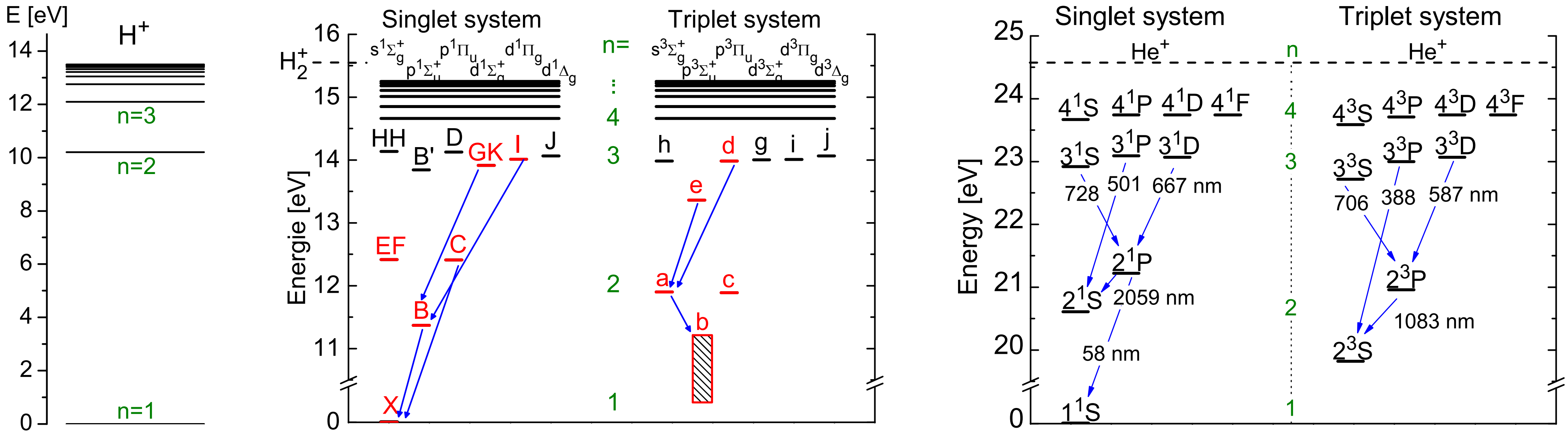
Application and Evaluation of Data in Population Models for

H H_2 and He

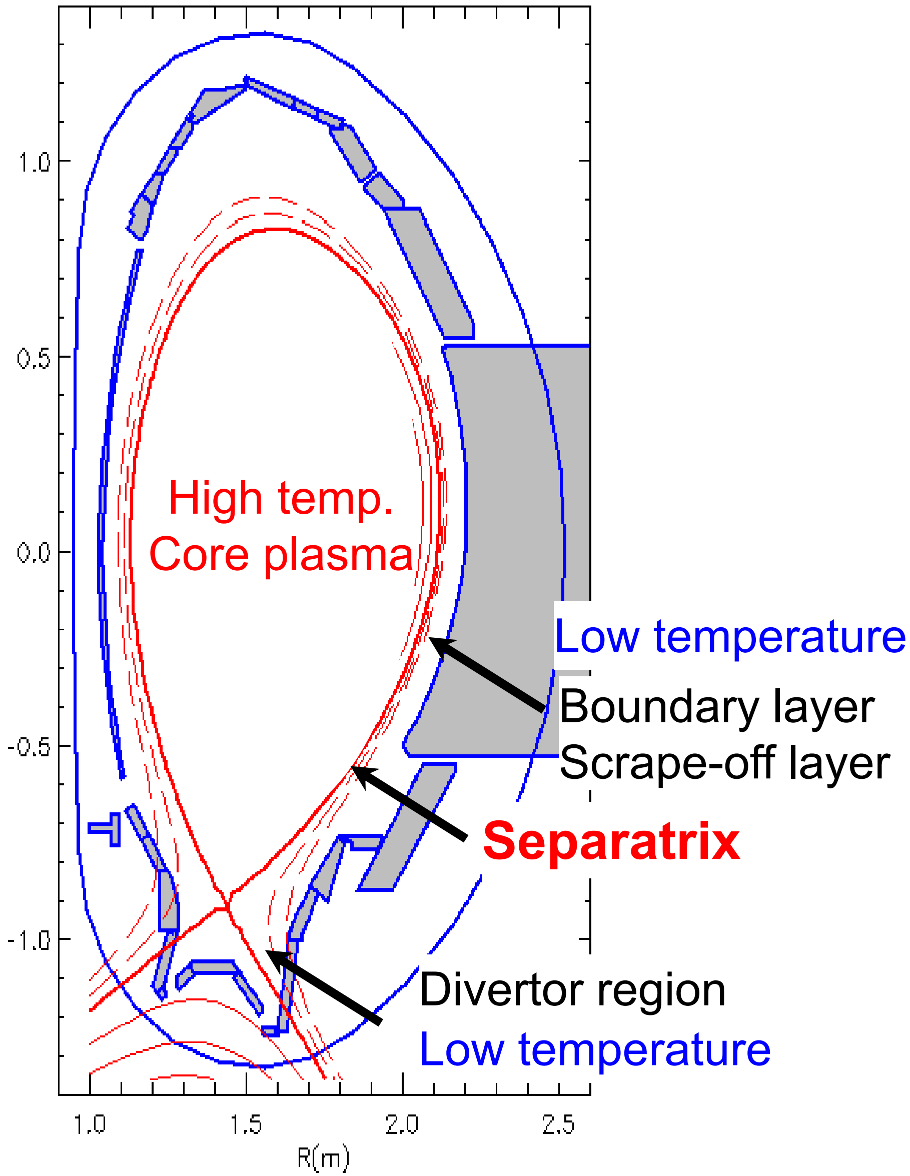


Ursel Fantz and Dirk Wünderlich

CRP on

"Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma"

Cold plasma edge: SOL, limiter and divertor plasmas



- **operate in different recycling regimes**

wide parameter range

$T_e \approx 50$ eV ⟶ few eV ⟶ below 1 eV

$n_e \approx 10^{18} - 10^{21}$ m^{-3}

ionising plasma ⟶ recombining plasma

- **are similar to laboratory plasmas**
  low temperature, low pressure plasmas

- **require diagnostics and modelling**

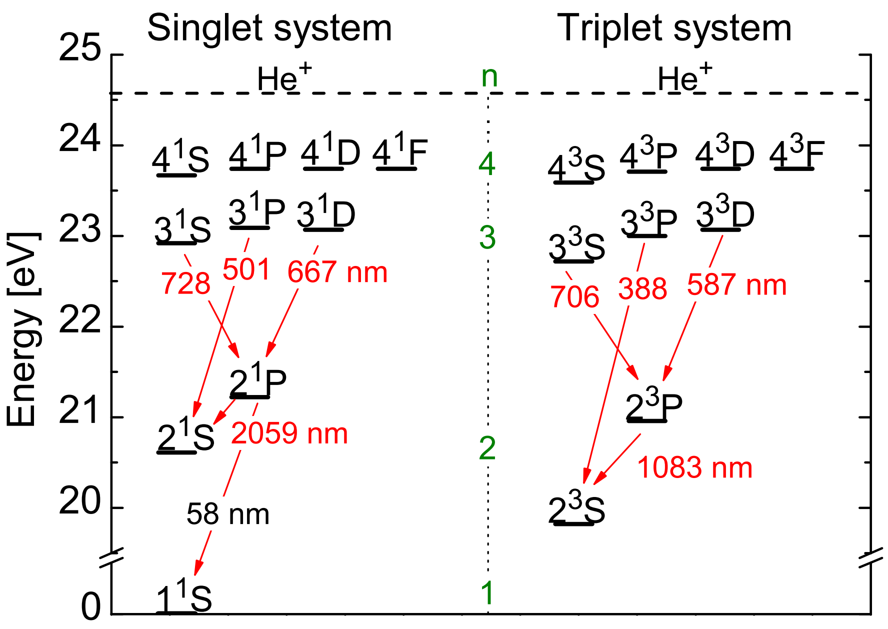
Population densities:
modelling and experiments

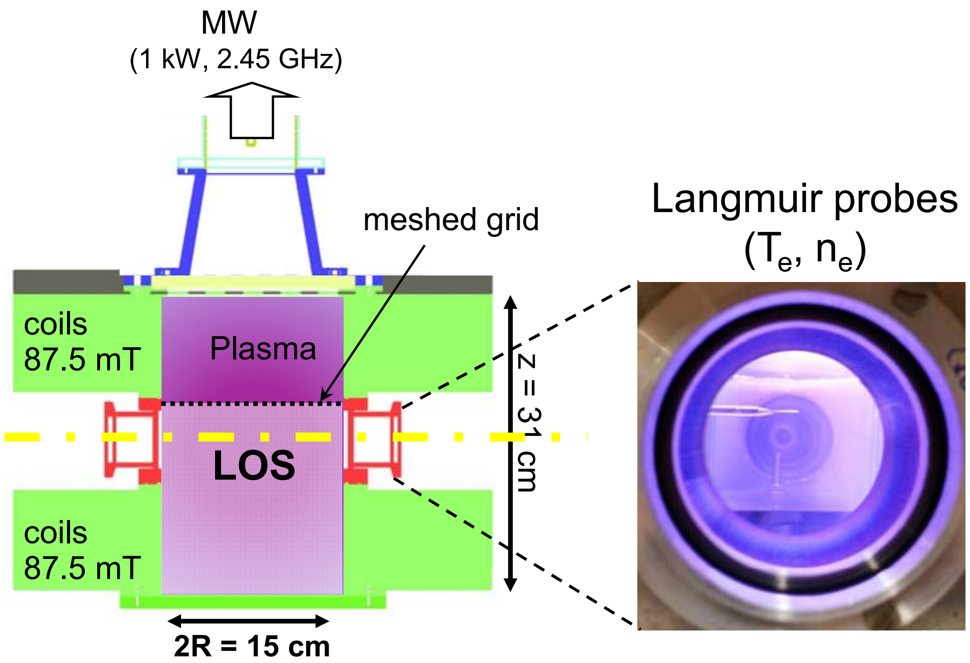
basis: atomic & molecular data

Population densities: modelling and experiments

Collisional radiative models → n(p) ↔ n(p) A_{pk} ← Experiments

= f (T_e, n_e, …)





Flexible code Yacora ↔ Spectroscopic diagnostics

Flexible code Yacora

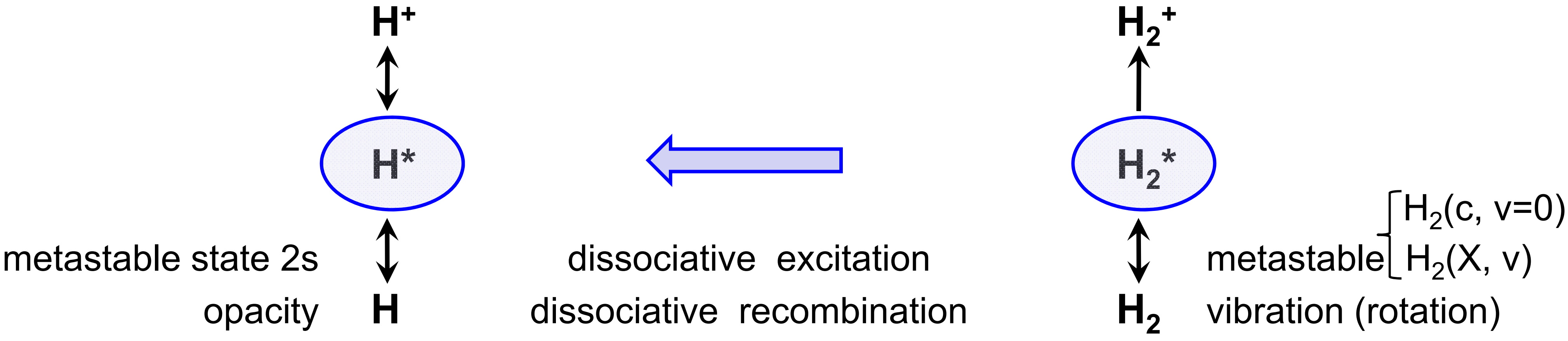
- simple change of input data
- based on cross sections (EEDF)
- easy to extend for new processes
- electron collisions & heavy particle collisions & radiation (opacity)

Spectroscopic diagnostics

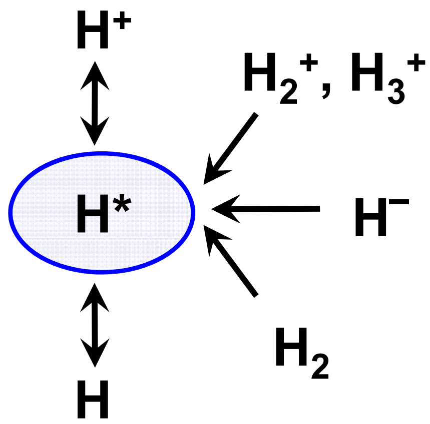
- line of sight (LOS) averaged
- emission spectroscopy
- absorption spectroscopy
- manifold of levels accessible (vibrational & rotationally resolved)

Check data & identify relevance of individual processes

CR model for atomic and molecular hydrogen



Extended CR model for atomic hydrogen



Molecules

- manifold of levels and transitions
  - electronic
  - vibrational and
  - rotational levels
- isotope effects

Data base ?

Vibrational resolution in ground state and electronically excited states

- n=2 and n=3 electronically resolved
- n=2 and selected states in n=3 vibrationally resolved
- rotational resolution neglected

Based on data from

Sawada: K. Sawada and T. Fujimoto, J. Appl. Phys. 78 (1995) 291

Janev: R. Janev, D. Reiter, U. Samm, Juel-Report 4105 (2003)

Miles: W. Miles, R. Thompson , A. Green, J. Appl. Phys. 43 (1972) 678

Extension of data base

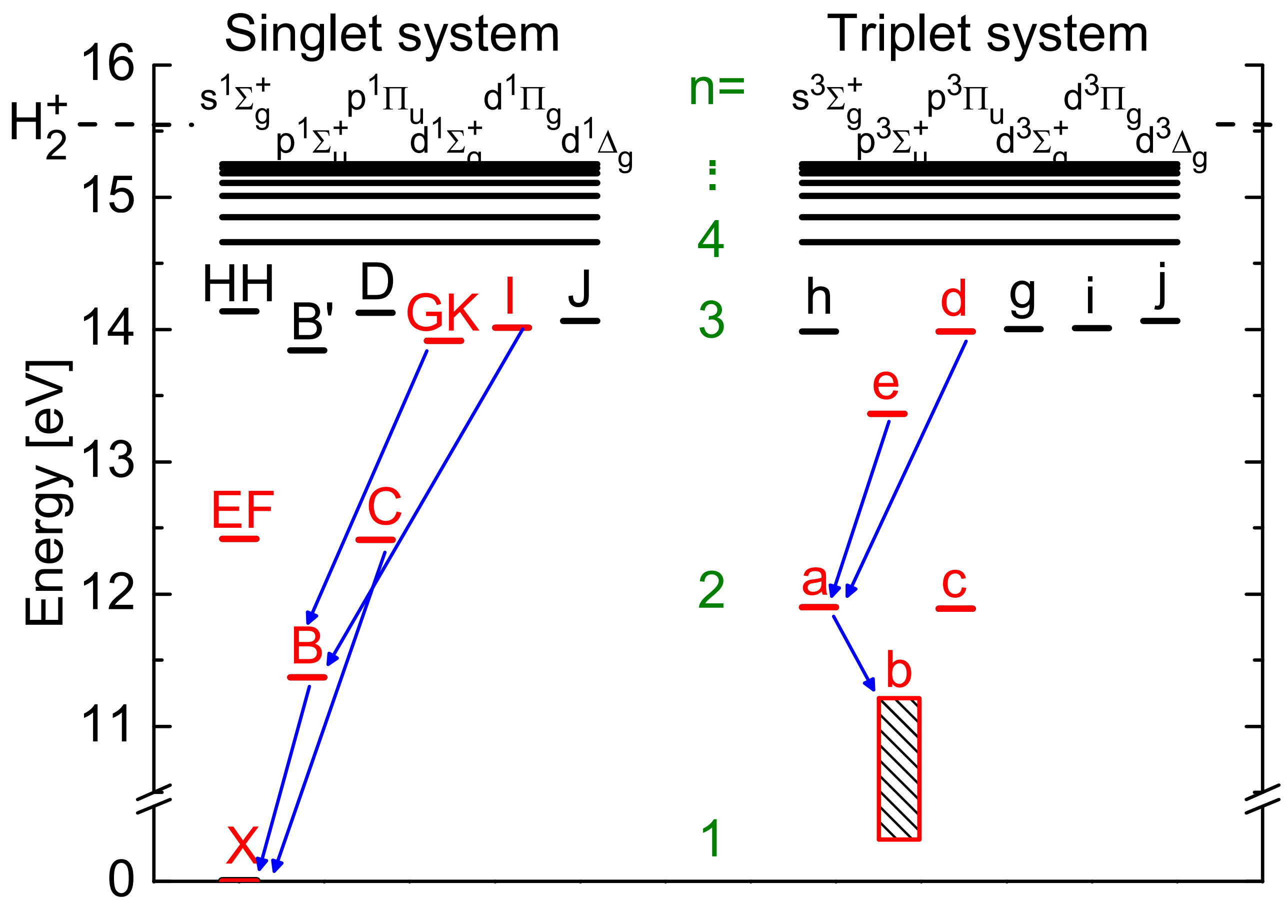
- Gryzinski method

$$\sigma_{vv'}^{pp'} = q_{v'v}^{p'p} \cdot F(E_e)$$

- Impact parameter method

$$\sigma_{vv'}^{pp'} = S(A_{v'v}^{p'p}) \cdot D(E_e)$$

- predissociation, autoionisation, quenching, ….



