Quantum mechanics and stellar spectroscopy

Towards high-accuracy stellar abundances

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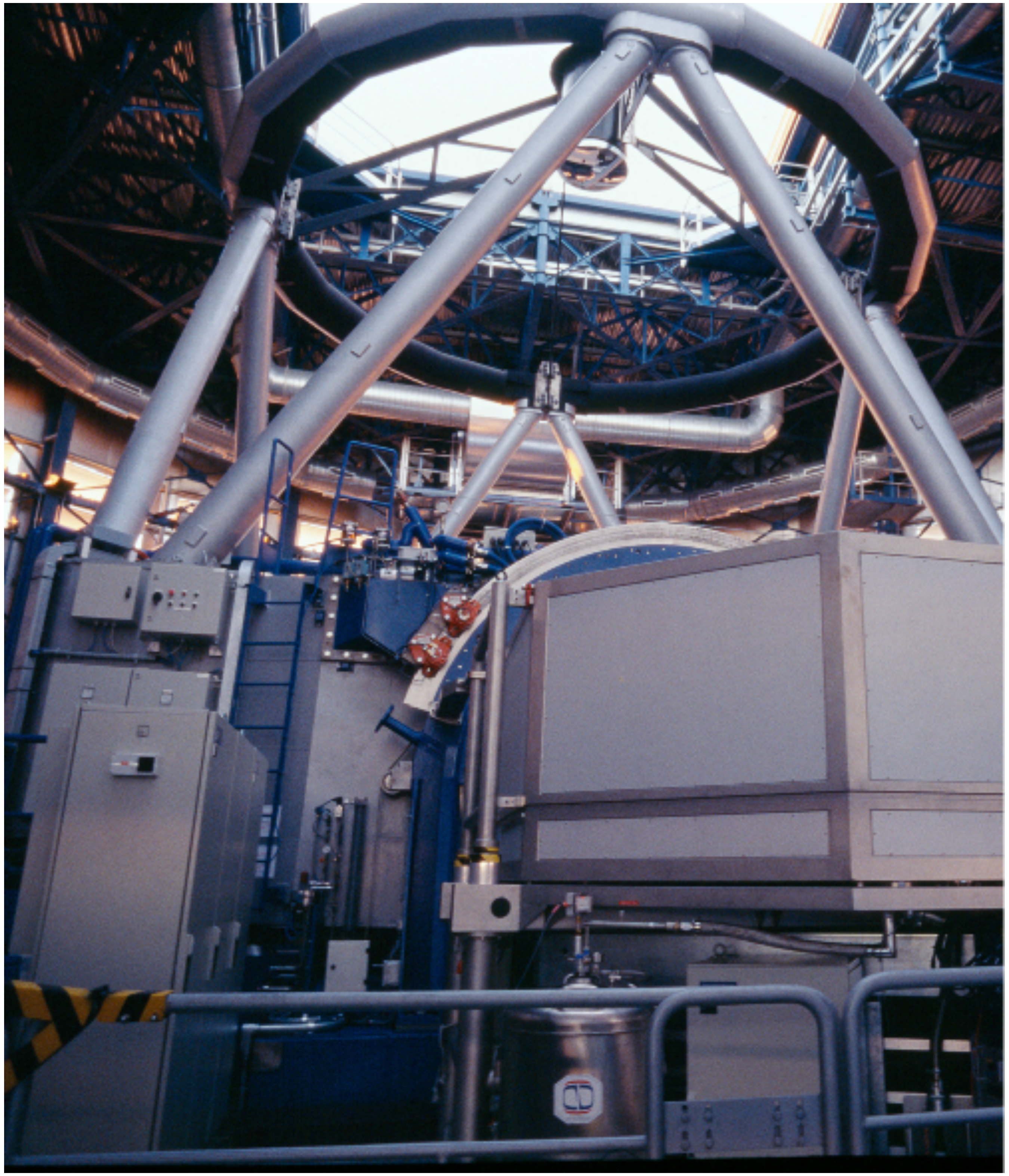
Accurate stellar spectroscopy pioneered in Uppsala by Ångström

Accurate stellar spectroscopy pioneered in Uppsala by Ångström

Modern observations improved in many dimensions

- resolution
- wavelength coverage
- signal-to-noise ratio
- distance of objects
- number of objects



UVES @ 8m VLT in Chile

Quantum mechanics and stellar spectroscopy have a long history

Williamina Flemming

LETTERS TO THE EDITOR.

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The Spectra of Helium and Hydrogen.

RECENTLY Prof. Fowler (Month. Not. Roy. Astr. Soc., December, 1912) has observed a number of new lines by passing a condensed discharge through mixtures of hydrogen and helium. Some of these lines coincide closely with lines of the series observed by Pickering in the spectrum of the star ζ Puppis, and attributed to hydrogen in consequence of its simple numerical relation to the ordinary Balmer series. Other lines coincide closely with the series predicted by Rydberg and denoted as the principal series of the hydrogen spectrum. The rest of the new lines show a very simple relation to those of the latter series, but apparently have no place in Rydberg's theory.

Niels Bohr

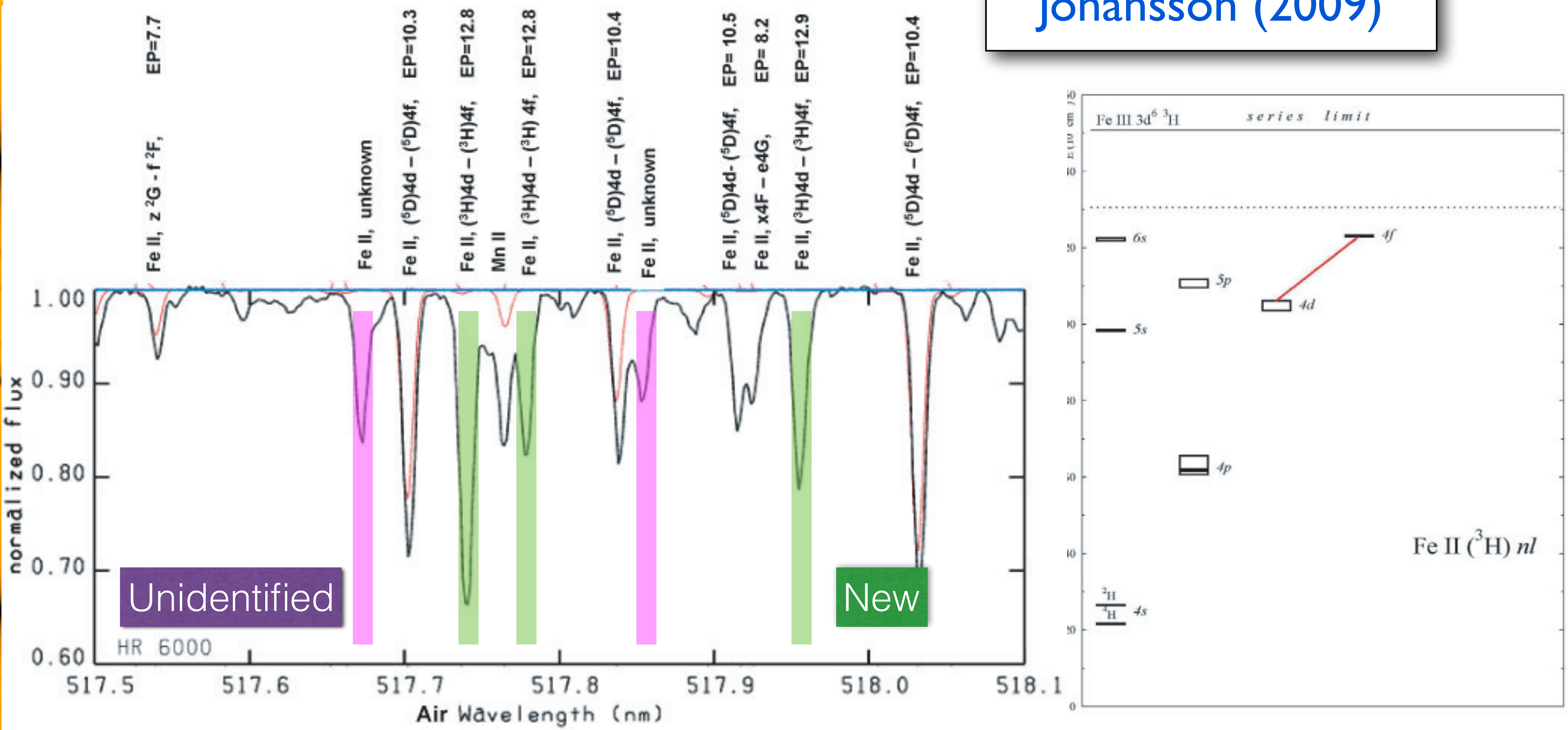
Bohr (1913)

The identification of lines observed by Flemming in zeta Puppis (O4If star) as being from He II was a major piece of the puzzle in Bohr's model.

This is a textbook example of interaction between astronomy, experimental and theoretical physics.

Quantum mechanics and stellar spectroscopy have a long history

Johansson (2009)



Identification of a 4d-4f multiplet of Fe II in HR6000 (Bp star with [Fe/H]~0.7), which had not been seen in lab spectra

Why do such things still exist?

"in principle"

$$i\hbar\frac{\partial}{\partial t}\Psi = H\Psi$$

$$H\Psi = E\Psi$$

"in practice"

- Atomic structure
- Interactions with photons
- Collisions

all still very active fields of research (laboratory astrophysics)

What can we do with accurate elemental abundances?

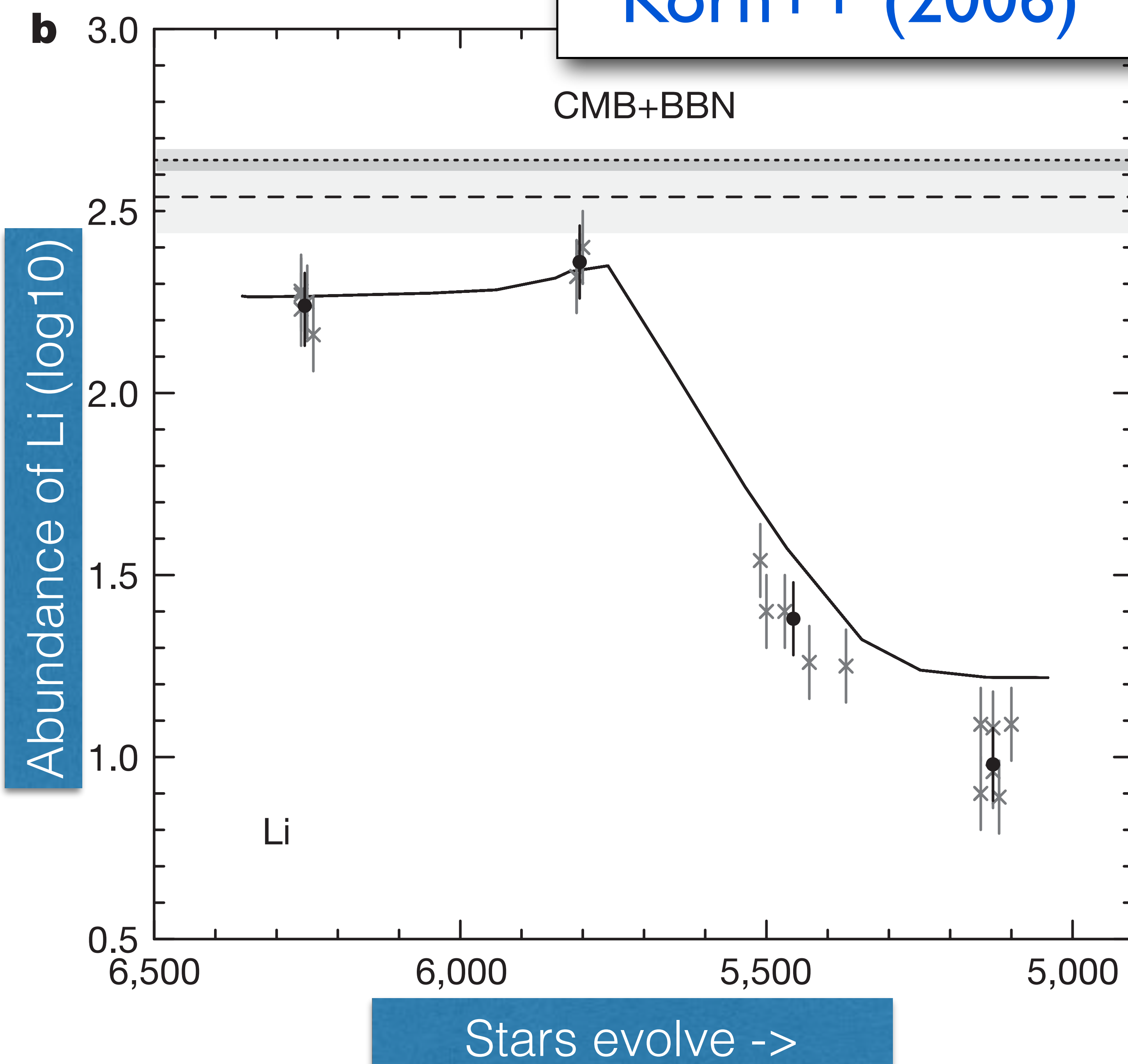
Abundances in stars provide “fossil” information in astrophysics.

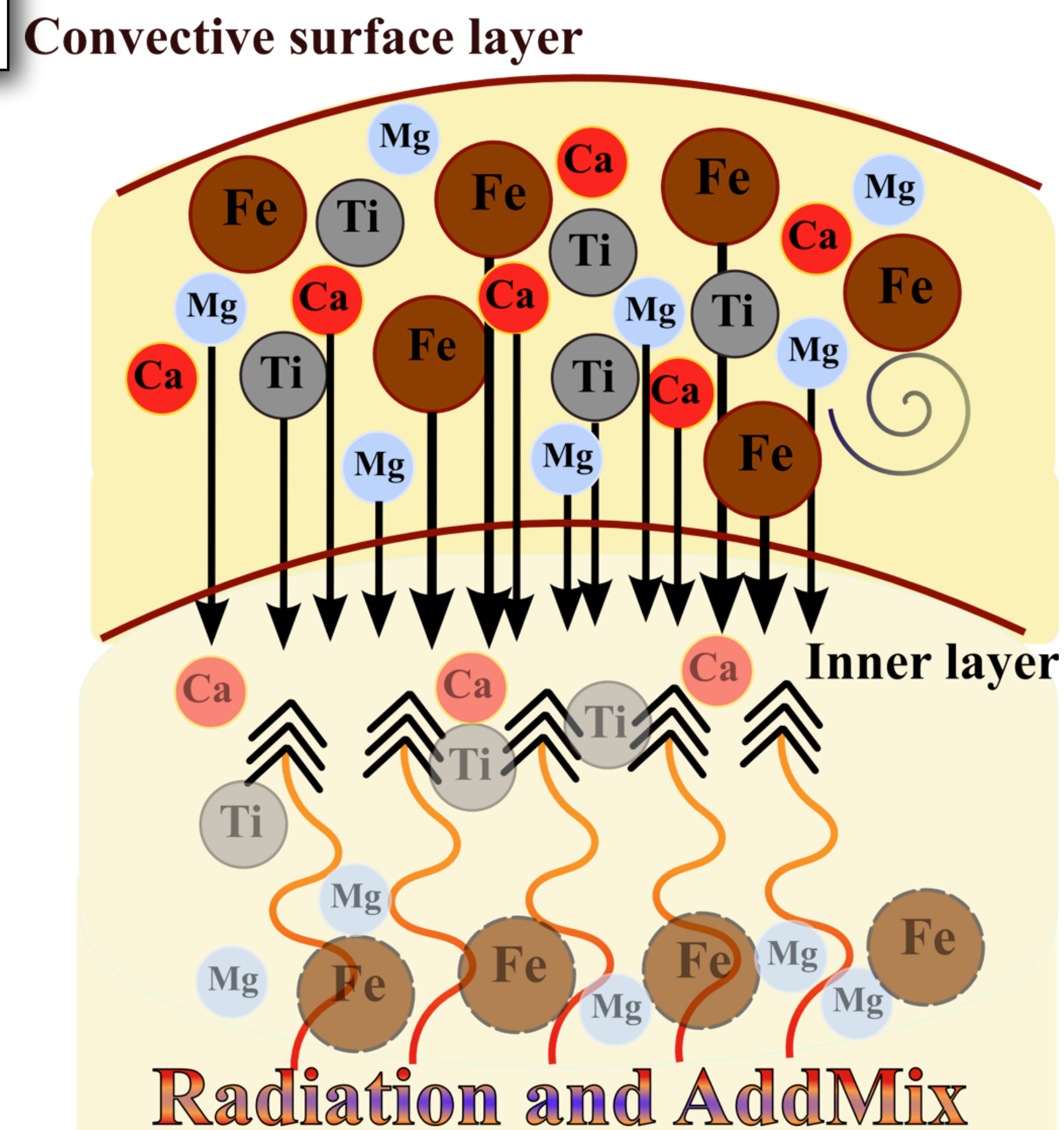
We can probe:

- stars themselves
- stellar populations
- the cosmic matter cycle
- planetary systems

Example application 1:
Probing (Big Bang) nucleosynthesis

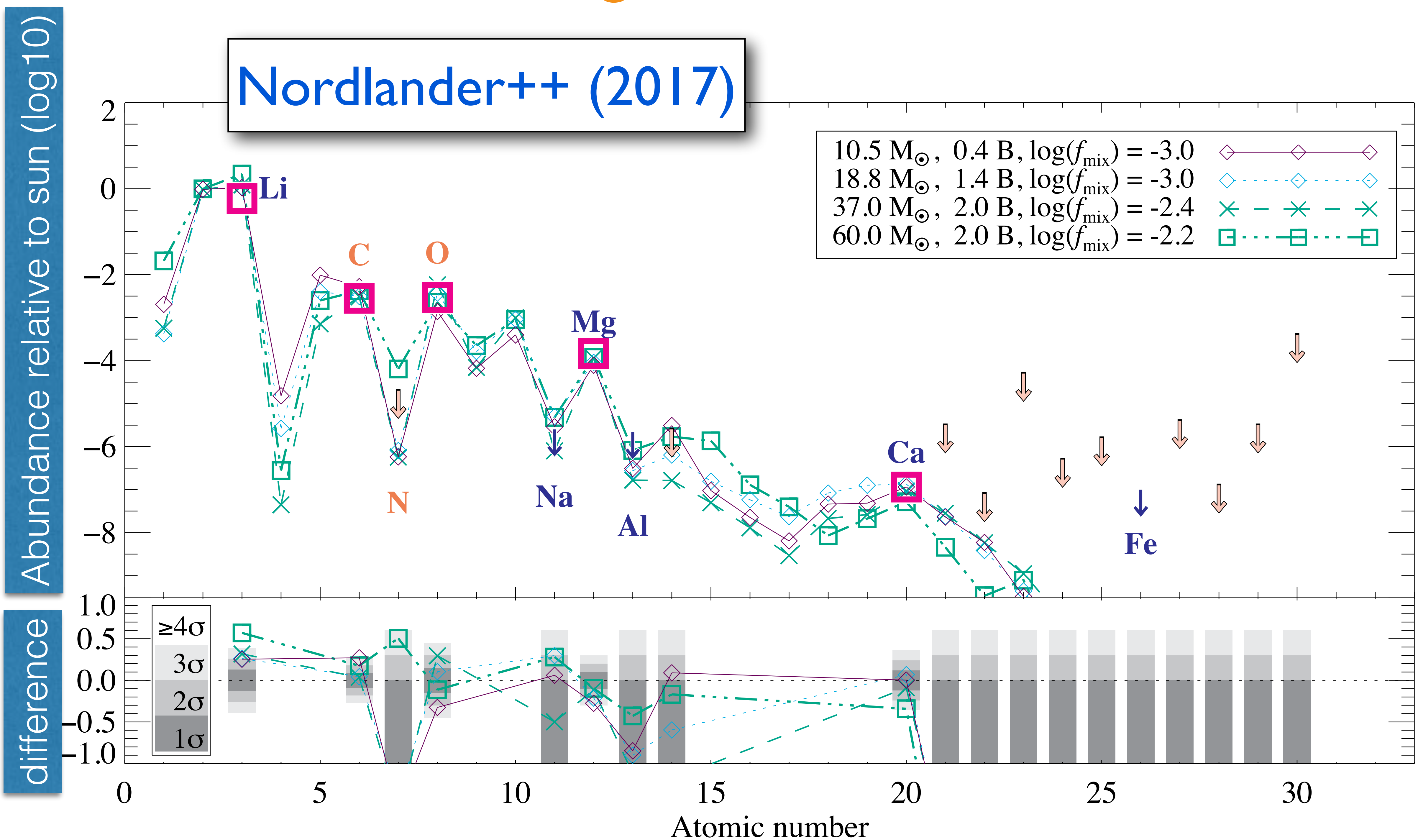
Korn++ (2006)





