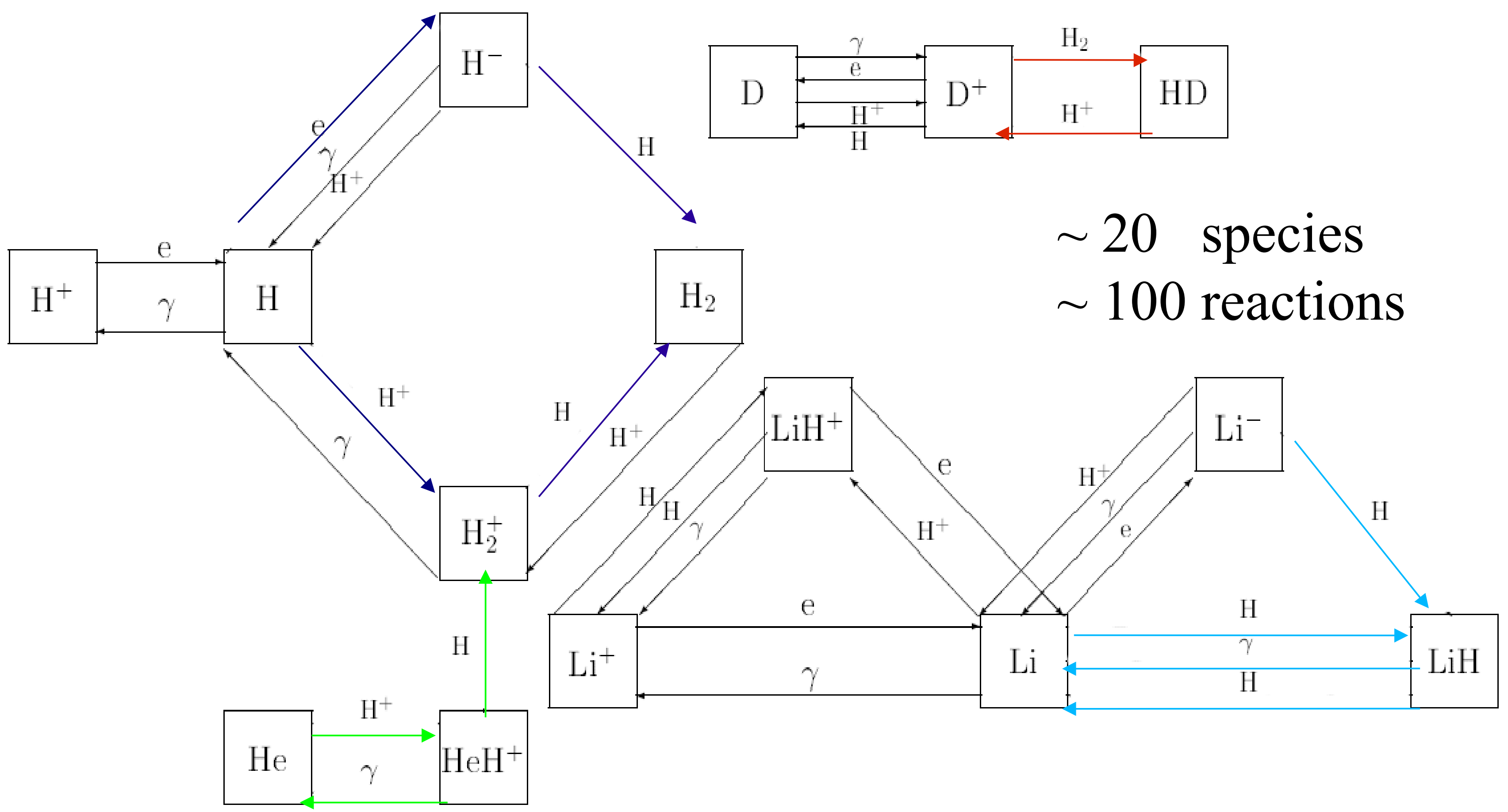
CosmoRec

Rubiño Martín et al.

2010, MNRAS, **403**, 439-452



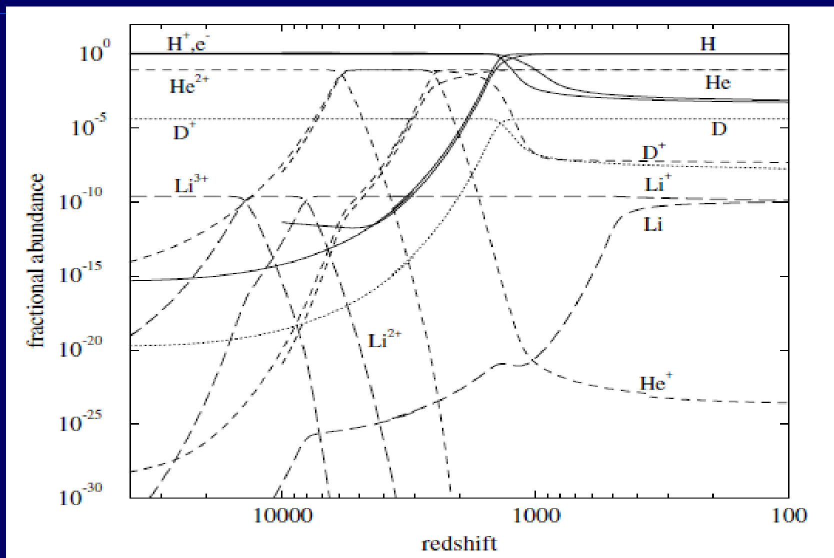
KINETIC MODEL: CHEMICAL PROCESSES (VI)



~ 20 species
~ 100 reactions

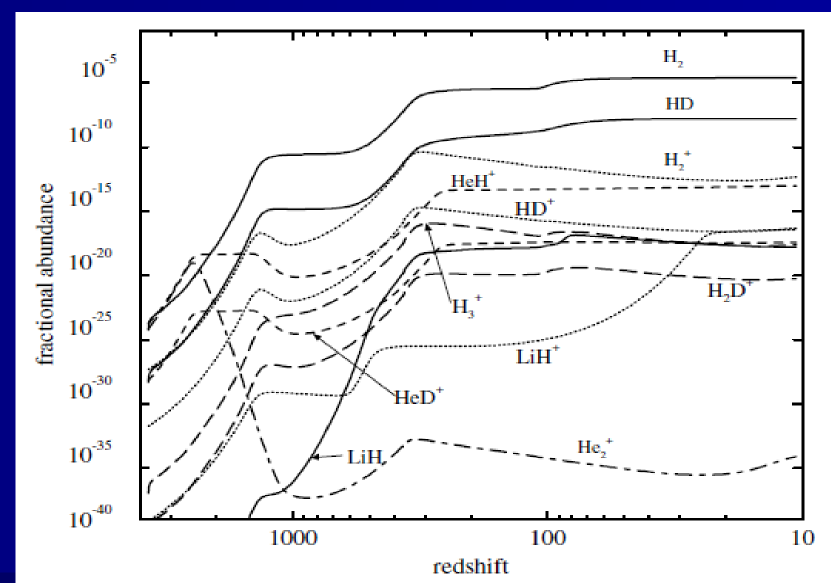
Galli & Palla, 1998, A&A, **335**, 403–420

KINETIC MODEL: FRACTIONAL ABUNDANCES (VII)



Lepp, Stancil &Dalgarno,

2002, J. Phys. B: At. Mol. Opt. Phys. **35**, R57–R80



BEYOND THE “STANDARD” KINETICS...