214 (elec. & vib.) levels; 21645 reactions

Vibrational resolution in ground state and electronically excited states

- n=2 and n=3 electronically resolved
- n=2 and selected states in n=3 vibrationally resolved
- rotational resolution neglected

Based on data from

Sawada: K. Sawada and T. Fujimoto
J. Appl. Phys. 78 (1995) 291

Janev: R. Janev, D. Reiter, U. Samm
Juel-Report 4105 (2003)

Miles: W. Miles, R. Thompson , A. Green
J. Appl. Phys. 43 (1972) 678

Extension of data base

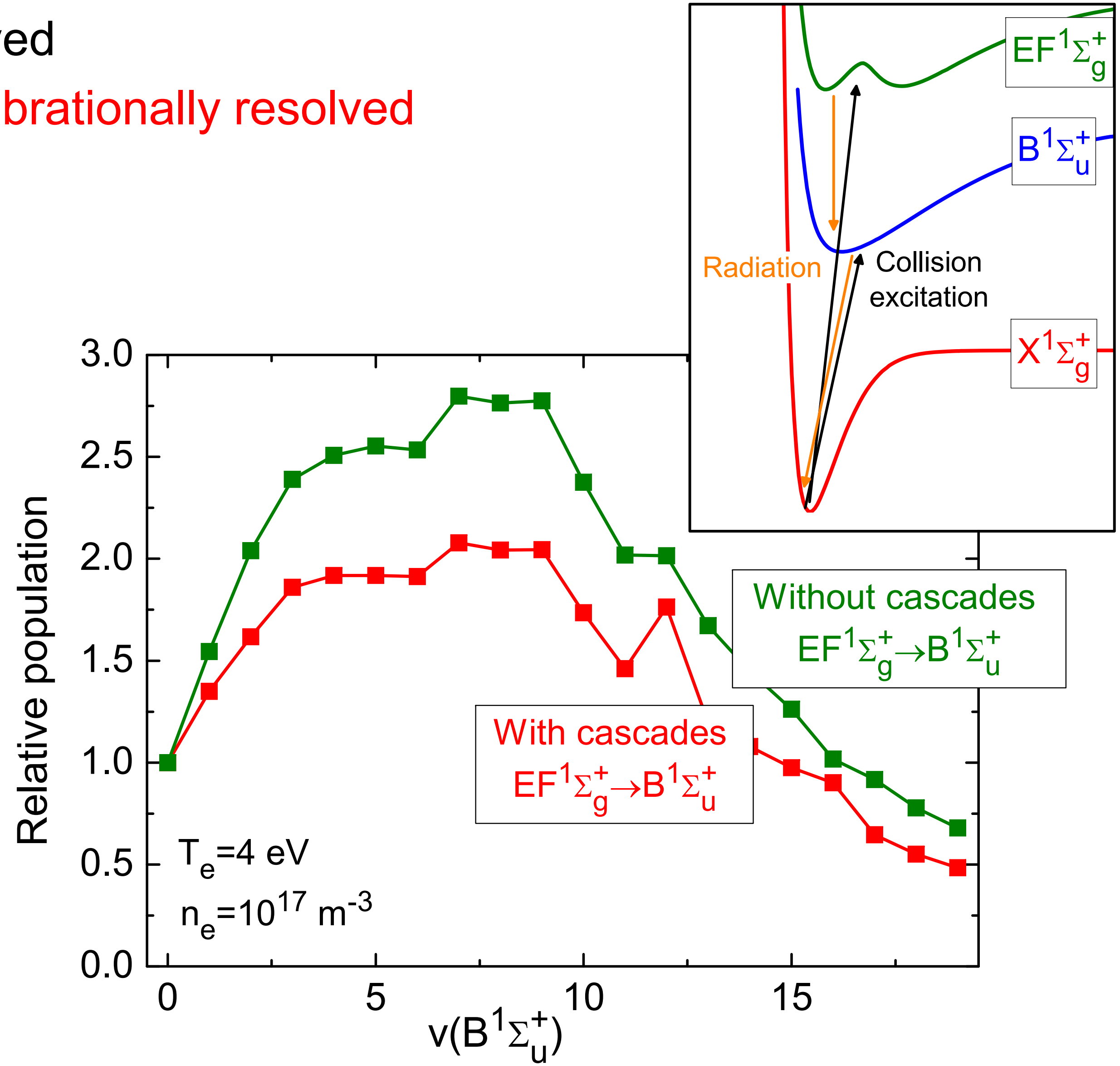
- Gryzinski method

$$\sigma_{vv'}^{pp'} = q_{v'v}^{p'p} \cdot F(E_e)$$

- Impact parameter method

$$\sigma_{vv'}^{pp'} = S(A_{v'v}^{p'p}) \cdot D(E_e)$$

- predissociation, autoionisation, quenching, ….



Vibrational distribution in excited state

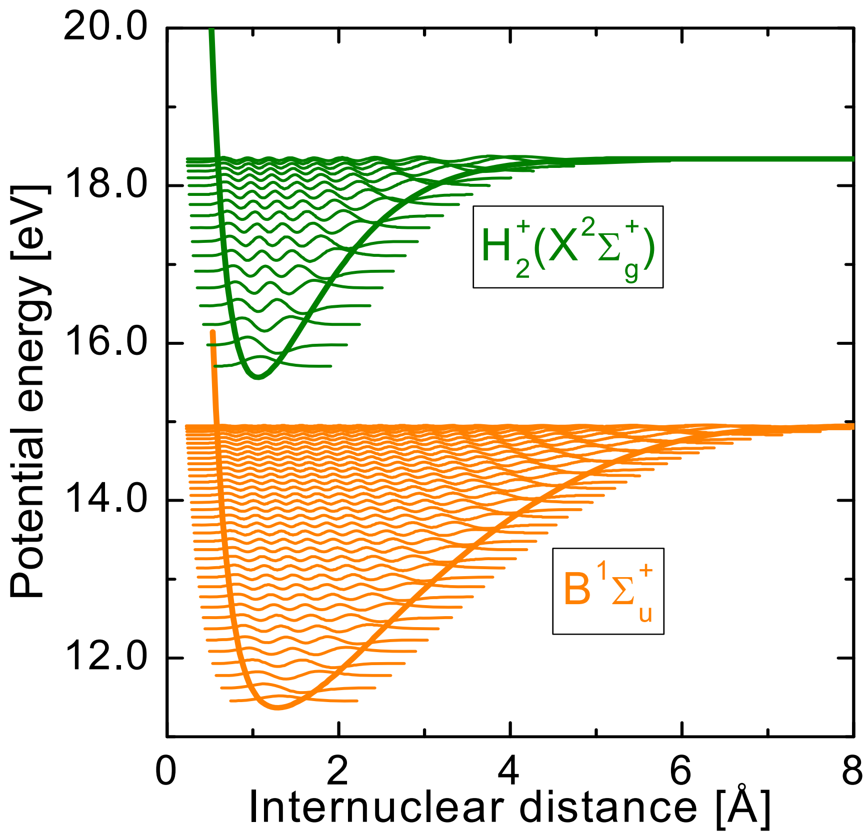
TraDiMo for Franck Condon factors and transition probabilities

U. Fantz and D. Wünderlich, ADNDT 92 (2006) 853

$H_2^*(v)$ - $H_2^+(v)$ transitions: data up to n=4

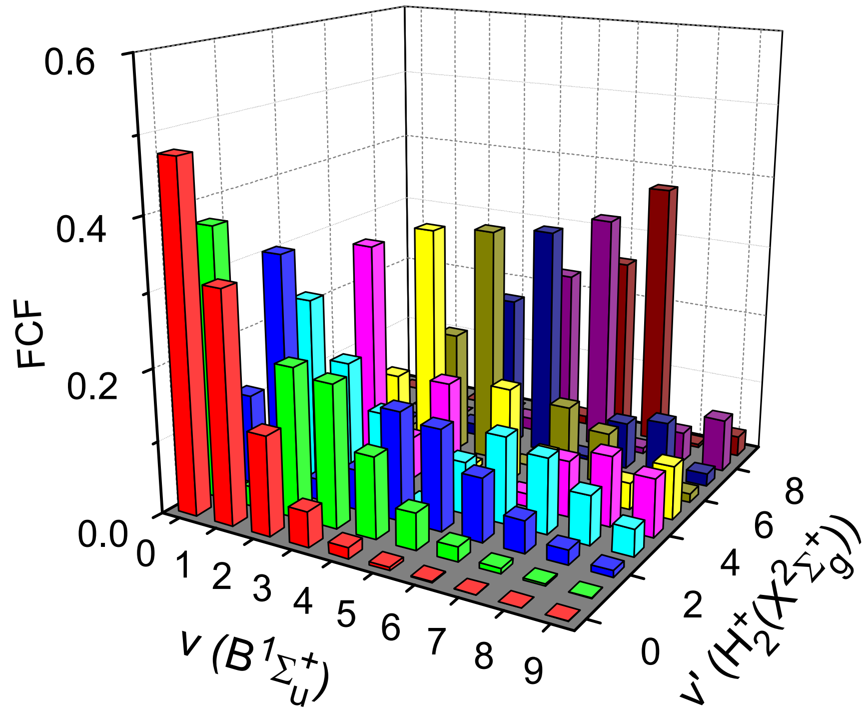
D. Wünderlich and U. Fantz, ADNDT 97 (2011) 152

Example: $B\ ^1\Sigma_u^+ \rightarrow H_2^+(X\ ^2\Sigma_g^+)$



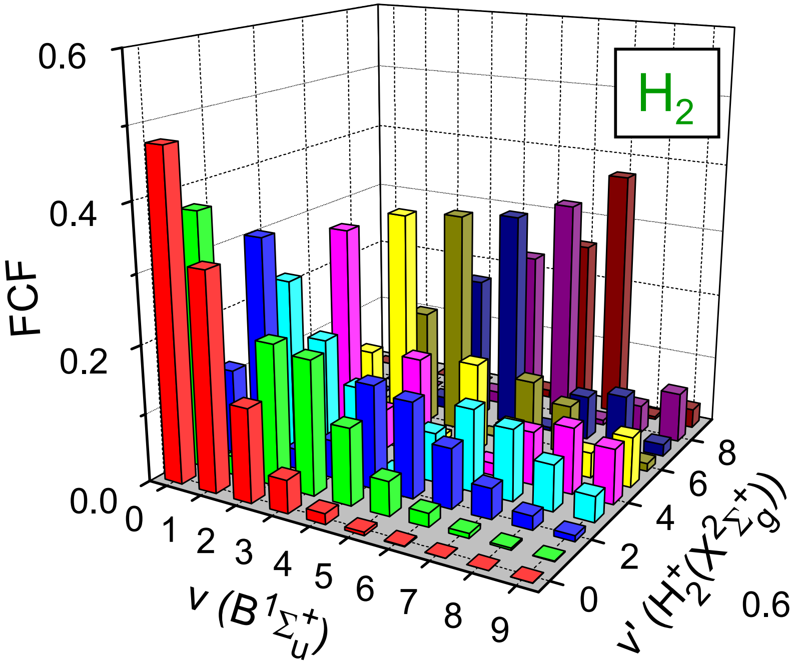
v →, v' ↓

q	0	1	2	3	4
0	4.76E-01	3.17E-01	1.36E-01	4.82E-02	1.54E-02
1	3.75E-01	2.73E-02	2.07E-01	1.96E-01	1.12E-01
2	1.26E-01	3.32E-01	2.93E-02	5.59E-02	1.51E-01
3	2.10E-02	2.53E-01	1.75E-01	1.15E-01	6.82E-04
4	1.56E-03	6.44E-02	3.22E-01	5.91E-02	1.49E-01
...					



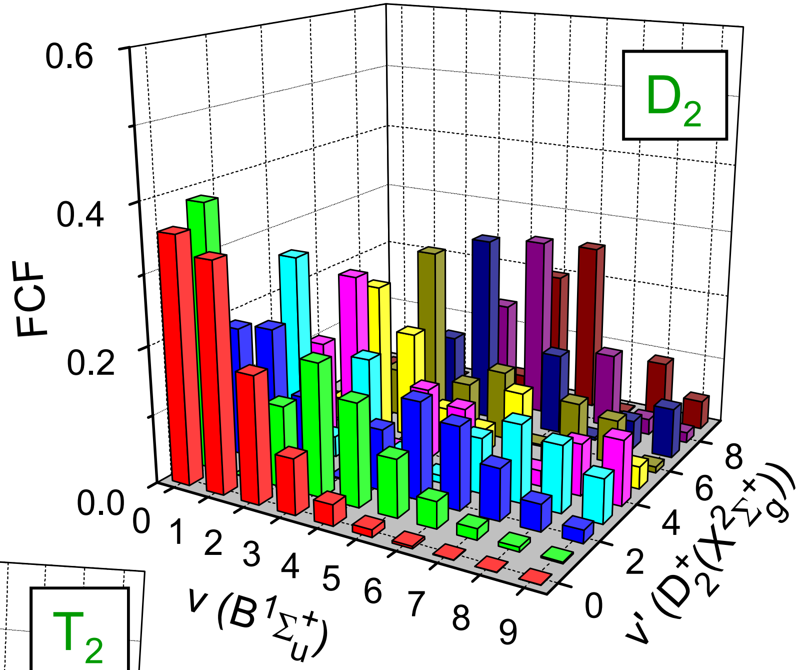
Yacora for molecular hydrogen

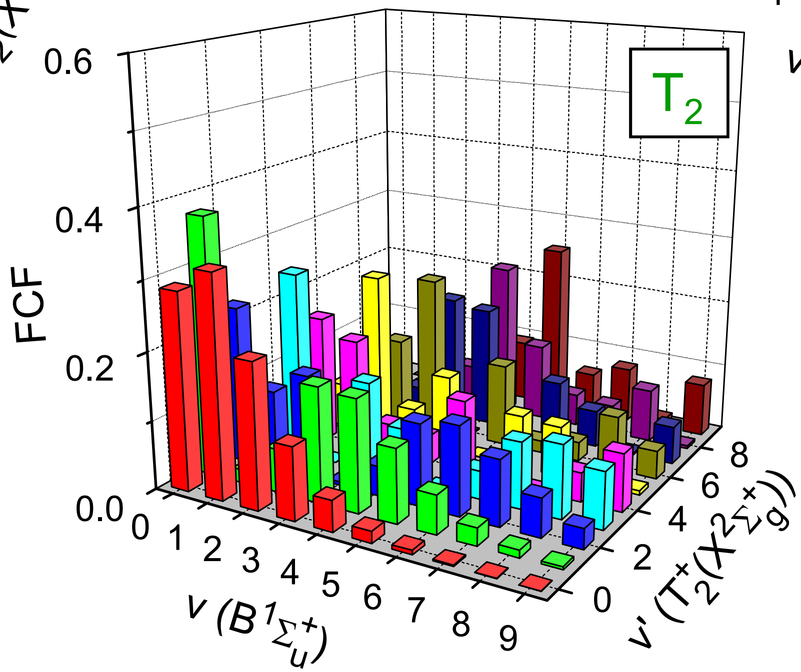
TraDiMo: $H_2^*(v)$ - $H_2^+(v)$ transitions: data up to n=4



$B\ ^1\Sigma_u^+ \rightarrow H_2^+(X\ ^2\Sigma_g^+)$

Isotope shifts



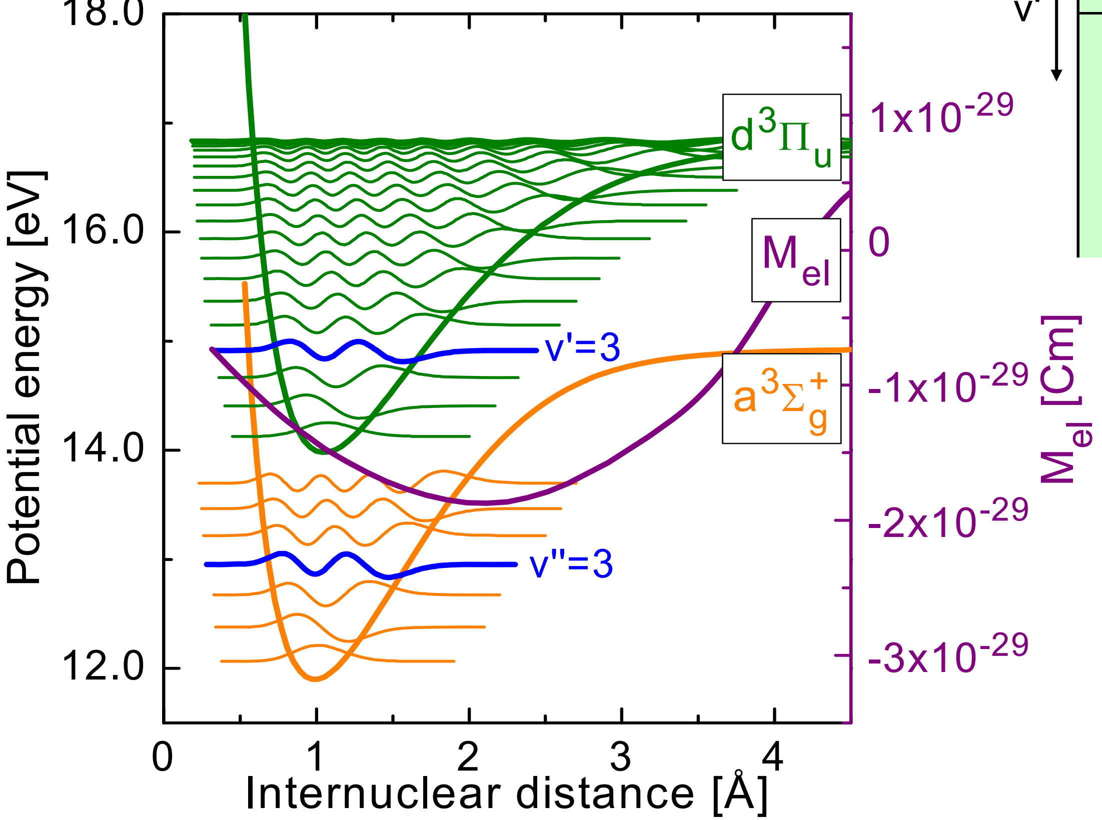


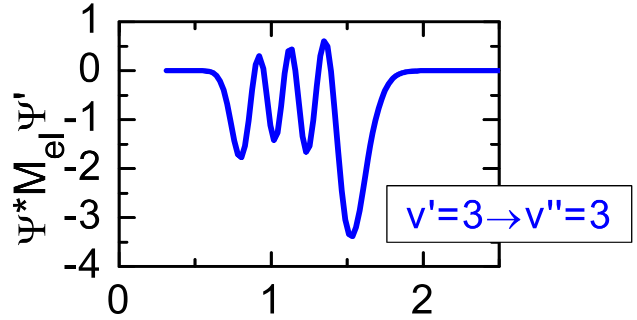
Yacora for molecular hydrogen

TraDiMo for Franck Condon factors and transition probabilities

$d\ ^3\Pi_u \rightarrow a\ ^3\Sigma_g^+$
Fulcher band

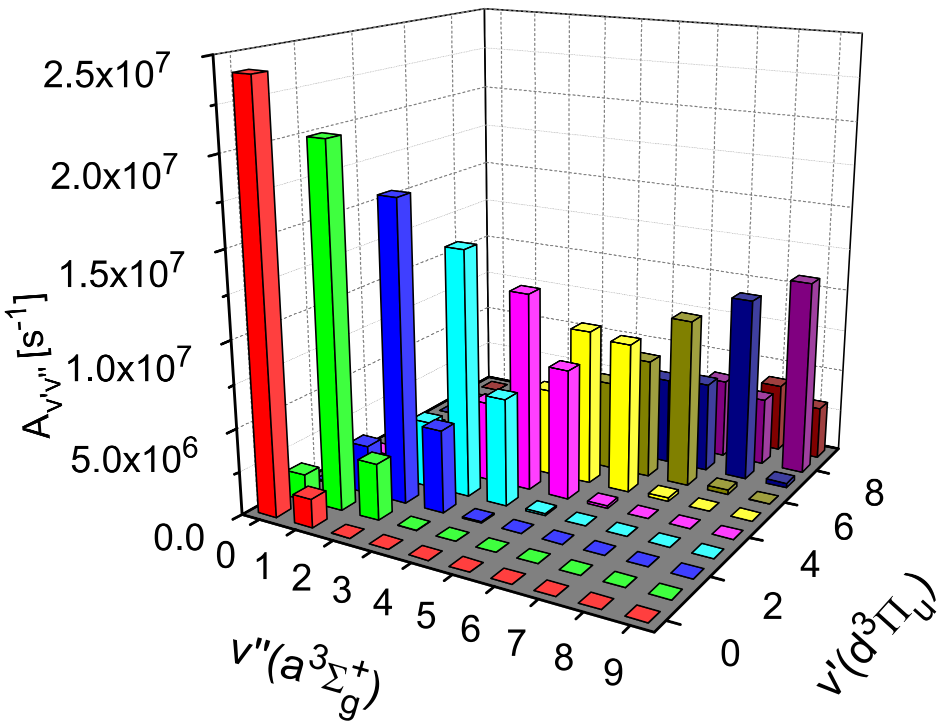
U. Fantz and D. Wünderlich, ADNDT 92 (2006) 853.





v'' →, v' ↓

q	0	1	2	3	4
0	2.41E+07	1.66E+06	9.27E+03	7.75E-02	5.62E-02
1	1.53E+06	2.07E+07	3.26E+06	2.97E+04	2.82E+00
2	1.07E+05	2.84E+06	1.74E+07	4.80E+06	6.23E+04
3	8.40E+03	3.19E+05	3.89E+06	1.43E+07	6.24E+06
4	5.87E+02	3.64E+04	6.22E+05	4.64E+06	1.15E+07
...					