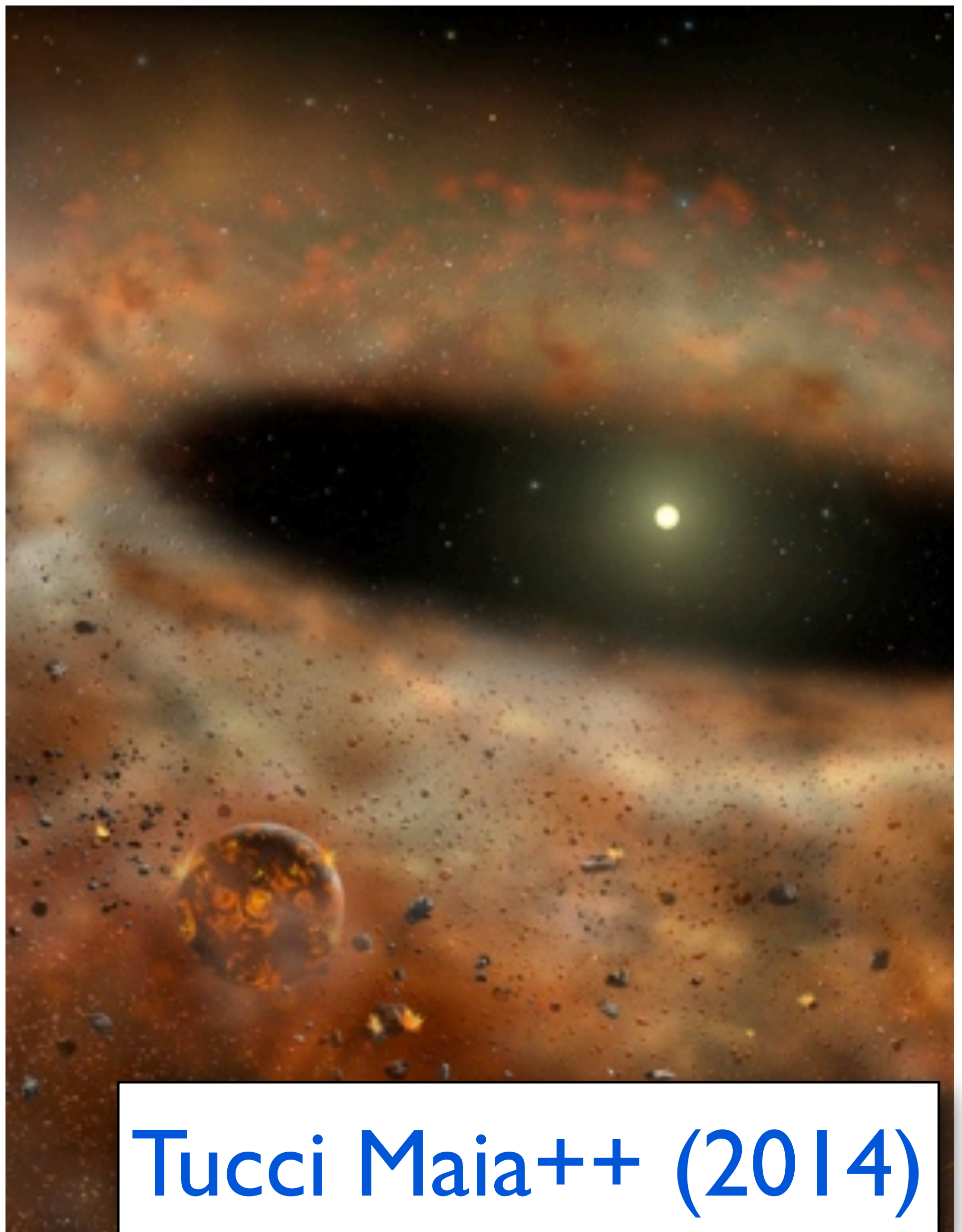
Abundances across evolutionary stages in globular cluster support that Li has been depleted in the atmosphere due to settling in old stars

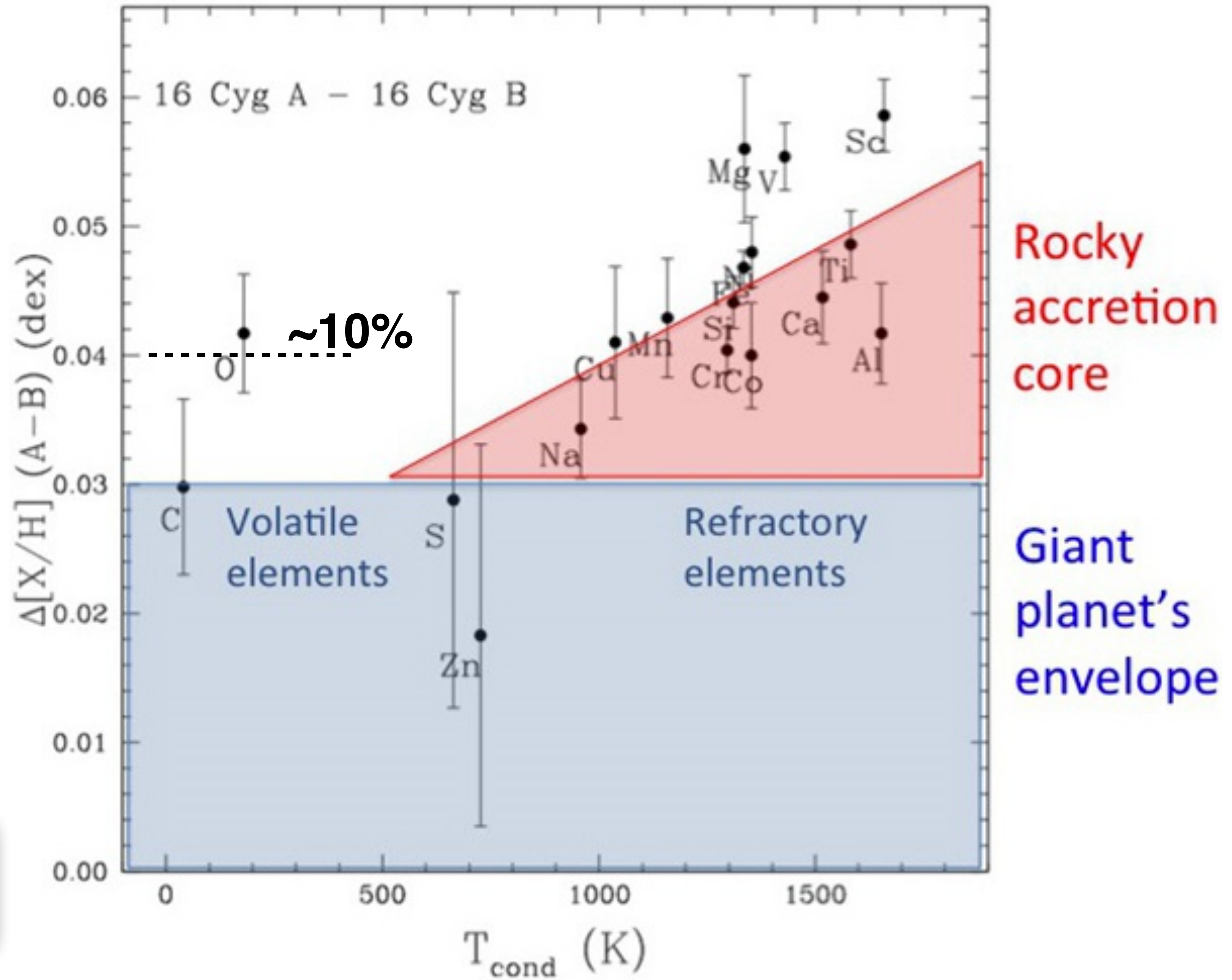
Example application 2: Probing the first stars



Abundances provide no support for first stars being supermassive

Example application 3:
Probing planetary system formation





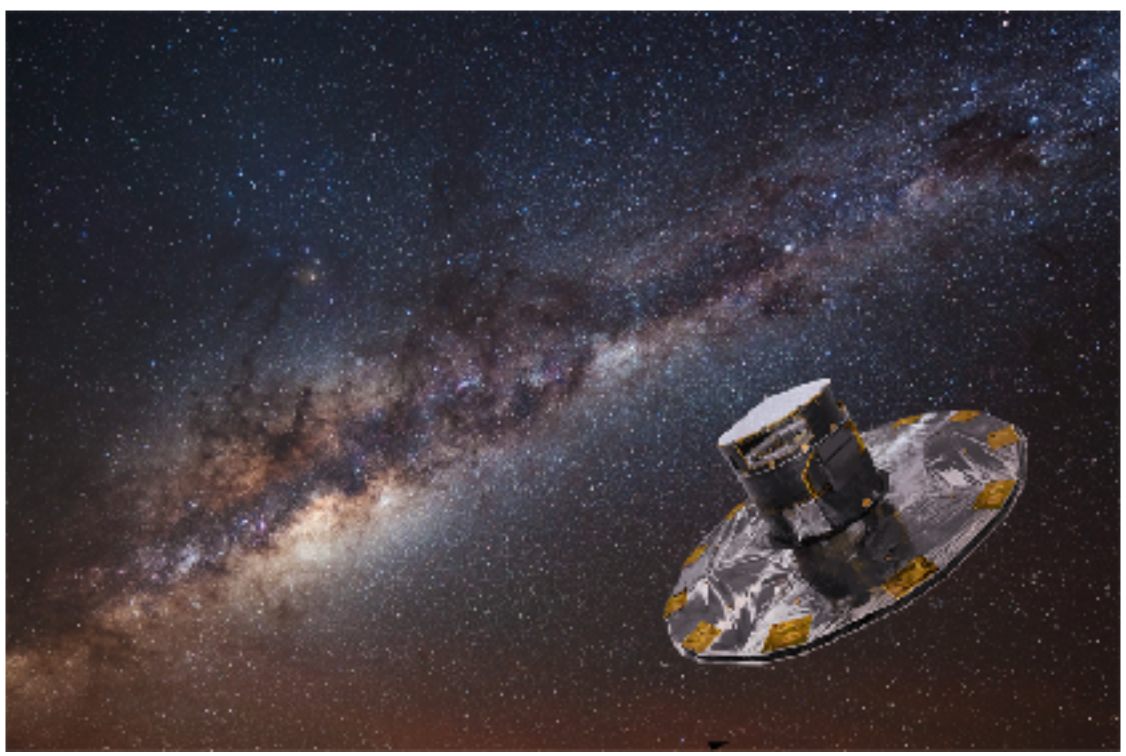
Two solar-type stars in binary, 16 Cyg B with 2.4 M_J planet

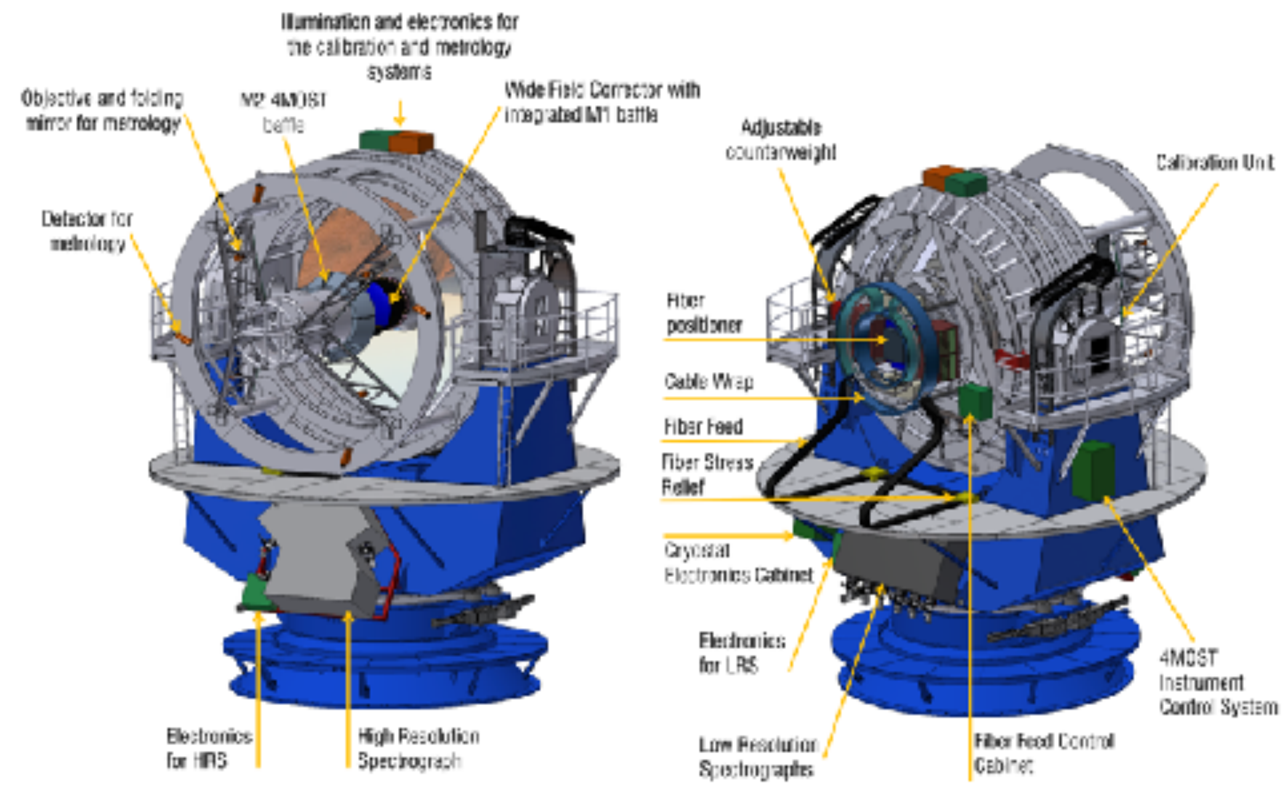
Abundances tell us planet probably has a rocky core