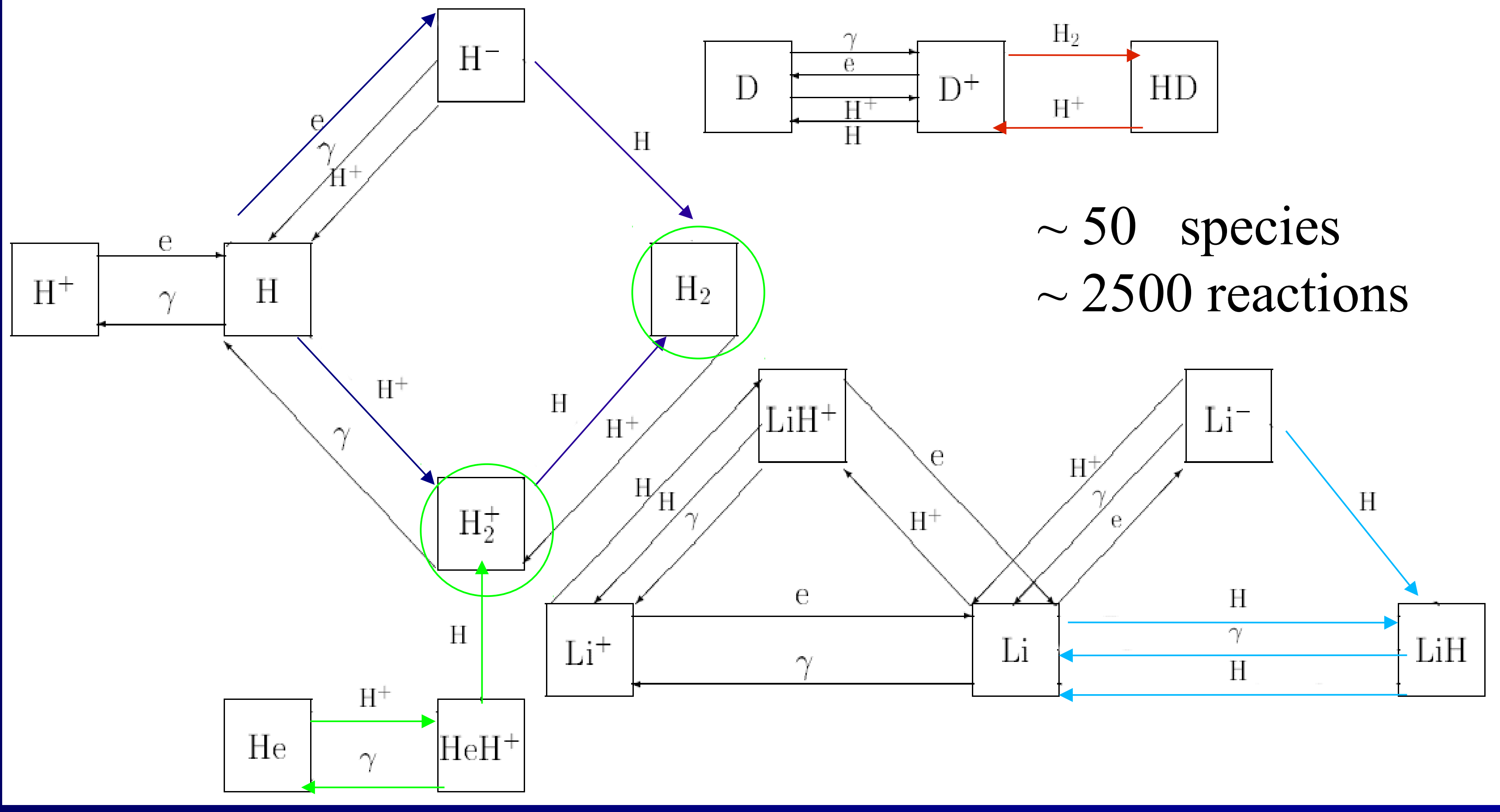
Non-equilibrium effects:

- state-to-state kinetics → Maxwell-Boltzmann's distributions

?

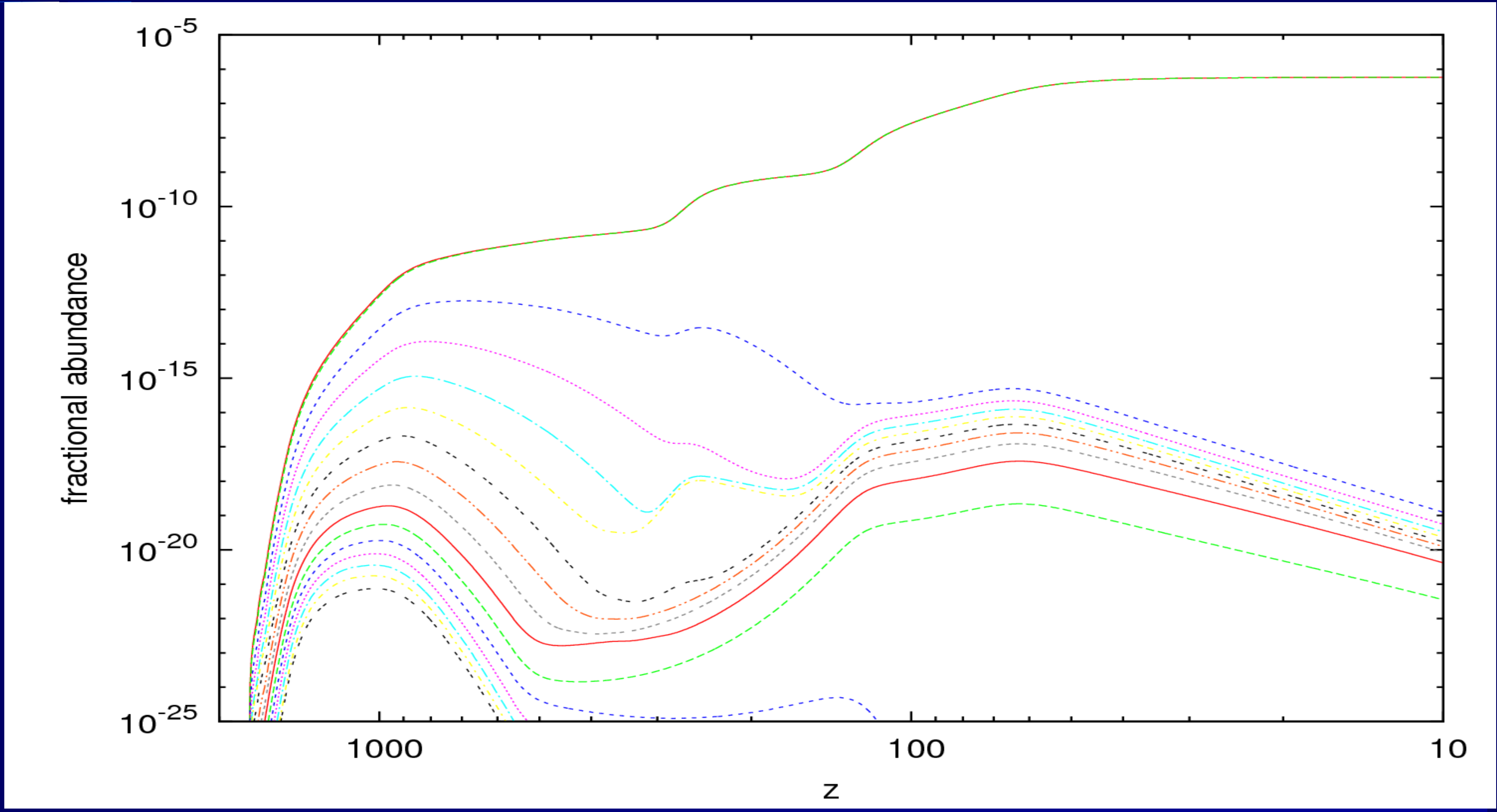
- CMB photons → Planck's distributions

KINETIC MODEL: STATE-TO-STATE KINETICS (I)



