MAX-PLANCK-INSTITUT
FÜR PLASMAPHYSIK

Collisional radiative modelling of H_2 with Yacora and steps needed for D_2

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EUROfusion

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Collisional radiative (CR) modelling for hydrogen plasmas

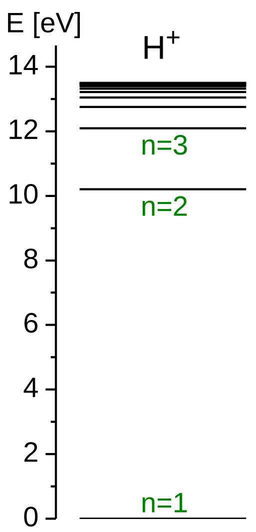
Population density of excited state p

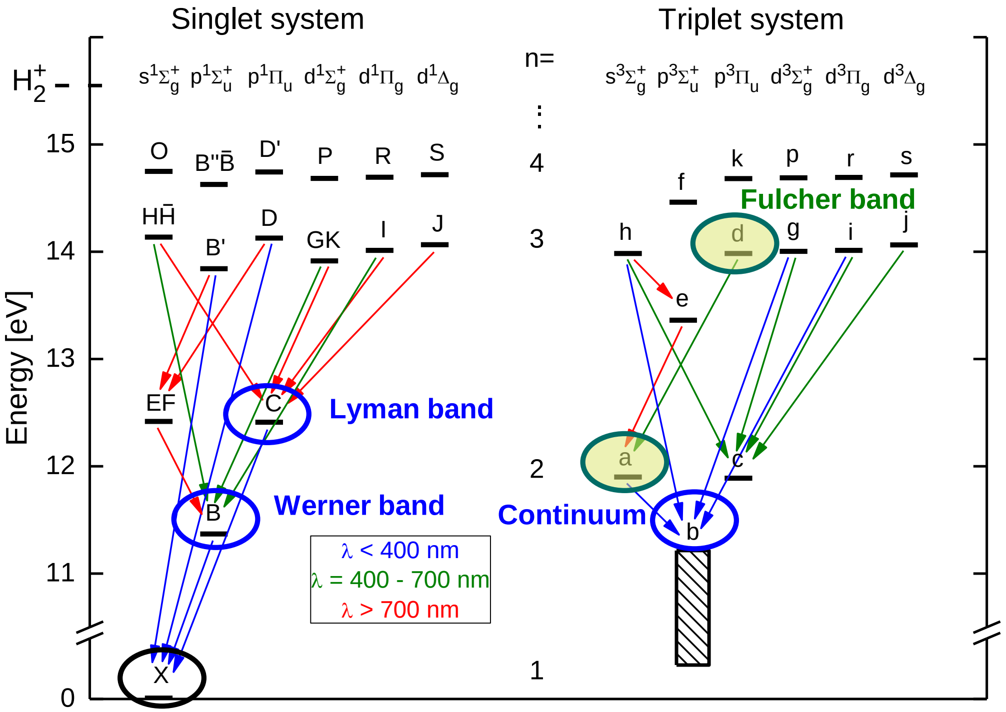
populating processes | de-populating processes

$$\frac{dn_p}{dt} = n_e[n_X X_{Xp}(T_e) + \sum_{q<p} n_q X_{qp}(T_e) + \sum_{q>p} n_q X_{qp}(T_e)] + \sum_{q>p} n_q A_{qp} - n_e[\sum_{q<p} n_p X_{pq}(T_e) + \sum_{q>p} n_p X_{pq}(T_e)] - \sum_{p>q} n_p A_{pq} - \sum_{i} n_i n_p X_{i,loss}(T_e)$$

direct excitation | stepwise exc. | coll. cascades | rad. cascades | down coll. | up coll. | radiation | further losses

Hydrogen atom & molecule





Set of ordinary differential equations
→ flexible solver Yacora

Quality of results correlates with
accuracy of reaction probabilities

Status 2014:

Yacora-H: based on ADAS data

Yacora-H2: electronically resolved, based on Janev and Miles data

and Yacora-H2(X1,v)

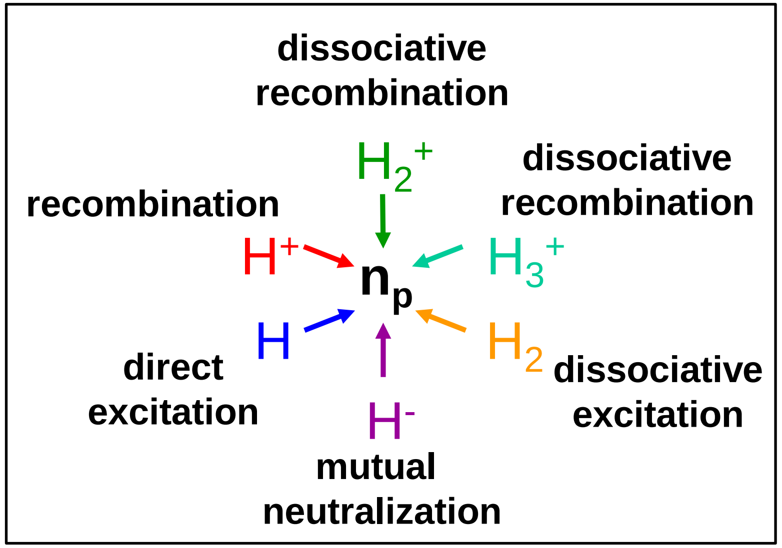
2019 → YOTW (Yacora on the Web)

Wünderlich et al.: JQSRT 240 (2020) 106695

Extended model for atomic hydrogen – Coupling to other species

Ionising and recombining plasma regions & ion-ion plasma

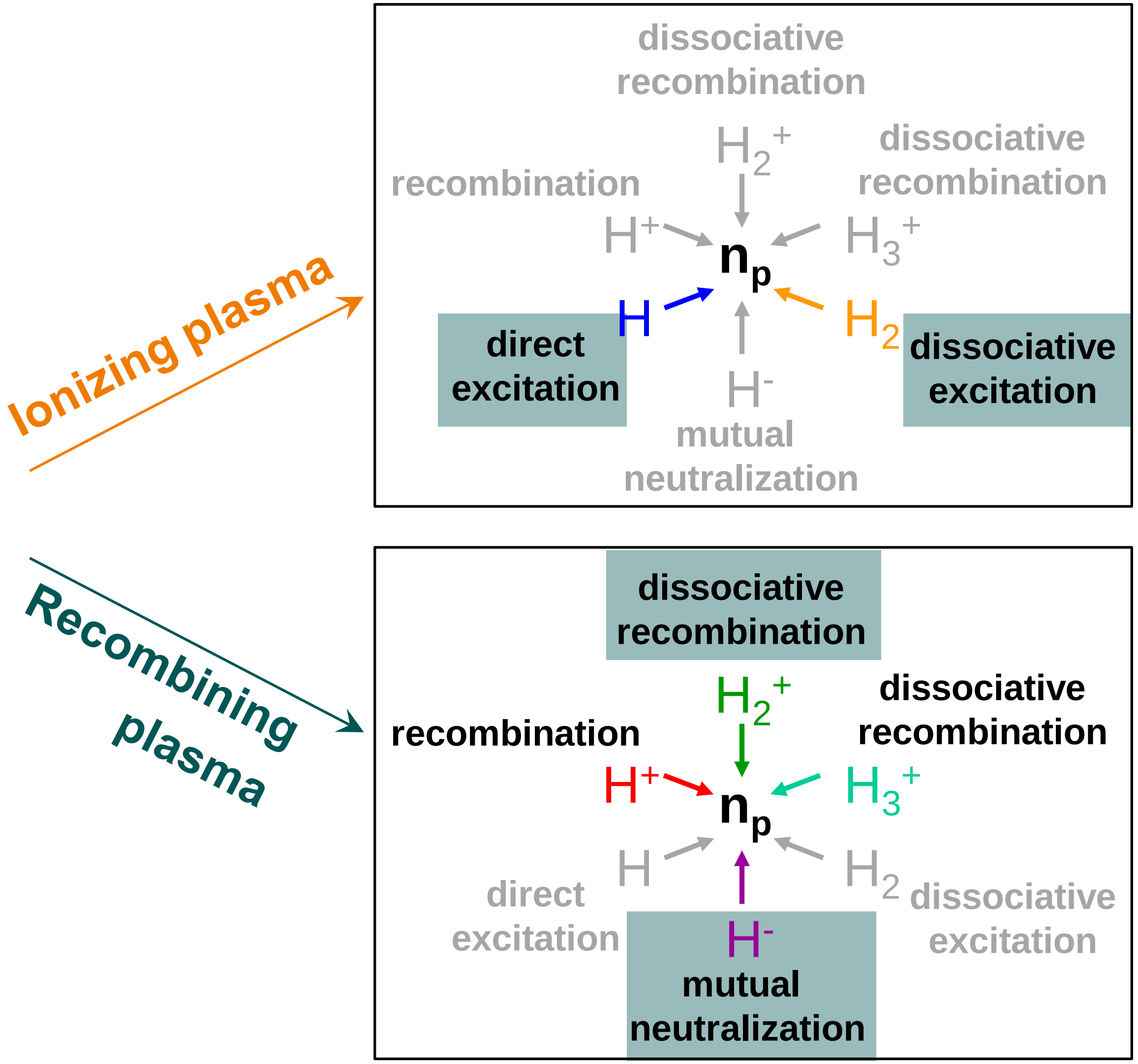
Requires coupling to all hydrogen species in a CR model