Accuracy will be important for galactic archeology

gaia

Knut och Alice Wallenbergs Stiftelse

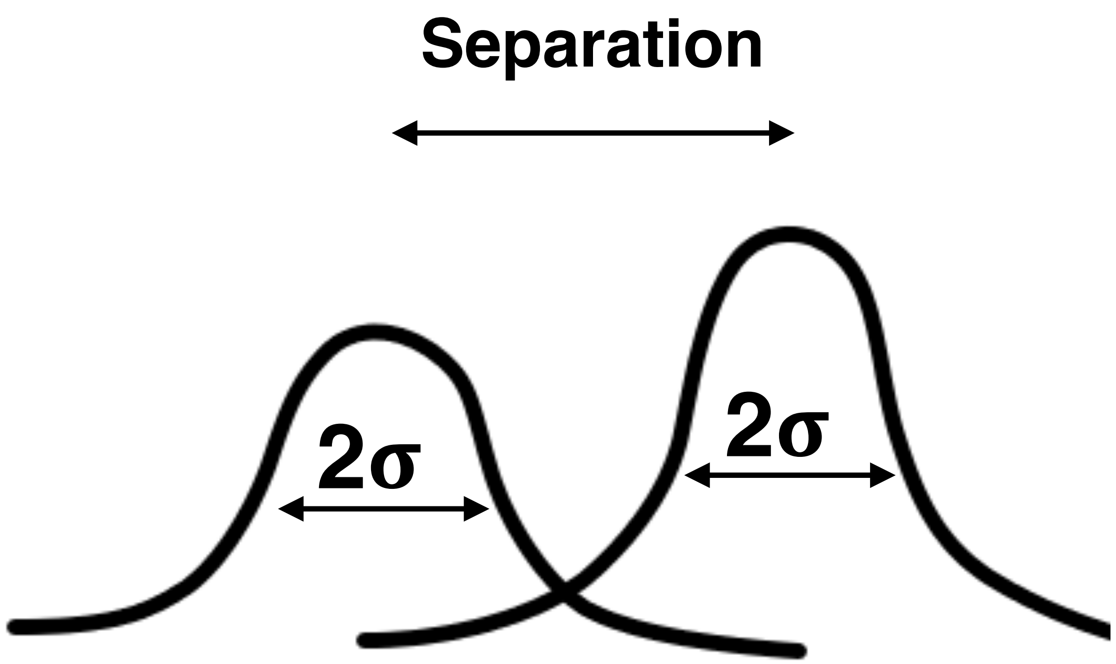


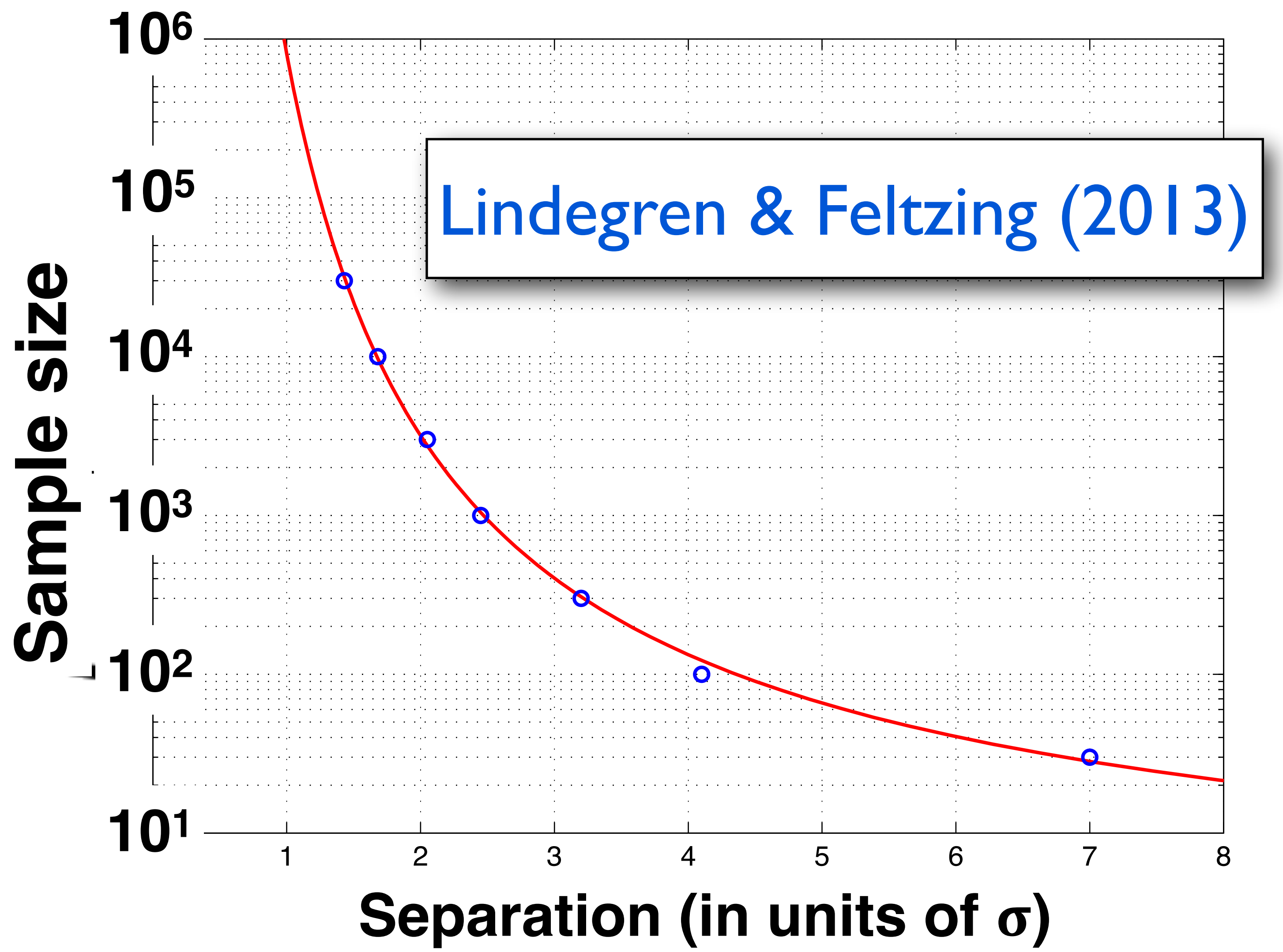


Accurate astrometry for $>10^9$ stars

High S/N and R spectra for $2x10^6$ stars

Accuracy more powerful than numbers

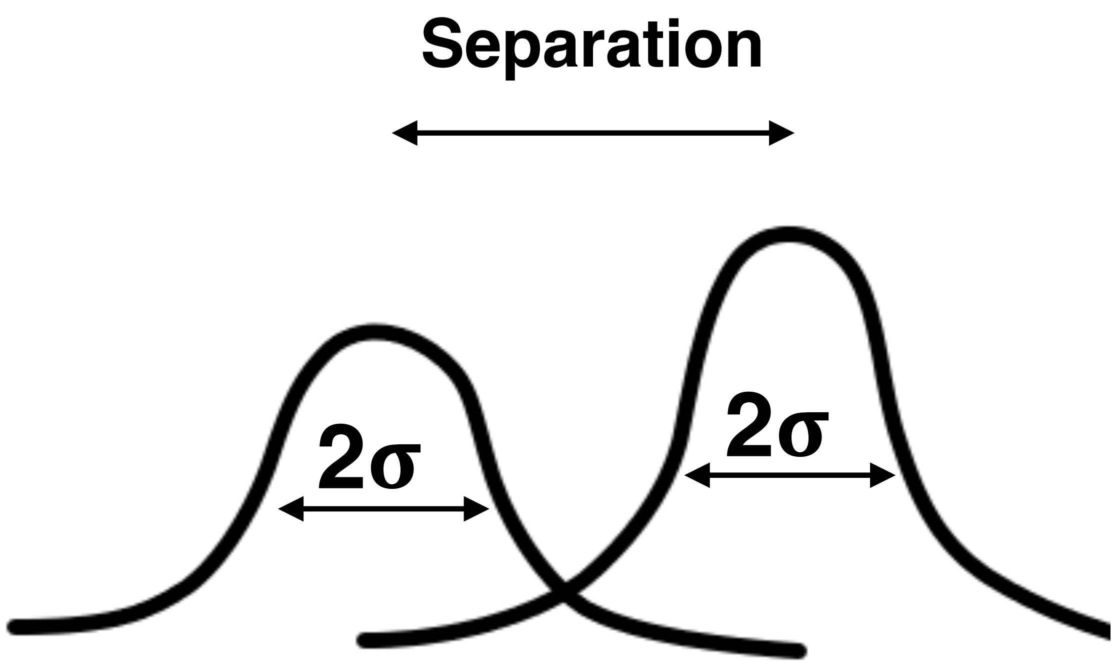


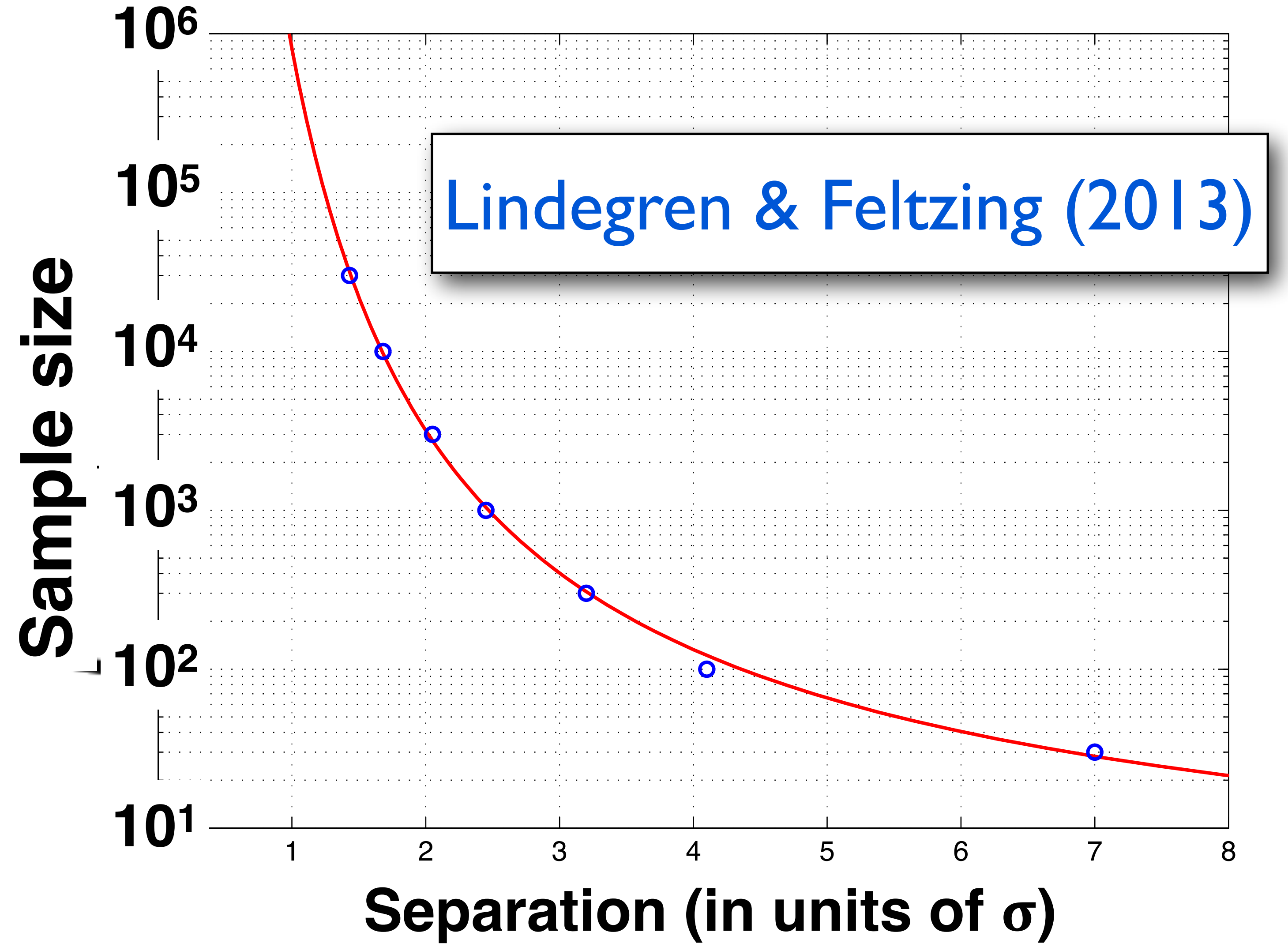


Present →

Accuracy (σ)	Resolve 0.2 dex (25%)	Resolve 0.1 dex (12%)	Resolve 0.01 dex (2%)
0.1 dex (25%)	10^3	10^6	$>>10^9$
0.09 dex (23%)	700	10^5	$>>10^9$
0.05 dex (12%)	100	10^3	$>>10^9$
0.01 dex (2%)	~2	~2	10^6

Accuracy more powerful than numbers

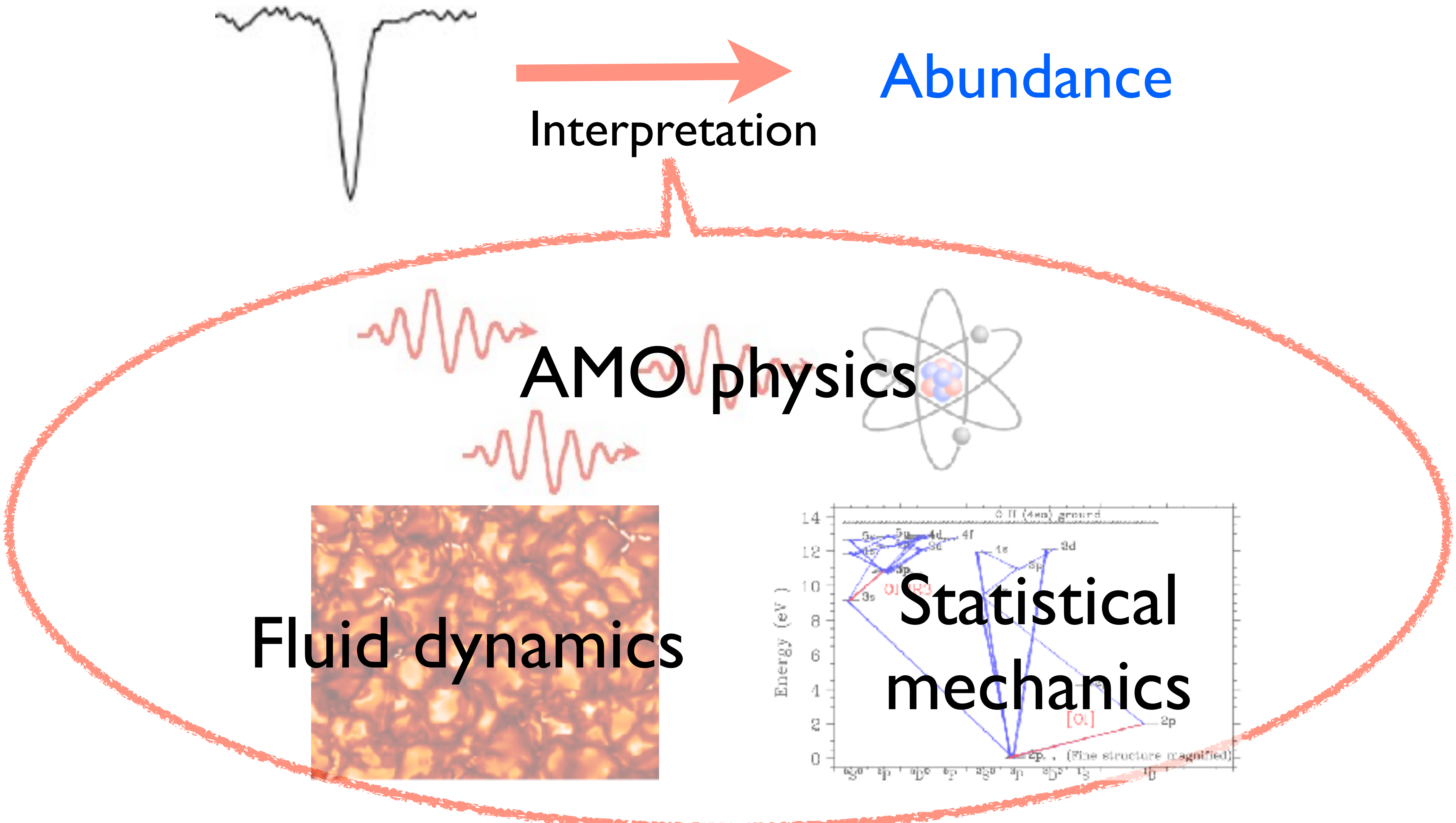




Or with 10^6 stars and 0.1 dex typical separation

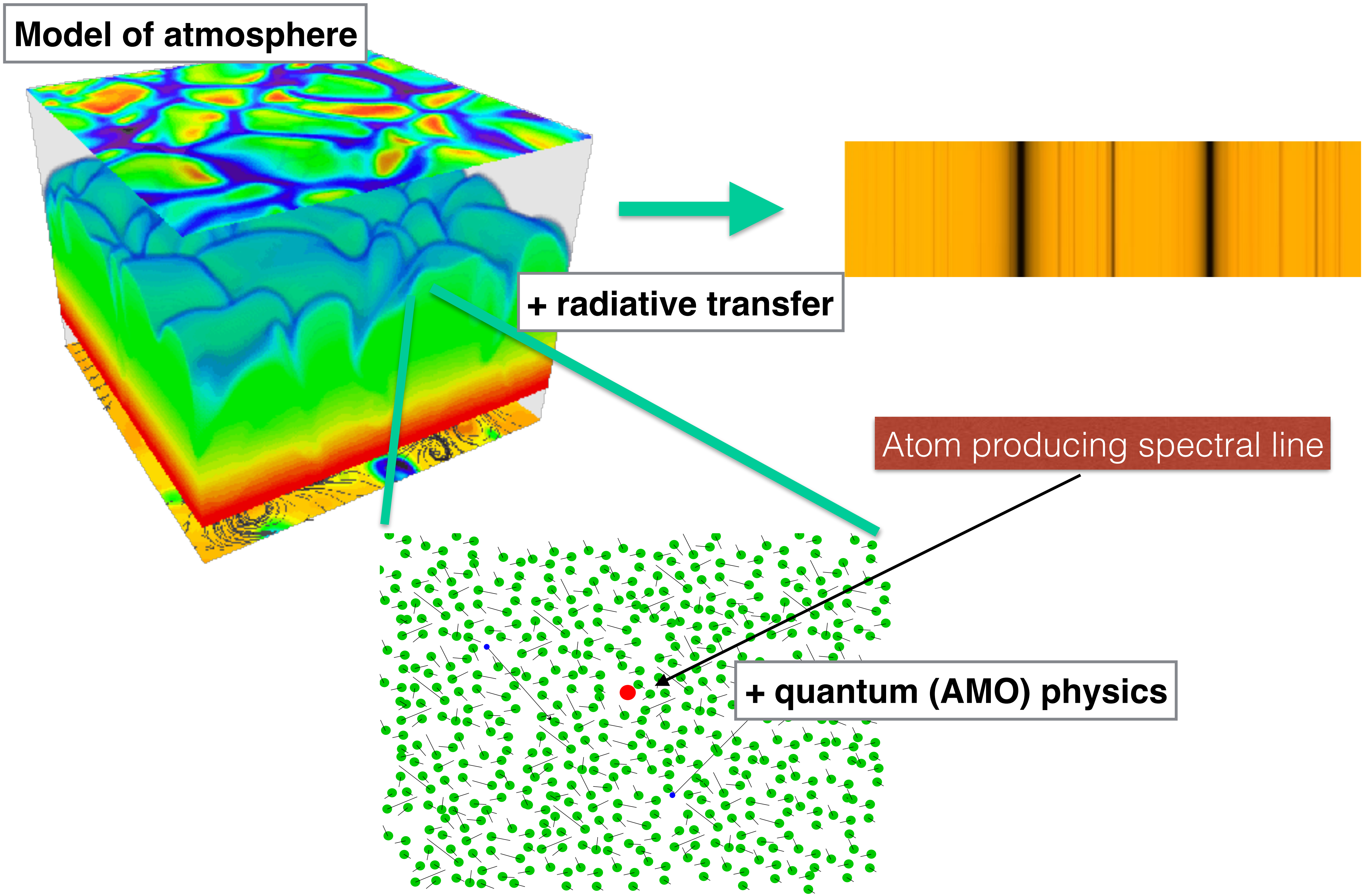
Accuracy (σ)	Resolve
0.1 dex (25%)	1 population
0.09 dex (23%)	10 populations
0.05 dex (12%)	1000 populations
0.01 dex (2%)	10^6 populations

Observations can be interpreted in terms of stellar properties e.g. elemental abundances



Uncertainties dominated by systematic errors in physics
We measure lines to ~1% (0.01 dex), but abundances have uncertainties of ~20% (0.1 dex)

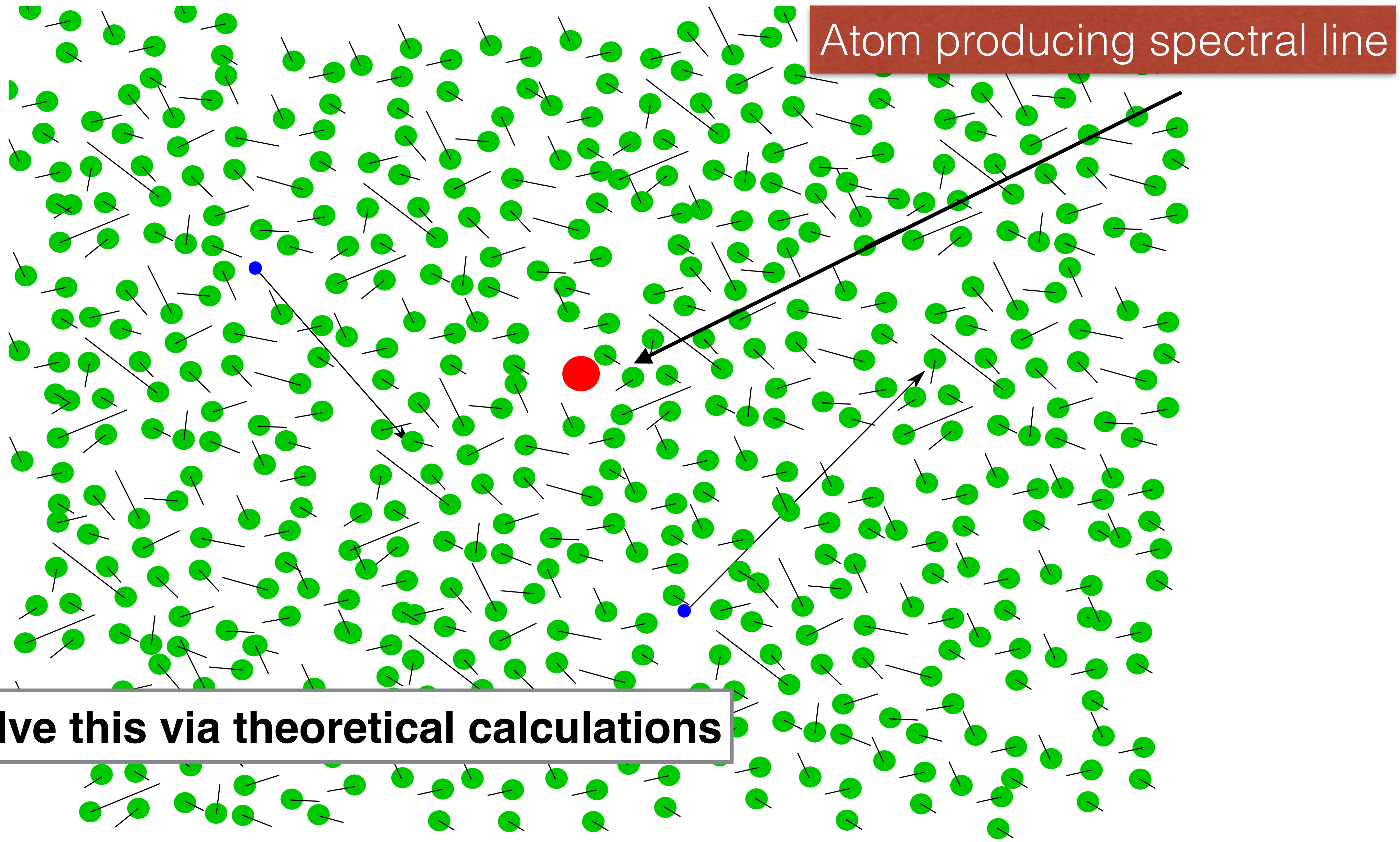
Modelling stellar spectra



Structure and interaction with radiation very important - collisions comparatively poorly known

The problem in modelling solar-type stars:

Effect of universe's most common element has often been missing or poorly known!