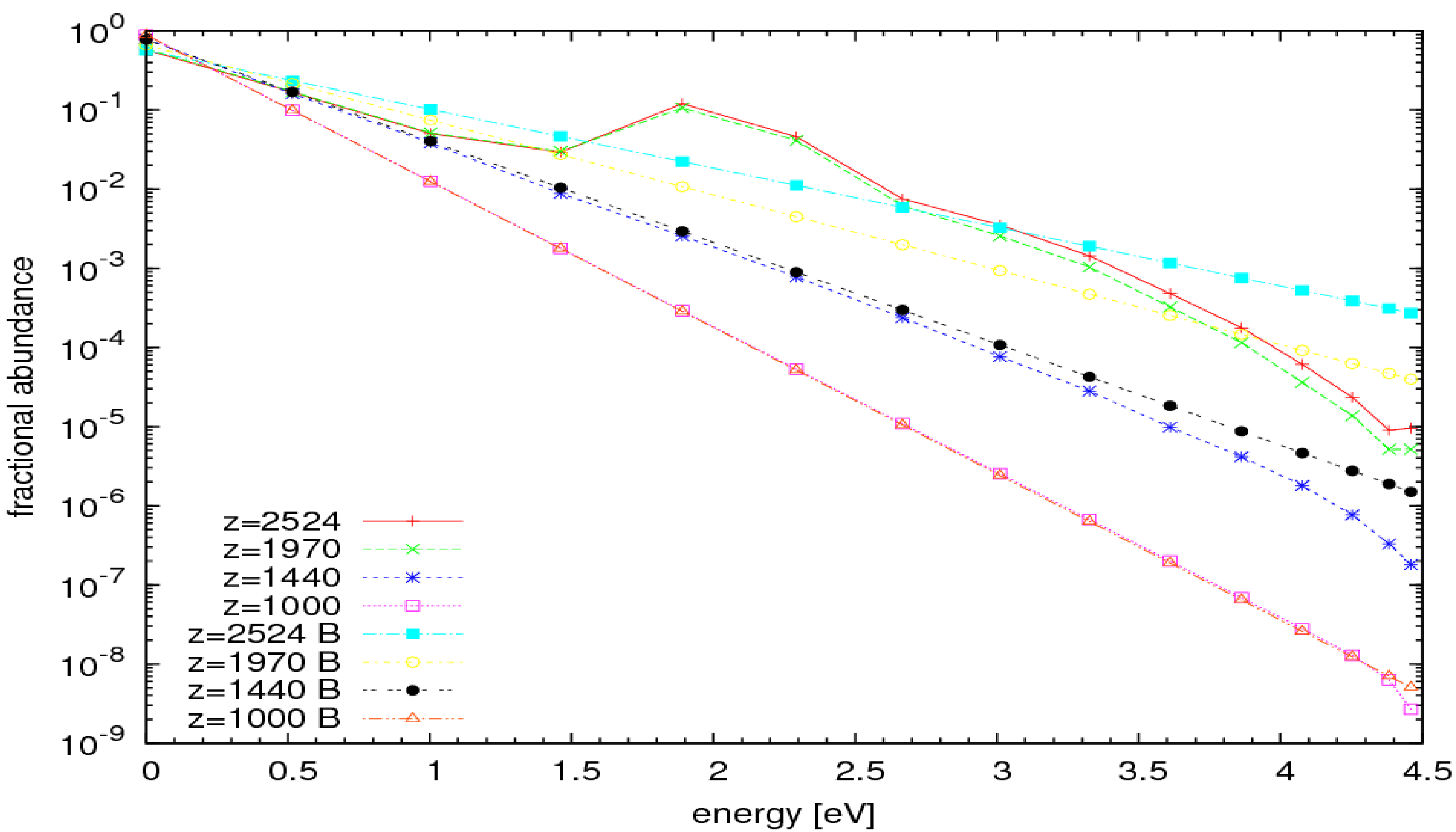
Galli & Palla, 1998, A&A, **335**, 403–420

RESULTS: VDF H_2 (I)



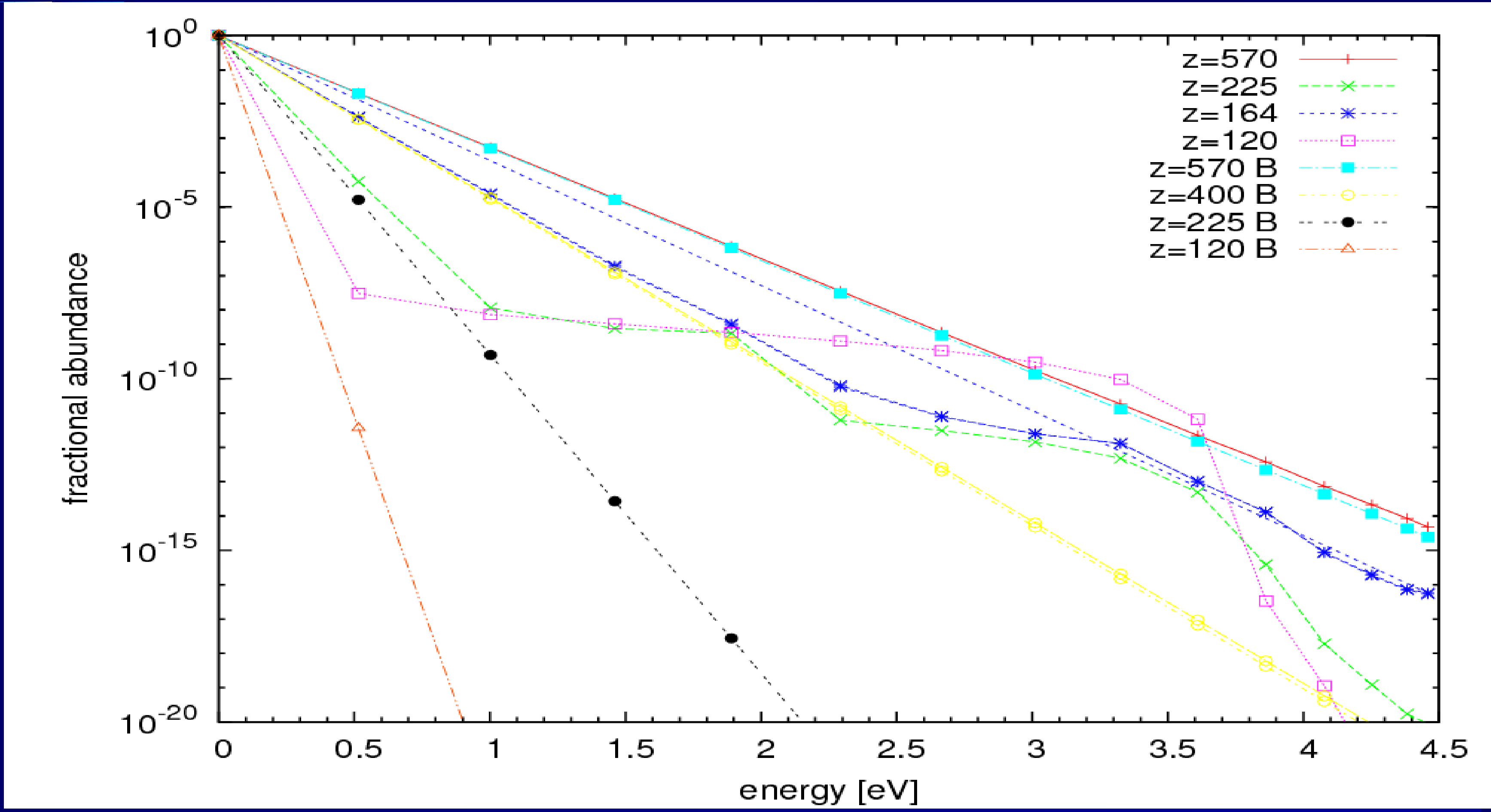
Coppola, Longo, Capitelli, Palla, Galli, 2011, ApJS, **193**, 7-18

RESULTS: VDF H_2 (II)