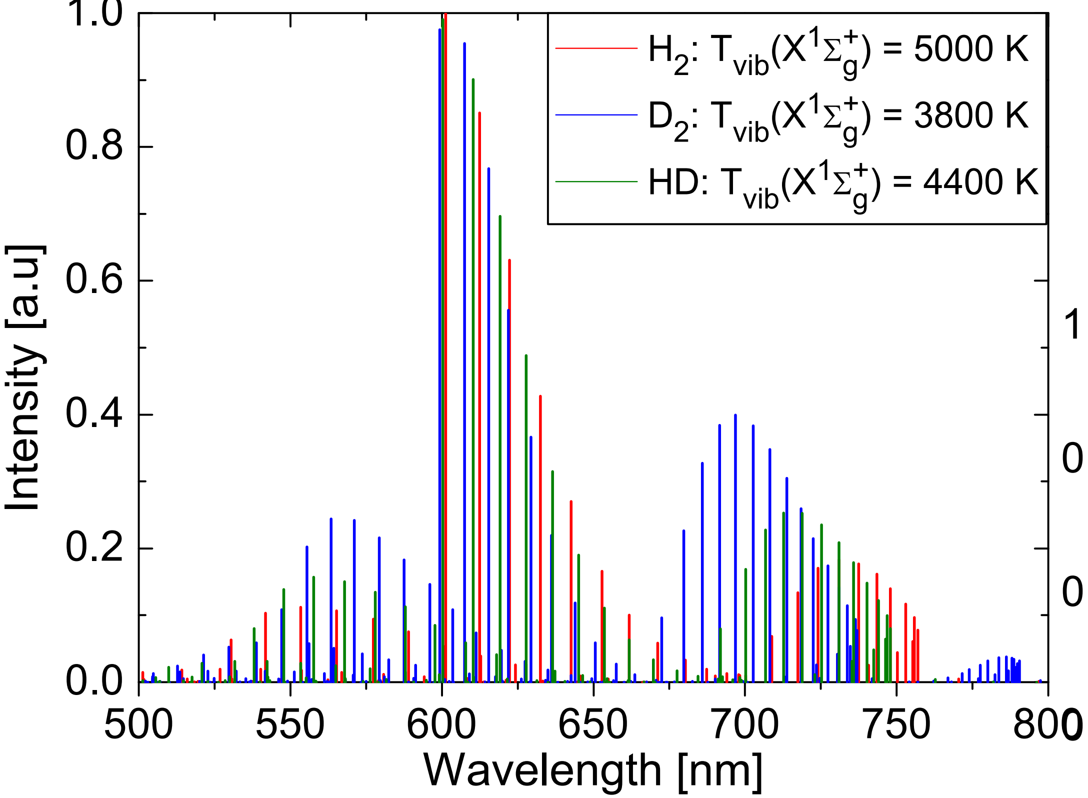


Franck Condon excitation $X\ ^1\Sigma_g, v \rightarrow d\ ^3\Pi_u, v'$ followed by spontaneous emission

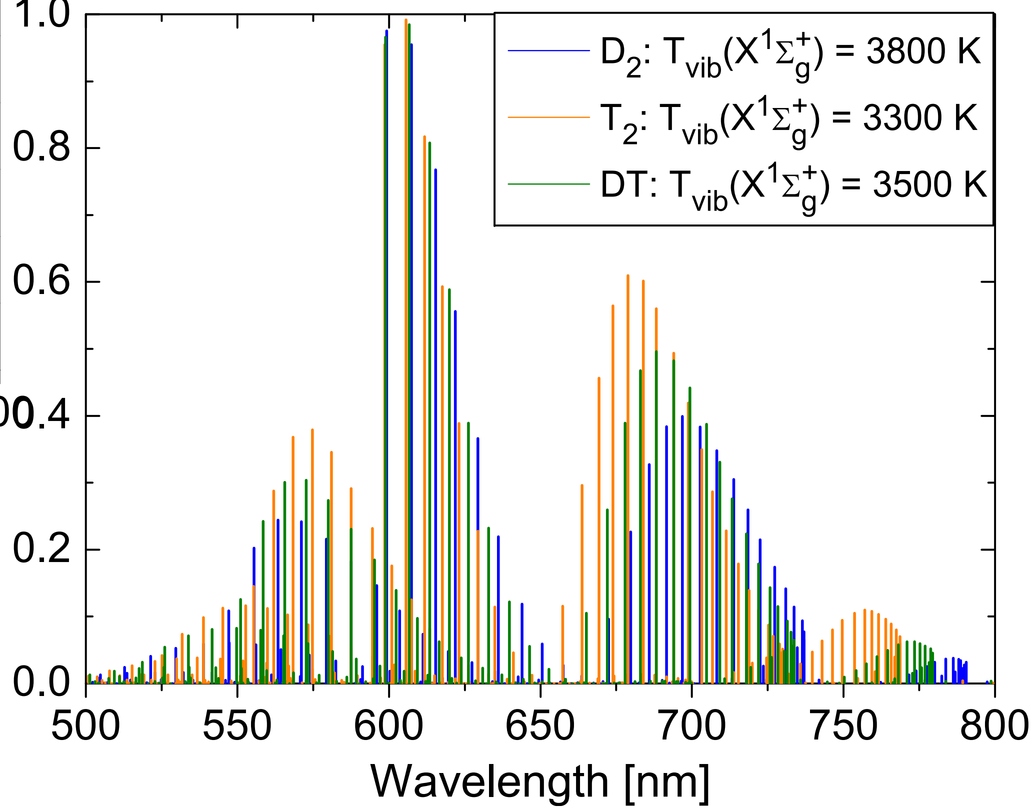
$d\ ^3\Pi_u, v' \rightarrow a\ ^3\Sigma_g^+, v''$

Fulcher band

H_2, D_2 and HD



D_2, T_2 and DT



assuming similar vibrational population in the ground state

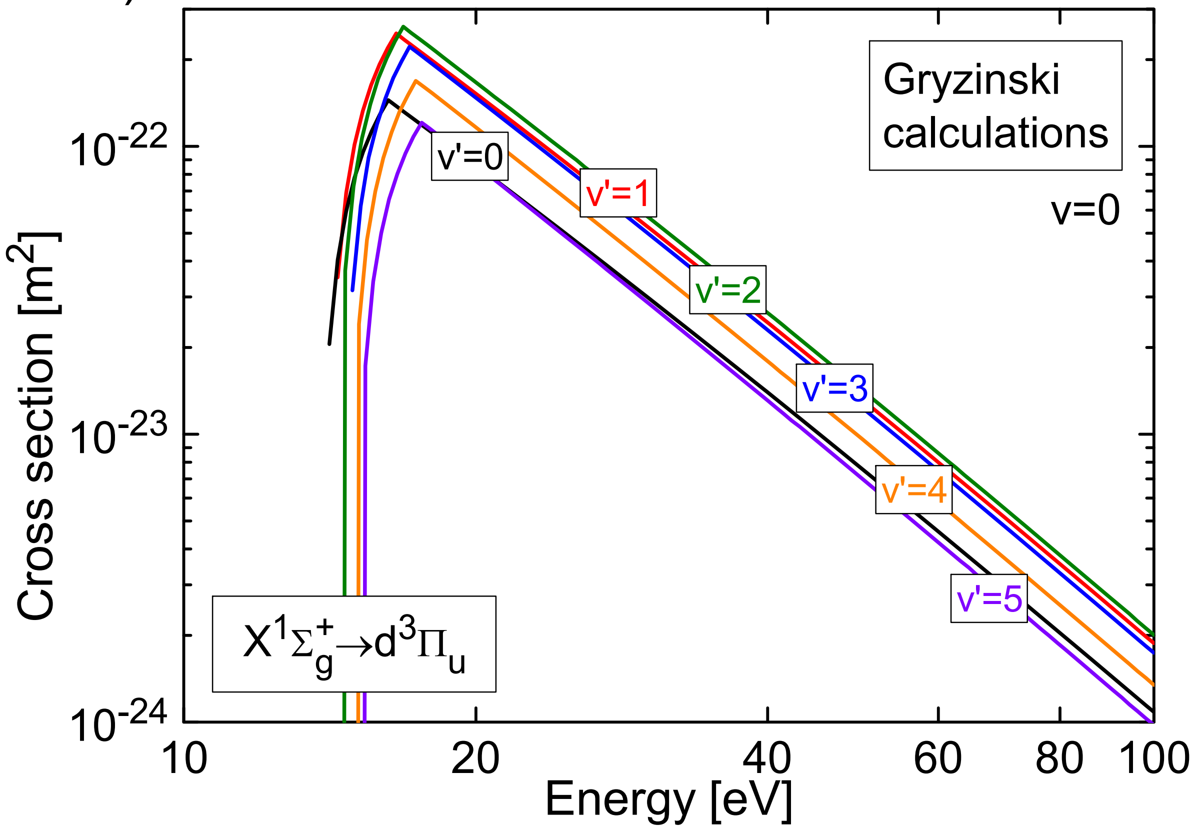
Gryzinski method for forbidden transition

M. Gryzinski, Phys. Rev. 138 (1965) A336
E. Bauer, C.D. Bartky, J. Chem. Phys. 43(1965) 2466

- classical method
- vibrational resolution by combination with Franck Condon theory
- in principle very simple method
- some obscurities, like definition of "next allowed level" (difficult in molecules)

Example: Fulcher band excitation

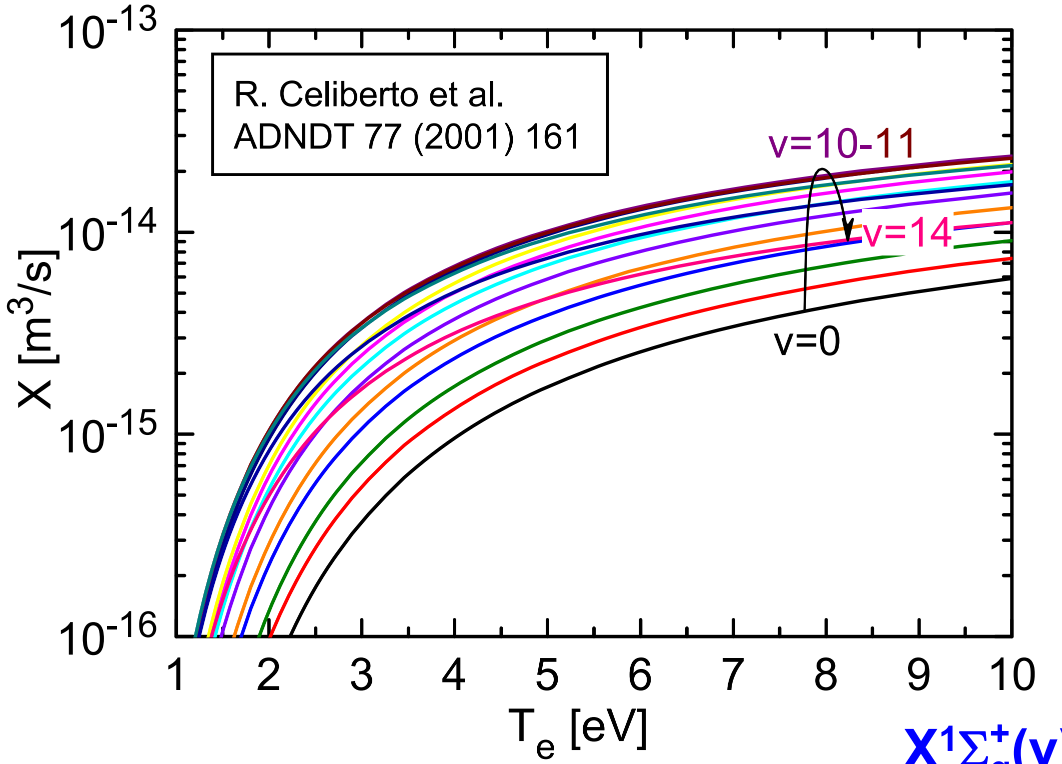
$X\ ^1\Sigma_g, v \rightarrow d\ ^3\Pi_u, v'$

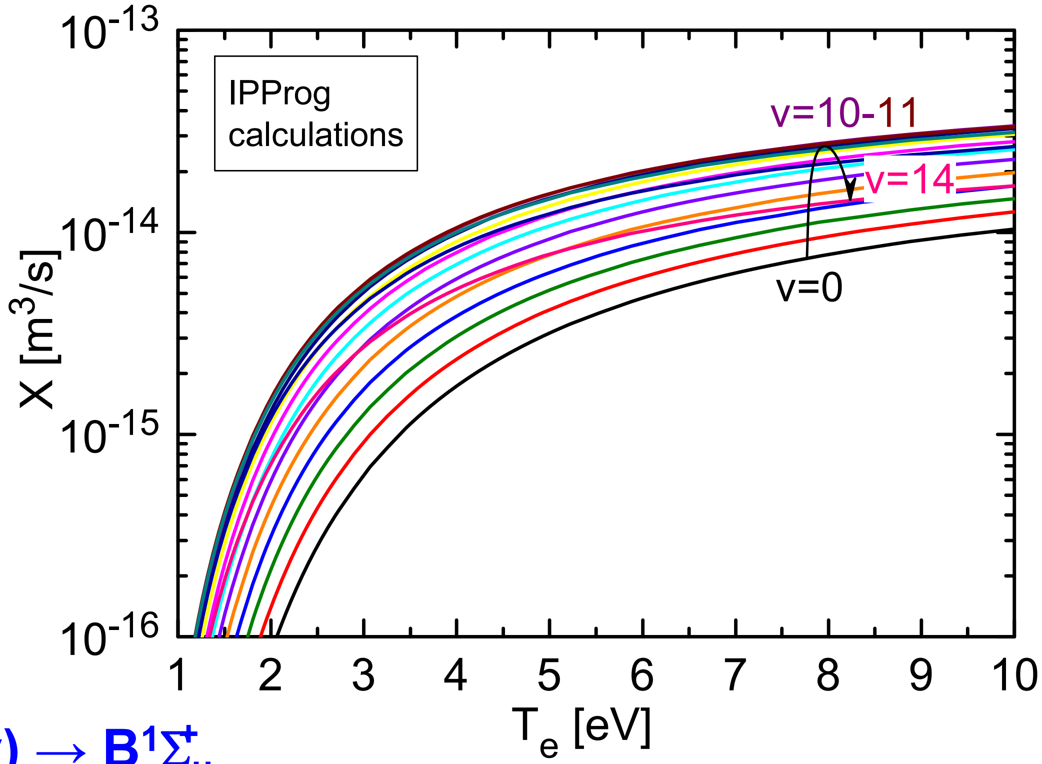


Yacora for molecular hydrogen

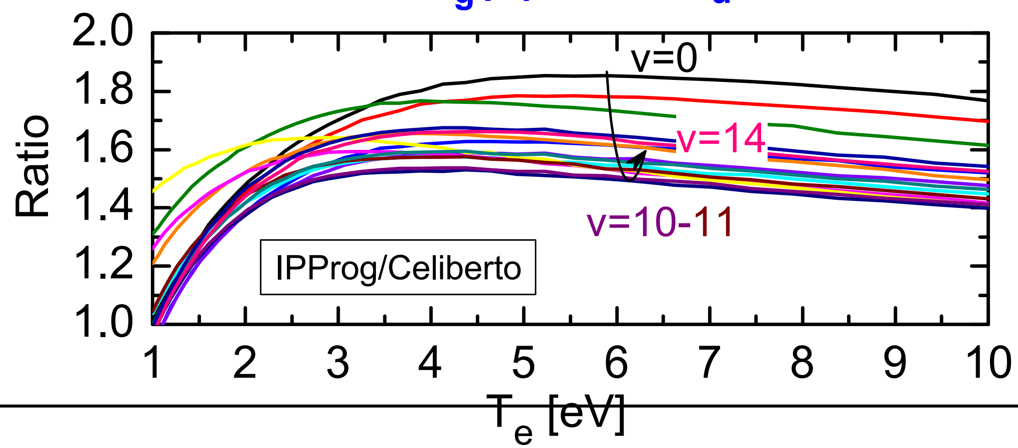
Impact parameter method (IPProg) for optically allowed transitions

A. Burgess, H. P. Summers, Mon. Not. R. Astr. Soc. 174 (1976) 345





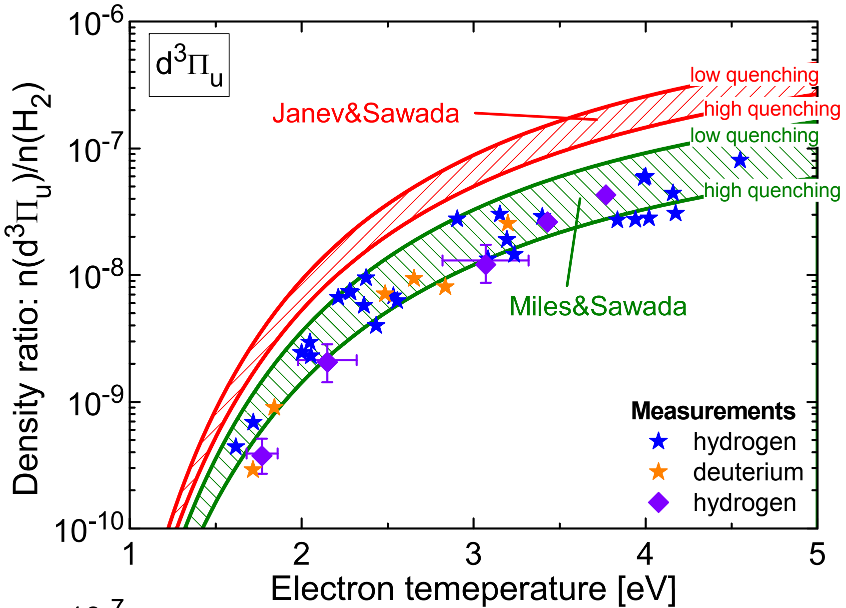
$X^1\Sigma_g^+(v) \rightarrow B^1\Sigma_u^+$