We try to solve this via theoretical calculations

$$N_H : N_e : N_p \sim 10^4 : 1 : 1$$

present day

$$N_H : N_e : N_p \sim 10^6 : 1 : 1$$

old stars

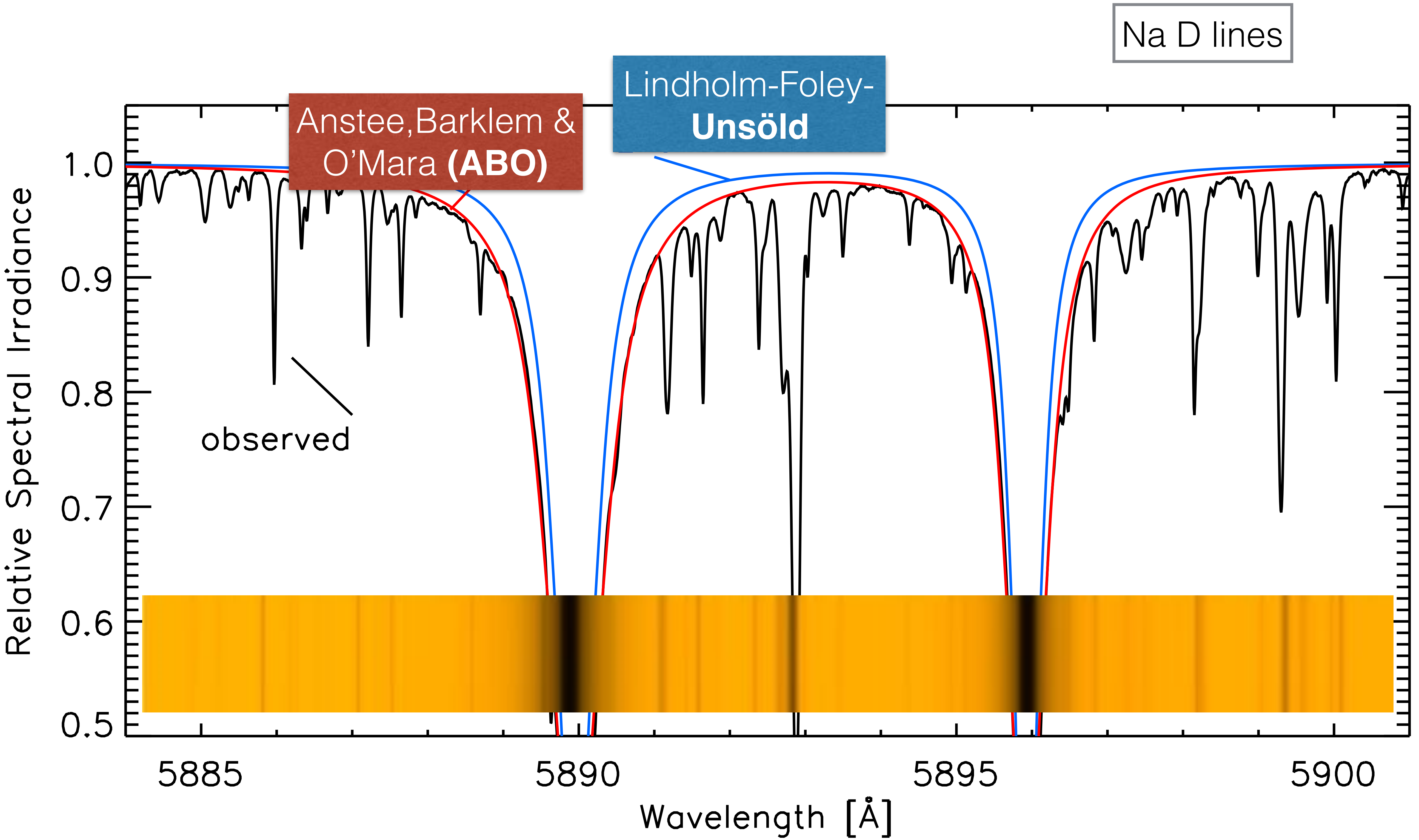
Two basic types

Elastic processes: clear hydrogen most important, unless there is degeneracy (e.g. H accidental degeneracy -> linear Stark)

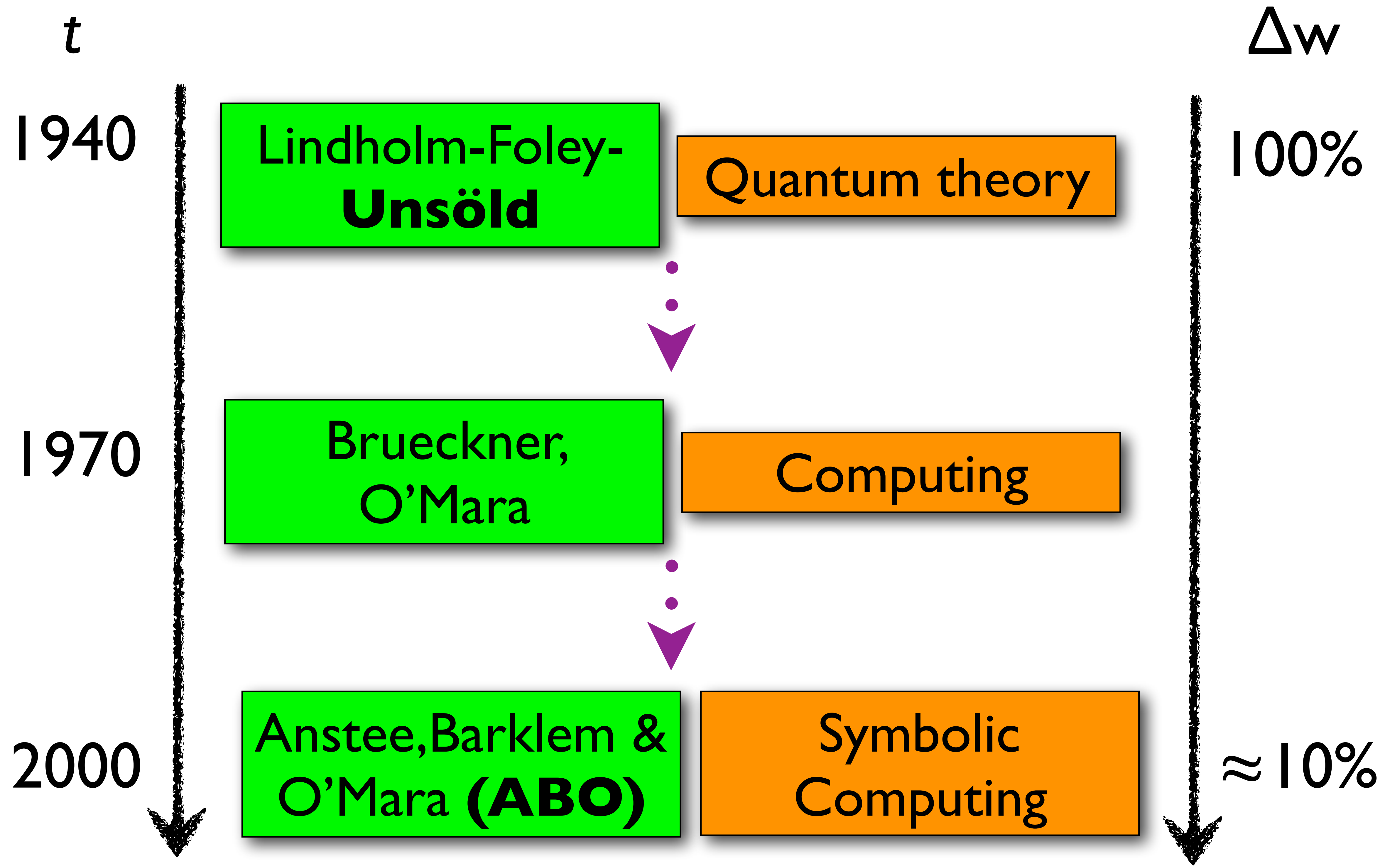
Inelastic processes: electrons important, but numbers mean hydrogen must be accounted for.

Tried to answer the question about importance of hydrogen collisions over the last 20 years

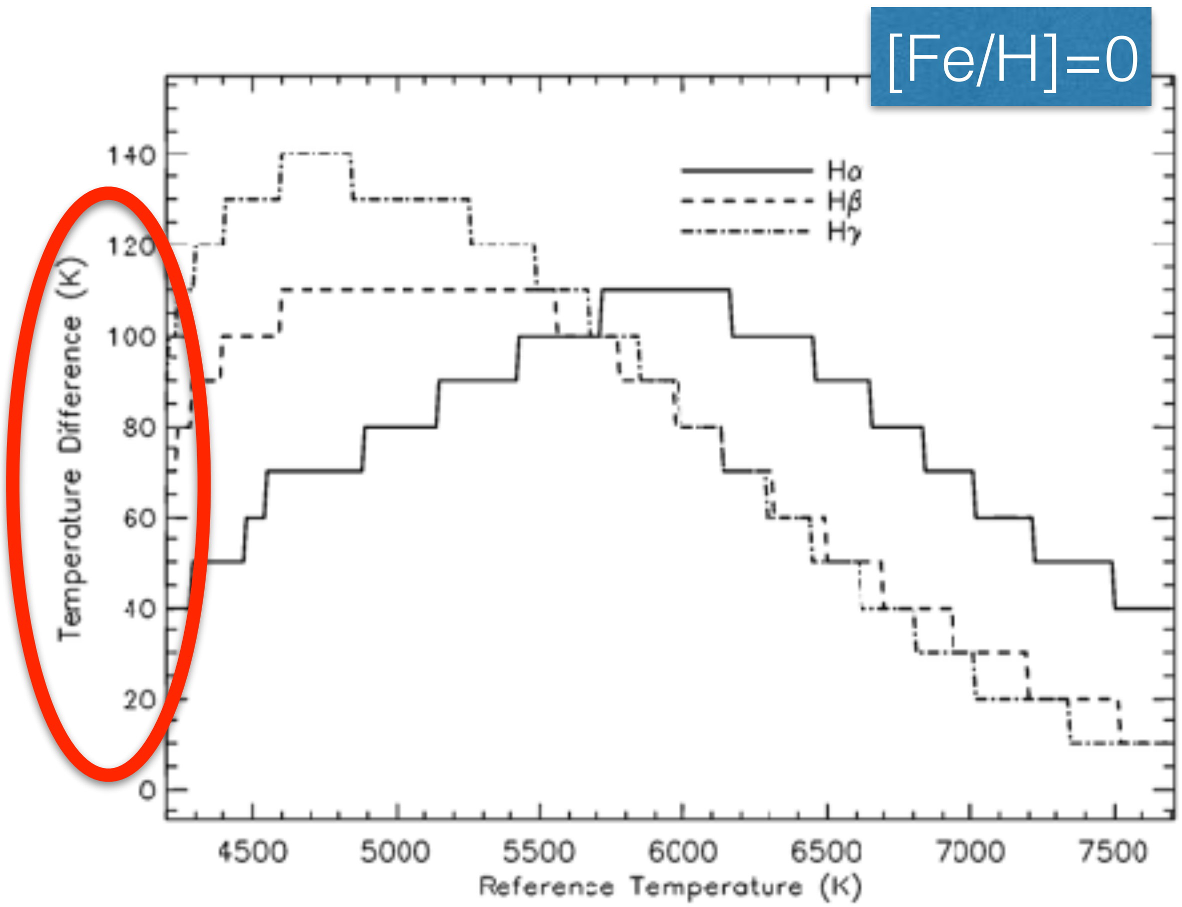
Elastic H impacts broaden spectral lines



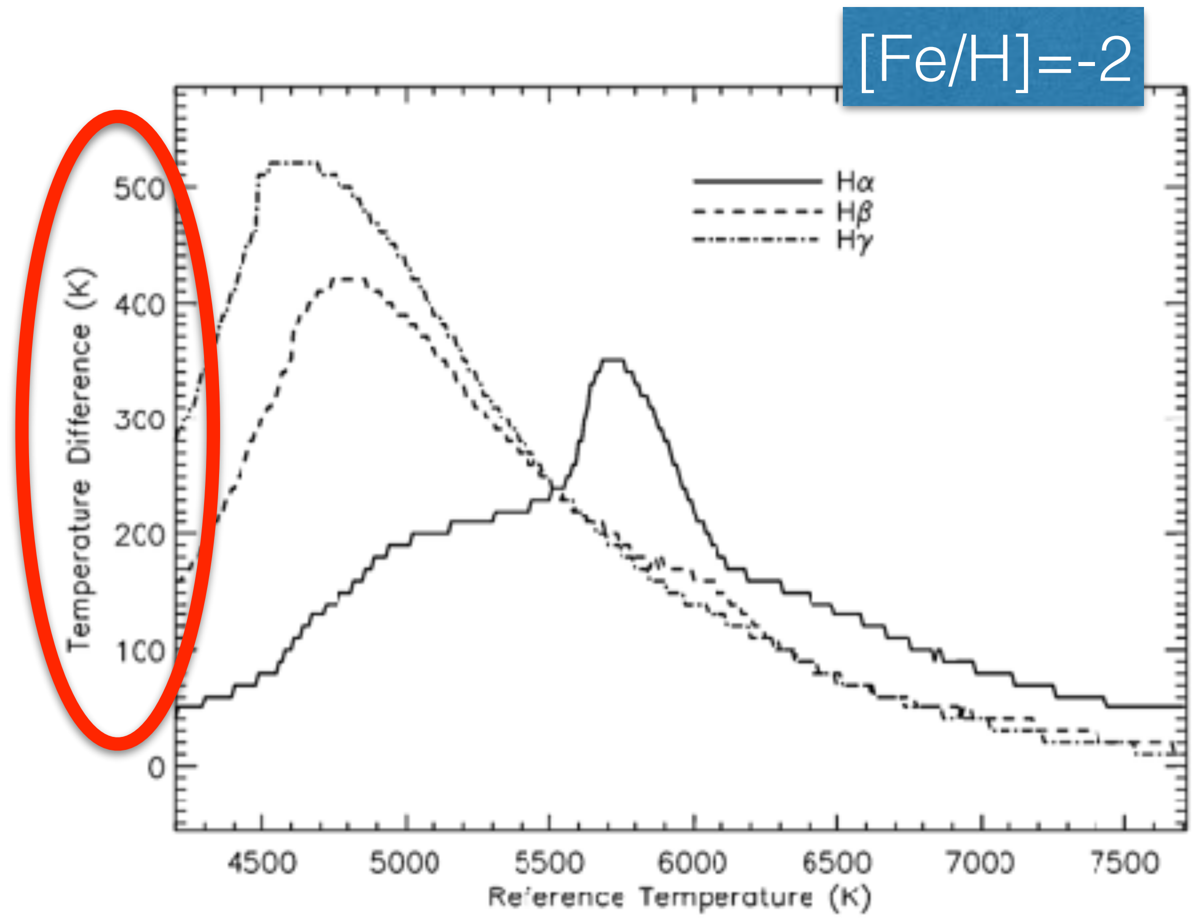
Development of line broadening theories for H impacts



Theory extended to H lines showed large changes in measured effective temperatures