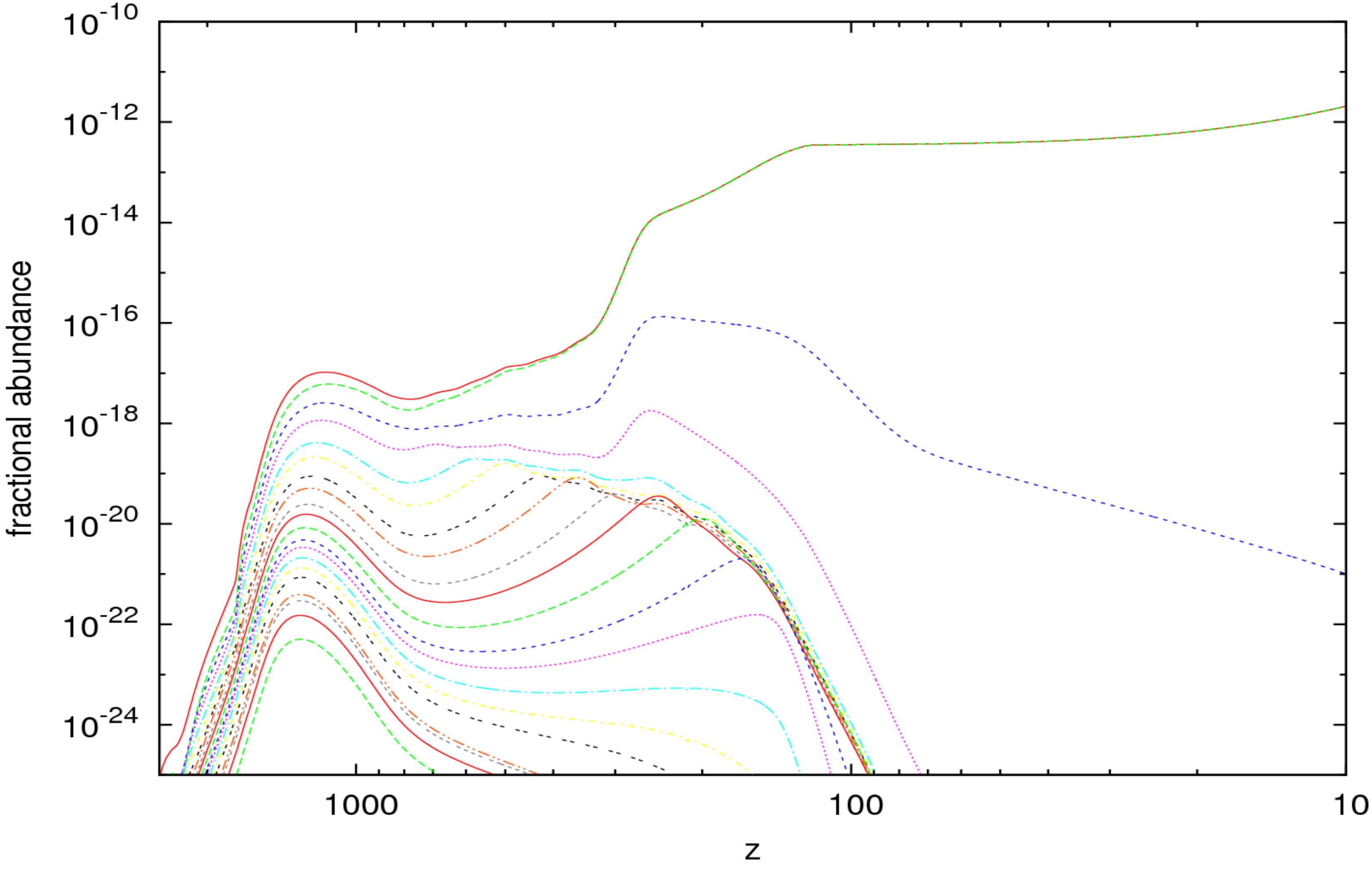
Coppola, Longo, Capitelli, Palla, Galli, 2011, ApJS, **193**, 7-18

RESULTS: VDF H_2 (III)