CR model: Yacora H

Wünderlich et al. Atoms. 4 (2016)26

Yacora on the Web: www.yacora.de



2024: The Yacora family

Towards a (ro-) vibrationally resolved CR model for (entire) H_2 system

Richard Bergmayr, PhD thesis in preparation

- **Electronic CR models**
  - Triplet system
  - Singlet system
  - Combined electronic model
- **Vibrationally resolved CR models**
  - Vibrationally resolved CR model for X[1]
  - Vibrationally resolved CR model for entire H_2 system
- **Ro-vibrationally resolved models**
  - Corona model for Fulcher-α band
  - Extended corona model

Benchmarking: negative ion sources (BATMAN Upgrade, ELISE), laboratory experiments, linear devices, divertor plasmas, EIRENE code, SOLPS-ITER code

Improvement in the input data basis
Electronic CR models

Electronic CR models
- **Triplet system**
- **Singlet system**
- **Combined electronic model**

Electron impact excitation

$e + H_2(n) \rightarrow e + H_2(n')$

❶ Miles data set: semi empiric cross sections
Miles et al, J. Appl. Phys. 43 (1972) 678

❷ Janev: summary of measurements and calculations
Janev et al, Report JÜL-4105 (2003)

❷ Celiberto: calculations for a few transitions, 2001.
Celiberto et al. ADNDT 77, (2001)

} significant inconsistencies

❸ MCCC: molecular convergent close-coupling method in the adiabatic-nuclei formulation, fully quantum mechanical
Scarlett et al, ADNDT 137 (2021) 101361

→ close collaboration with Fursa group, Curtin University, Australia

Improvement in the input data basis
Electronic CR models

Electronic CR models

- **Triplet system**
- **Singlet system**
- **Combined electronic model**

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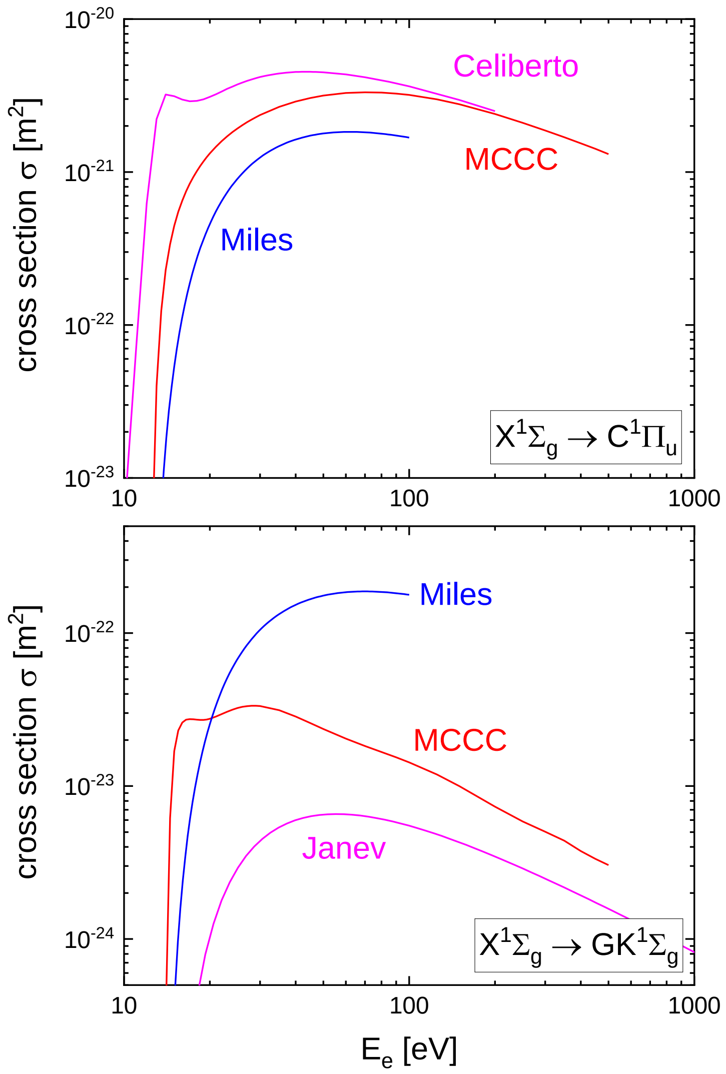
Celiberto et al. ADNDT 77, (2001)

❸ MCCC:

Scarlett et al, ADNDT 137 (2021) 101361

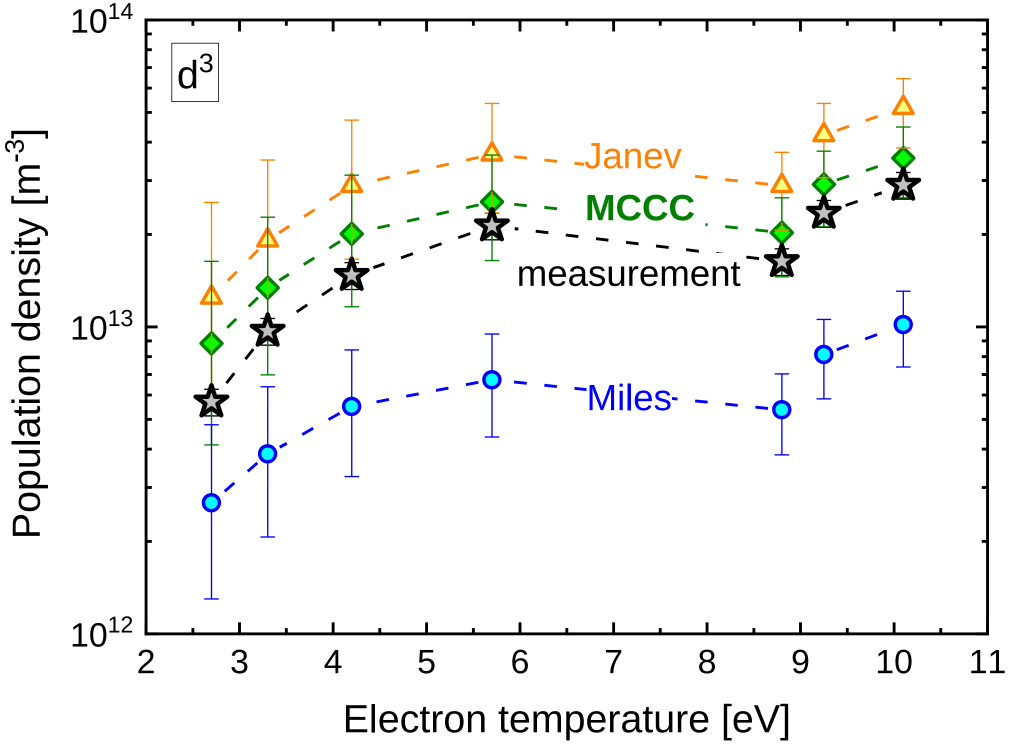


Improvement in the input data basis

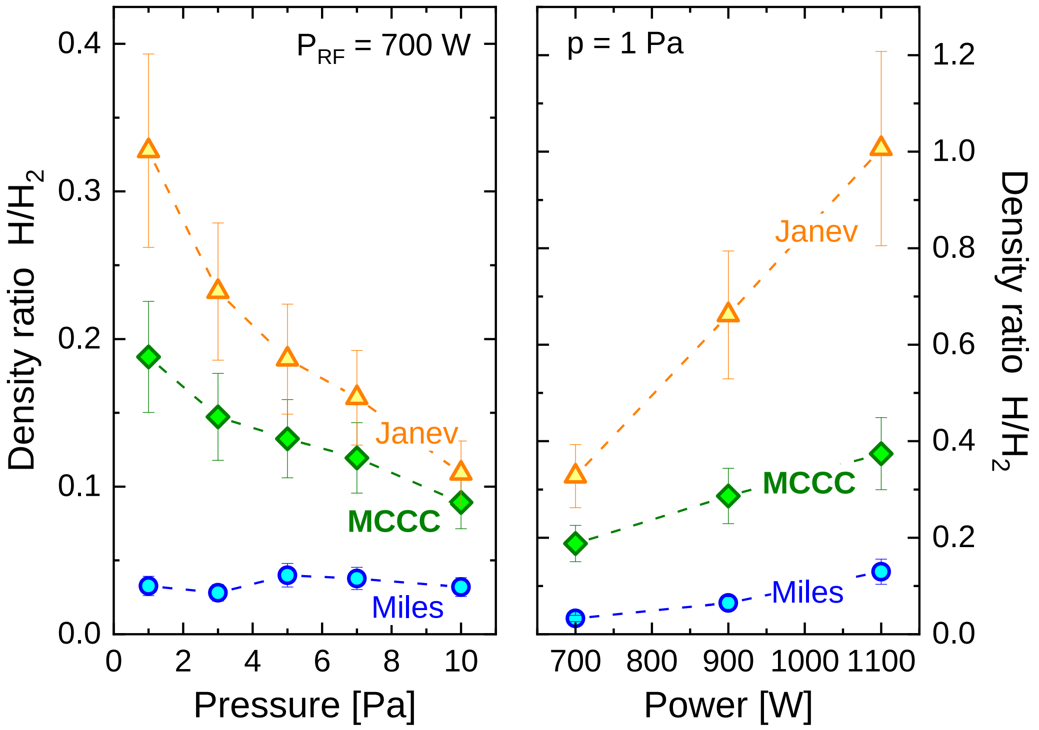
Electronic CR models – Benchmark

Low pressure, low-temperature lab experiment Wünderlich et al. J. Phys. D 54 (2021) 115201

- T_e and n_e from Langmuir probe
- Electron densities < 10^{17} m^{-3}

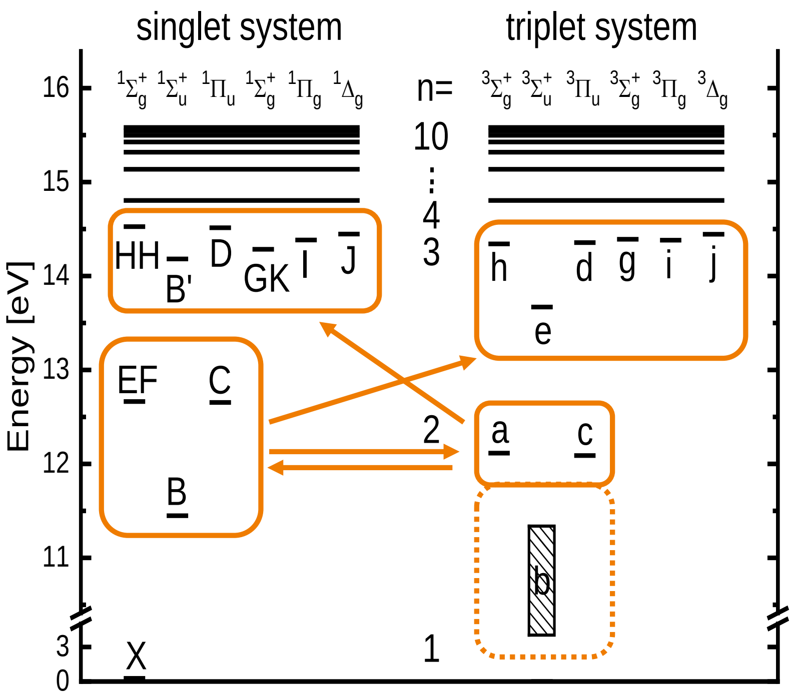


Impact of data used in the analysis on density ratio



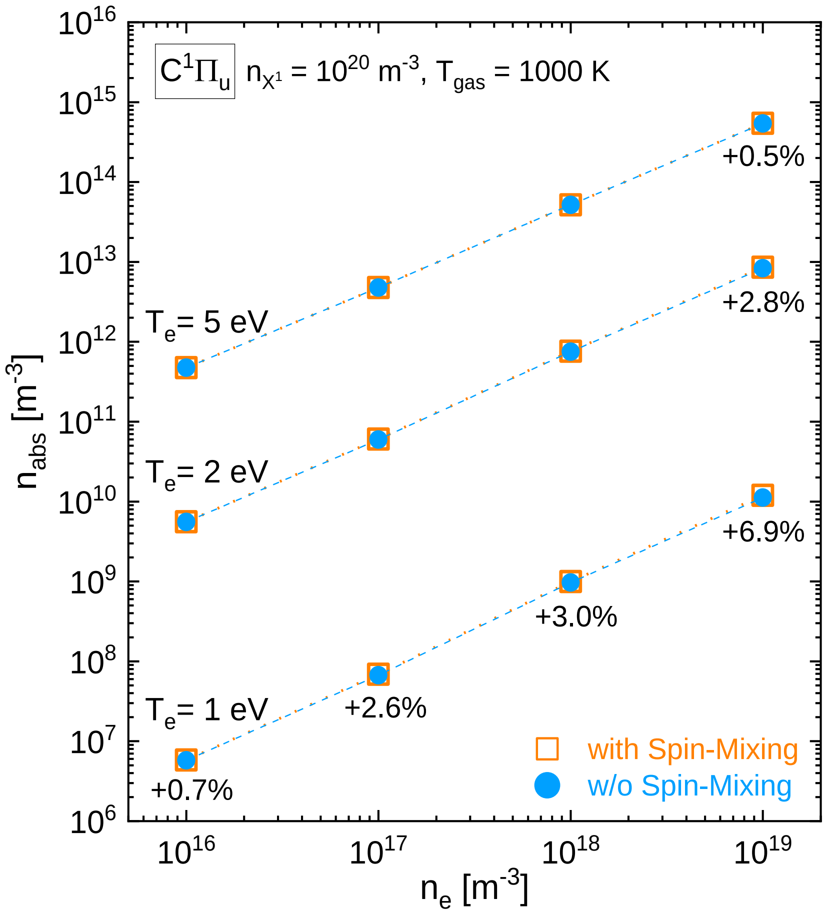
Improvement in the input data basis

Electronic CR models – Spin mixing



e + $H_2(n=2)_{singlet}$ → e + $H_2(n=2,3)_{triplet}$

e + $H_2(n=2)_{triplet}$ → e + $H_2(n=2,3)_{singlet}$



$$\frac{(n_{with} - n_{without})}{n_{without}}$$

Influence rather small but most pronounced for low T_e and high n_e.