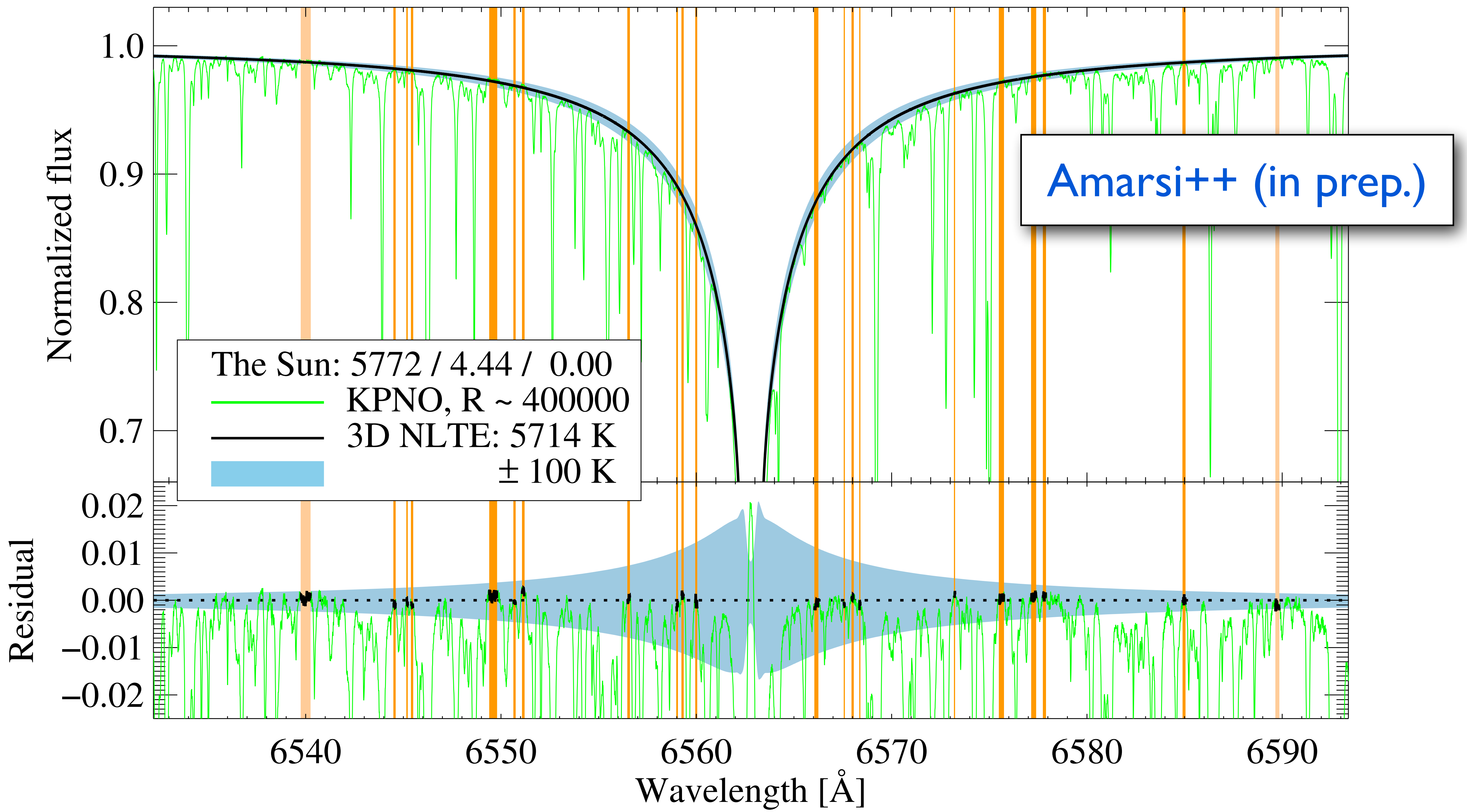


~100 K



~300 K

Agreement with observation is ~1% in 3D non-LTE



unfortunately 1% -> ~100 K

Summary: Elastic collisions - spectral line broadening

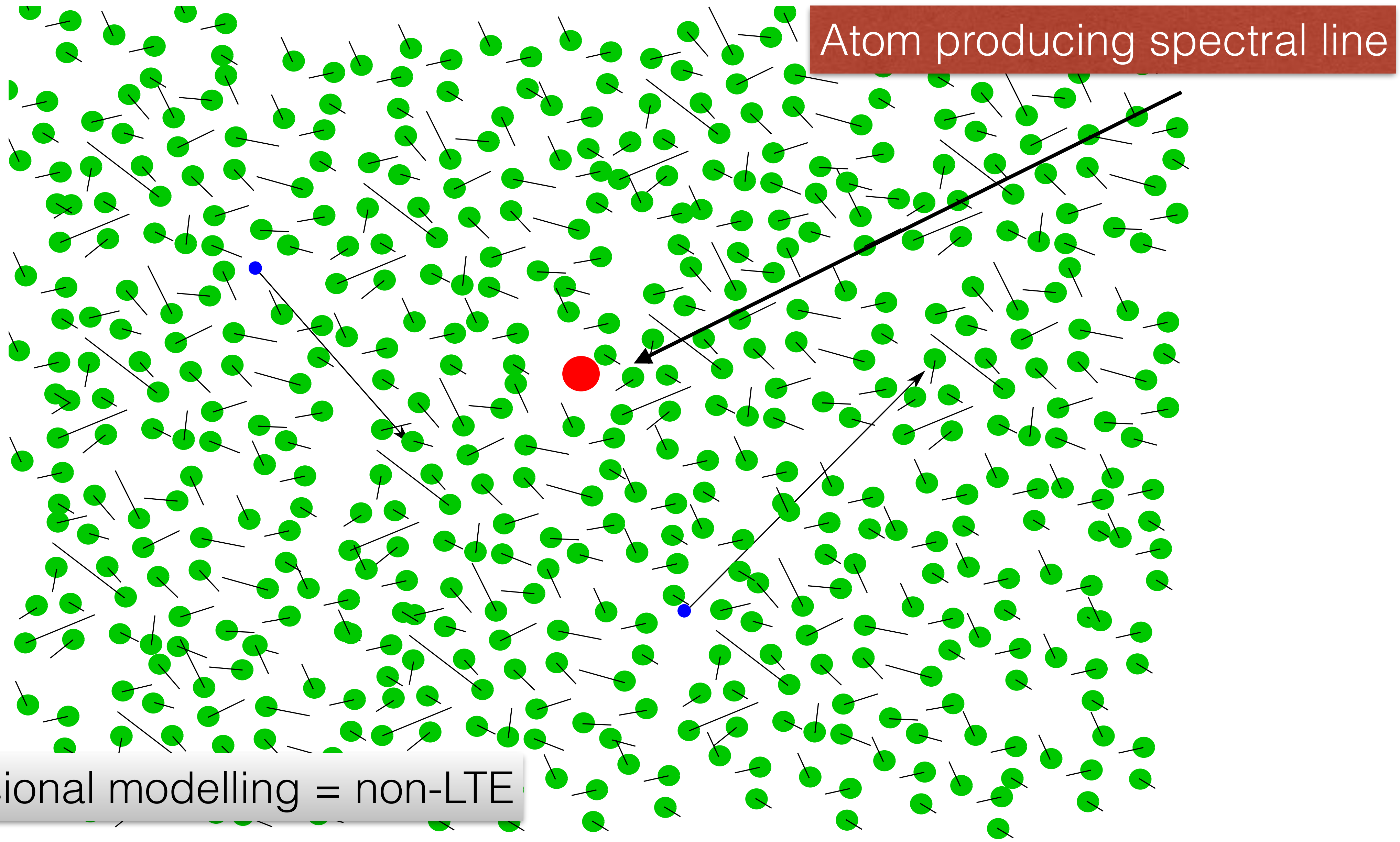
- ABO theory “improves” all tested cases.
- Agreement with astrophysical spectra and detailed calculations suggests error ~10%
- Data for ~43000 lines in VALD
- Freely available codes for H line opacities

Inelastic collisions and non-LTE

The introduction of the physics of atomic collision processes into the interpretation of astronomical phenomena took Astronomy beyond simple considerations of local thermodynamic equilibrium [i.e. non-LTE] into the discipline of Astrophysics.

Dalgarno (2001)

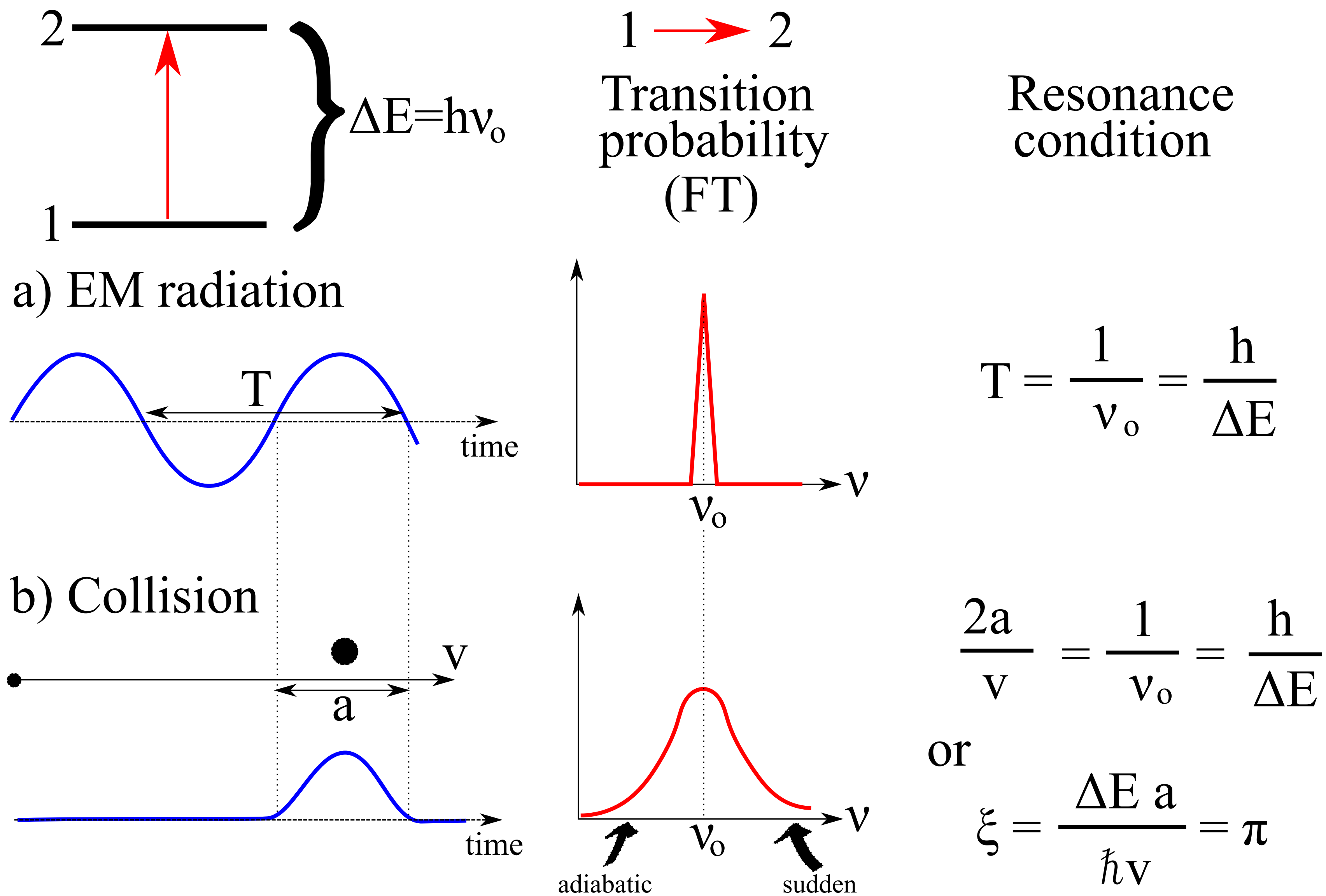
Which inelastic collisions?



$$N_H : N_e : N_p \sim 10^4 : 1 : 1$$ **present day**

$$N_H : N_e : N_p \sim 10^6 : 1 : 1$$ **old stars**

Which inelastic collisions? Massey criterion:



At collision velocities in stellar atmospheres, electrons expected to be near resonance, heavy particles adiabatic (=inefficient)

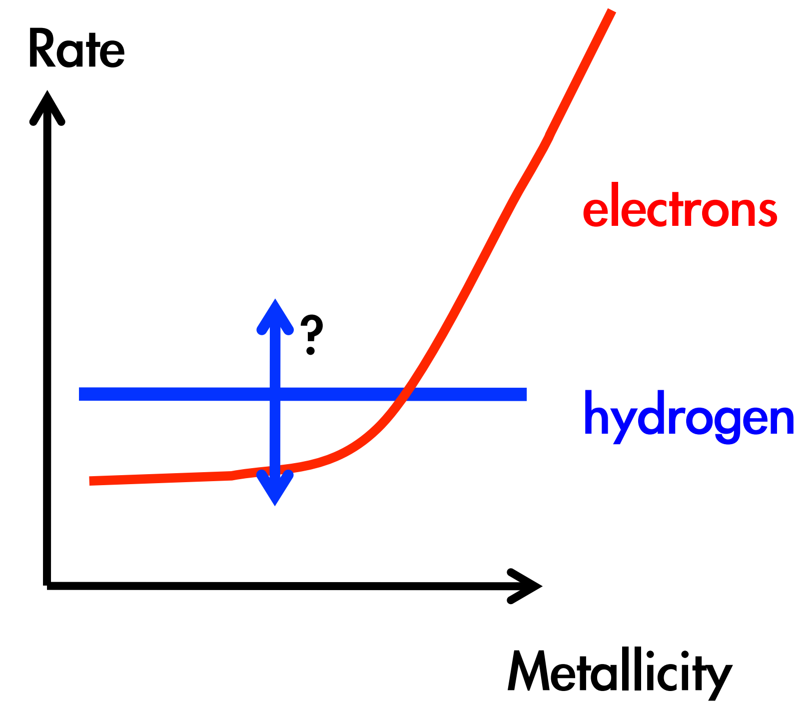
Which inelastic collisions?

$N_H/N_e \approx 10^4 - 10^6$

- do numbers overcome efficiency?

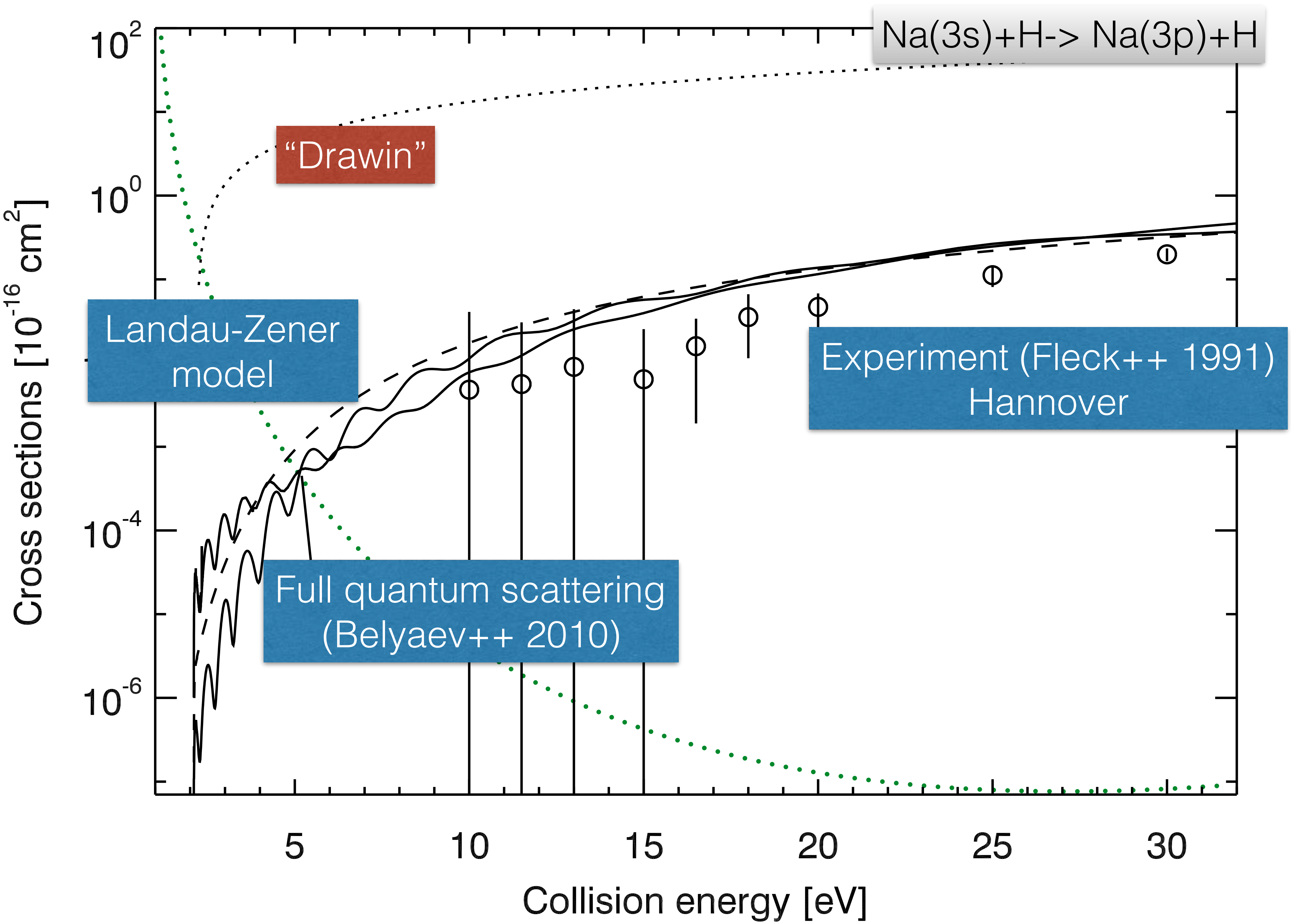
$N_p/N_e \approx 1$

- protons can probably be neglected

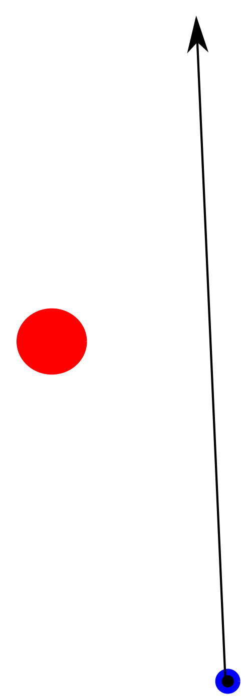


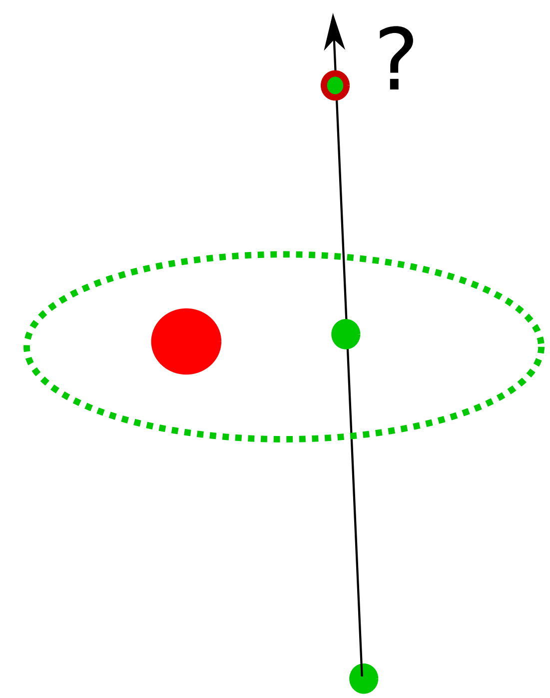
Note: considering only excitation/de-excitation here...

Steenbock & Holweger (1986) introduced the "Drawin" formula (modified classical Thomson)



Physics: The classical picture is wrong!