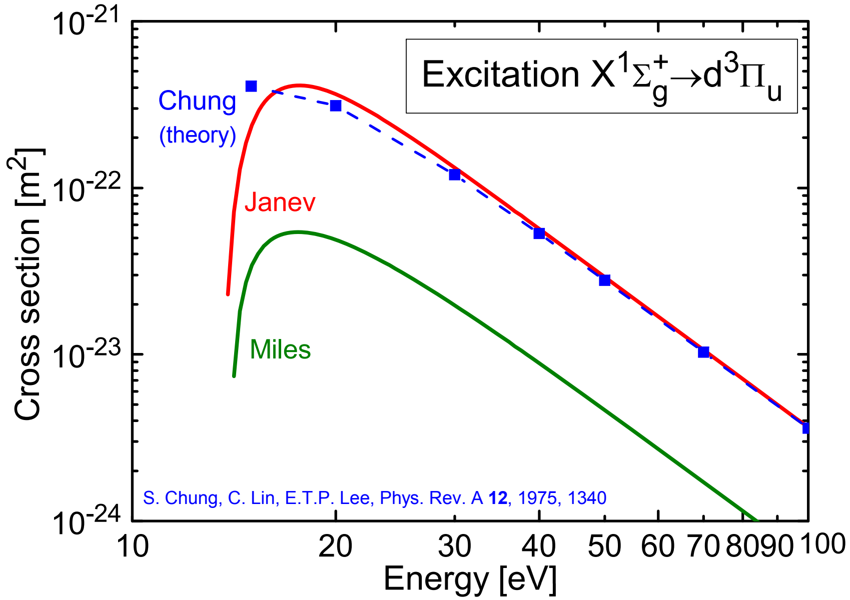


reasonable agreement

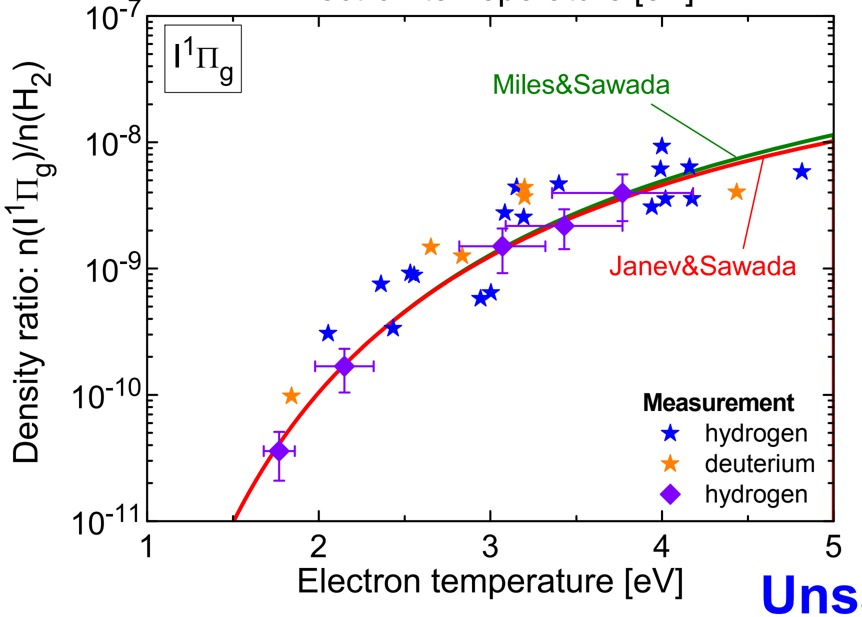
CR model for molecular hydrogen

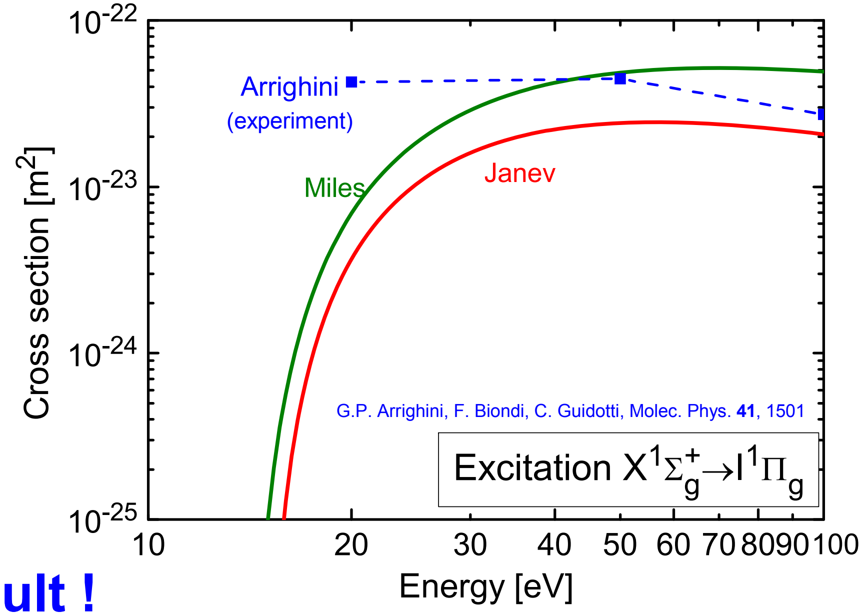
Population densities: comparison with measurements (low and high quenching)





Triplet system





Singlet system

Unsatisfying result !

Yacora for molecular hydrogen

Unsatisfying result

Disagreement of measurements with most recent and accurate cross sections (Janev)

Identify possibly missing reaction channels ⇨ ongoing work

Candidate: effective mixing of electronic levels in n=3 (small energy differences)

- vibrational resolution → statistical distribution not applicable
- extend database by cross sections for mixing processes (Gryzinski method)
- extend database (and check existing data) for ionizing processes (Gryzinski method) ⇨ H_2^+

Yacora for atomic hydrogen

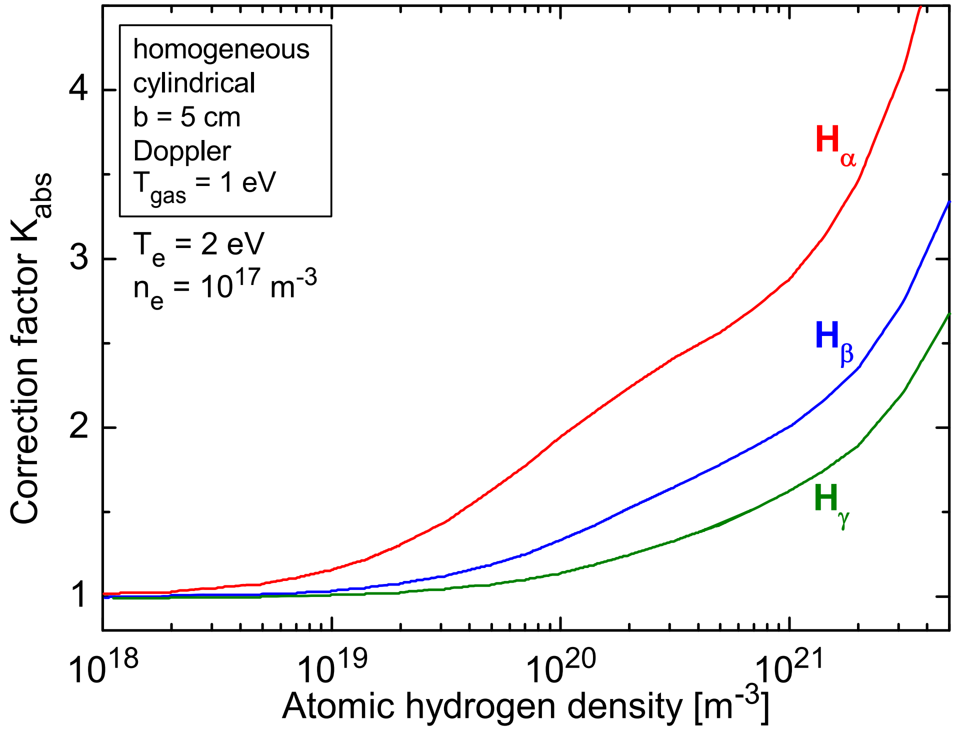
Opacity and dissociative recombination

opacity of Lyman lines enhances Balmer radiation

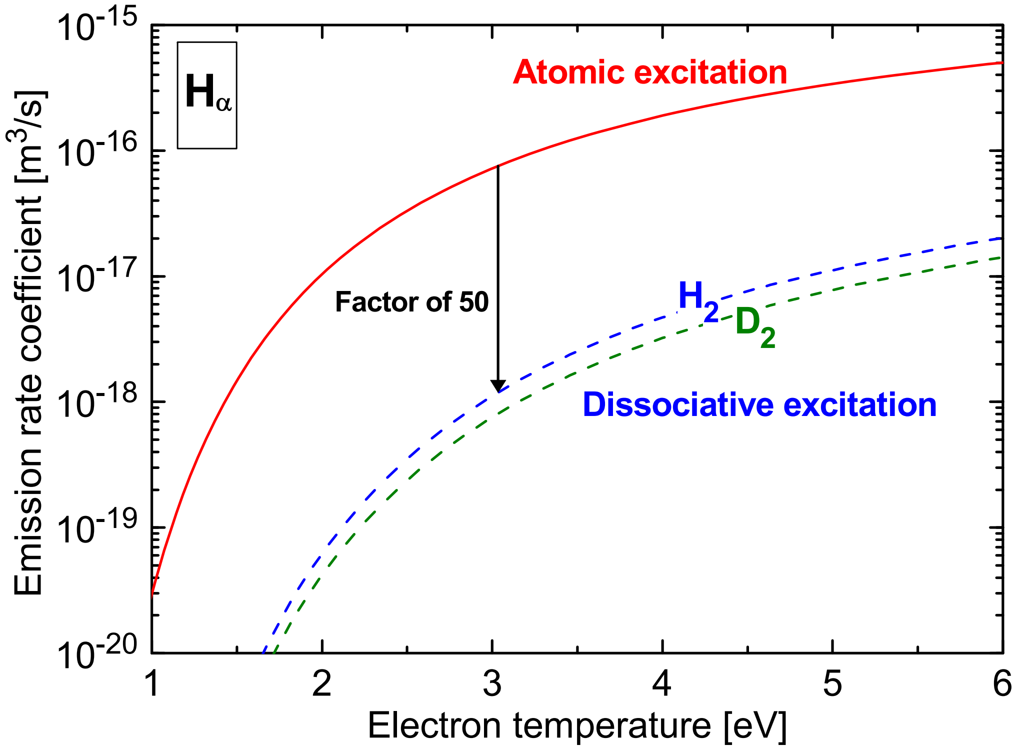
$$\varepsilon_{H_\alpha} = n_H n_e X(T_e, n_e) \frac{A_{3,2}}{(A_{3,2} + A_{3,1}\Theta_{L_\beta})}$$

population escape factor: $0 < \Theta_{p,k} < 1$

$e + H_2 \rightarrow H_2^* \rightarrow H\ (n > 1) + H + e$



Influence on Balmer line ratios



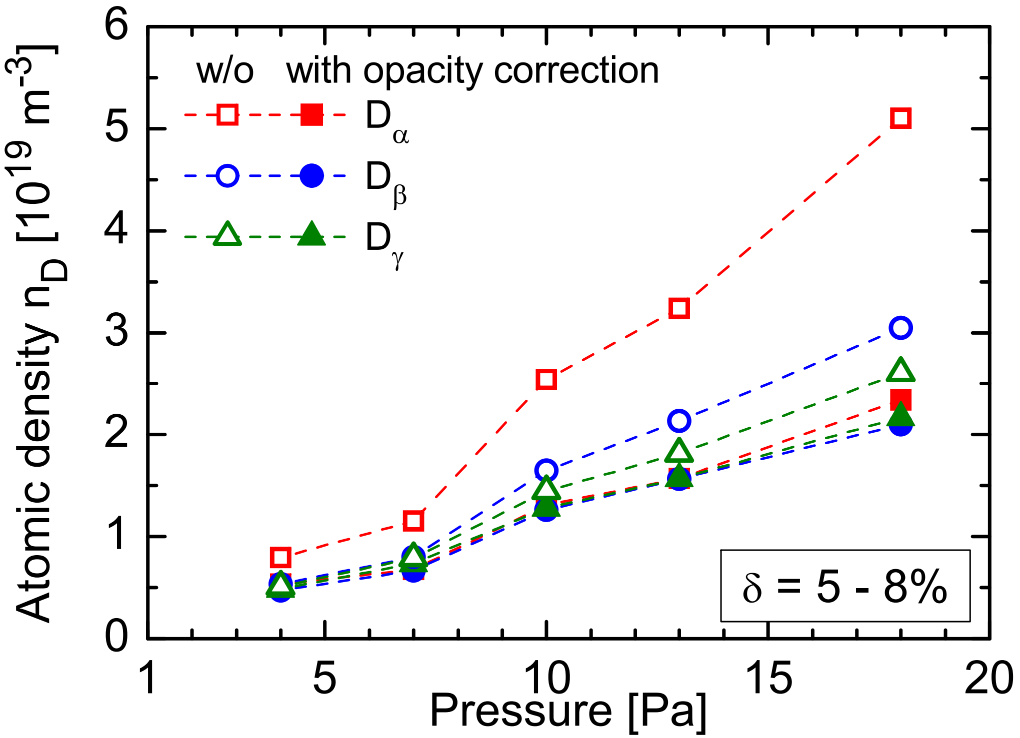
Different contributions for the isotopes H_2 and D_2

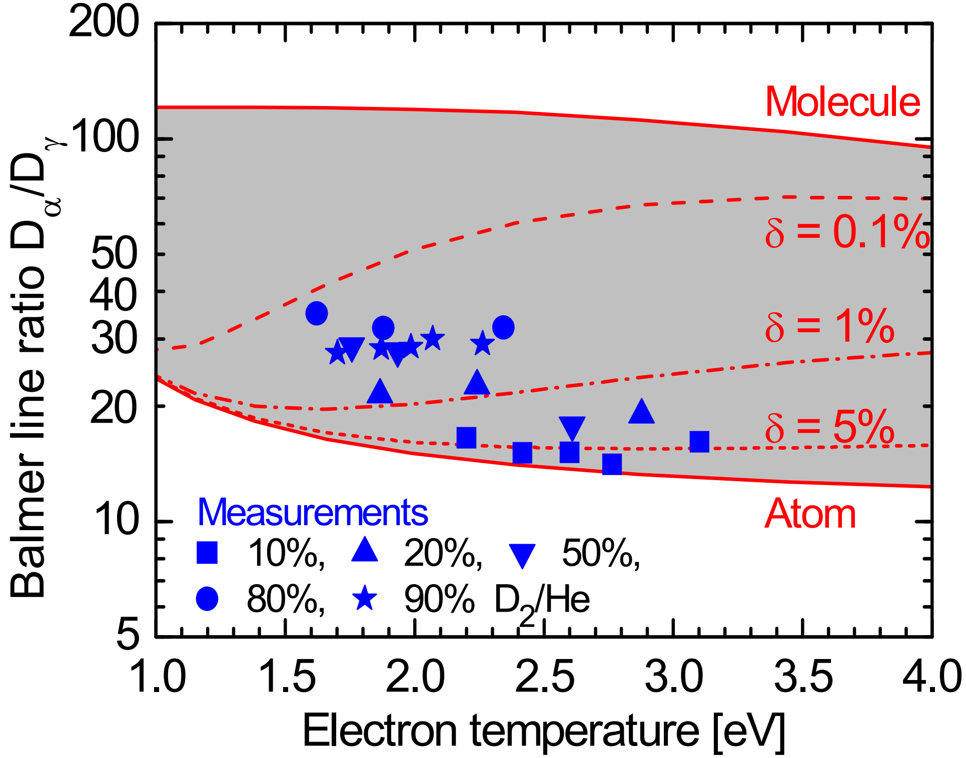
Yacora for atomic hydrogen

Opacity and dissociative recombination

K. Behringer, U. Fantz, New Journal of Physics **2** (2000) 23

ECR discharge: $n_e = 10^{17}$ m^{-3}, T_e = 2- 4 eV





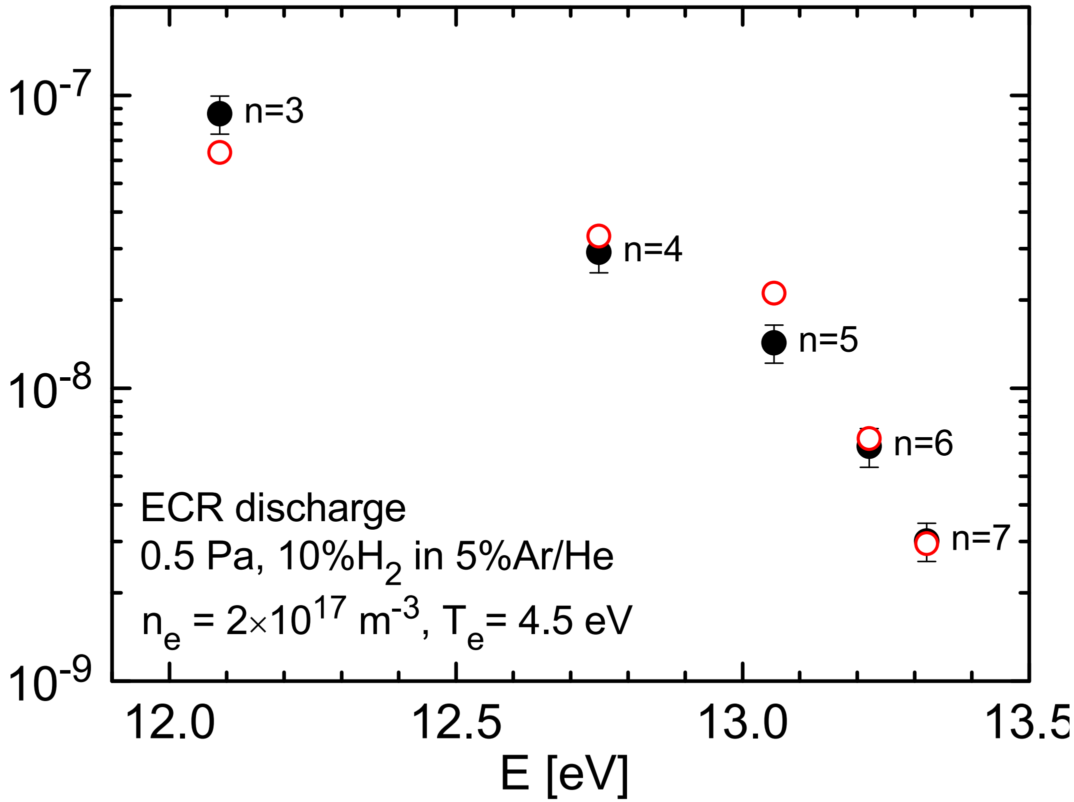
Agreement among the Balmer lines

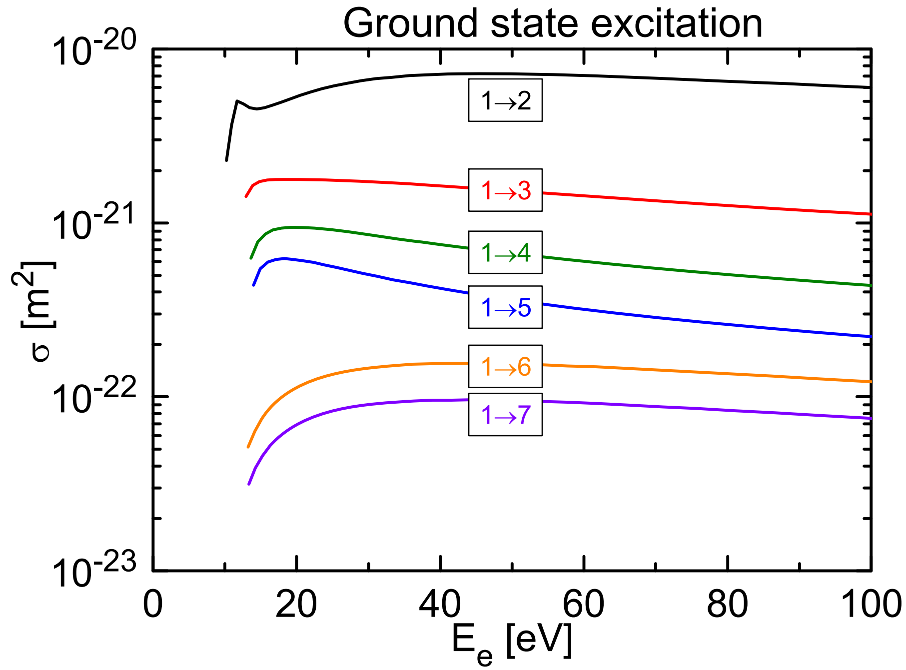
Line ratios are sensitive for low degree of dissociation