Use of separate electronic models (singlet and triplet) sufficient

Improvement in the input data basis
Vibrationally resolved CR model for X^1 – Yacora-H2(X1,v)

Richard Bergmayr,
PhD thesis in preparation

Reaction		Model 2004	Model 2022
Electron Impact (De-) Excitation (EIE)	$e + H_2(v) \rightarrow e + H_2(v')$	Buckman 1985	replaced
Electron Impact Dissociation (EID)	$e + H_2(v) \rightarrow e + H_2(n>1) \rightarrow e + H + H$	Celiberto 1999	MCCC
Dissociative Attachment (DA)	$e + H_2(v) \rightarrow H + H^-$	Bardsley 1979	Horacek 2004, Laporta
Charge Exchange (CX)	$H^+ + H_2(v) \rightarrow H + H_2^+$	Janev 2008	replaced
Non-Dissociative Ionization (NDI)	$e + H_2(v) \rightarrow e + e + H_2^+$	Wünderlich 2021	no change
Radiative Recombination (RR)	$e + H_2^+ \rightarrow H_2(v)$	Sawada 1995	no change
Collisional 3 Particle Recombination (C3PR)	$e + e + H_2^+ \rightarrow e + H_2(v)$	Sawada 1995	no change
Transitions via B and C	Electron Impact (De-)Excitation Spontaneous Emission	Celiberto 2001, Janev 2003 Fantz 2006	MCCC no change
Dissociative Ionization (DI)	$e + H_2(v) \rightarrow e + e + H + H^+$	-	✓
Proton Impact (De-) Excitation (PIE)	$H^+ + H_2(v) \rightarrow H^+ + H_2(v')$	-	✓
Proton Impact Dissociation (PID)	$H^+ + H_2(v) \rightarrow H^+ + H + H$ $H^+ + H_2(v) \rightarrow H + H^+ + H$	-	✓
H- Associative Detachment (H-AD)	$H^- + H \rightarrow H_2(v') + e$	-	✓
Hydrogen Atom Impact Dissociation (HAID)	$H + H_2(v) \rightarrow H + 2\,H$	-	✓
Hydrogen Molecule Impact Excitation (HMIE)	VT: $H_2(v) + H_2(w) \rightarrow H_2(v\pm1) + H_2(w)$ VV: $H_2(v) + H_2(w+1) \rightarrow H_2(v+1) + H_2(w)$	-	✓
H_3^+ Dissociative Recombination (H3+DR)	$e + H_3^+ \rightarrow H + H_2(v')$	-	✓
Hydrogen Atom Impact (De-) Excitation (HAIE)	$H + H_2(v=0) \rightarrow H + H_2(v'>0)$	-	✓

Improvement in the input data basis

Vibrationally resolved CR model for X[1] – Yacora-H2(X1,v)

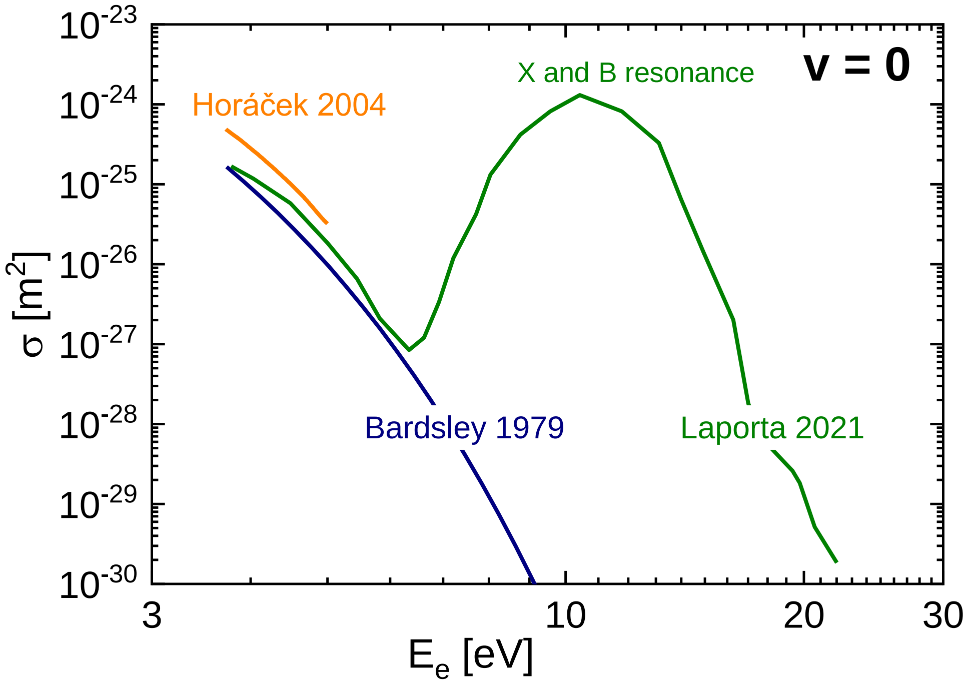
Dissociative Electron Attachment DEA

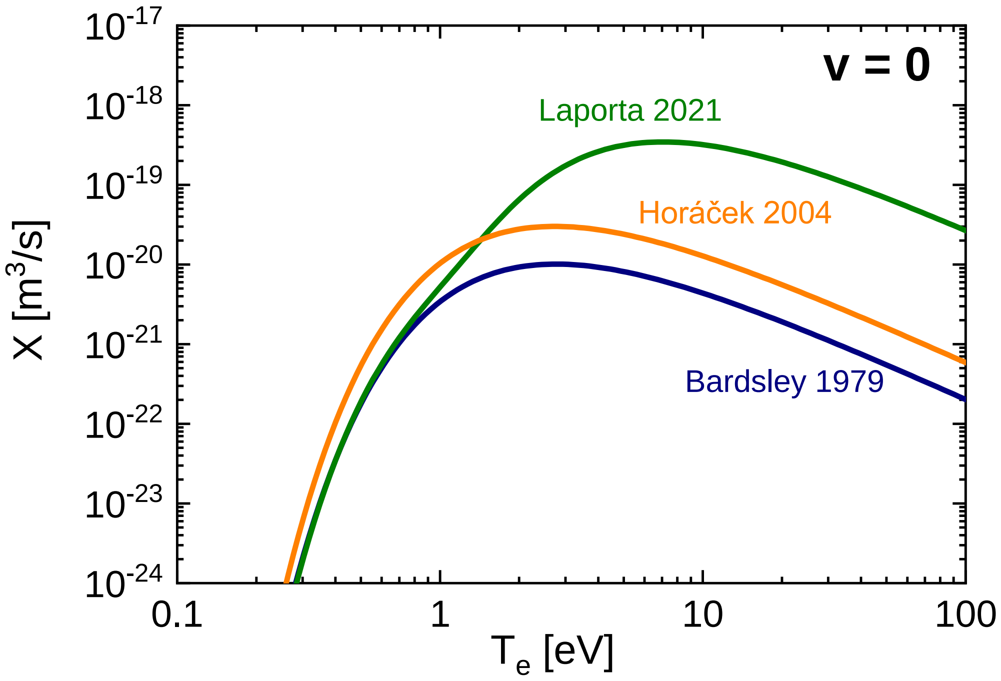
$e + H_2(v) \rightarrow H_2^- \rightarrow H + H^-$