Classical impact
leads to excitation or ionisation via energy transfer through Coulomb interactions

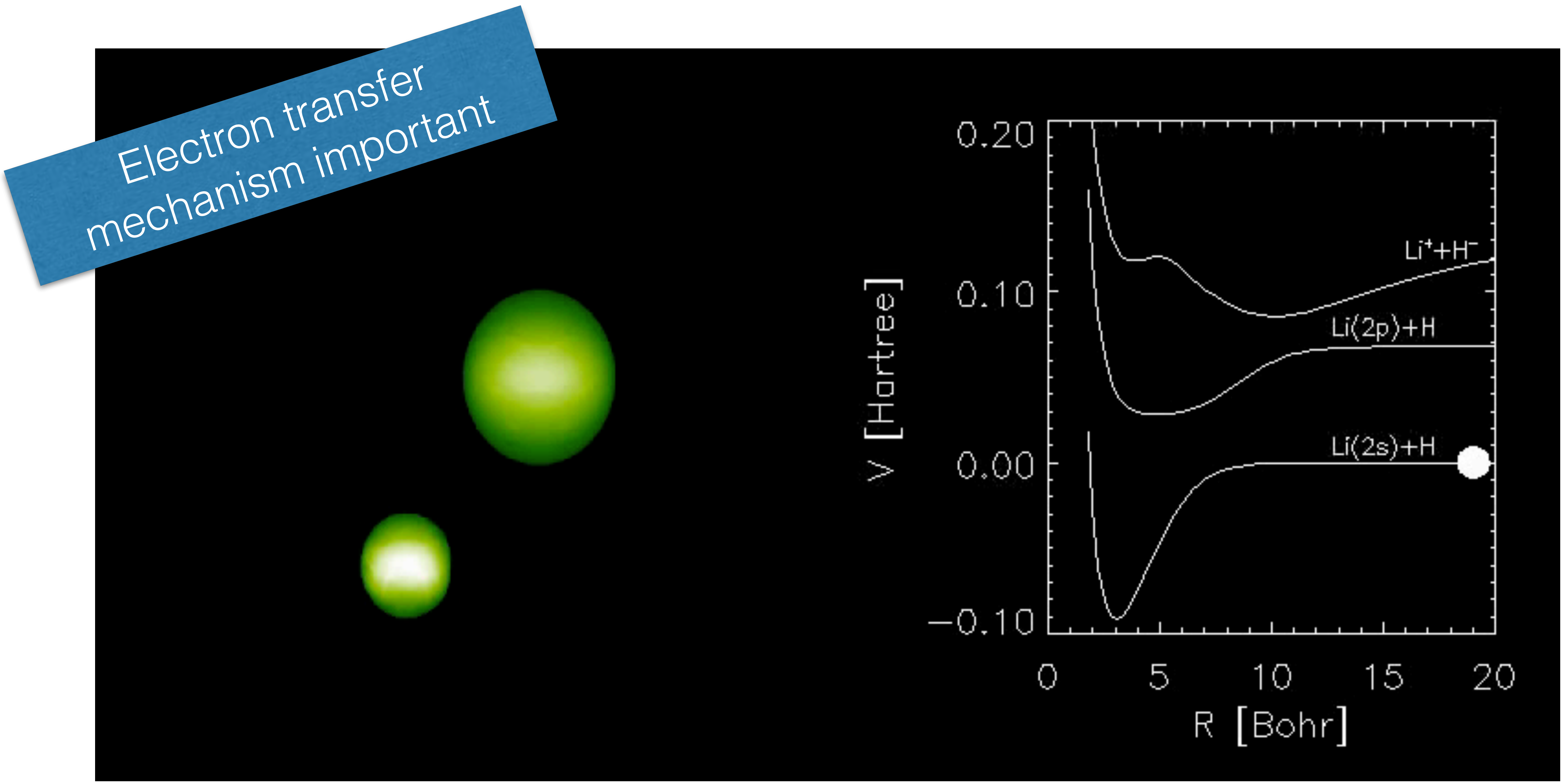
Quantum collision
leads to quasi-molecule and possible rearrangement of electrons, which can lead to energy transfer

and heavy particle collisions are fundamentally different to electron collisions

Inelastic processes due to H impact influence the state populations

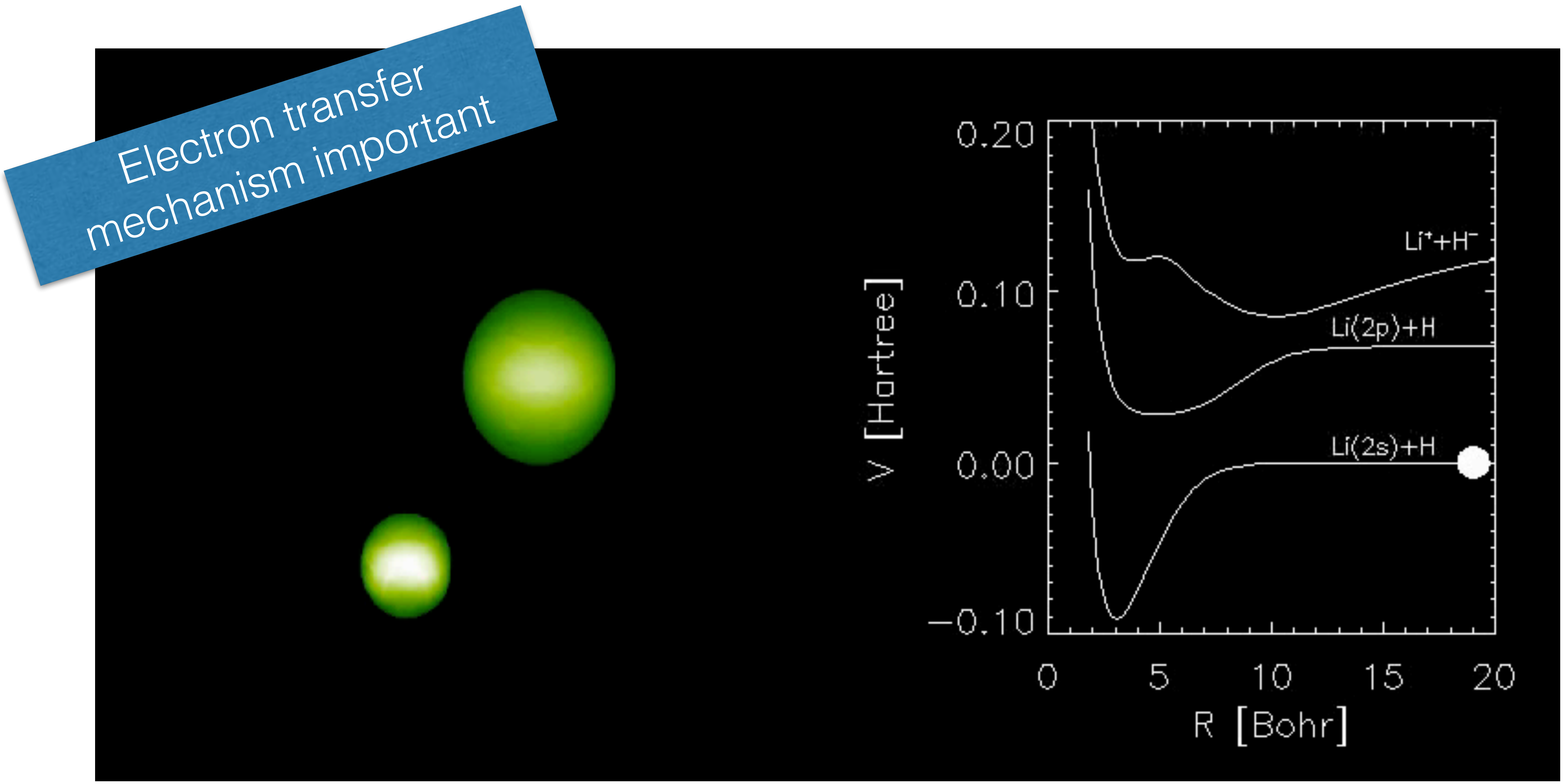
$$\mathrm{X}(nl) + \mathrm{H} \rightleftharpoons \mathrm{X}(n'l') + \mathrm{H}$$

$$\mathrm{X}(nl) + \mathrm{H} \rightleftharpoons \mathrm{X}^{+} + \mathrm{H}^{-}$$

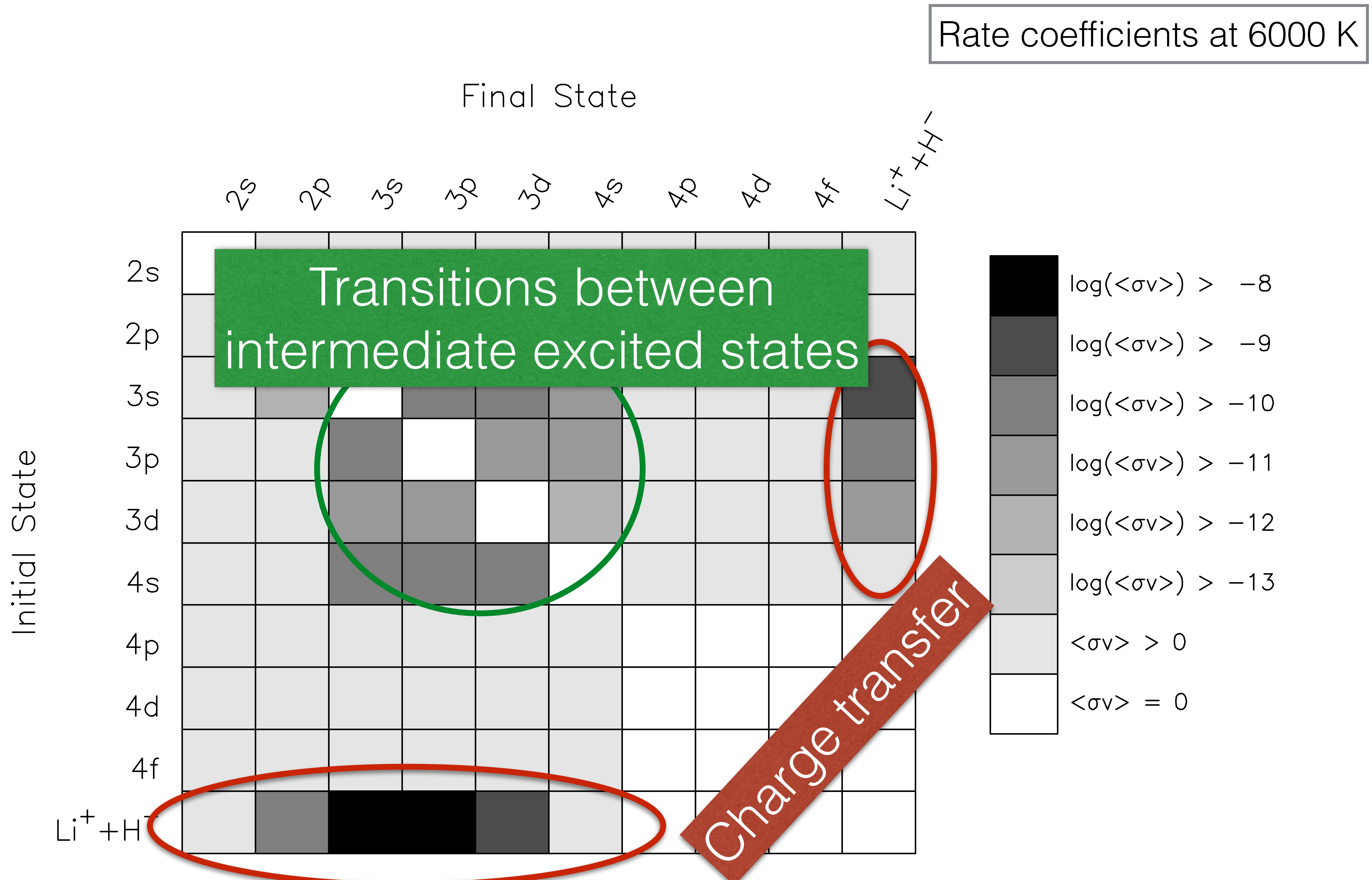


Inelastic processes due to H impact influence the state populations

$$X(nl) + H \rightleftharpoons X(n'l') + H$$
$$X(nl) + H \rightleftharpoons X^{+} + H^{-}$$

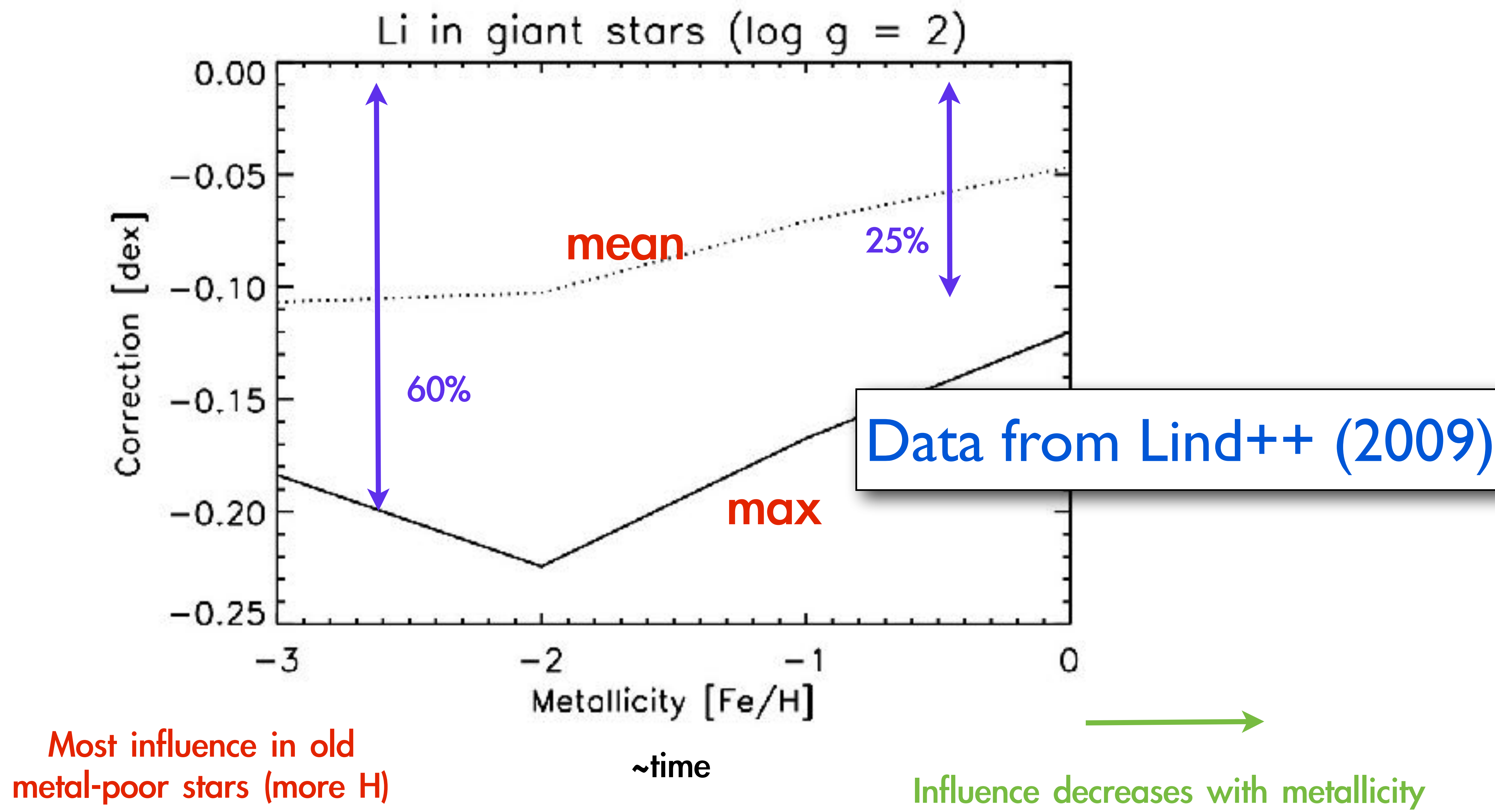


Li+H data: charge transfer processes important

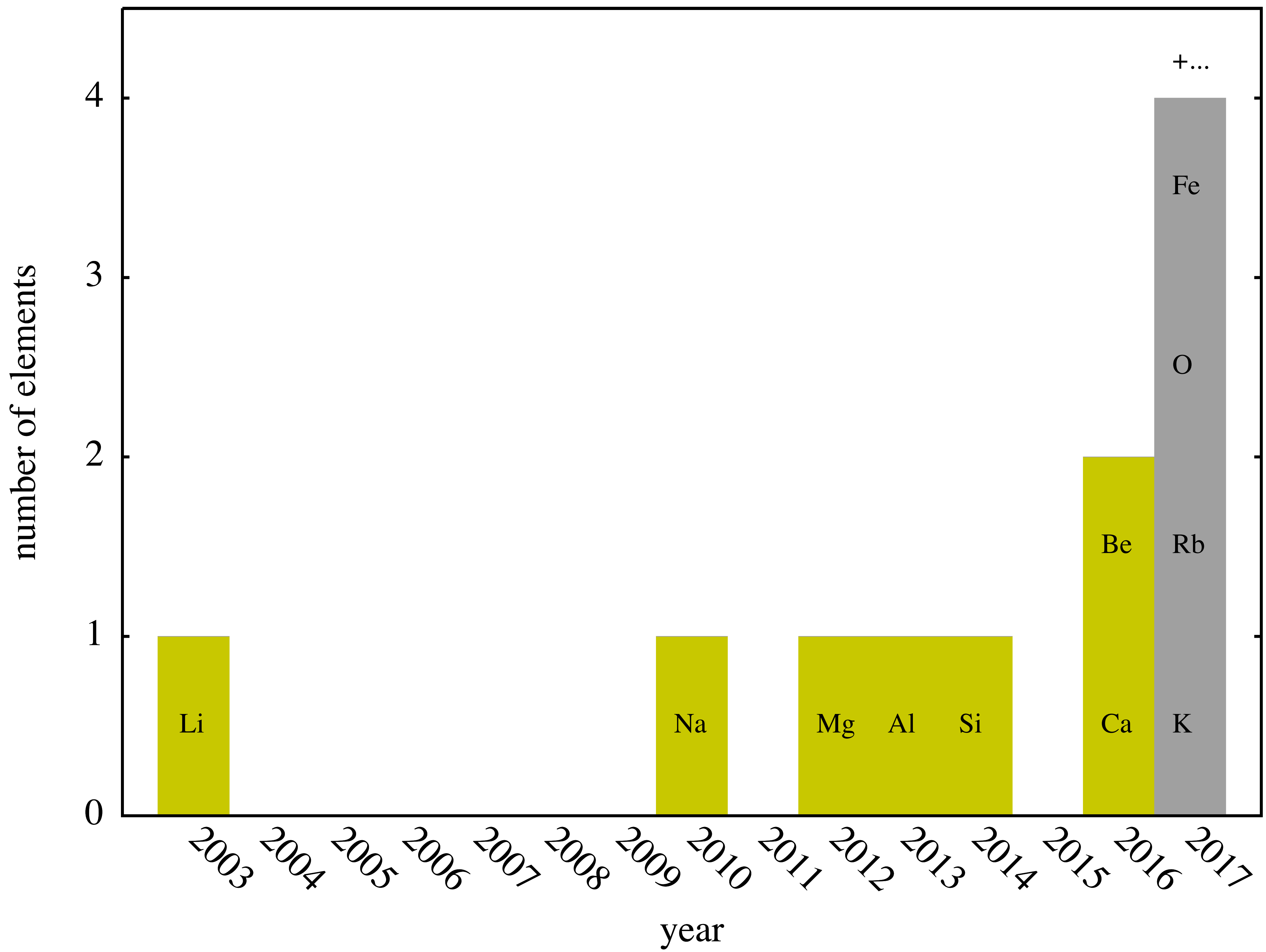


Charge transfer processes change interpreted abundances

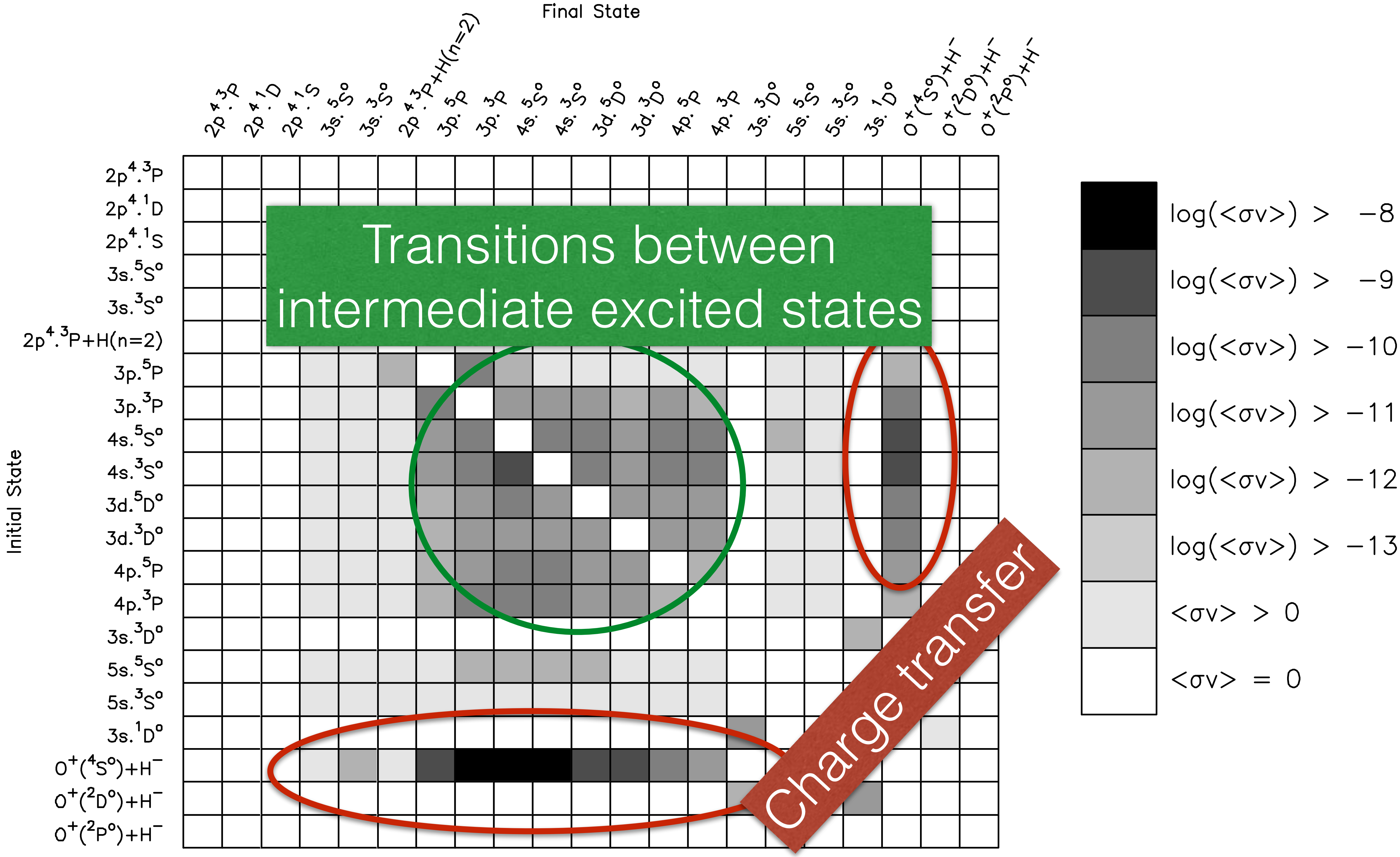
- Charge transfer is the dominant process for Li and Na
- Abundances overestimated by as much as 60% (0.2 dex) if not included