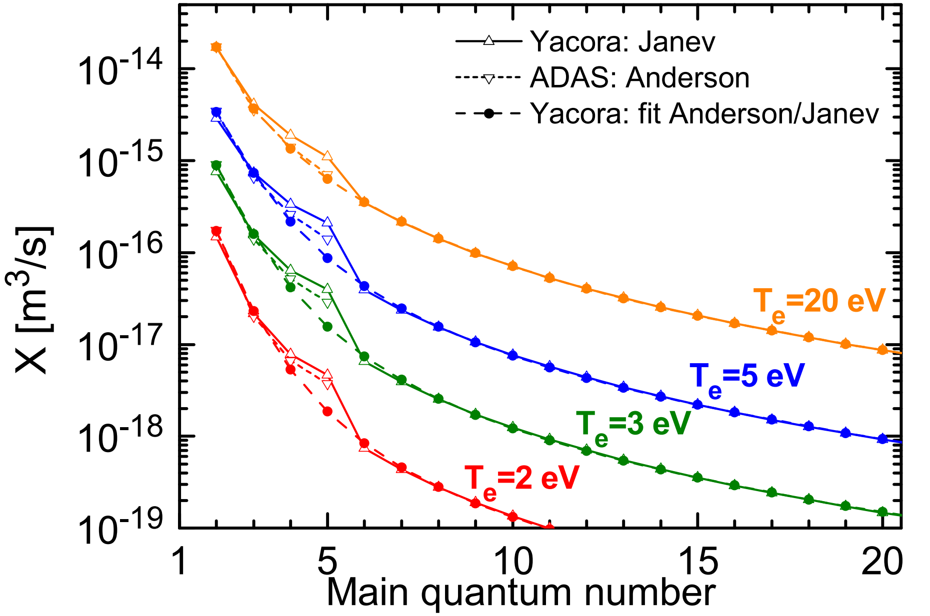
Comparison with measurements:

check cross sections for direct excitation

Balmer lines: Boltzmann plot $n_p/n_0/g_p$







Cross sections

R. Janev, D. Reiter, U. Samm: Juel-Report 4105 (2003)

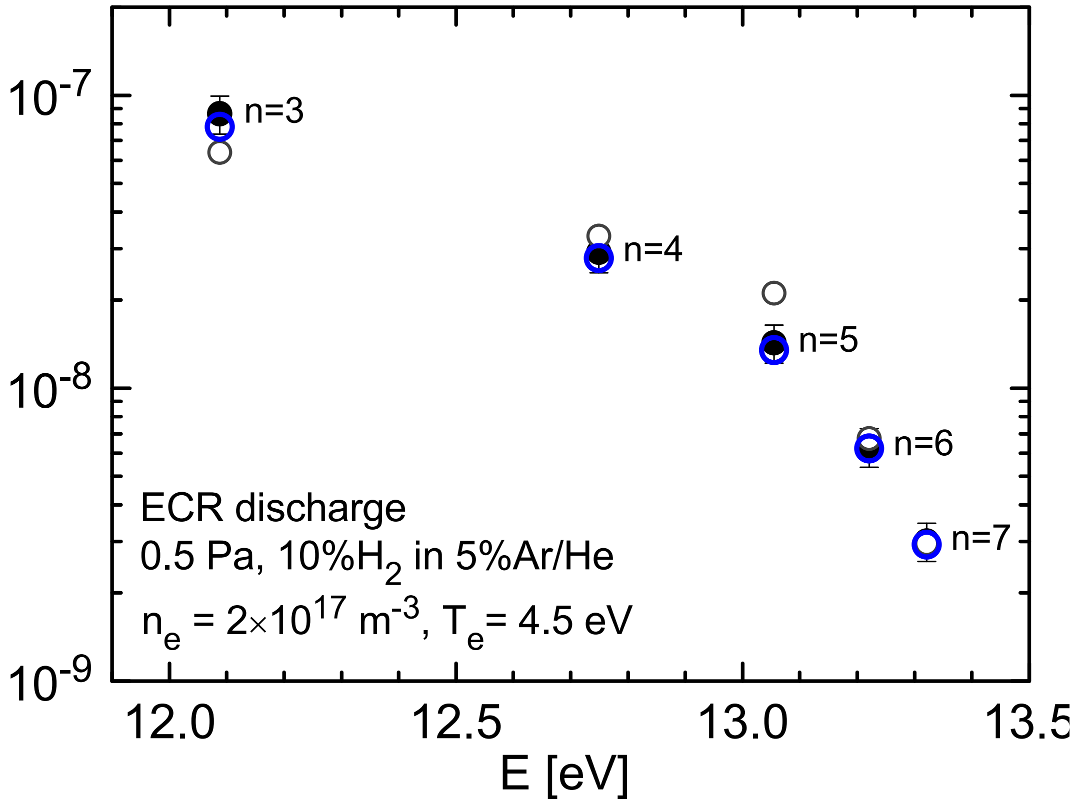
H. Anderson, C. P. Ballance, N. R. Badnell, H. P. Summers, J. Phys. B. 33 (2000) 1255

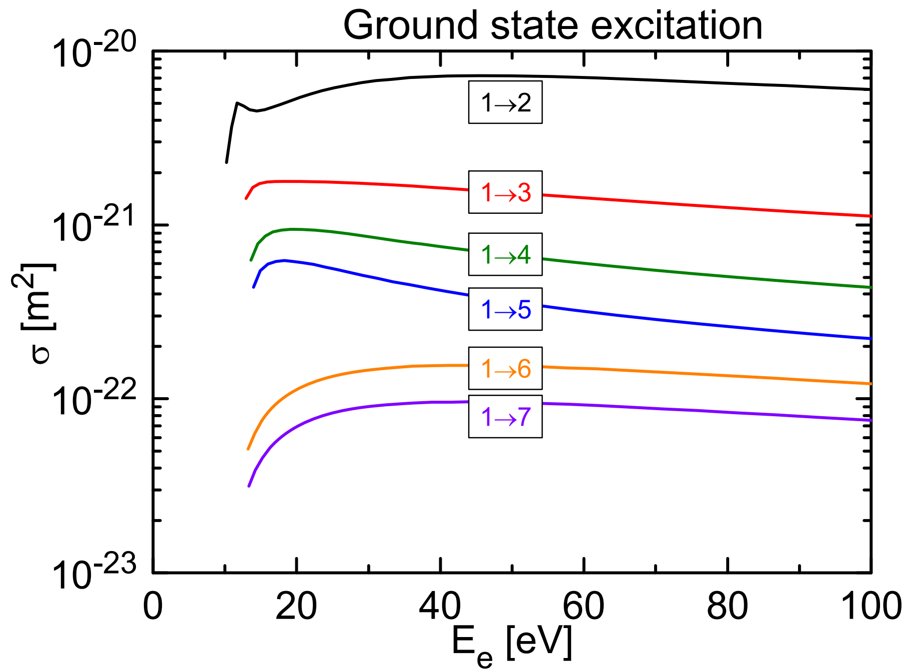
IPP

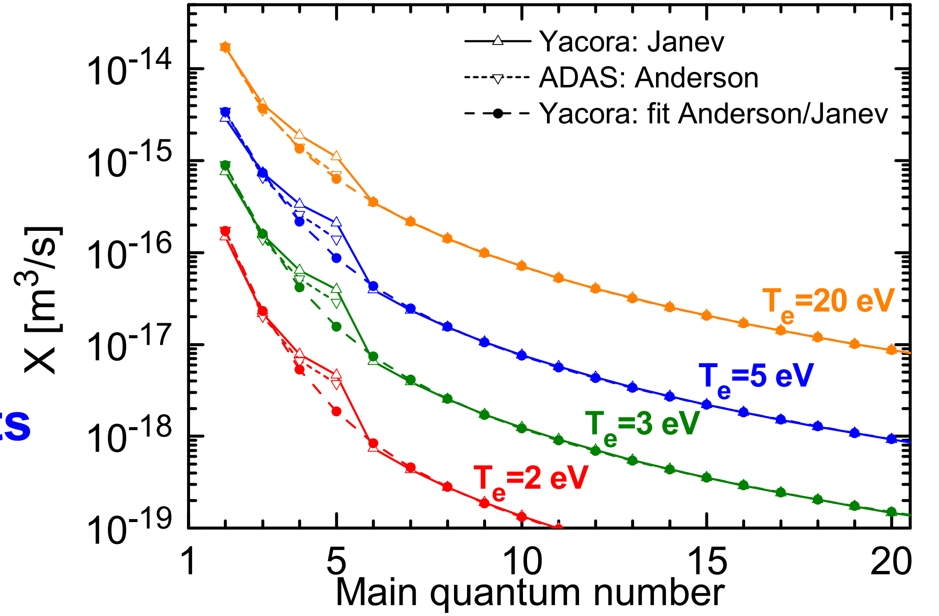
Comparison with measurements:

check cross sections for direct excitation

Balmer lines: Boltzmann plot $n_p/n_0/g_p$





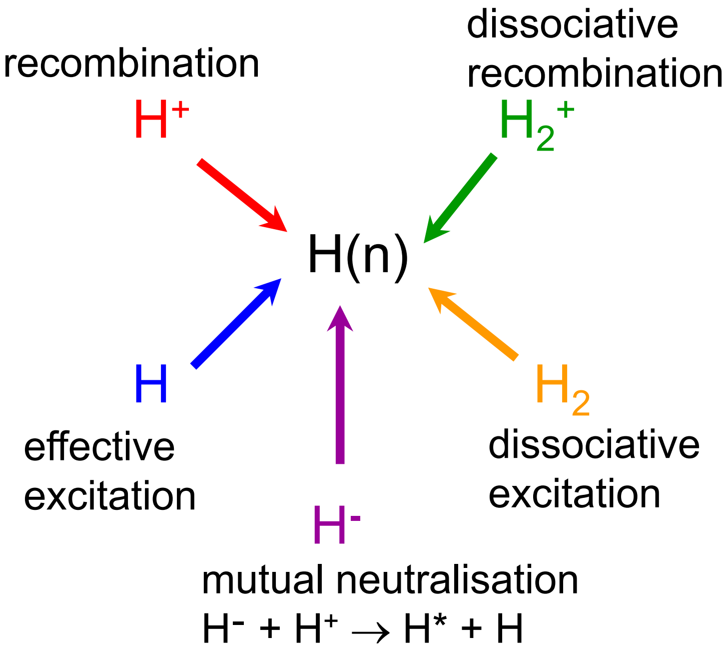


Yacora now in agreement with experiments

D. Wünderlich et al. JQSRT 110 (2009) 62

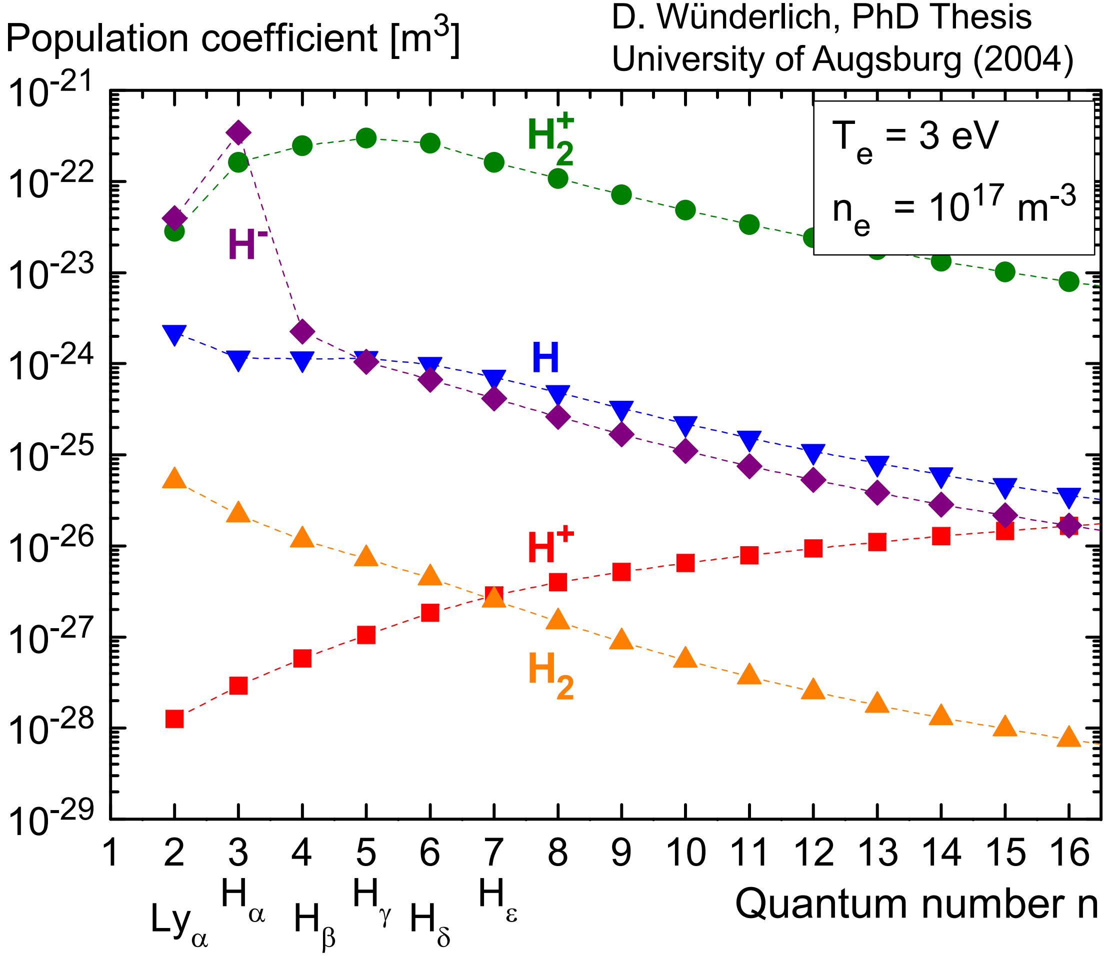
Yacora for atomic hydrogen

Coupling to other hydrogen species

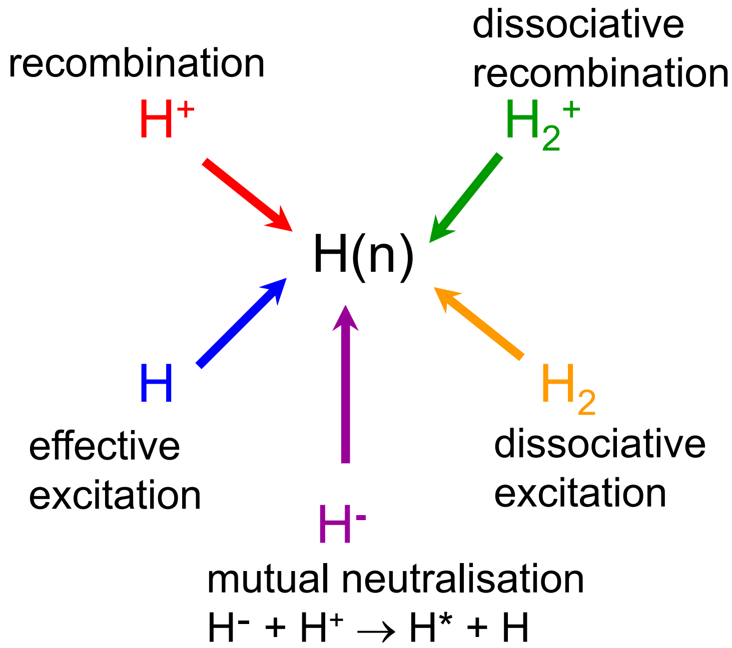


$$
\begin{aligned}
n(p) = & R_H(p)\, n_H\, n_e \\
& + R_{H^+}(p)\, n_{H^+}\, n_e \\
& + R_{H_2}(p)\, n_{H_2}\, n_e \\
& + R_{H_2^+}(p)\, n_{H_2^+}\, n_e \\
& + R_{H^-}(p)\, n_{H^-}\, n_e
\end{aligned}
$$