- Process can proceed via several resonances $H_2^-(X^2\Sigma_u^+, B^2\Sigma_g^+, C^2\Sigma_g^+)$
- Previously only channel via $H_2^-(X^2\Sigma_u^+)$ included
- Laporta 2021: consideration of other resonances

→ implementation of Horáček 2004, replaced then by Laporta data 2024 [private communication]

Bardsley and Wadehra, Phys. Rev. A 20 (1979) 1398
Horáček et. al, Phys. Rev. A 70 (2004) 052712
Laporta et al, Plasma Phys. Contr. Fus. 63 (2021) 085006





Improvement in the input data basis

Vibrationally resolved CR model – Yacora-H2(v)

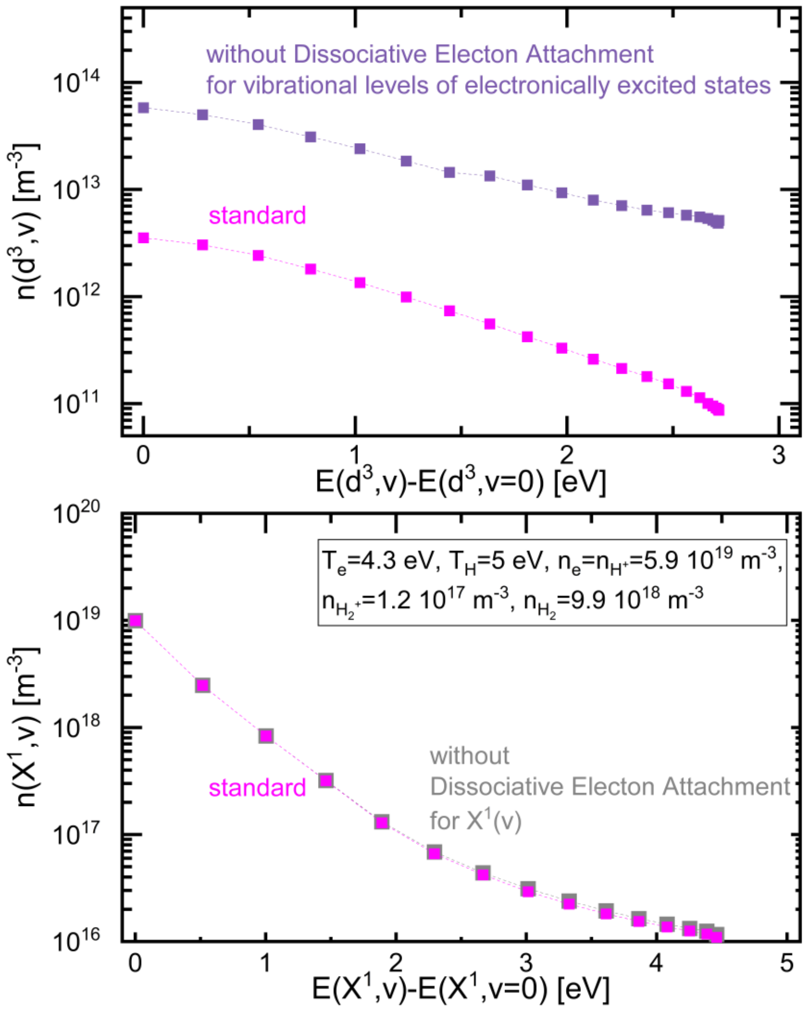
Dissociative Electron Attachment DEA for (vibrational levels of) electronically excited states

- Studies and input data in literature scarce!
- Constant rate coefficients (motivated by measurements) applied
  - $X_{DEA}(n=2) = 1 \cdot 10^{-15}$ m^3/s
  - $X_{DEA}(n=3) = 6 \cdot 10^{-11}$ m^3/s

Hiskes, Applied Physics Letters 69 (1996) 755
Datskos et al., Phys. Rev.. A, 55 (1997) 4131

- Comparison of (d^3,v)-densities between standard Yacora-H2(v) calculation and calculation without DEA for vibrational levels of electronically excited states shows discrepancy by one order of magnitude (for given plasma parameters)
- (Preliminary) benchmarks with measurements suggest smaller but not neglectable $X_{DEA}(n=3)$

$$e + H_2(n\Lambda_\sigma,v) \rightarrow H_2^- \rightarrow H + H^-$$



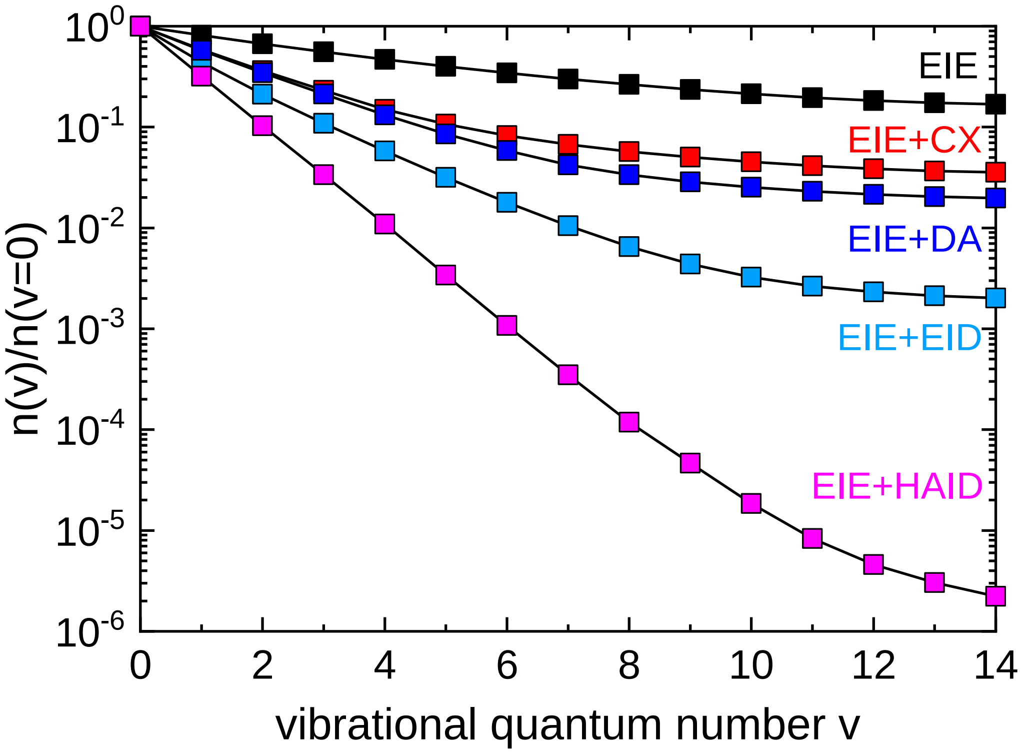
R.C. Bergmayr et al., Nuclear Materials and Energy, submitted