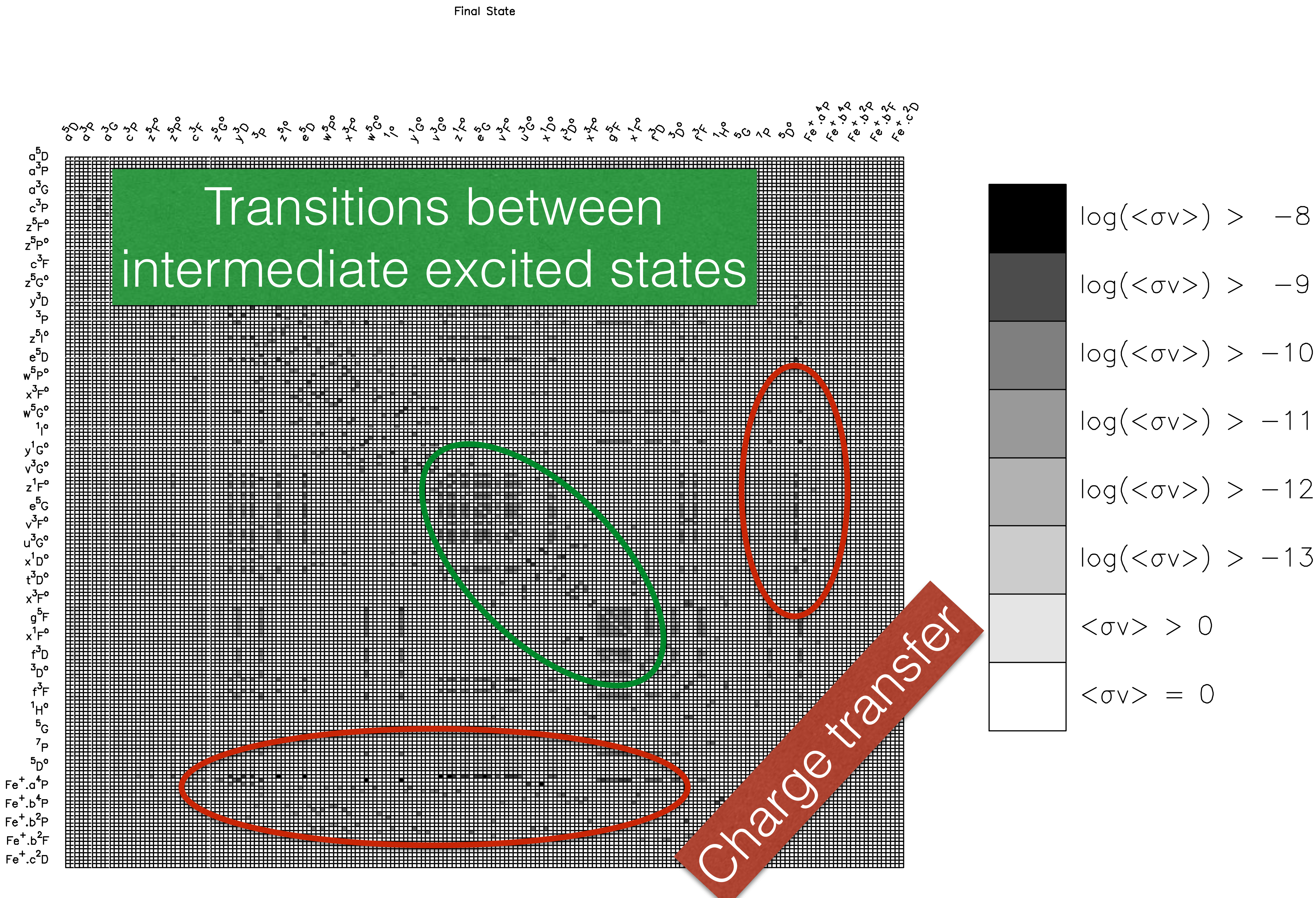
Progress speeding up and complex atoms now possible



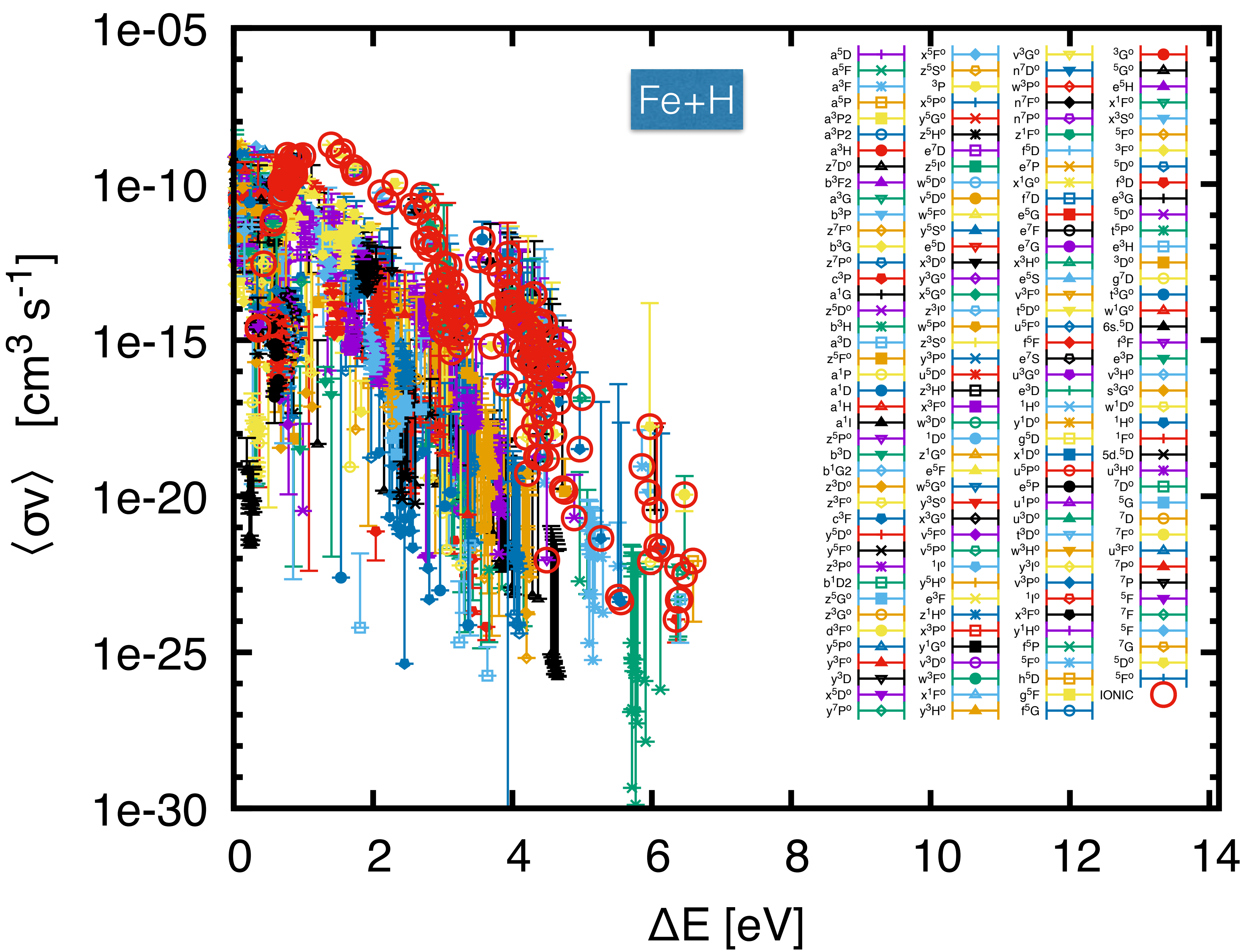
O+H data


Final State
Initial State
$2p^{4}.^{3}P$
$2p^{4}.^{1}D$
$2p^{4}.^{1}S$
$3s.^{5}S^{o}$
$3s.^{3}S^{o}$
$2p^{4}.^{3}P+H(n=2)$
$3p.^{5}P$
$3p.^{3}P$
$4s.^{5}S^{o}$
$4s.^{3}S^{o}$
$3d.^{5}D^{o}$
$3d.^{3}D^{o}$
$4p.^{5}P$
$4p.^{3}P$
$3s.^{3}D^{o}$
$5s.^{5}S^{o}$
$5s.^{3}S^{o}$
$3s.^{1}D^{o}$
$O^{+}(^{4}S^{o})+H^{-}$
$O^{+}(^{2}D^{o})+H^{-}$
$O^{+}(^{2}P^{o})+H^{-}$
log(<σv>) > −8
log(<σv>) > −9
log(<σv>) > −10
log(<σv>) > −11
log(<σv>) > −12
log(<σv>) > −13
<σv> > 0
<σv> = 0
Transitions between intermediate excited states
Charge transfer

Fe+H data


Final State
Transitions between intermediate excited states
Charge transfer
log(<σv>) > −8
log(<σv>) > −9
log(<σv>) > −10
log(<σv>) > −11
log(<σv>) > −12
log(<σv>) > −13
<σv> > 0
<σv> = 0

Error estimates -> “Fluctuations”



Quantum mechanical processes are important in going from ~20% to ~1%

Together with collaborators have shown the importance of quantum mechanical processes such as:

- charge transfer via tunnelling
- spin transfer via exchange interaction

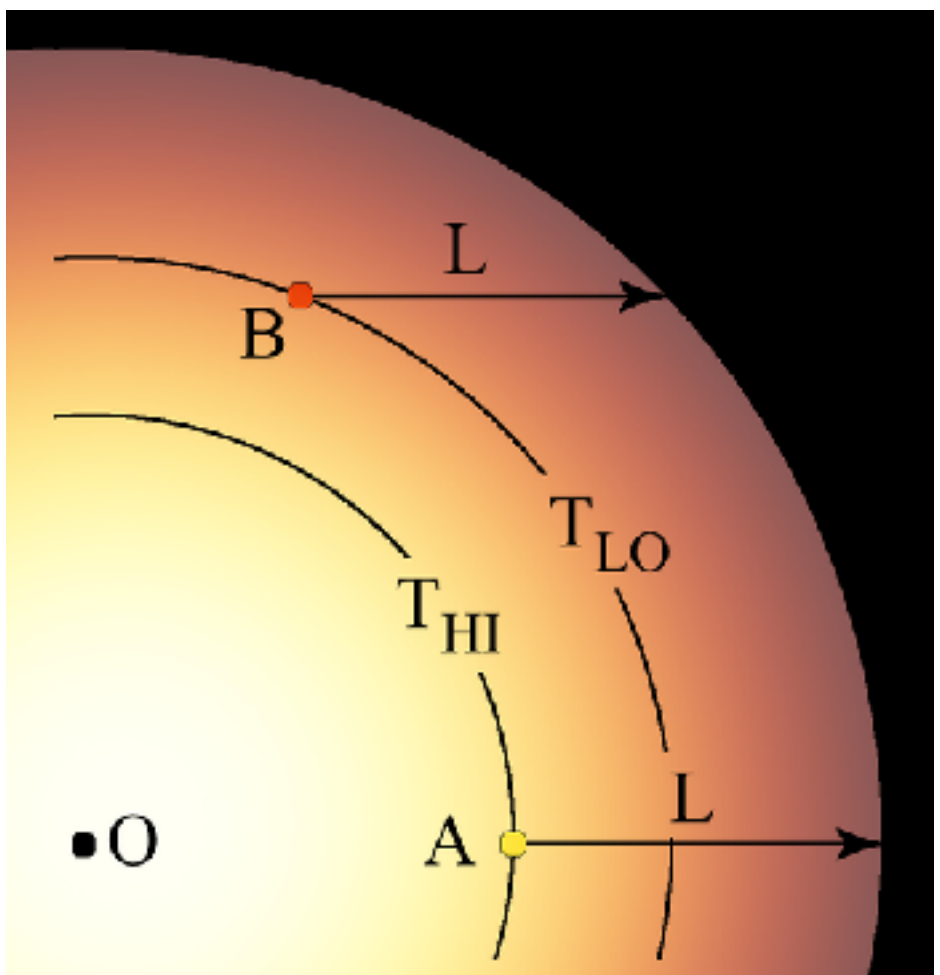
in the accurate interpretation of stellar spectra.

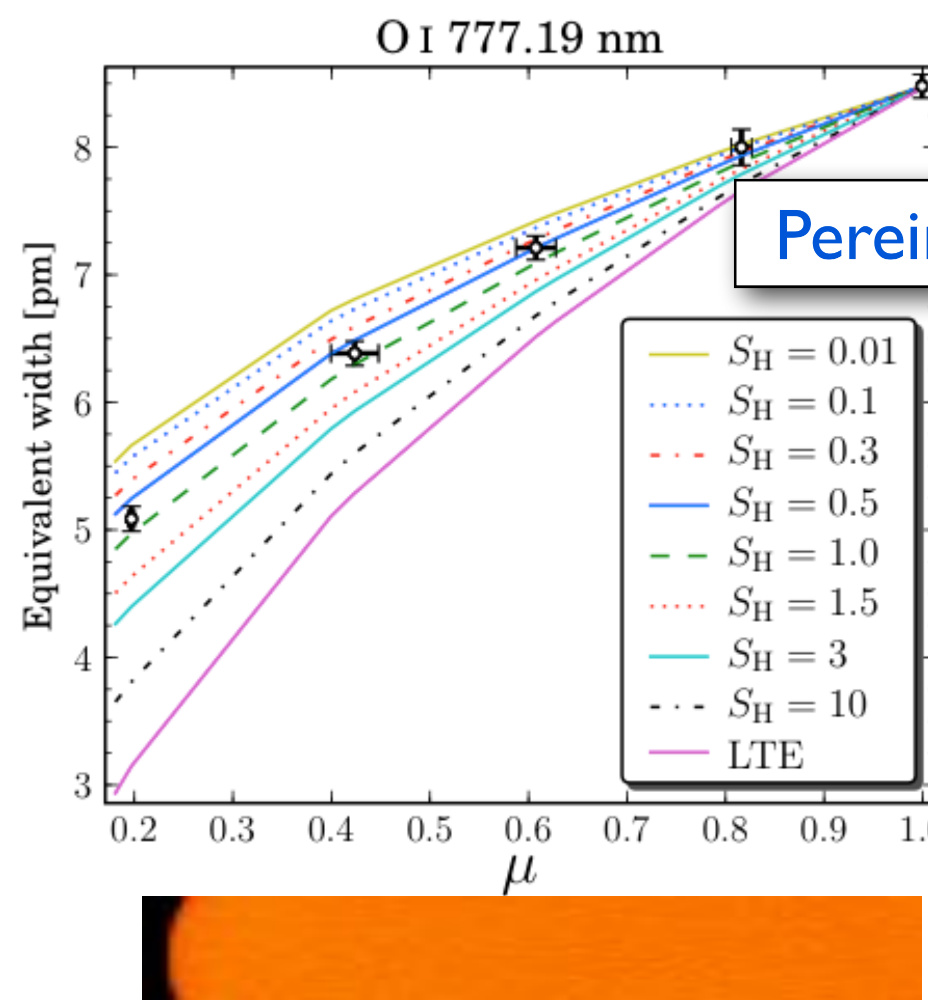
And developed methods to do such calculations at the levels of accuracy and completeness needed for astrophysics (?).