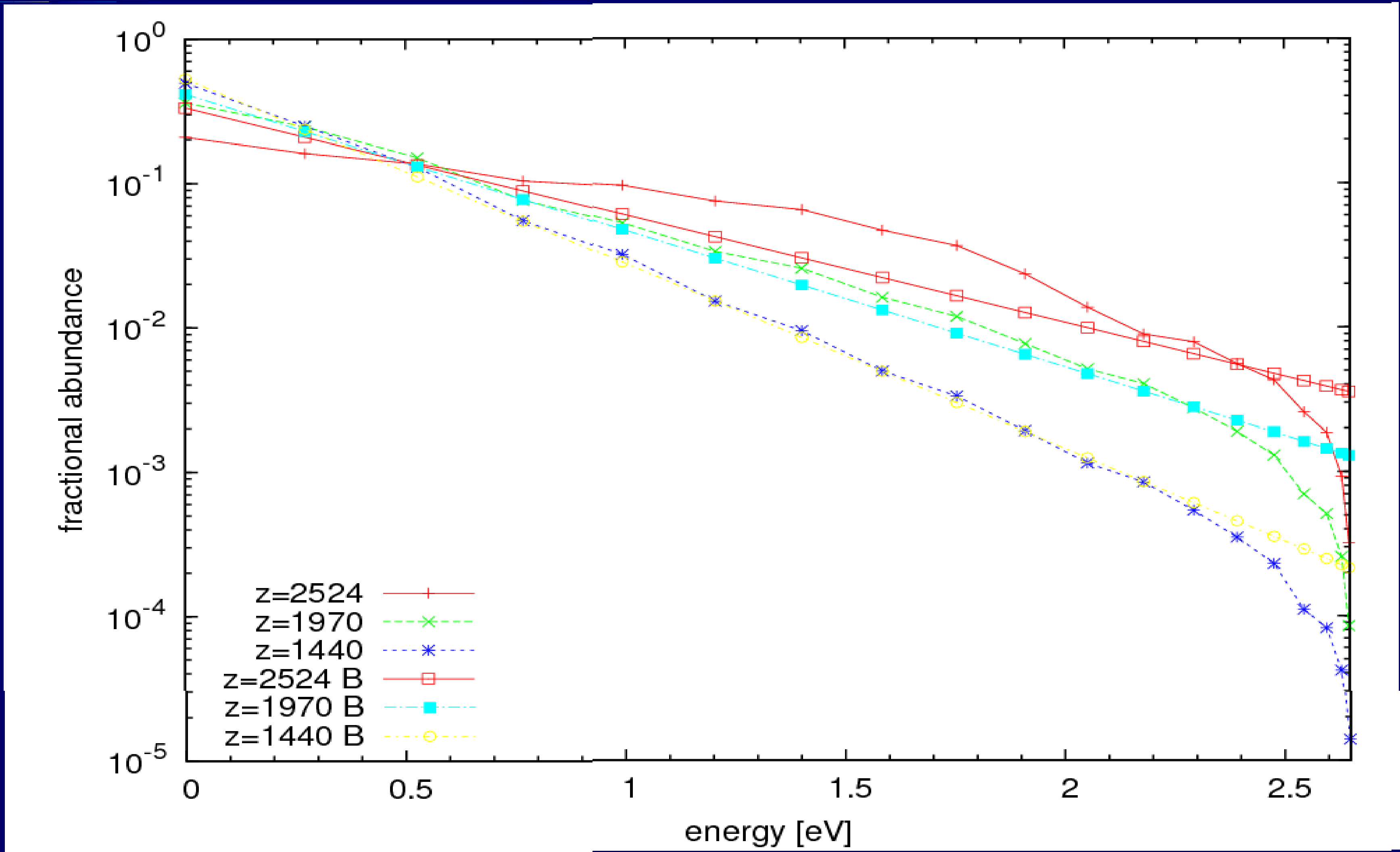


Coppola, Longo, Capitelli, Palla, Galli, 2011, ApJS, **193**, 7-18

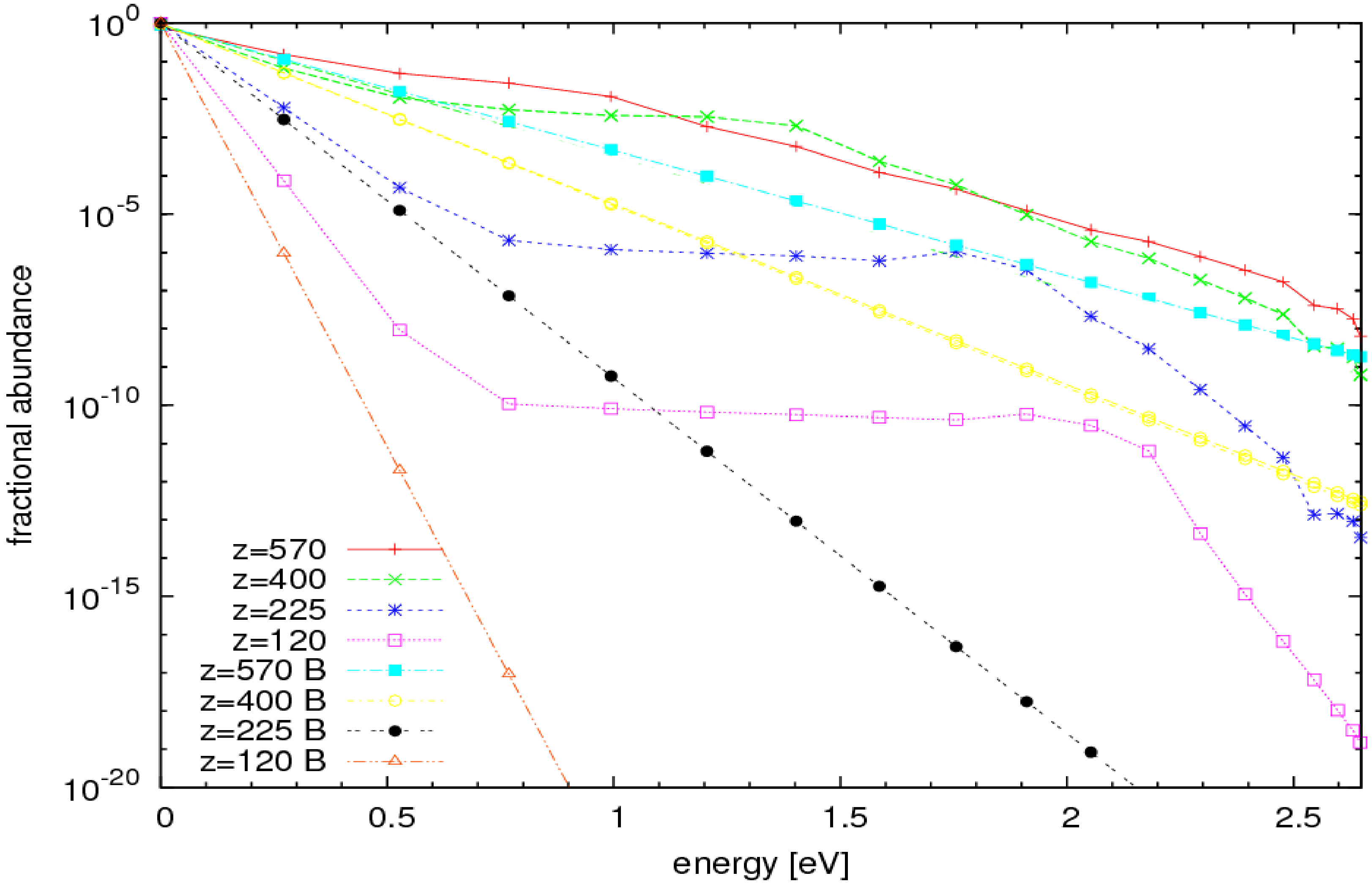
RESULTS: VDF H_2^+ (I)



RESULTS: VDF H_2^+ (II)



RESULTS: VDF H_2^+ (III)



BEYOND THE “STANDARD” KINETICS... (II)

MASSIVE PARTICLES SCATTERING

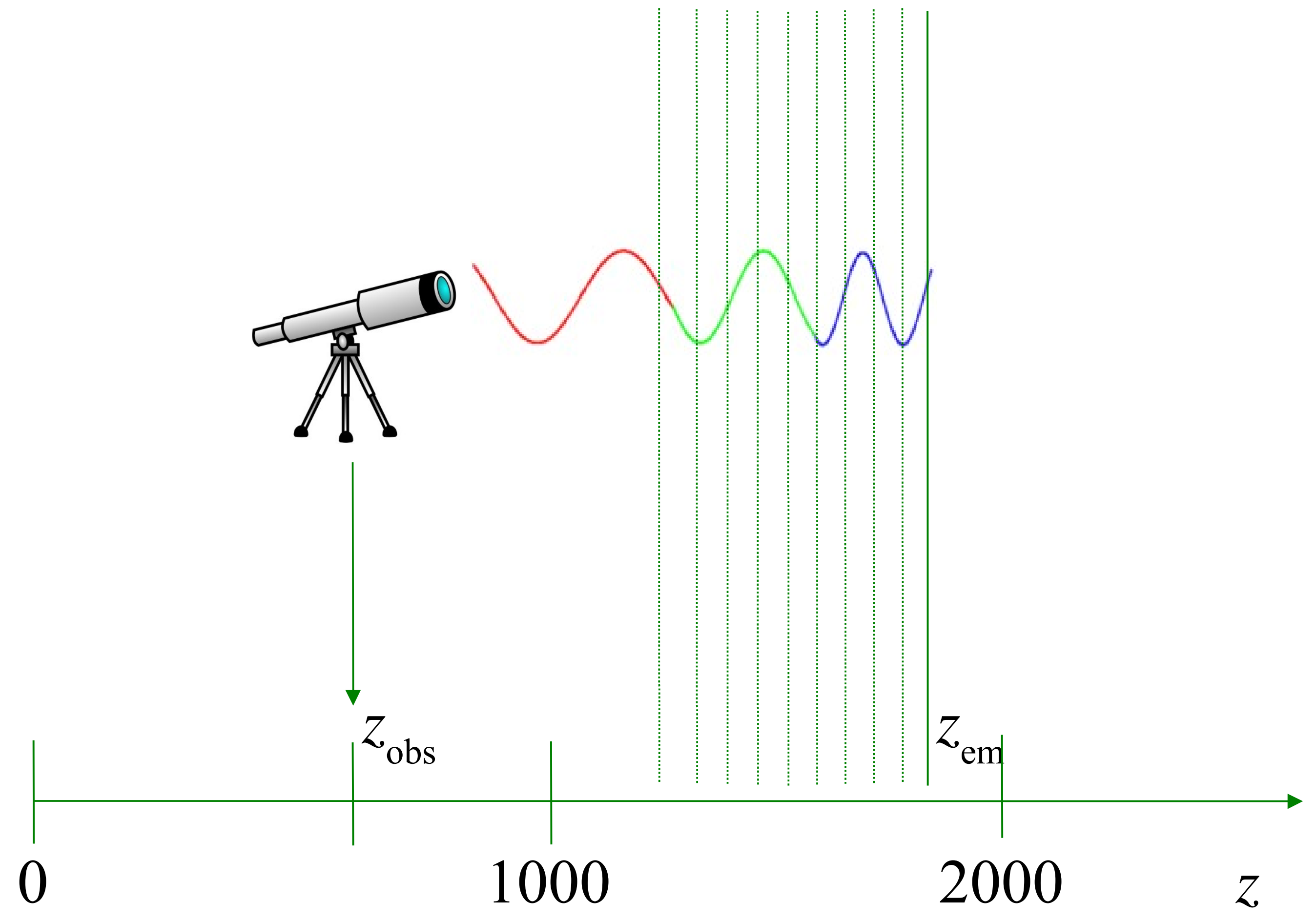
PHOTONIC PROCESSES

$$k(T) = \left(\frac{2}{k_B T}\right)^{3/2} \frac{1}{\sqrt{\mu\pi}} \int_0^\infty dE\ E\ e^{-\frac{E}{k_B T}} \sigma(E)$$

$$k_{photo}(z) = 4\pi \int_0^\infty \frac{\sigma(\nu)}{h\nu} \left[B_z(\nu) + \sum_{i \to j} I_{ij}^z(\nu)\right] d\nu.$$

$$n_b = 1.123 \times 10 \cdot (1 - Y_p)\Omega_b h^2 (1+z)^3 \quad [m^{-3}]$$

SPECTRAL DISTORTIONS (I)



SPECTRAL DISTORTIONS (II)

$$j_{\nu_{ij}}(z) = h\nu_{ij}\Delta R_{ij}(z)\phi(\nu(z))$$

$$\Delta R_{ij}(\nu) = A_{ij}N_i \frac{e^{h\nu_{ij}/kT_r}}{e^{h\nu_{ij}/kT_r}-1}\left[1-\frac{N_j}{N_i}e^{-h\nu_{ij}/kT_r}\right]$$

$$I_{ij}^{z_{obs}}(\nu) = \frac{c}{4\pi}\int_{z_{em}}^{z_{obs}} \frac{j_{\nu_{ij}}(z)}{(1+z)^3}(1+z_{obs})^3\left|\frac{dt}{dz}\right| dz$$

$$I_{ij}^{z_{obs}}(\nu) = \frac{ch}{4\pi}\frac{\Delta R_{ij}(z_{em})}{H(z_{em})}\frac{(1+z_{obs})^3}{(1+z_{em})^3}$$