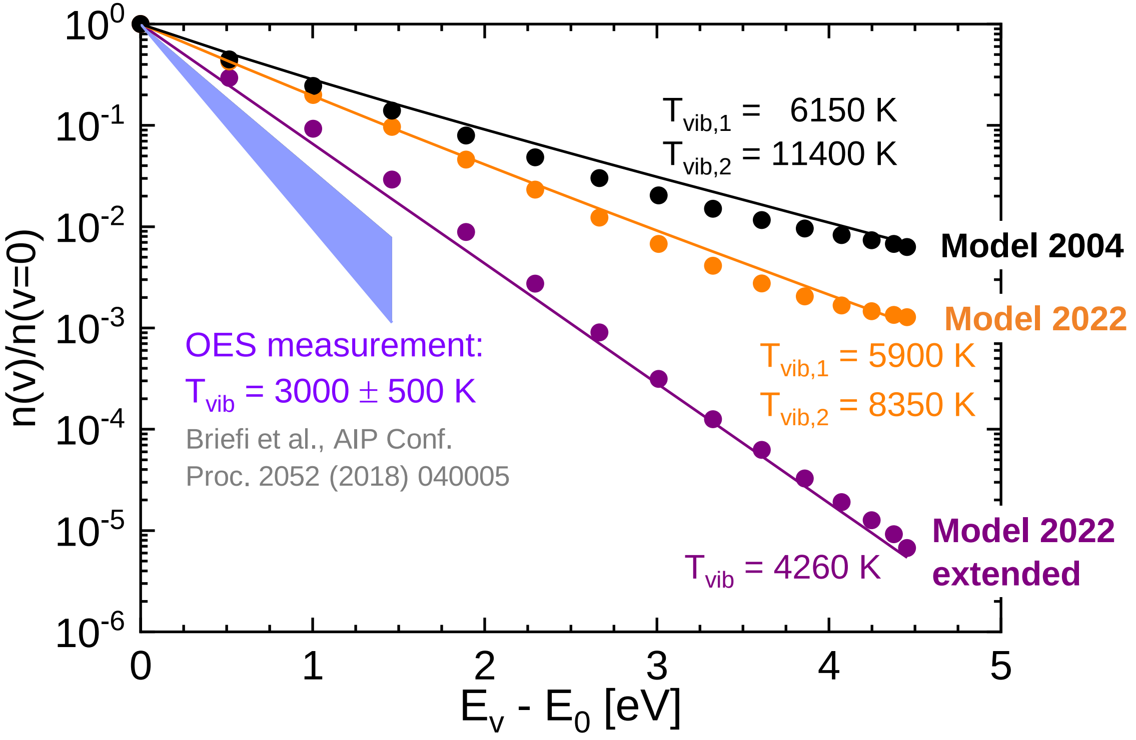
Improvement in the input data basis

Vibrationally resolved CR model for X^1 – Yacora-H2(X1,v) – Benchmark

Negative hydrogen ion source, low temperature plasma

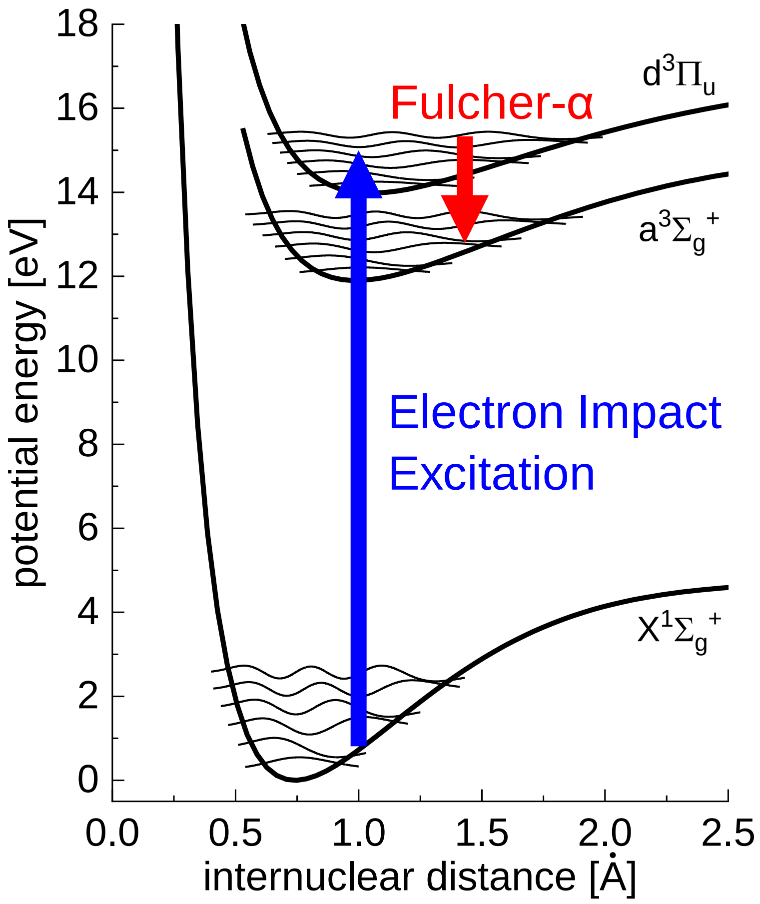
$T_e = 2.5$ eV	$n_e = 6 \cdot 10^{16}$ m^{-3}	$n_{H^-} = 10^{17}$ m^{-3}
$T_H = T_{H^-} = T_{H^+} = 0.8$ eV	$n_{H_2} = 3 \cdot 10^{19}$ m^{-3}	$n_{H^+} = n_{H_2^+} = 2.4 \cdot 10^{16}$ m^{-3}
$T_{H_2} = T_{H_2^+} = T_{H_3^+} = 0.1$ eV	$n_H = 10^{19}$ m^{-3}	$n_{H_3^+} = 1.2 \cdot 10^{16}$ m^{-3}





Improvement in the input data basis

Ro-vibrationally resolved Corona model – Yacora-H2(v,N)-Fulcher



- Ground state $n(X^1, v, N)$ according to two-temperature distribution

$$n(X^1, v', N') =$$
$$n_{H2}\left[(1-\beta)\,\tilde{n}_{rot}(v', N', T_{gas})\,\tilde{n}_{vib}(v', T_{vib1}) + \beta\,\tilde{n}_{rot}(v', N', T_{rot2})\,\tilde{n}_{vib}(v', T_{rot2})\right]$$

- Rate equation: $$\frac{dn_p}{dt} = \sum_{q<p} X_{qp} n_q n_e - \sum_{q<p} A_{pq} n_p$$

Electron Impact Excitation (EIE)
$e + H_2(X^1,v,N) \rightarrow e + H_2(d^3,v',N')$
Spontaneous Emission
$H_2(d^3,v',N') \rightarrow H_2(a^3,v'',N'') + hf$

- Separate treatment of $d^3(v,N)+$ and $d^3(v,N)-$ (selection rules)
- 45 259 fully ro-vibrationally resolved MCCC cross sections applied