Testing via astrophysics: comparing models with observations

- Standard stars - but still limited by f-values, and other factors

- SST - centre to limb variation of spectral lines





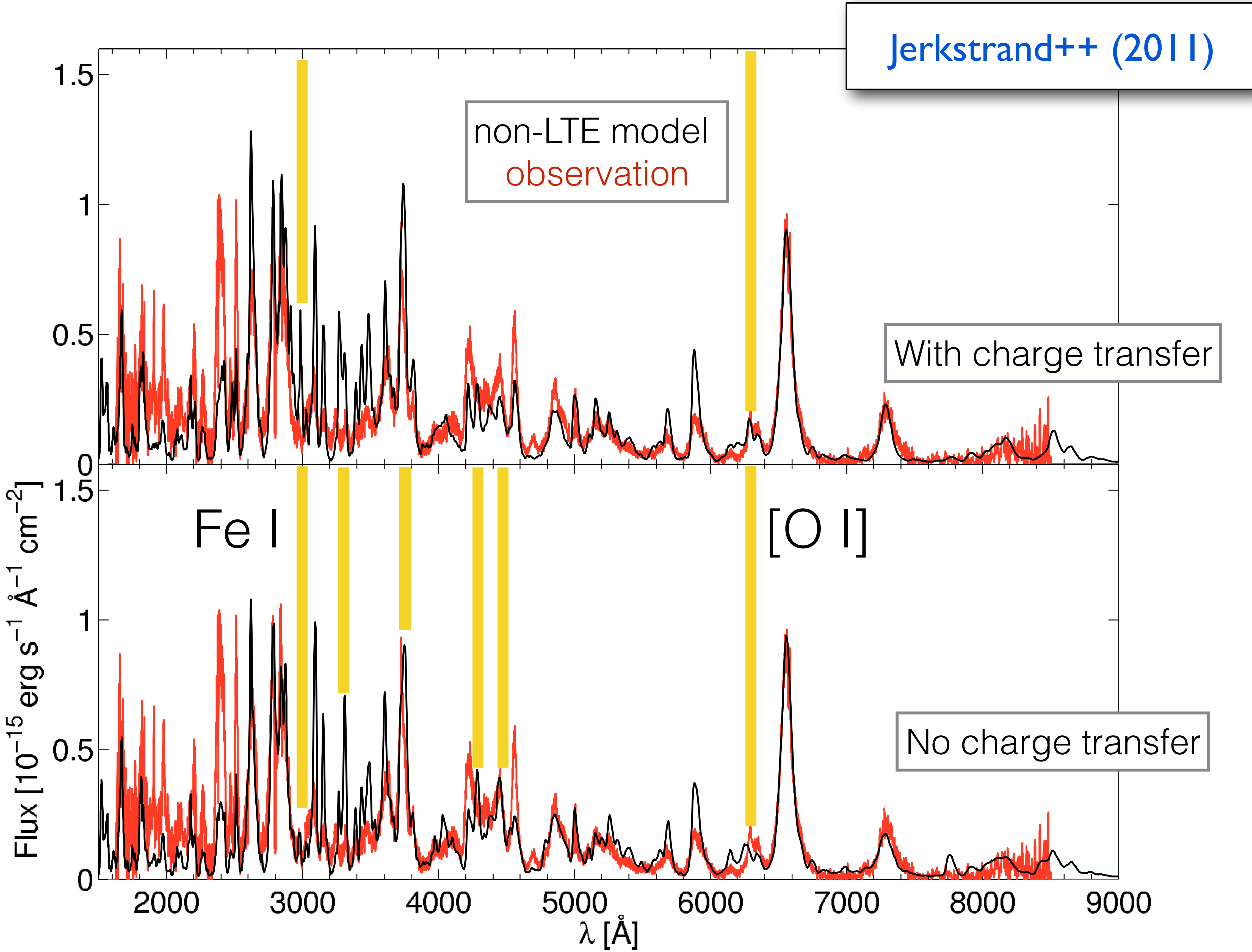
Pereira++(2009)

Testing via experiment: probing electron transfer reactions at the atomic level

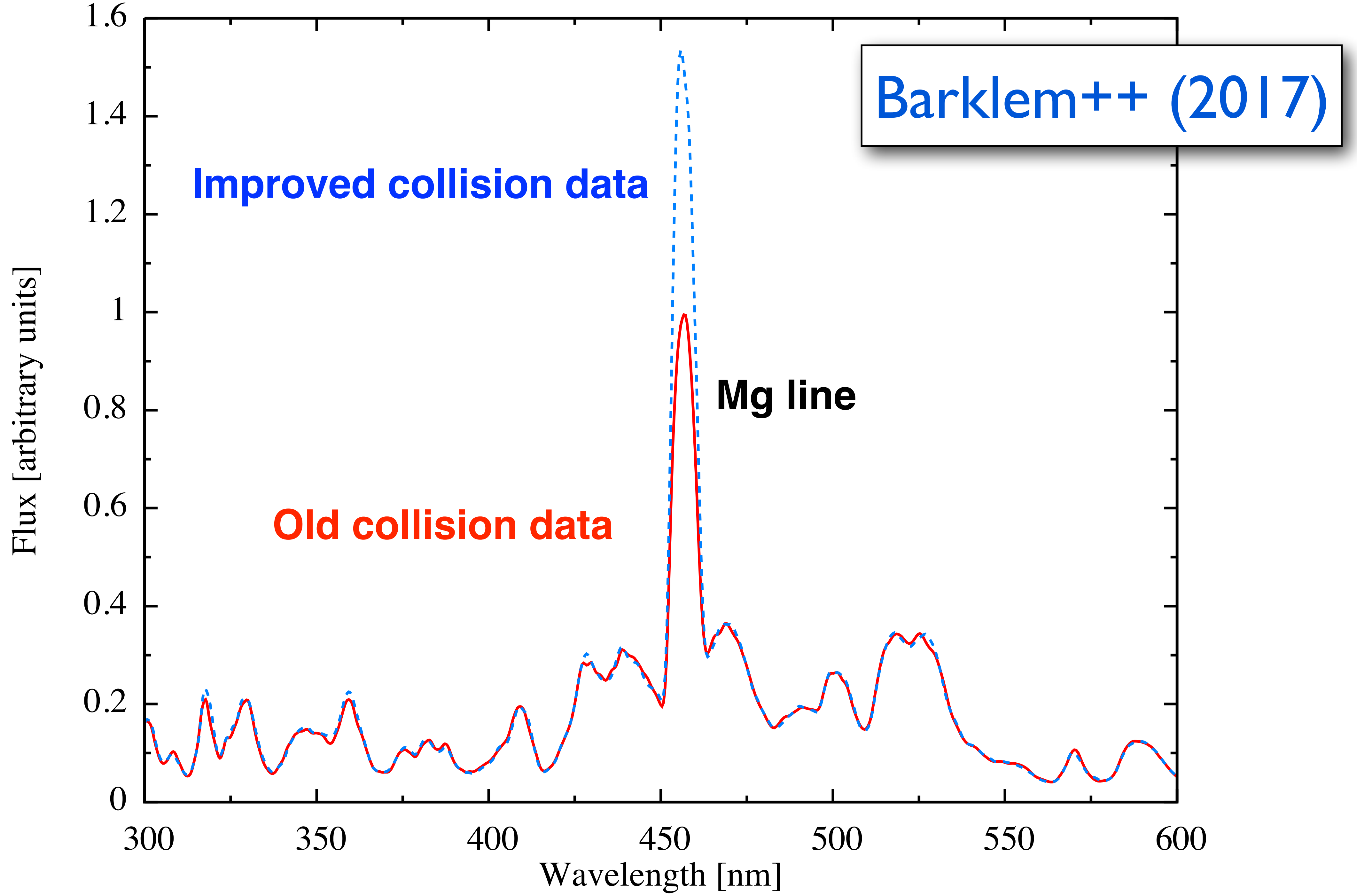
- low-energy
- quantum-state resolved

Double ElectroStatic Ion Ring ExpEriment (DESIREE) in Stockholm

Beyond stars: Supernova ejecta have similar conditions



Beyond stars: Supernova ejecta have similar conditions



Changes inferred amount of Mg produced by supernova by 50%

Beyond stars: *Kilonova* ejecta also have similar conditions

Kasen++ (2017)

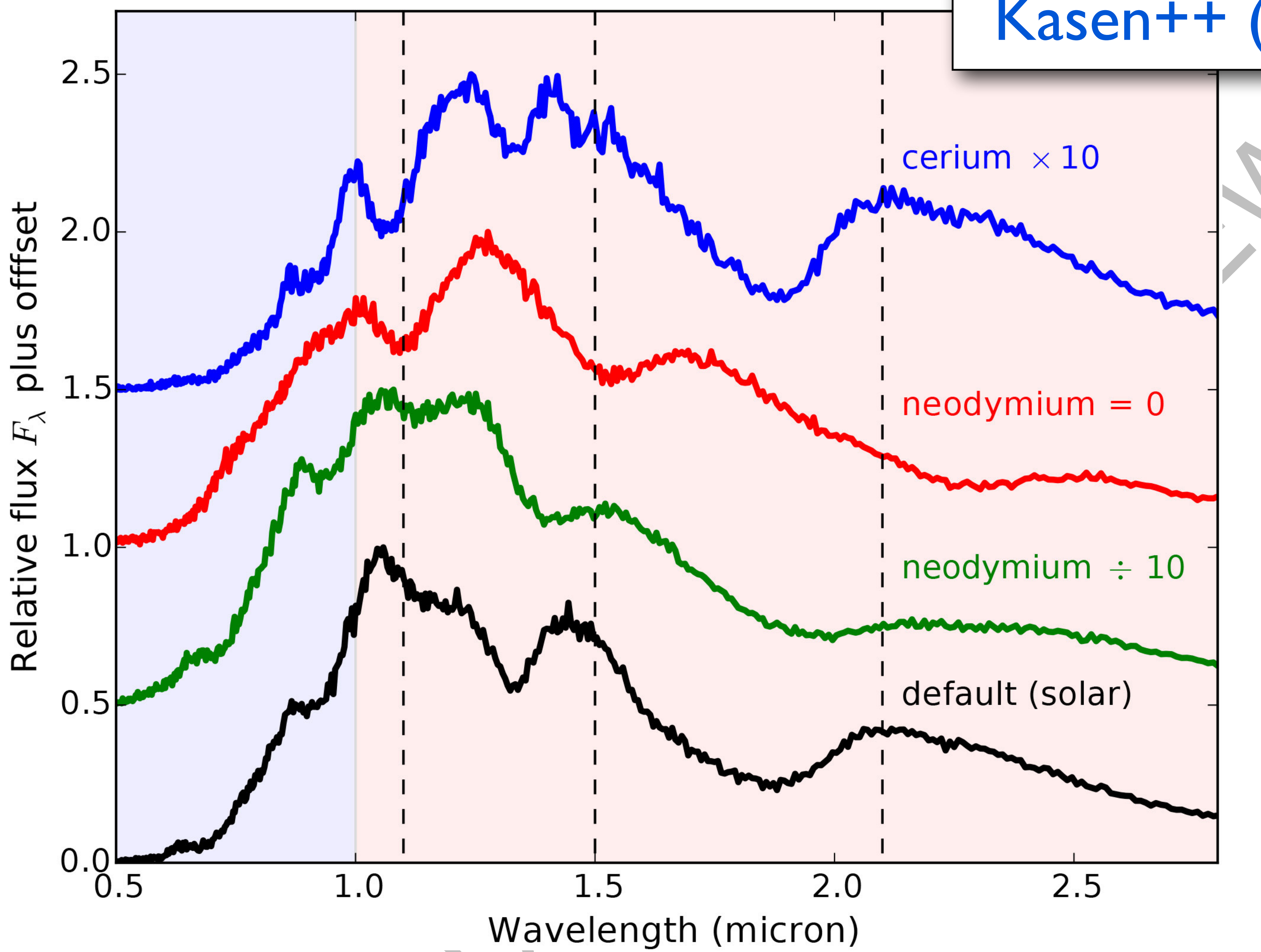


Figure 4 | Models demonstrating how kilonova spectral features probe the abundance of individual r-process elements. The spectral peaks in the models are due to blends of many lines, primarily those of the complex lanthanides species. The default model shown (parameters $M = 0.04 M_{\odot}$, $v_k = 0.15c$, $X_{lan} = 10^{-1.5}$) uses a solar distribution of lanthanides, and has spectral peaks near 1.1 µm, 1.5 µm and 2.0 µm (marked with dashed lines). These features are mainly attributable to neodymium ($Z = 60$) given that reducing or removing this species changes the feature locations. However, other lanthanides such as cerium ($Z = 58$) also affect the blended peaks. Uncertainties in the current atomic line data sources limit hinder spectral analysis, but with improved atomic inputs a more detailed compositional breakdown is within reach.

Concluding remarks

- To get the most out of current and future surveys (e.g. 4MOST) a lot can be gained by small increases in accuracy
- Quantum effects such as electron tunnelling and spin exchange are important in going to high accuracy abundances
- Providing error estimates (“fluctuations”) is important
- Many similarities in data needed for supernova and kilonova ejecta modelling to stellar atmospheres
- Combination of theory, experiment and observation crucial to progress

Future?

"Opacity/Iron project"

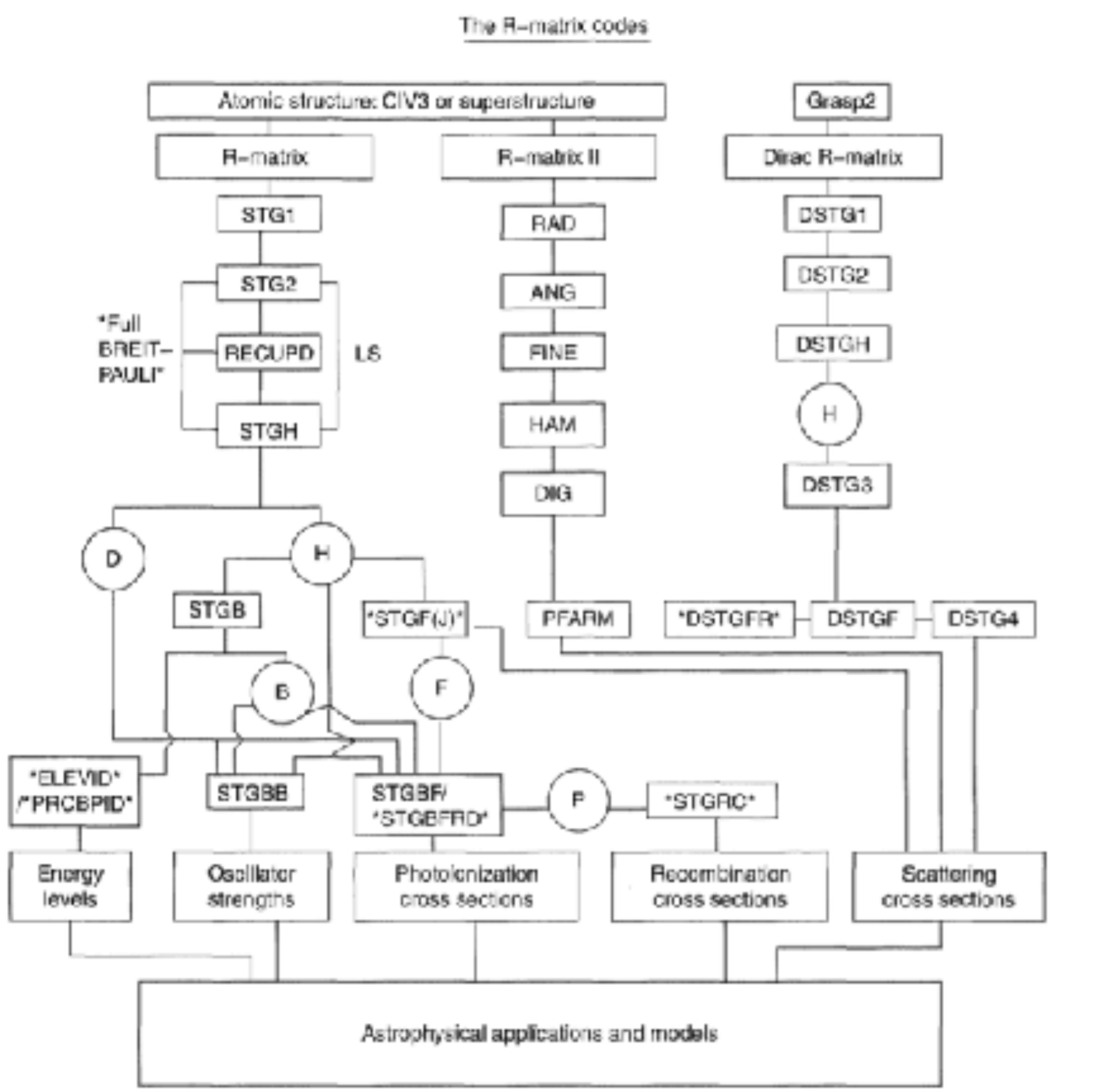
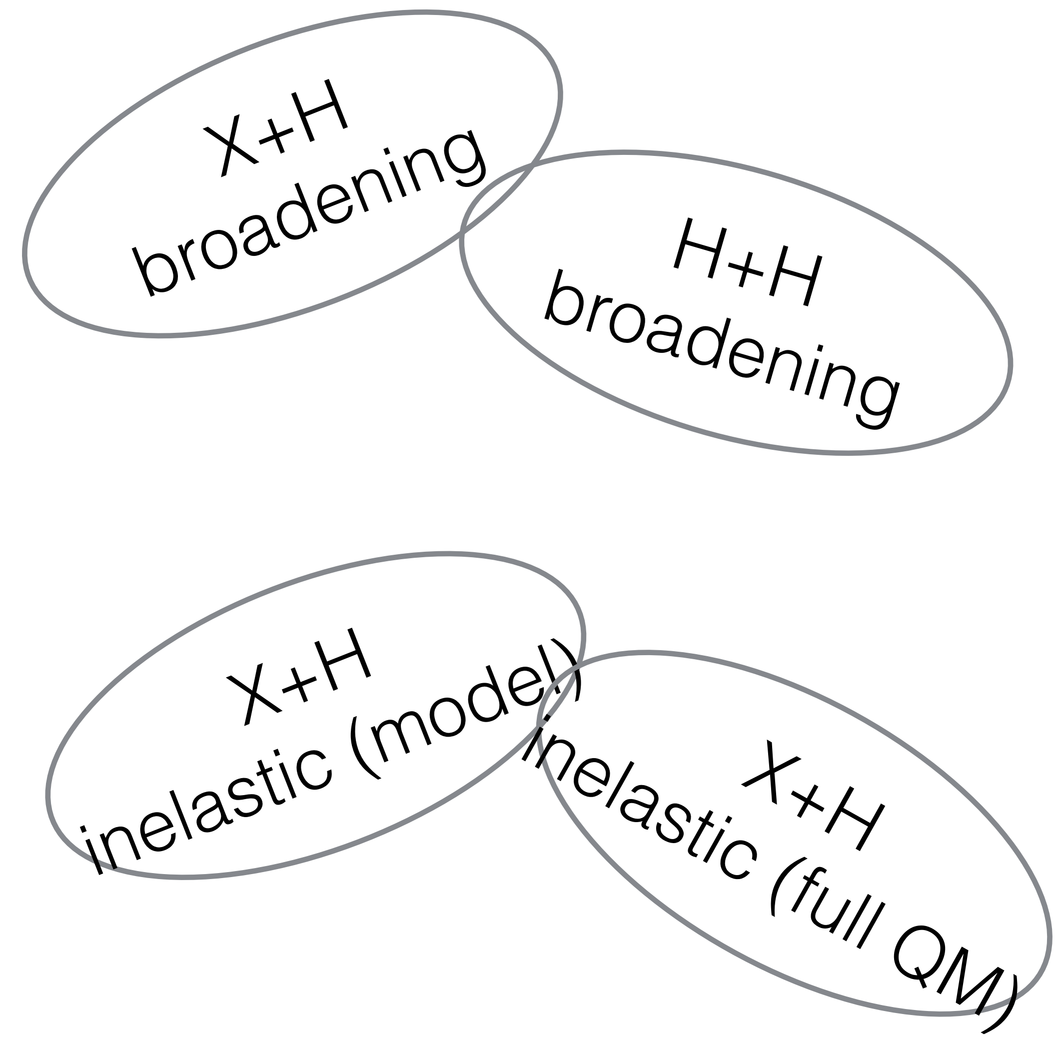


FIGURE 3.9 The three main branches represent different versions of the R-matrix package of close-coupling codes as described in the text.

"???? project"



And extend to other heavy particles…

Thank you!