SPECTRAL DISTORTIONS (III)

$$\frac{1}{c}\frac{\mathrm{d}J_\nu}{\mathrm{d}z} = \frac{\kappa_\nu J_\nu - j_\nu}{H_0(1+z)^2\sqrt{1+\Omega_0 z}} + \frac{3J_\nu}{c(1+z)}$$

$$\kappa_\nu = \frac{c^2}{8\pi\nu^2} n_1 A_{\mathrm{ul}} \frac{g_{\mathrm{u}}}{g_1}\left(1 - \frac{g_1 n_{\mathrm{u}}}{g_{\mathrm{u}} n_1}\right)\phi(\nu - \nu_{\mathrm{ul}})$$

$$j_\nu = \frac{h\nu}{4\pi} n_{\mathrm{u}} A_{\mathrm{ul}} \phi(\nu - \nu_{\mathrm{ul}})$$

$$\left.\frac{\Delta J_\nu}{J_\nu}\right|_{z=0} = [R(z_{\mathrm{i}}) - 1][1 - \mathrm{e}^{-\tau(z_{\mathrm{i}})}]$$

$$R(z_{\mathrm{i}}) = \left[\frac{g_{\mathrm{u}} n_1(z_{\mathrm{i}})}{g_1 n_{\mathrm{u}}(z_{\mathrm{i}})} - 1\right]^{-1}\left\{\exp\left[\frac{h\nu_{\mathrm{ul}}}{kT_{\mathrm{r}}(z_{\mathrm{i}})}\right] - 1\right\}$$

Bougleux, E. & Galli, D. **1997**
MNRAS, **288**, 638-648

SPECTRAL DISTORTIONS (IV)

- matter/antimatter annihilation
- decaying particles
- interaction with matter

…………

- primordial atomic recombination ($z \sim 1100$)