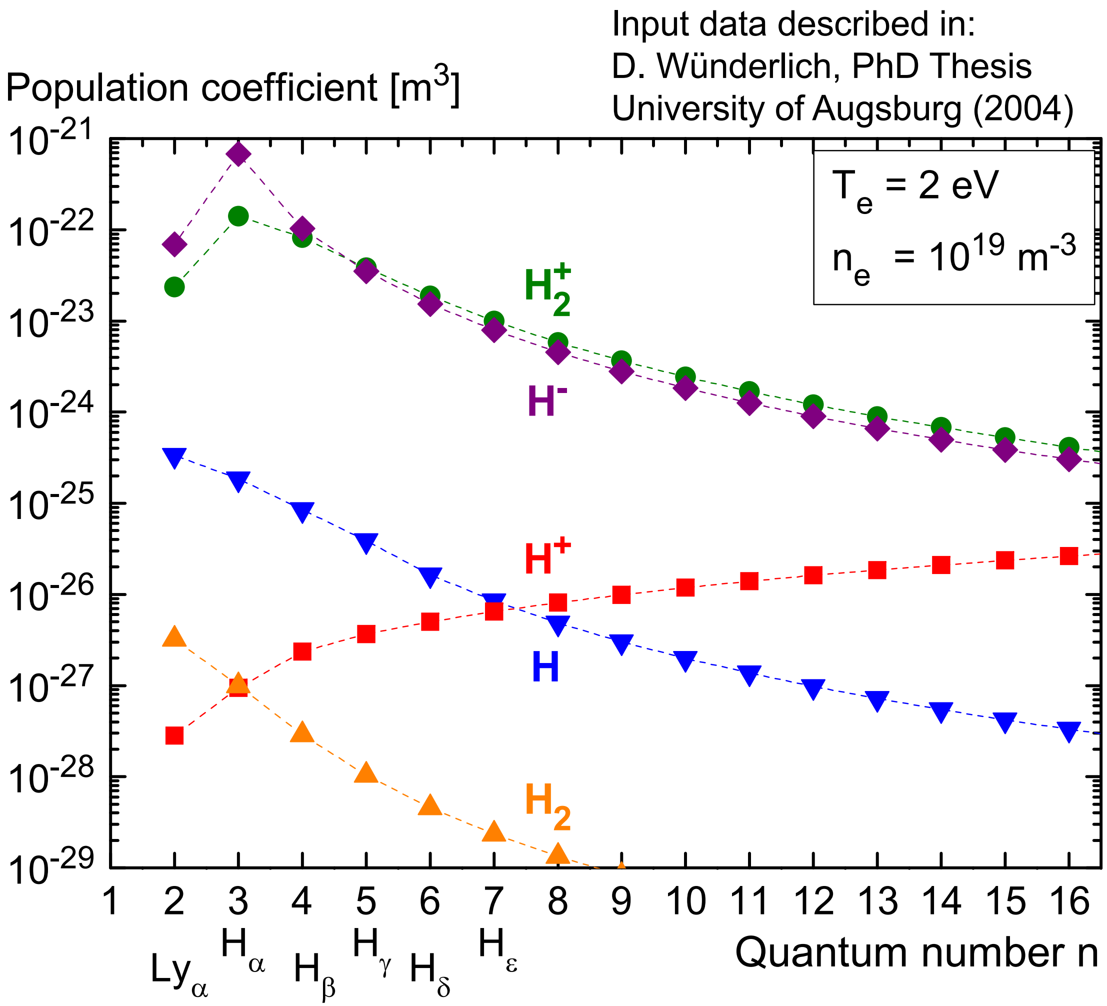
Input data described in:
D. Wünderlich, PhD Thesis
University of Augsburg (2004)



Coupling to other hydrogen species

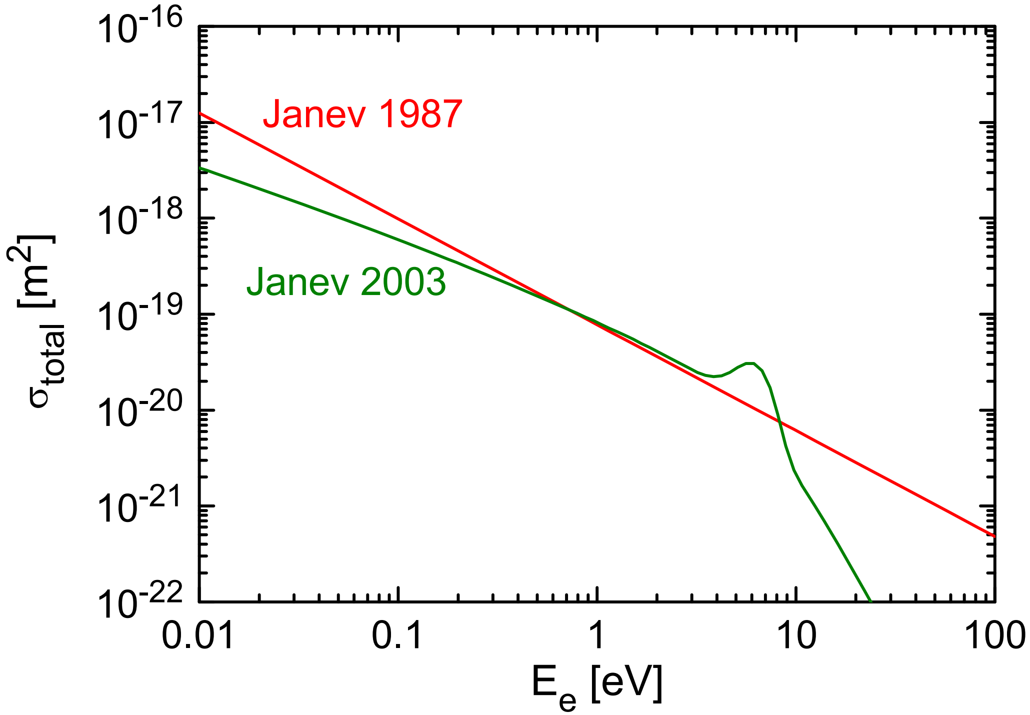


$$
\begin{aligned}
n(p) = {} & R_H(p)\, n_H n_e \\
& + R_{H^+}(p)\, n_{H^+} n_e \\
& + R_{H_2}(p)\, n_{H_2} n_e \\
& + R_{H_2^+}(p)\, n_{H_2^+} n_e \\
& + R_{H^-}(p)\, n_{H^-} n_e
\end{aligned}
$$



Change of relevance of individual processes

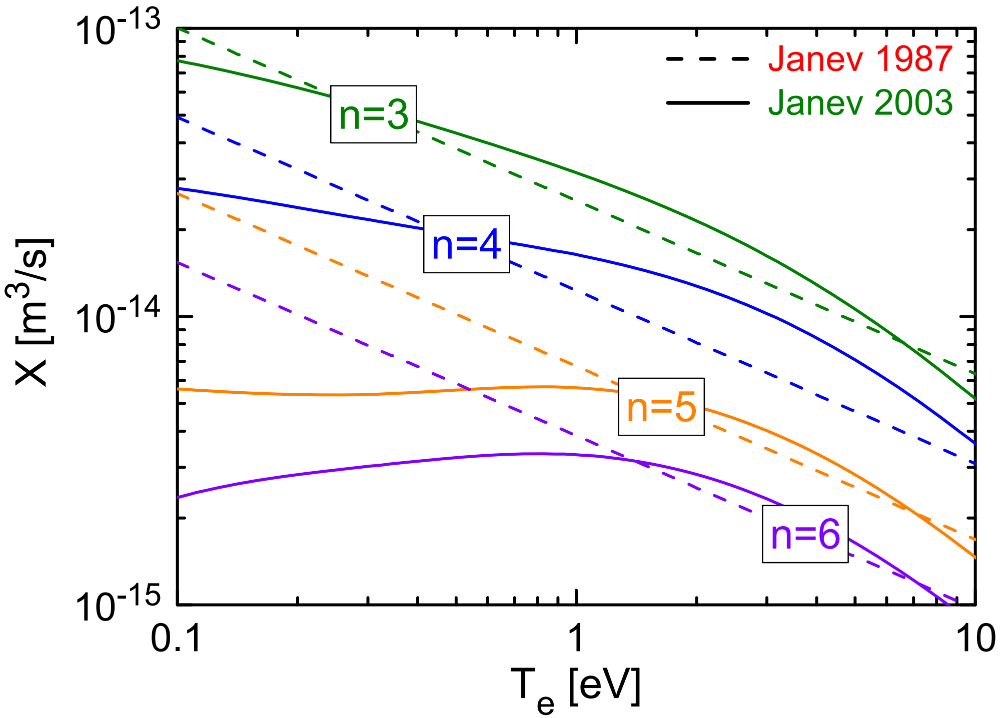
Relevance of dissociative recombination $H_2^+ + e \rightarrow H(n) + H$



R.K. Janev, W.D. Langer, J.K. Evans
D.E. Post *Elementary Processes in Hydrogen/Helium Plasmas*
Springer, Berlin (1987)

fixed branching ratio

n=2: 0.1	n=5: 0.12
n=3: 0.45	n=6: 0.69
n=4: 0.22	n>6: $10/n^3$



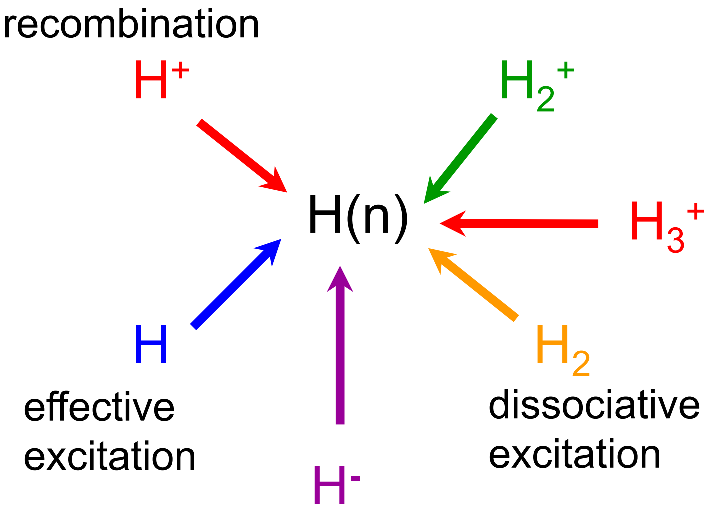
Data set changed

R. Janev, D. Reiter, U. Samm, Juel-Report 4105 (2003)

branching ratio vibrationally resolved and energy dependent

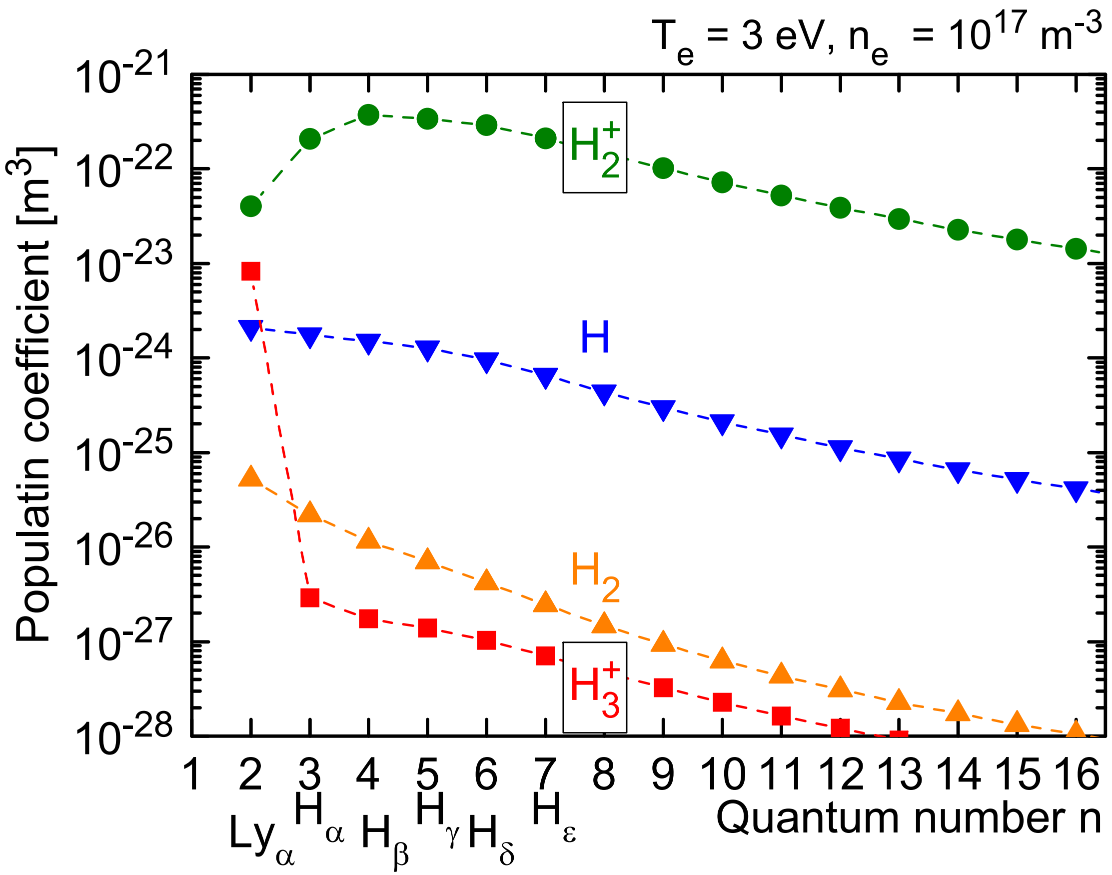
Yacora now in better agreement with experimental data (H^- sources)

Coupling to other hydrogen species



channel added

open issue: D_2^+, H_3^+, D_3^+



Dissociative recombination H_3^+

$H_3^+ + e \rightarrow H + H + H$ ①

$\rightarrow H_2 + H(n)$ ②

R. Janev, D. Reiter, U. Samm: Juel-Report 4105 (2003)

branching ratio ① well known

S. Datz et al., Phys. Rev. Lett. **74**(1995) 896

branching ratio ② not known

② all in n=2:

F.C: Kulander et al., J. Phys. B **12** (1979) L501

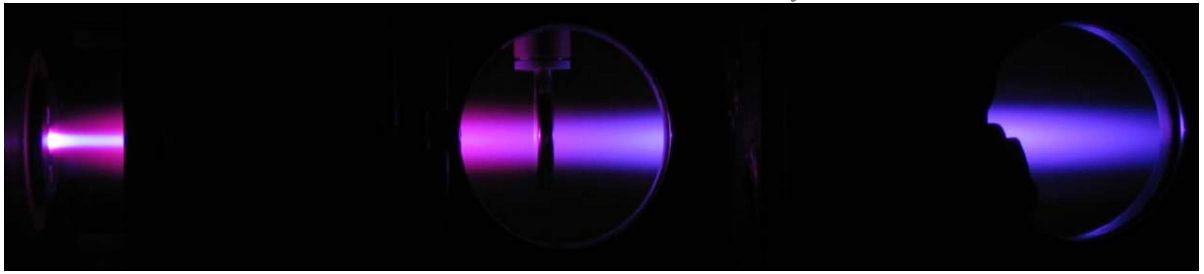
Application to ionising and recombining plasmas

Recombination by

Atoms and/or Molecules?

Transition from an ionising to a recombining plasma

courtesy: Pilot-PSI, FOM Institute

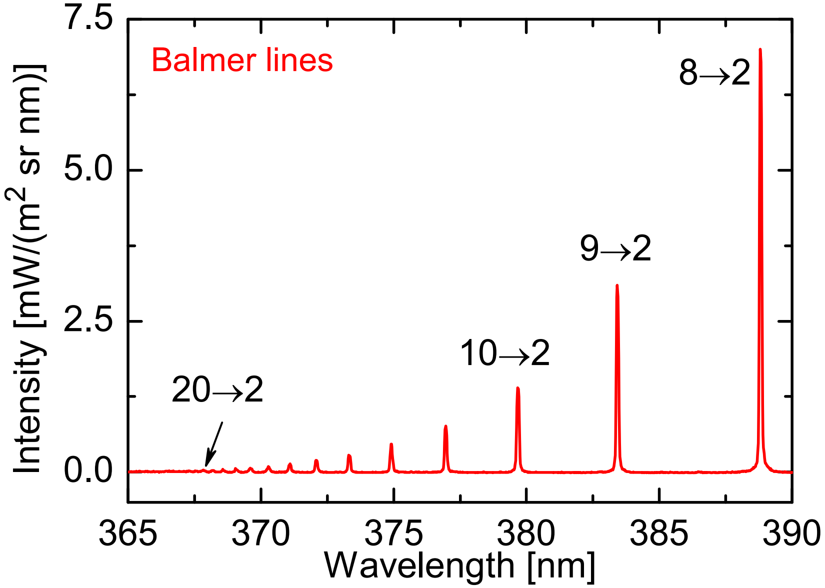


Electron Ion Recombination EIR

$H^+ + e + e \rightarrow H + e$ 3-body rec.

$H^+ + e \rightarrow H + h\nu$ radiative rec.

$n_e \approx 10^{20} - 10^{21}\ m^{-3}$, $T_e < 1.5$ eV



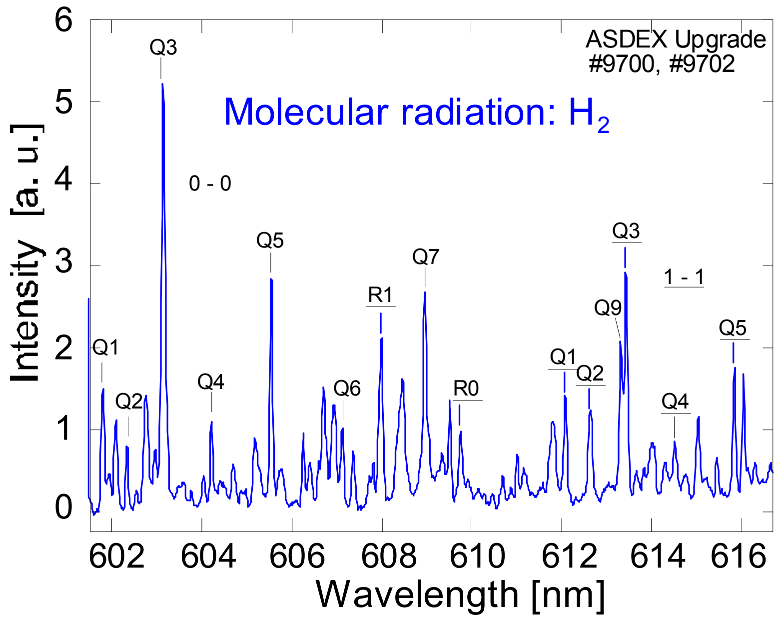
courtesy: PSI-2, Exp. Plasmaphysik, Berlin

Molecular Assisted Recombination MAR

$H_2(v) + H^+ \rightarrow H + H_2^+$ charge exchange

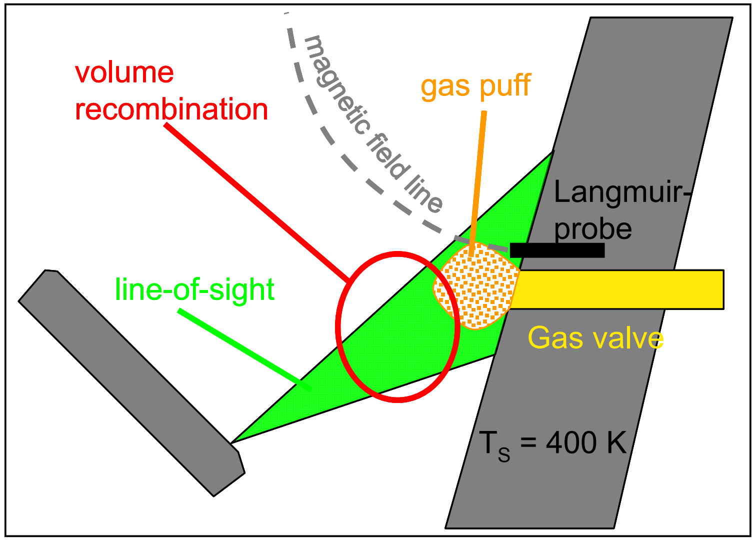
$H_2^+ + e \rightarrow H + H^*$ dissociative rec.