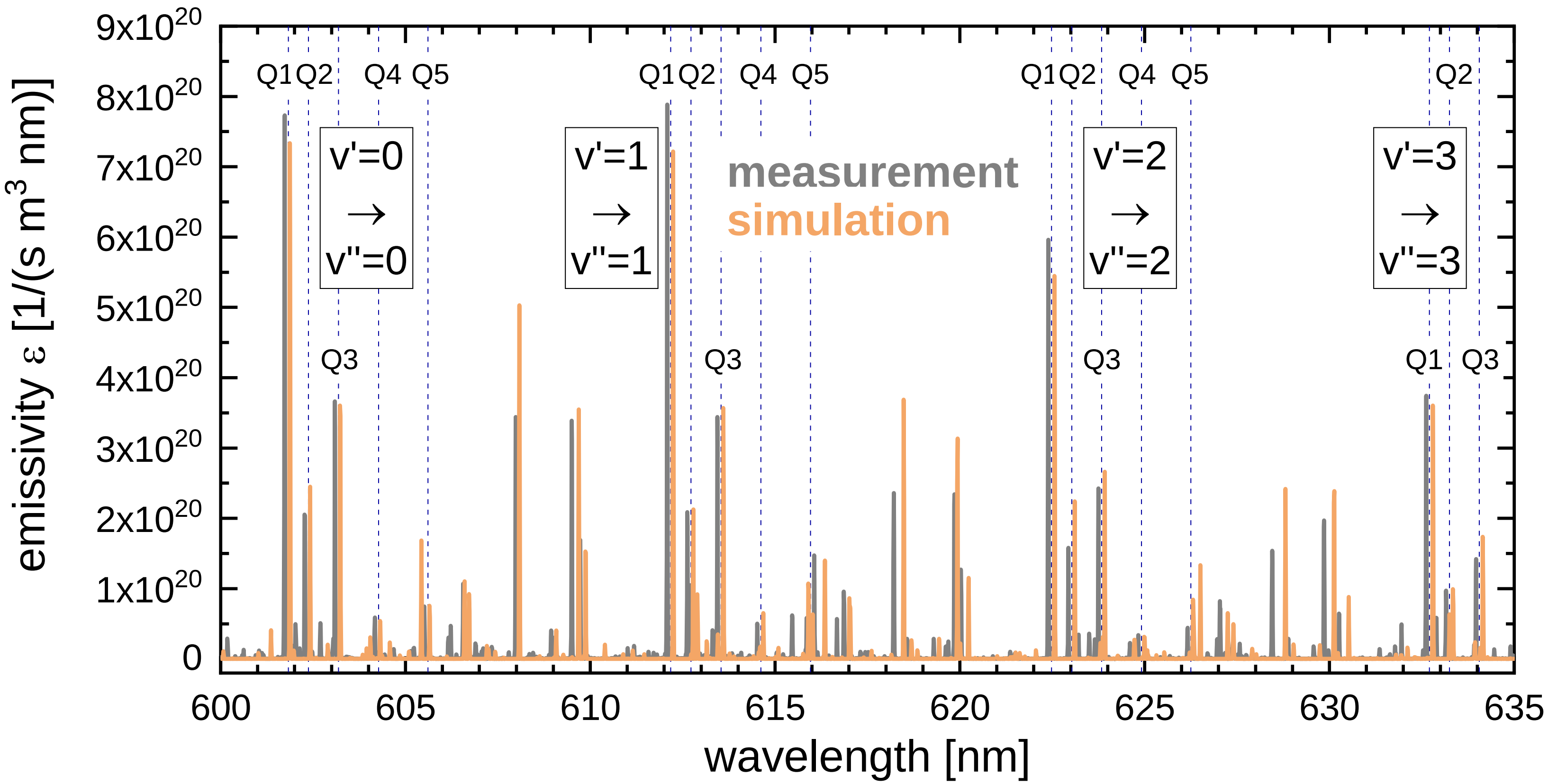
Scarlett et al., Phys. Rev. A 107 (2023) 06280

Improvement in the input data basis

Ro-vibrationally resolved Corona model – Yacora-H2(v,N)-Fulcher

Benchmark with spectra from lab experiment (ICP, p = 1.1 Pa, P_{RF} = 700 W)

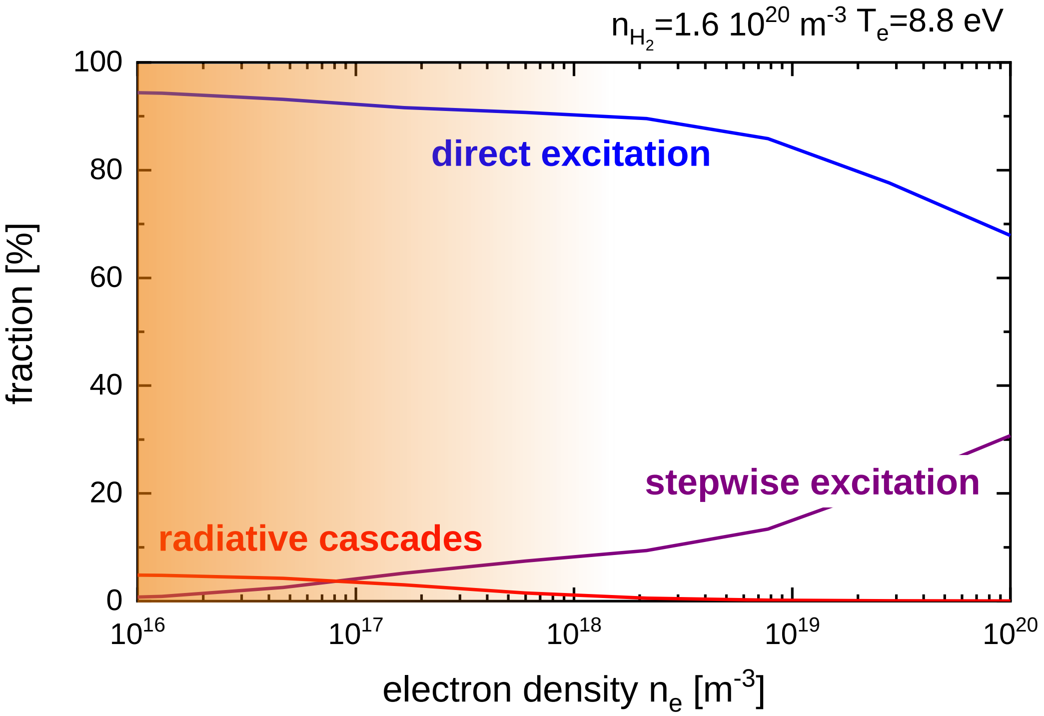
T_e = 8.8 eV, n_e=1.84 10^{16} m^{-3} from Langmuir probe