$$A^{+} + e^{-} \longrightarrow A + h\nu$$

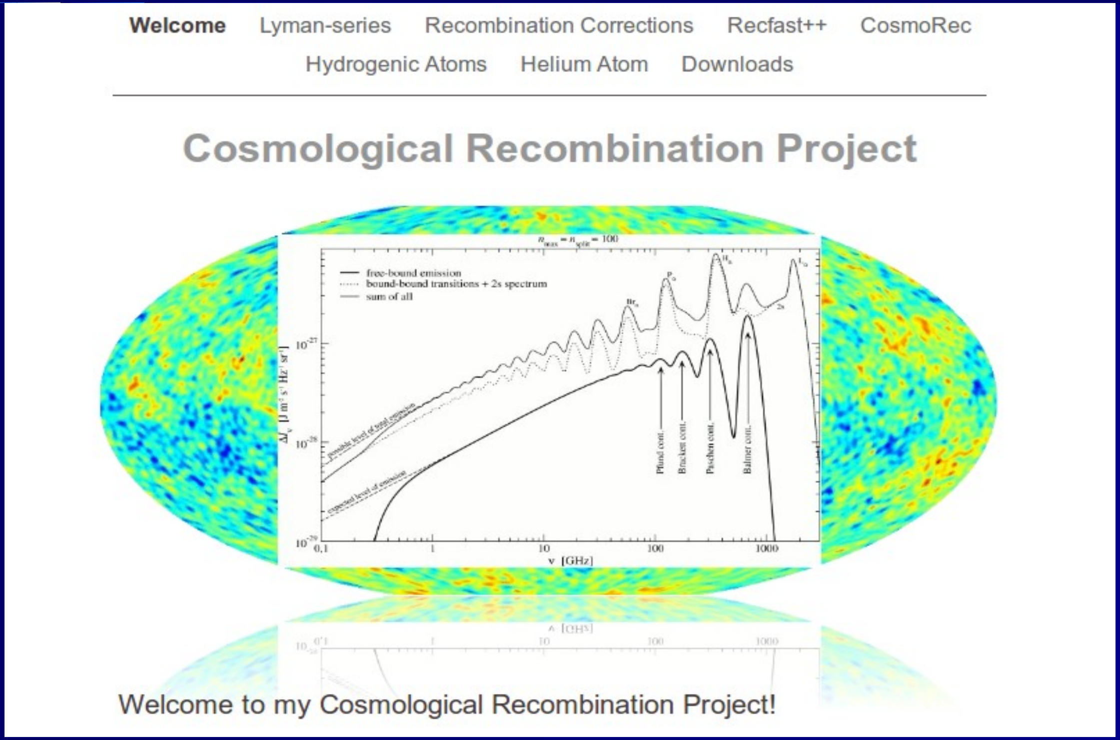
He^{++} He^{+}

H^{+}

- molecular radiative cascade

$$H_2(v) \longrightarrow H_2(v') + h\nu$$

PRIMORDIAL ATOMIC RECOMBINATION

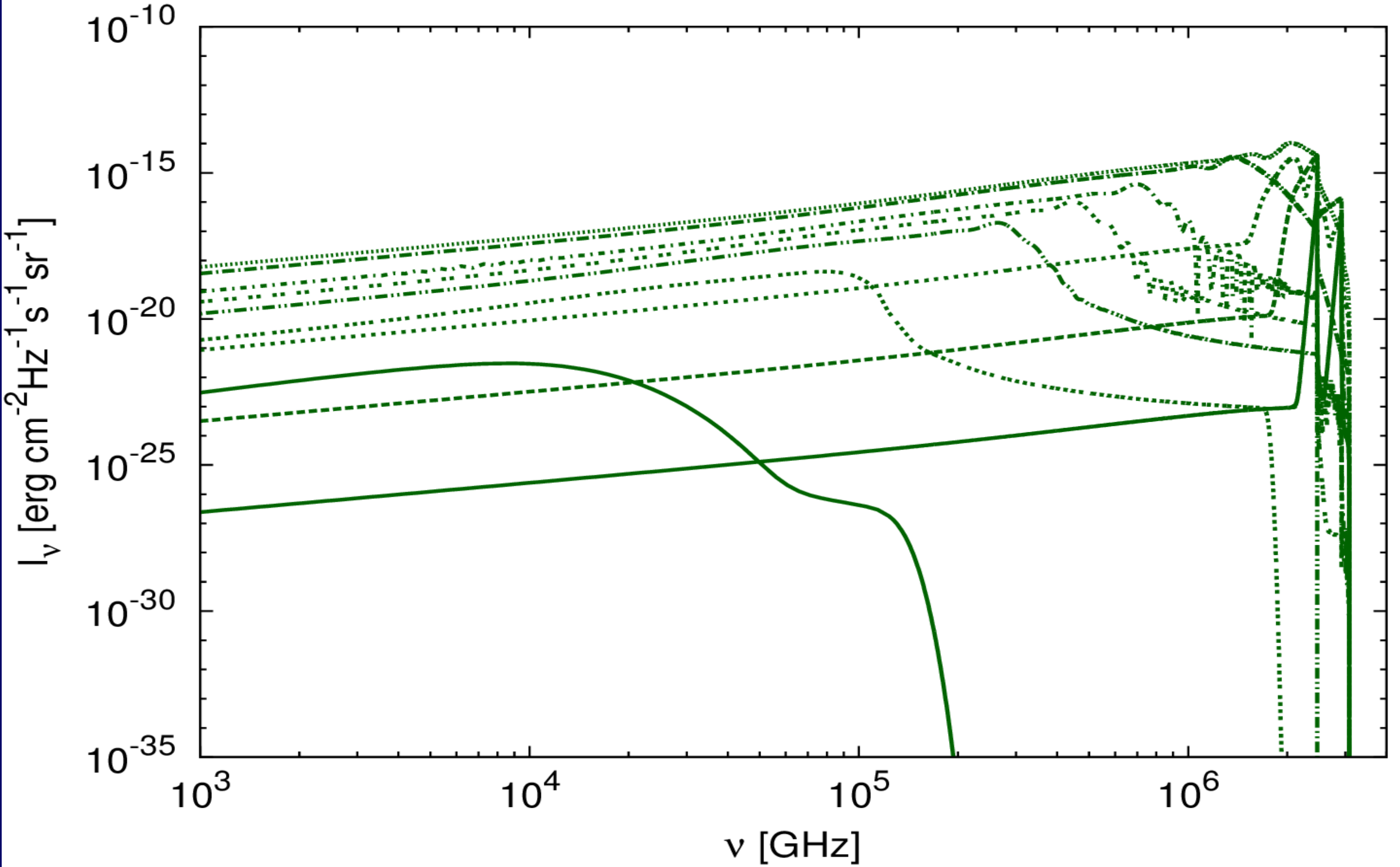


CosmoRec

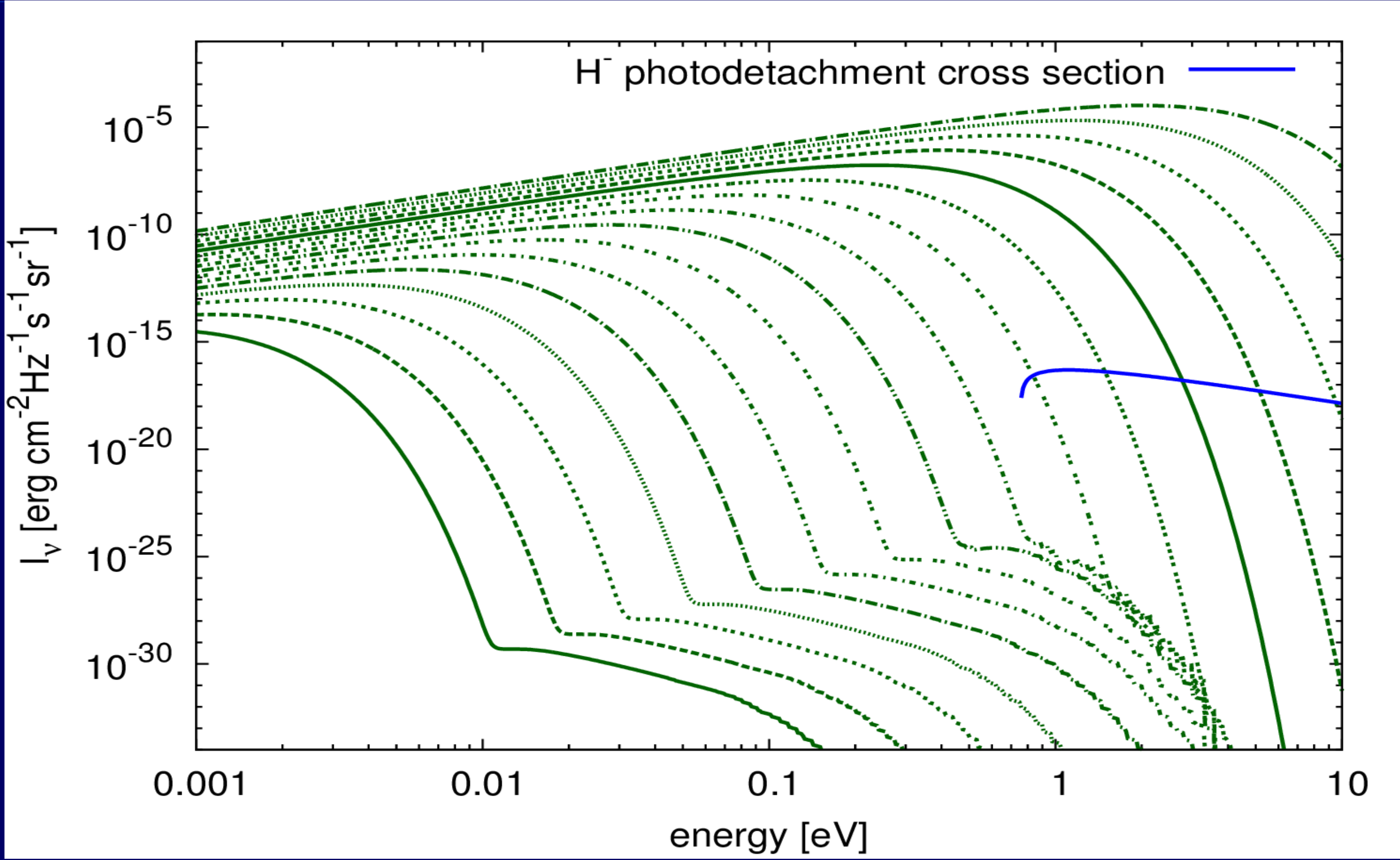
- effective multi-level approach;
- fast and accurate (~1.3 sec)
- solves a detailed radiative transfer problem for Ly-n
- available @ www.Chluba.de/CosmoRec

http://www.cita.utoronto.ca/~jchluba/Science_Jens/Recombination/Welcome.htm

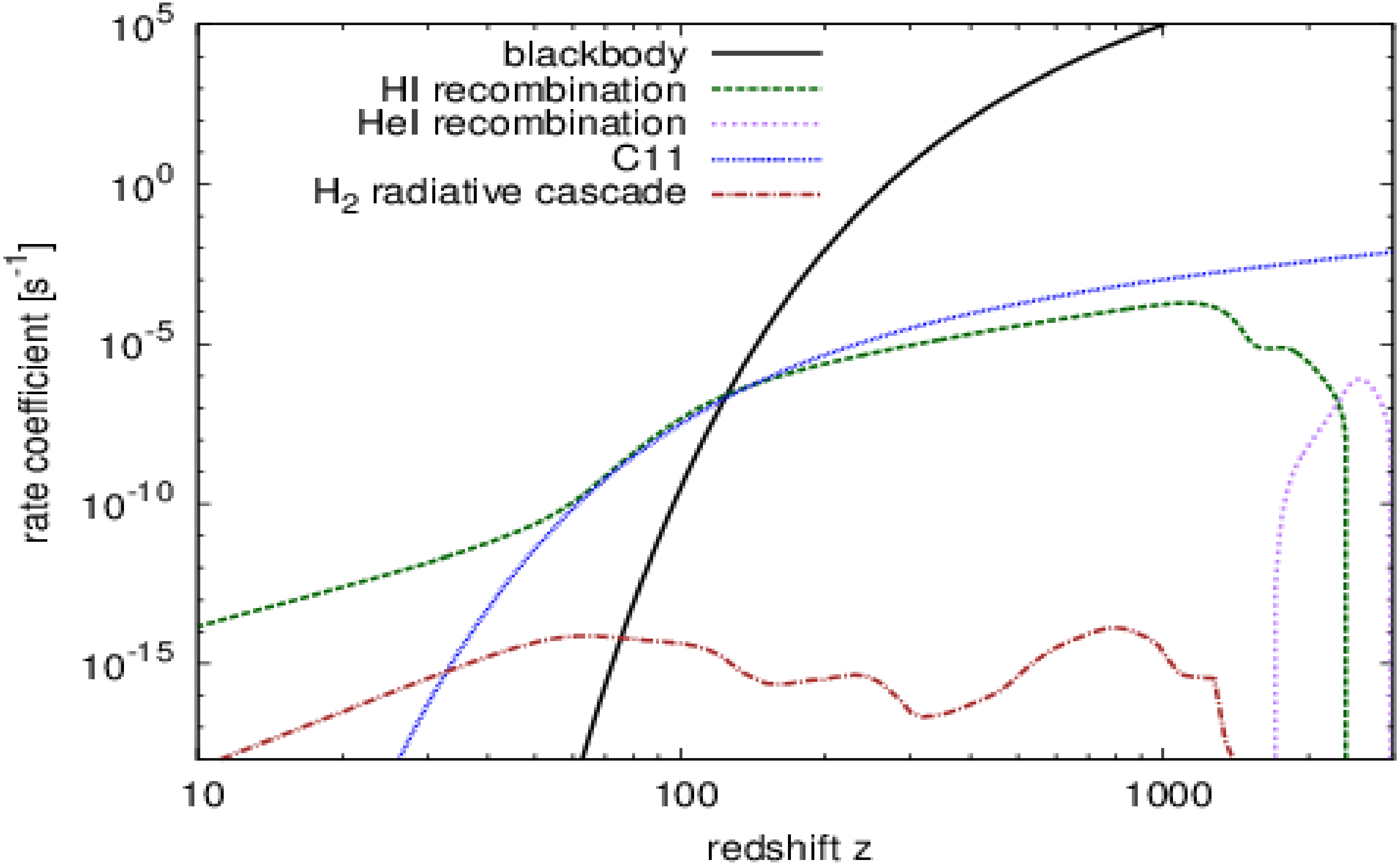
SPECTRAL DISTORTIONS (V)