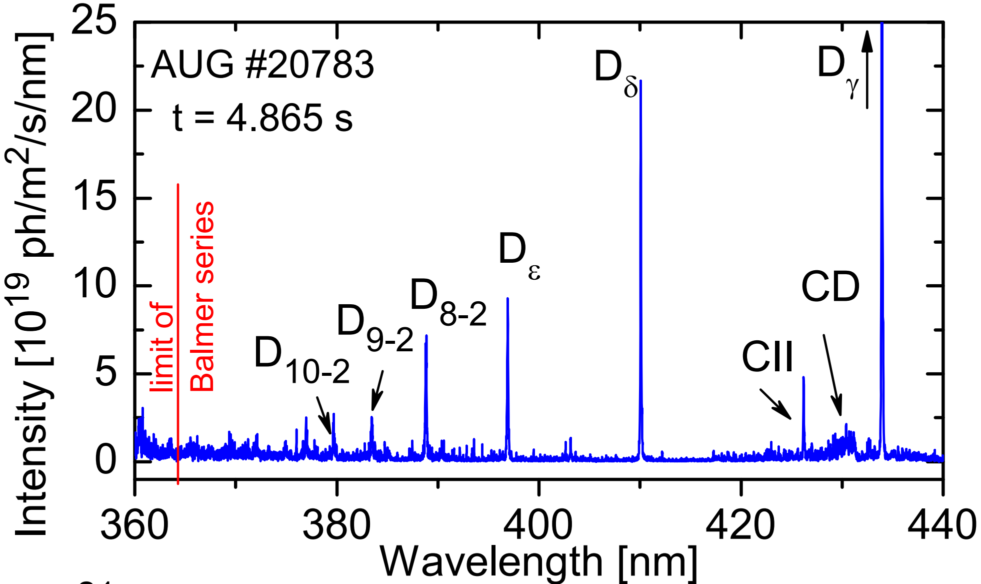
$n_e \approx 10^{19} - 10^{21}\ m^{-3}$, $T_e \approx 2 - 10$ eV

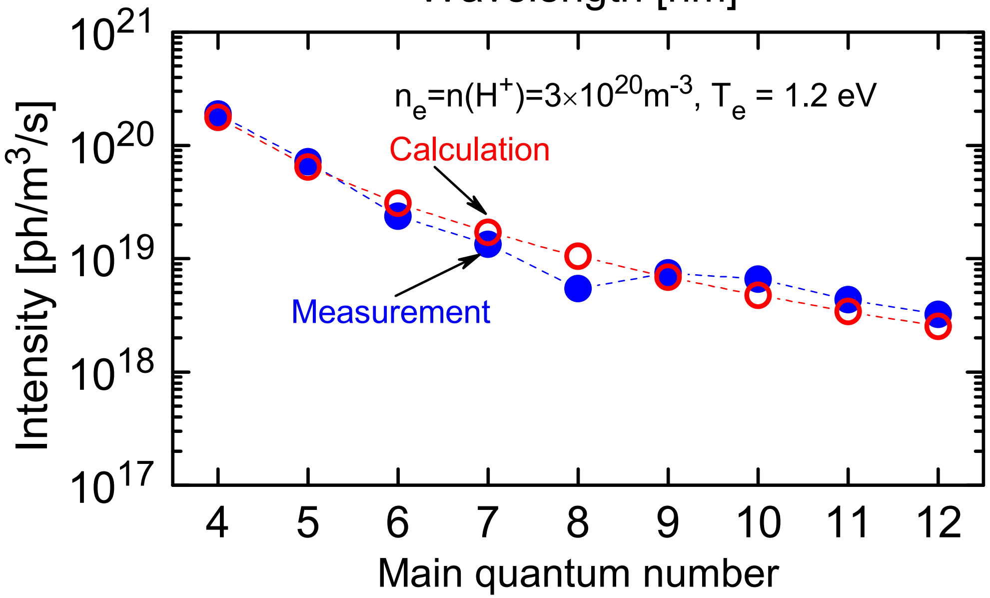


Experimental validation of recombination: outer divertor of ASDEX Upgrade

S. Brezinsek, R. Pugno, U. Fantz, A. Manhard et al.,
Phys. Scr. T118 (2007) 40







Langmuir probes:

T_e= 2 eV, n_e = 4×10^{18} m^{-3}

D_β Stark broadening:

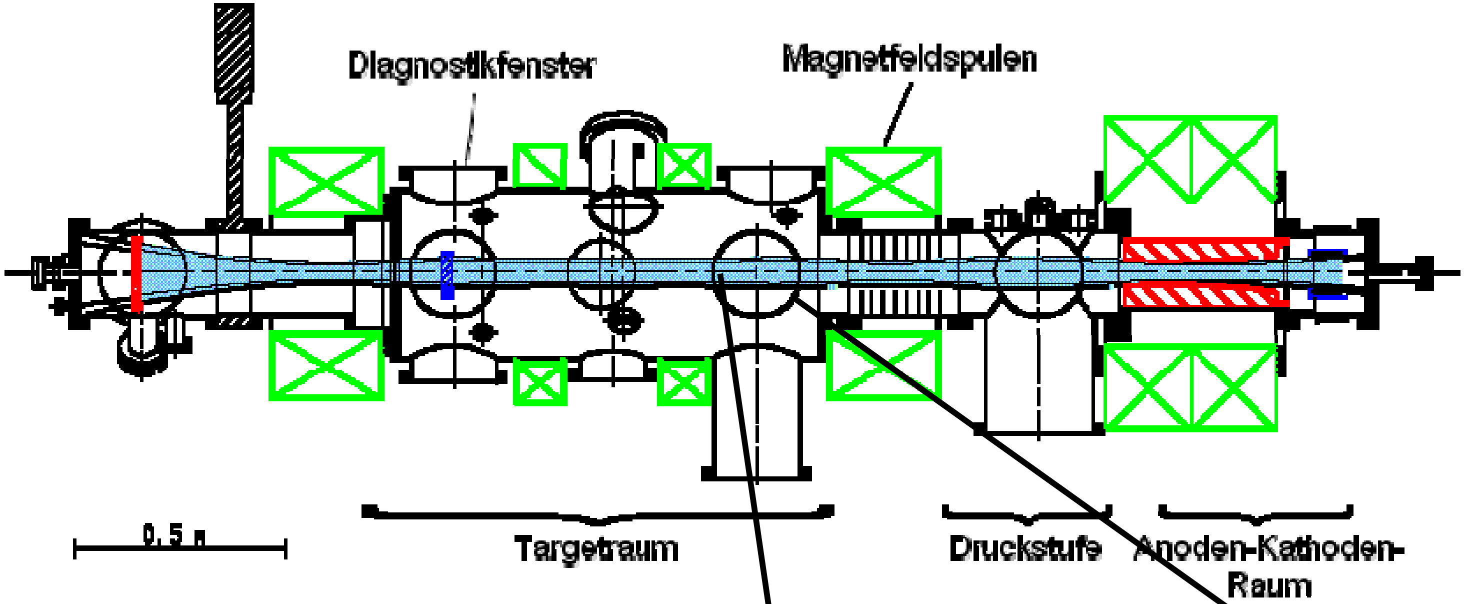
n_e = 3×10^{20} m^{-3}

OES+Yacora:

T_e= 1.2 eV, n_e = 3×10^{20} m^{-3} ✓

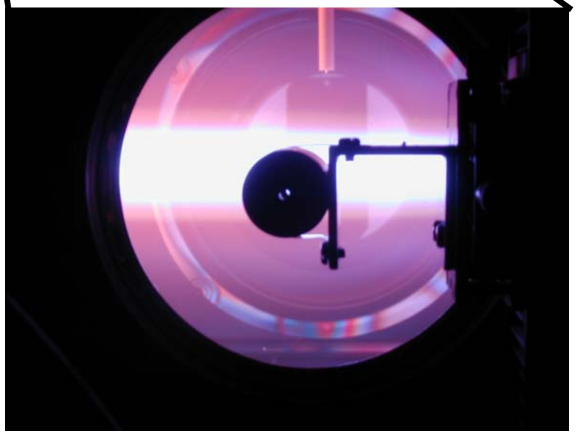
Linear plasma devices: contributions from particle species to Balmer radiation

Plasma generator PSI-2: Berlin ⇨ FZ Jülich (2010)



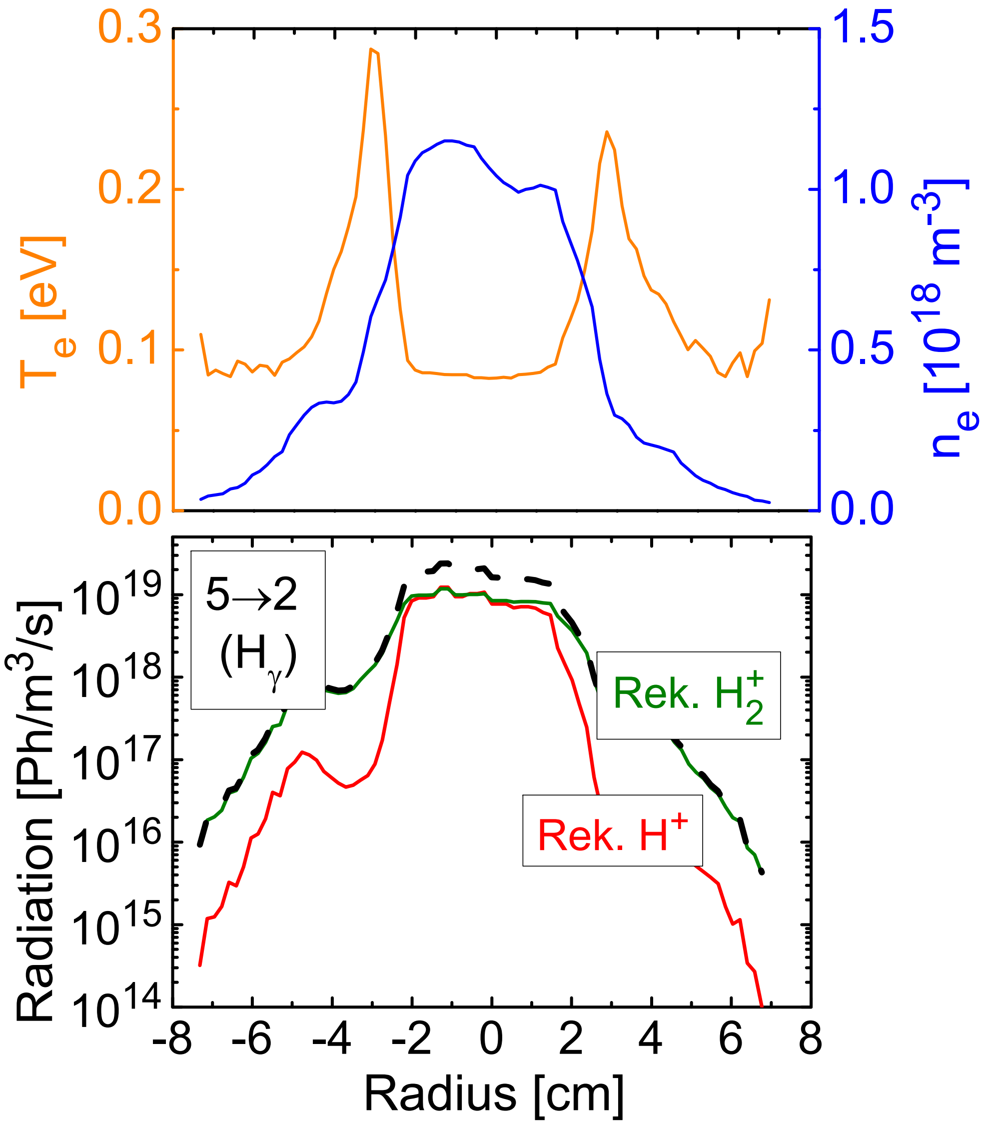
- hollow cathode
- magnetic field for confinement
- $n_e = 10^{17} - 10^{20}\ m^{-3}$
- $T_e = 0.1 - 10$ eV

recombining plasma by
gas puff in target chamber



Linear plasma devices: contributions from particle species to Balmer radiation

Radial profiles (T_e, n_e from probes)

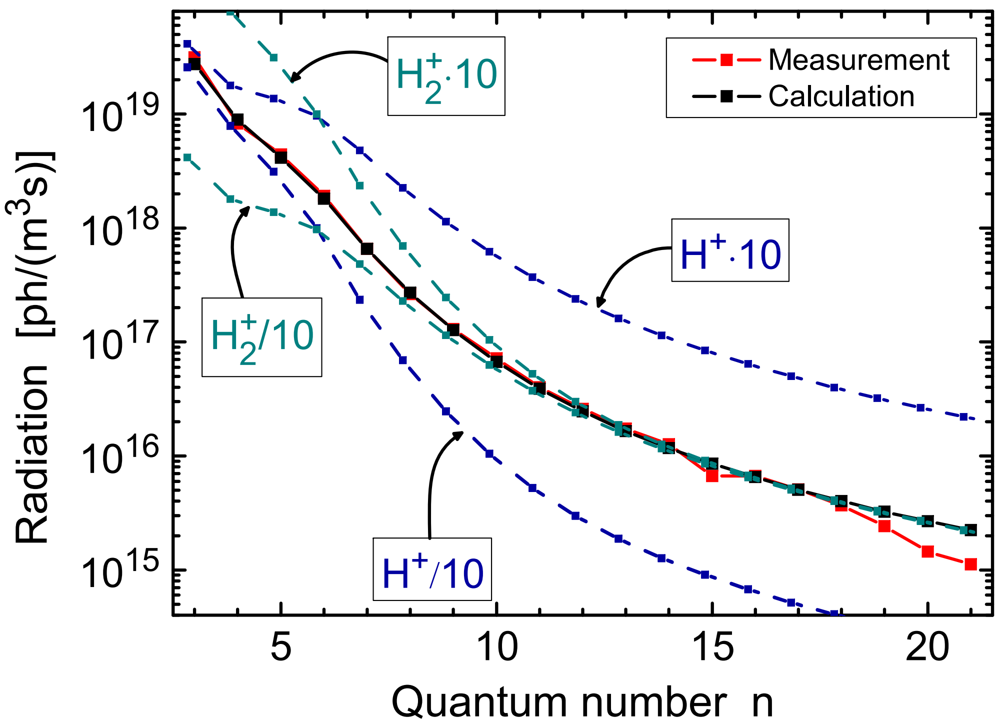


Relevance of ions

Sensitive method

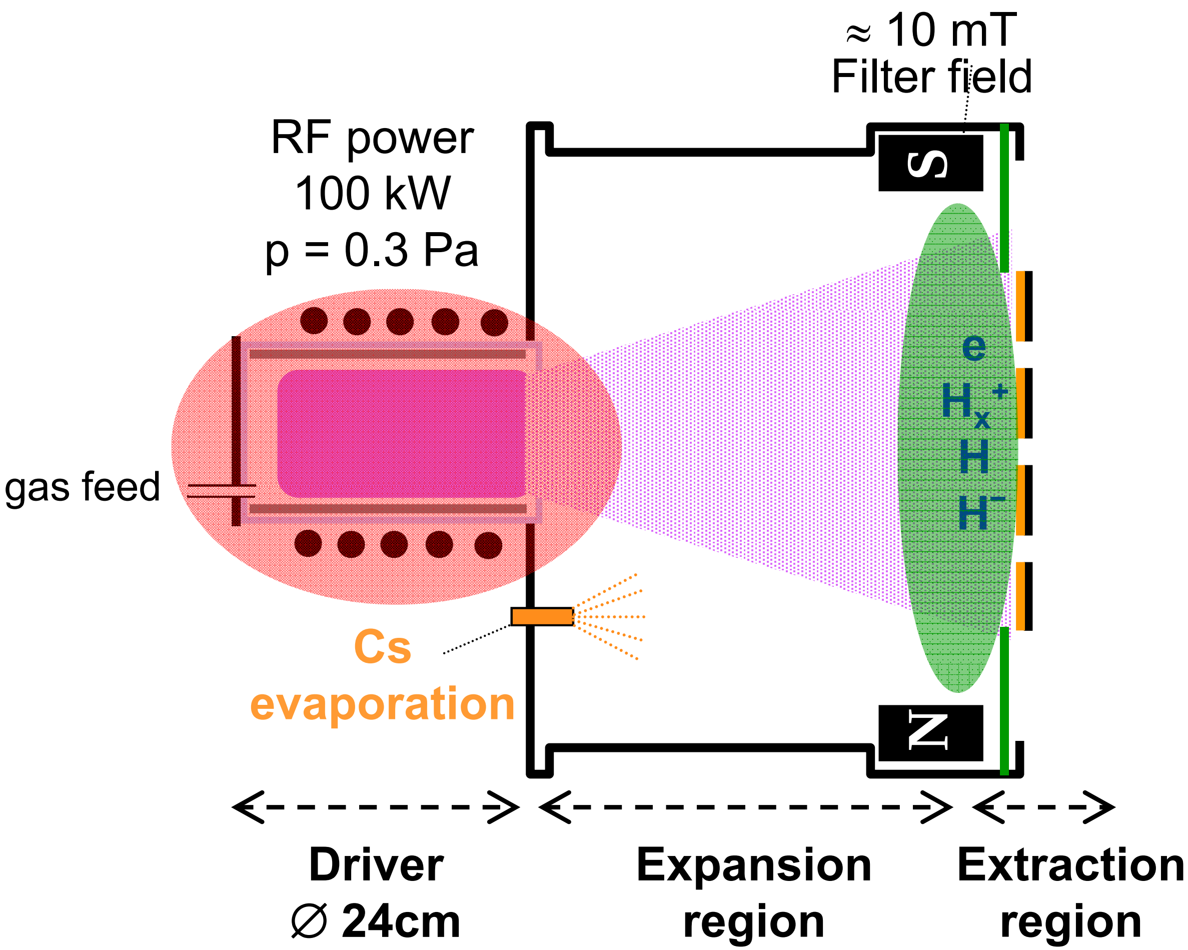
$n(H^+) \approx 5.2\times10^{17}\ m^{-3} \approx\ 50\%\ n_e$