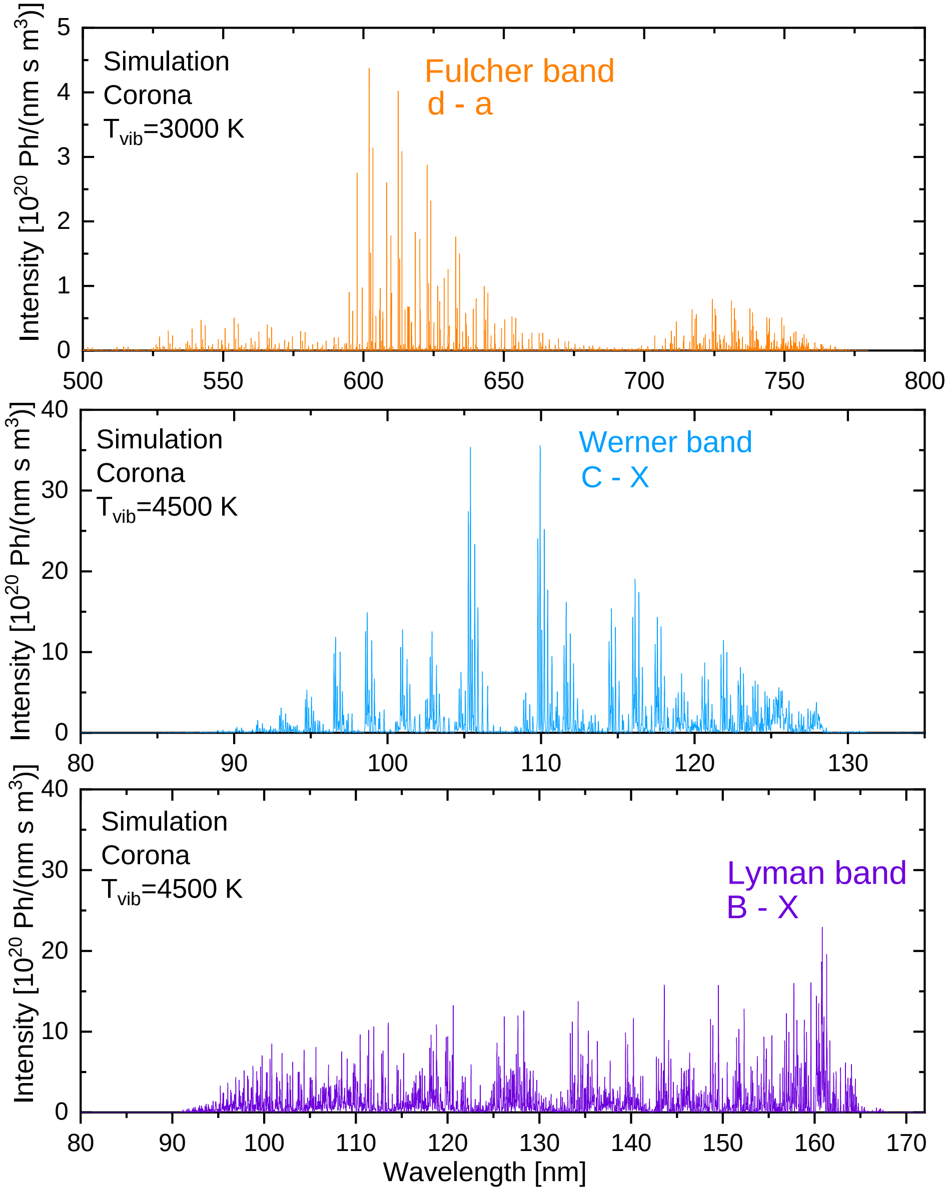


- Excellent agreement in absolute values
- Previous model → factor 3 higher emissivity
- Q-lines show general agreement

Improvement in the input data basis
Ro-vibrationally resolved Corona models

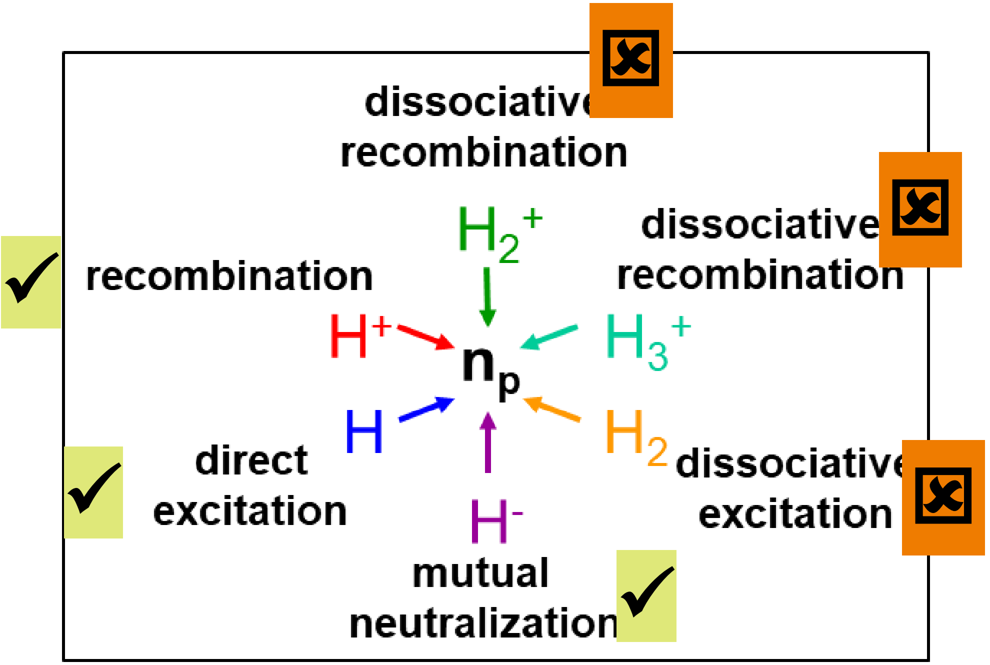
Applicability of Corona model
→ check with **electronic CR model**





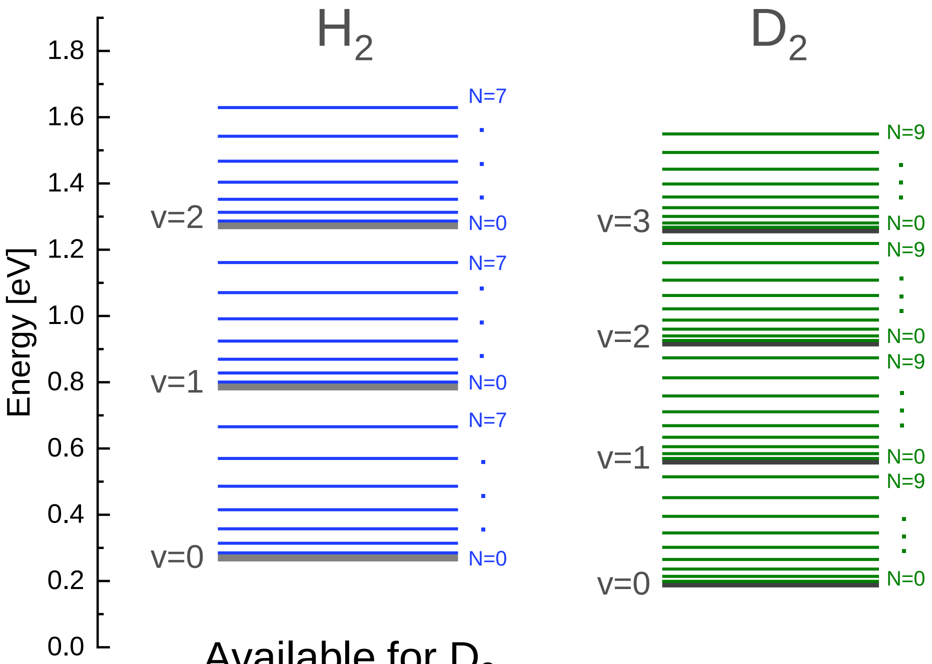
Towards deuterium

Atomic model



and opacity effects

Molecules



Available for D_2

- Transition probabilities A_{ik}
- Dissociative attachment (Laporta)
- Ionisation Gryzinski method and MCCC

In planning: Yacora-D2(v) with MCCC data
[private communication]

Summary

Recent progress of collisional radiative modelling of H_2 with Yacora

Electronic CR models
- Triplet system
- Singlet system
- Combined electronic model

Vibrationally resolved CR models
- Vibrationally resolved CR model for X[1]
- Vibrationally resolved CR model for entire H_2 system

Ro-vibrationally resolved models
- Corona model for Fulcher-α band
- Extended corona model

Accompanied by benchmarking to experimental data

Towards a (ro-) vibrationally resolved CR model for (entire) H_2 system and D_2

Atomic and molecular model
Status 2014/2019
YOTW
Yacora on the Web

Data status, availability and recommendations

Main messages from this talk

MCCC data is open available and their usage is benchmarked in different devices

- electronically resolved, for H_2 and its isotopomeres
- vibrationally resolved
- working on rot-vib resolved data ?

Implementation of MCCC data for hydrogen (deuterium) in fusion codes for neutrals like EIRENE, SOLPS, …

The Yacora family is benchmarked and available for further testing in extended parameter ranges

- coupling to H atom (and thus D as well) available
- low T_e down to 1 eV and low n_e done for H_2
- lower T_e and higher n_e @ Magnum PSI underway
- models and experimental data for D_2 are missing

Yacora can provide effective rate coefficients as look-up tables to be exchanged and tested against AMJUEL data, …

The currently used data set for A & M data for hydrogen **should be exchanged** by updated and recommended data **to catch the right physics** in low temperature fusion (relevant) plasmas).

The step to deuterium is essential.