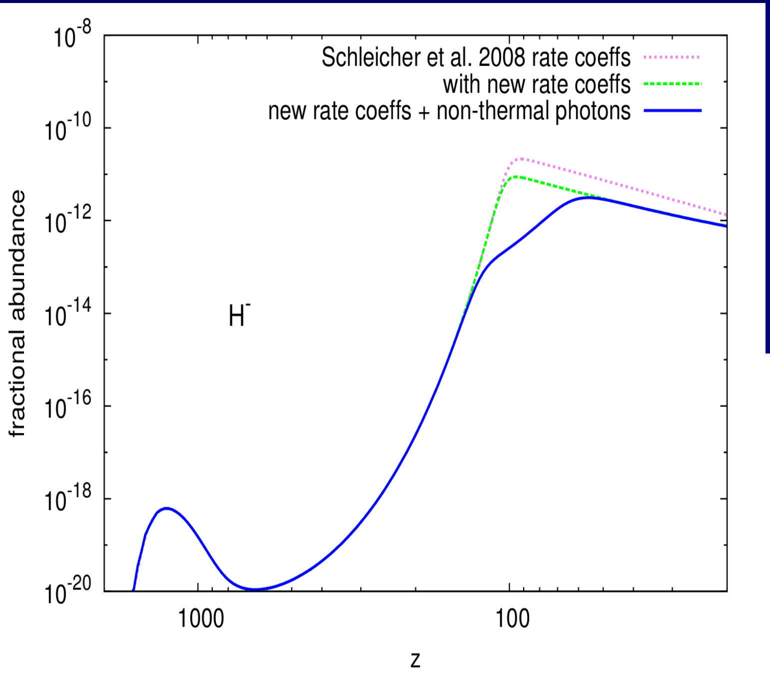
SPECTRAL DISTORTIONS (VI)

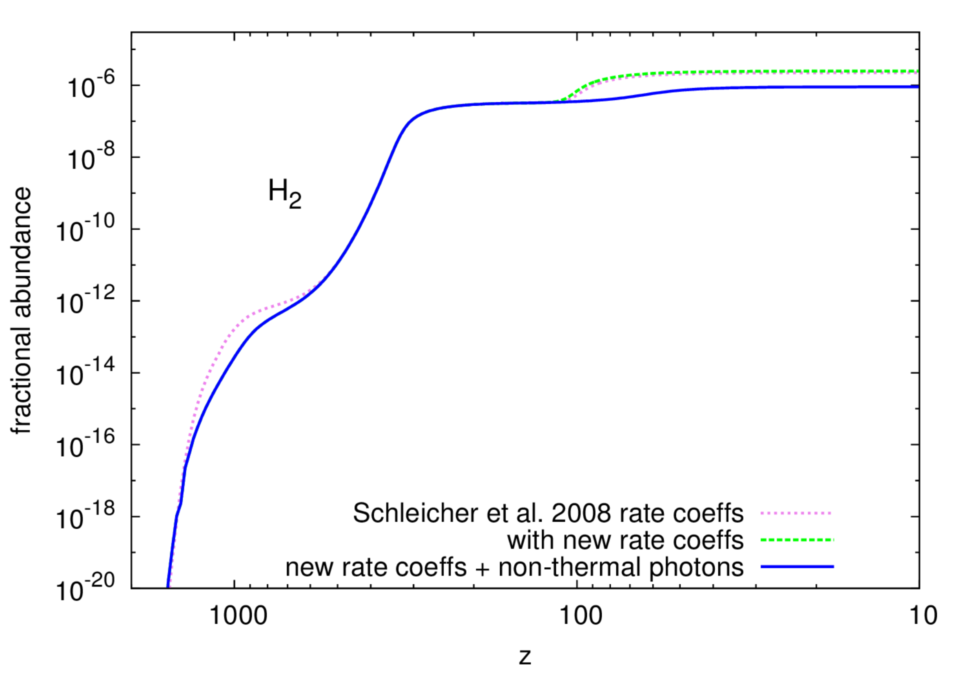


SPECTRAL DISTORTIONS (VII)

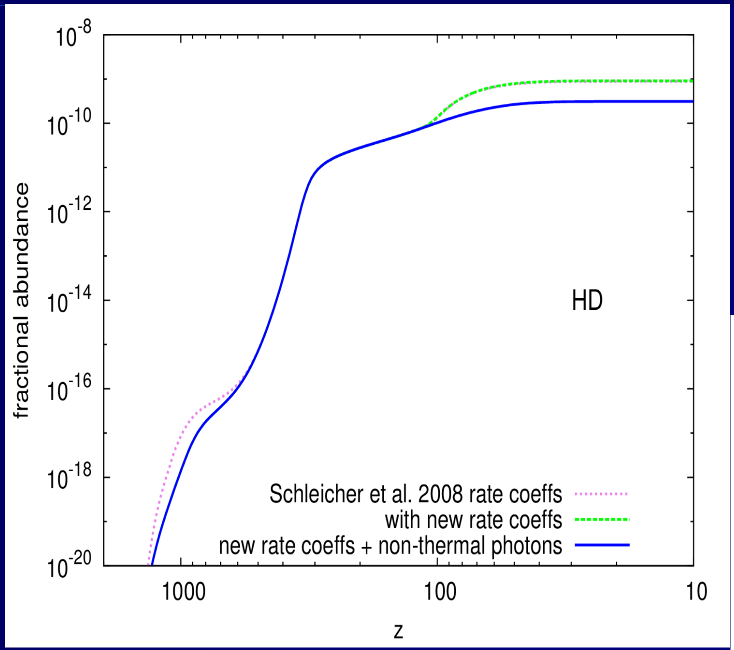


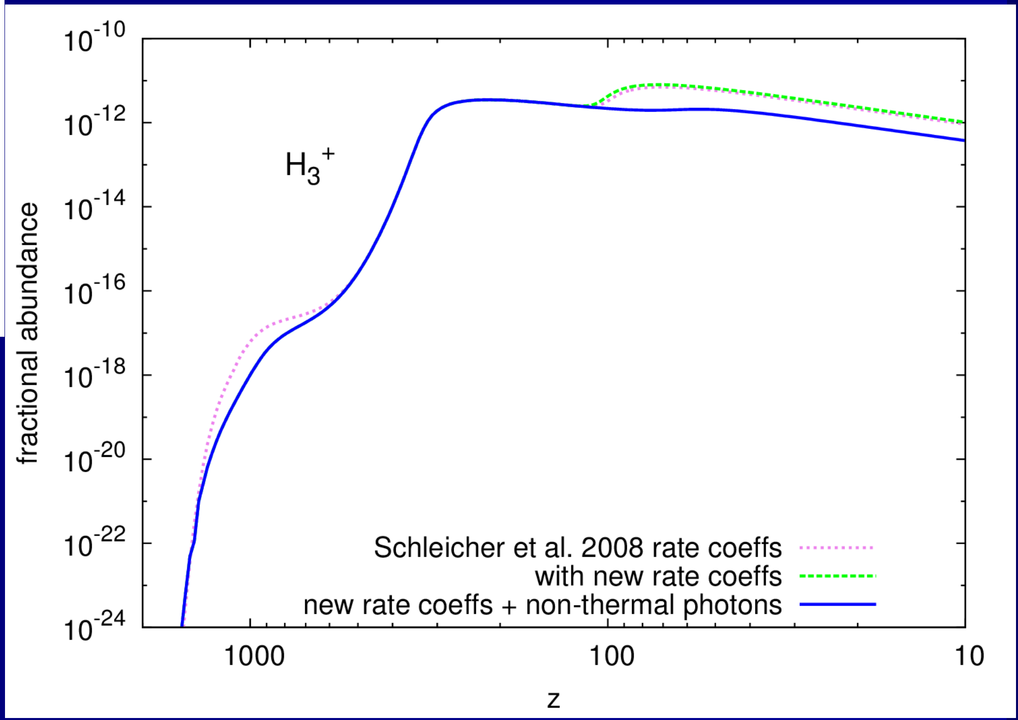
SPECTRAL DISTORTIONS (VIII)





SPECTRAL DISTORTIONS (IX)





CONCLUSIONS:

- non-equilibrium distributions:
  - → molecular vibration
  - → distortion photons
    - → atomic
    - → molecular

“origin”

- “chemical feedback on the chemistry”

...ACKNOWLEDGEMENTS...

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...workshop organizers...


Starry Night over the Rhone
Vincent van Gogh
THANKS...