$n(H_2^+) \approx 1.3\times10^{15}\ m^{-3} \approx 0.1\%\ n_e$



Ion sources for negative hydrogen ions: ionising – recombining plasma

H, H_x^+ + surface e^- → H^- Cs evaporation → low work function



Plasma generation
ionising plasma

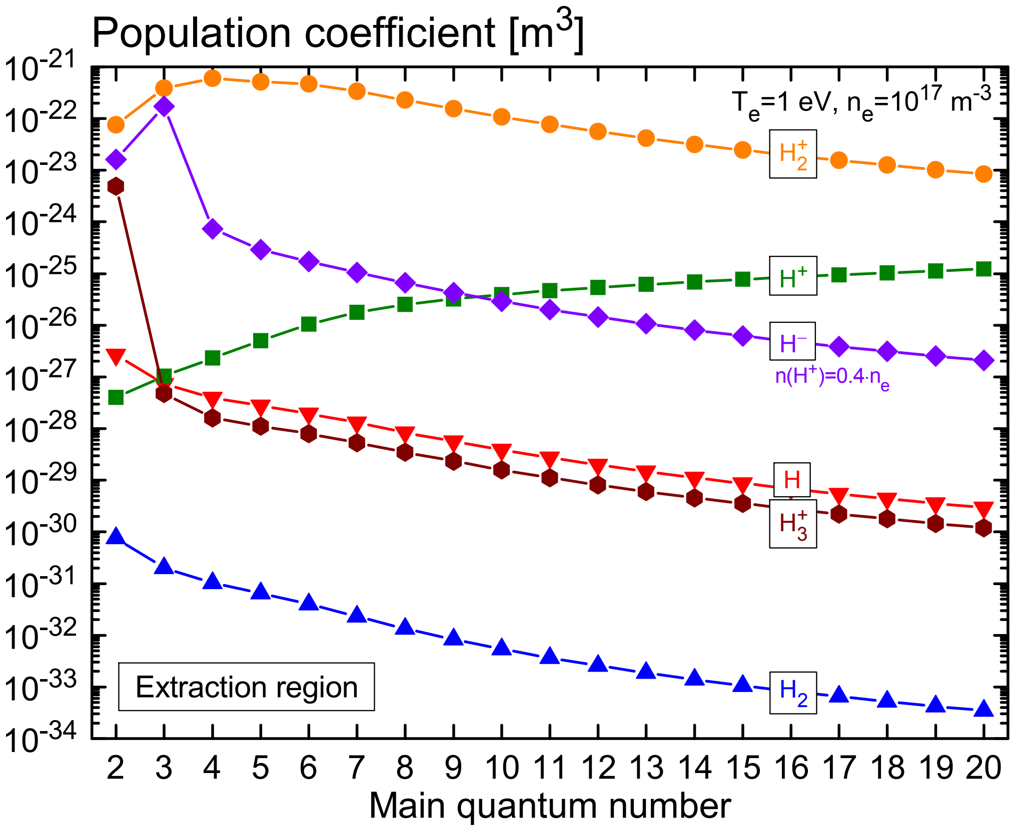
- ionisation: $\alpha \approx 0.1$
- dissociation: $\delta \approx 0.3$
- $T_e \approx 10$ eV
- $n_e \approx 5\times10^{18}\ m^{-3}$

H^- generation
recombining plasma

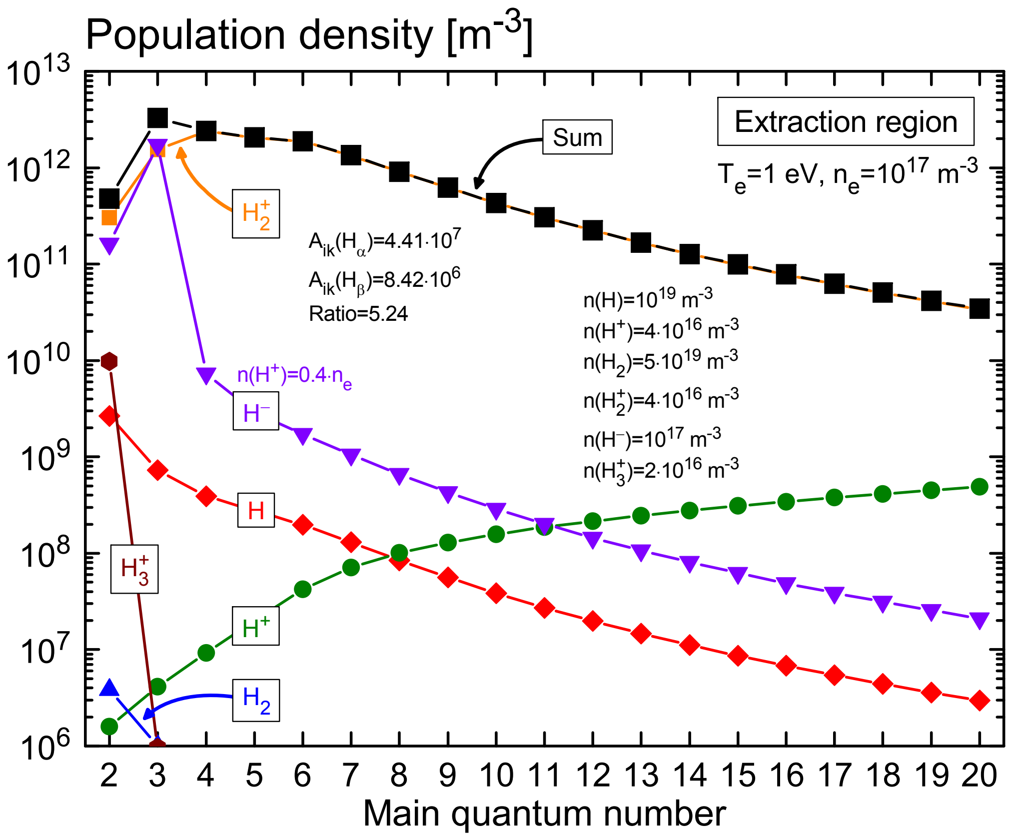
- $T_e \approx 1$ eV
- $n_e \approx 5\times10^{17}\ m^{-3}$
- $H^-/n_e \approx 0.1 – 5$
- $Cs^+/n_e \approx 0.01 – 0.1$

Physical understanding: diagnostics and modelling

Ion sources for negative hydrogen ions: recombining plasma

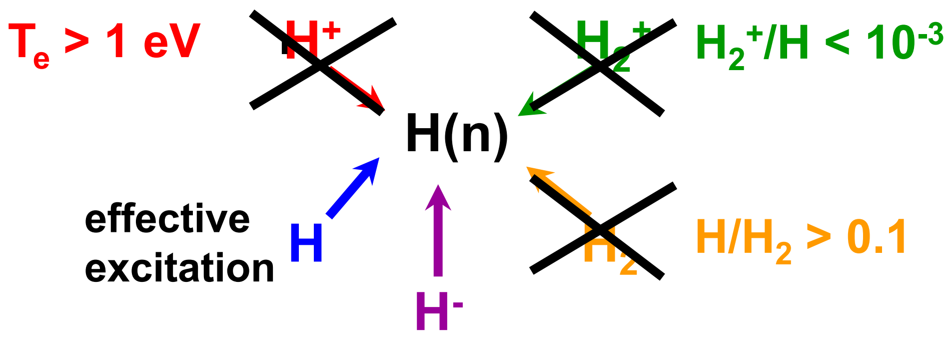


Relevance of H_2^+ and H^-



Ion sources for negative hydrogen ions: mutual neutralisation → H^- diagnostic

U. Fantz , D. Wünderlich NJP 8 (2006) 301

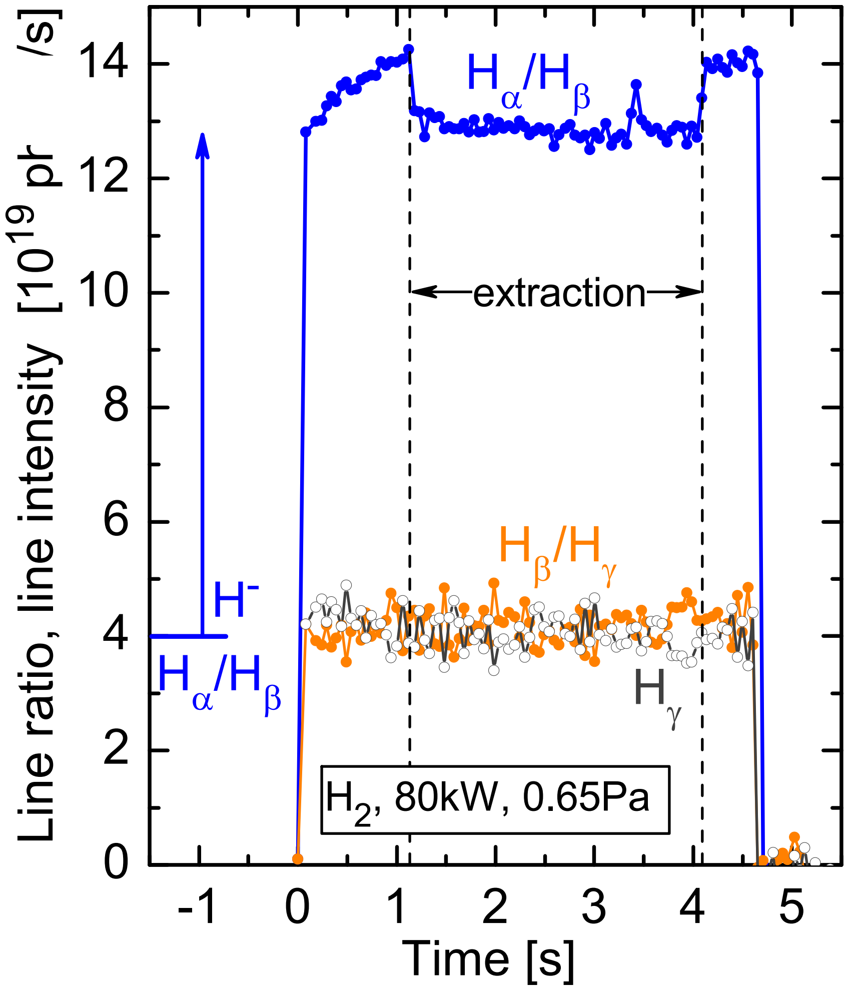


mutual neutralisation

$$H^+ + H^- \rightarrow H(n=3) + H$$

$$H(n=3) \rightarrow H_\alpha$$

Collisional radiative model



Measurement of Balmer line ratios

- **H_α/H_β depends on H^-/H**
- **H_β/H_γ reflects n_e and T_e**
- **high H_α/H_β ratio: $H^- = 10^{17}$ m^{-3}**
- **stable H_β/H_γ ratio, i.e. stable n_e and T_e**

Setup of the model

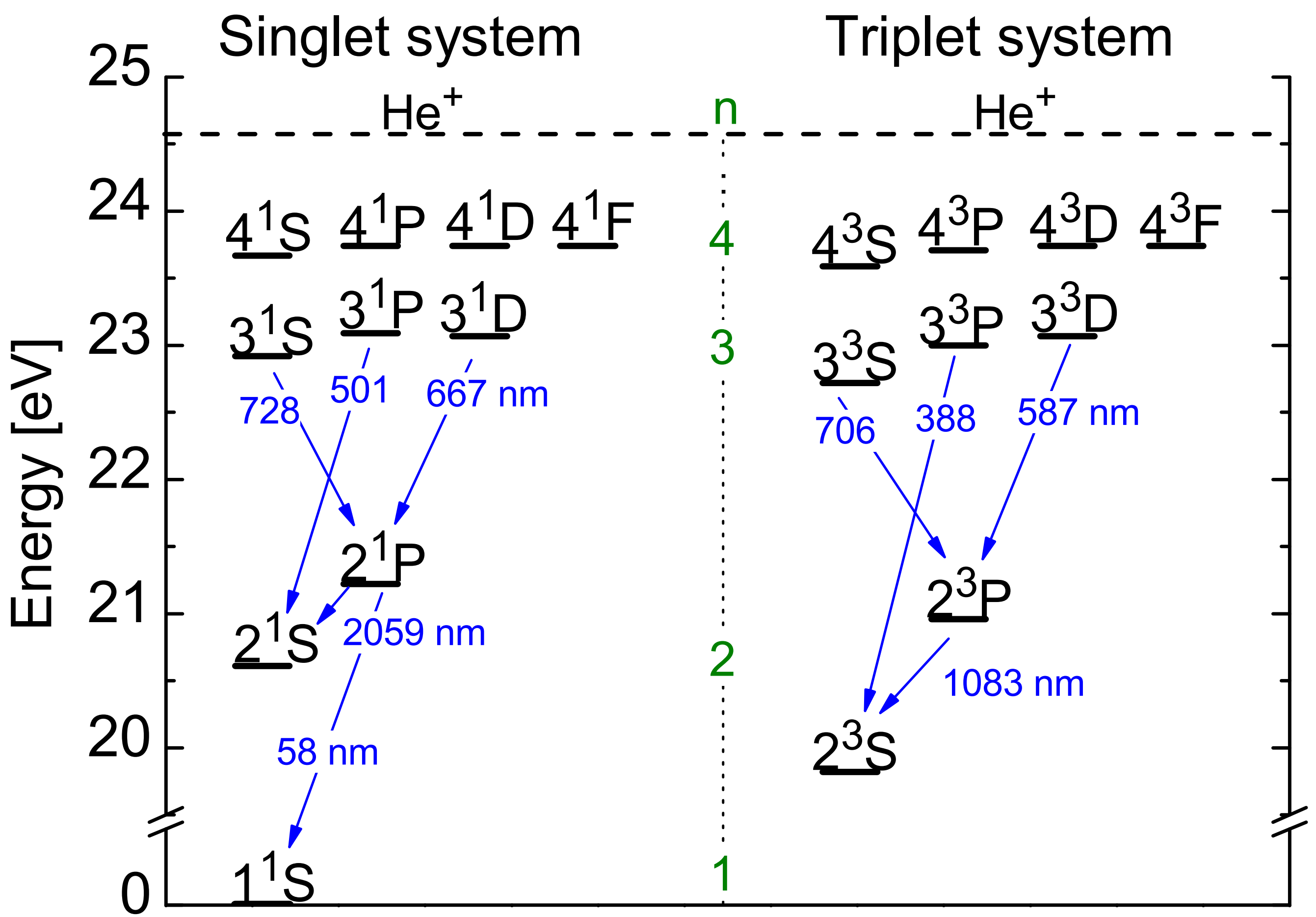
- cross sections for electron excitation and ionization from Ralchenko
- electronic states resolved up to n=4 in both multiplet systems
- angular momentum resolved
- 19 levels, 338 reactions

Yu. V. Ralchenko et al., NIFS-DATA-59 (2000)

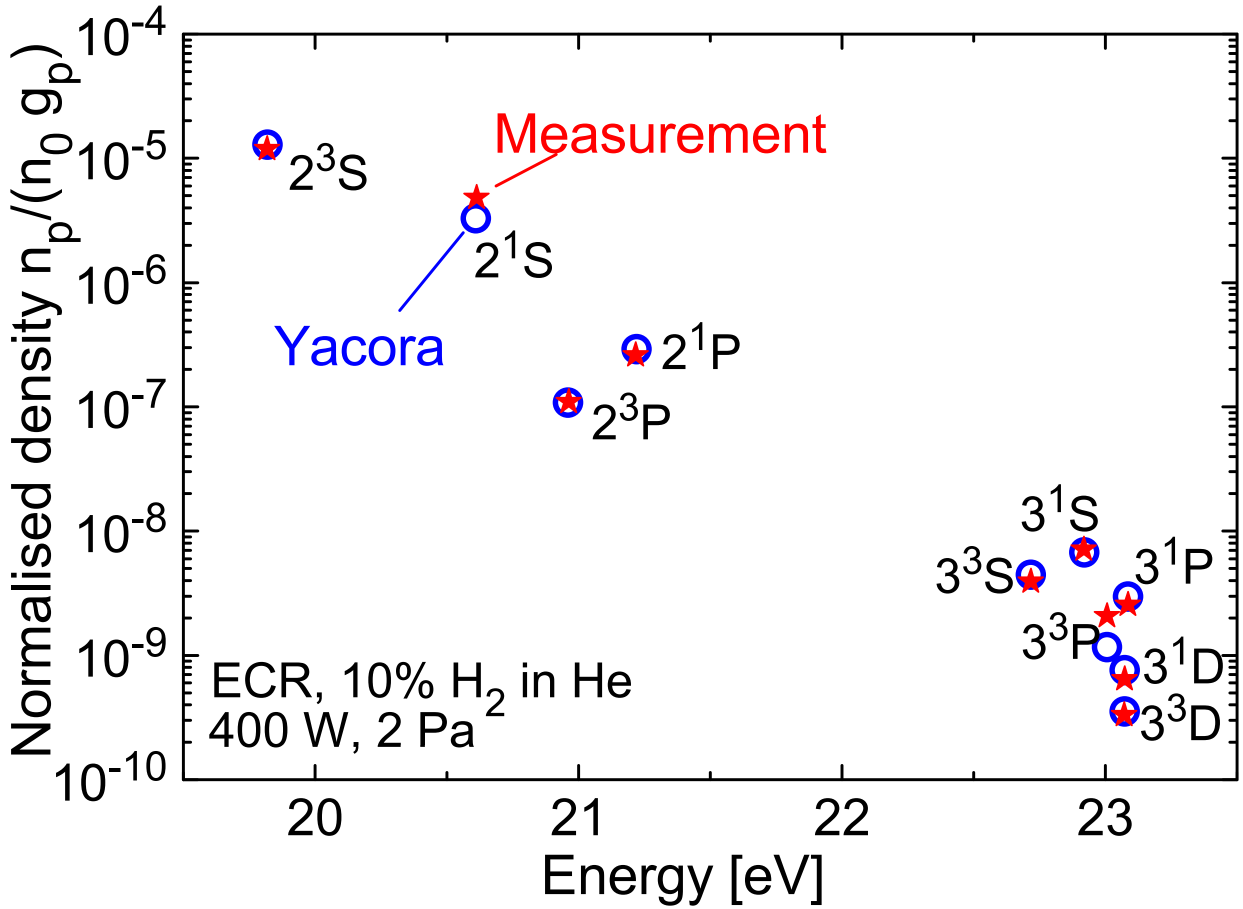
Cross checked with results from ADAS He

but more flexible

e.g. opacity



Comparison with experiment **Boltzmann plot**



Good agreement up to n=3

Importance of opacity and diffusion of metastable states

Next: n=4

Continuously updated & further checks with experiments

- investigations of He / H_2 (He/ D_2) mixtures
- measurements of **HeH^+** (HeD^+)

Summary

Work plan

- **Population densities: modelling and experiments** — **continue**
  - check data
  - identify relevance of individual processes
- **CR modelling for H_2 and H** — **continue + D_2**
  - status of Yacora modelling
  - continuous progress (H_2^+, H_3^+, ..)
  - coupling to different species
- **Applications to ionising and recombining plasmas** — **continue**
  - divertor plasmas
  - linear plasma devices
  - negative hydrogen ion sources — **+ beam data**
- **CR modelling for He and some applications** — **continue + HeH^+**
  - flexible model available (opacity)

isotope scaling