



MPG contribution to SP X.1 Atomic and molecular processes in attached/detached plasmas

TASK: Atomic and molecular hydrogen spectroscopy in ionizing and recombining plasmas
D0004: Interpretation spectroscopy results using spectra simulation and (CR) modelling with YACORA (MPG)

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Yacora: a flexible solver for Collisional Radiative models

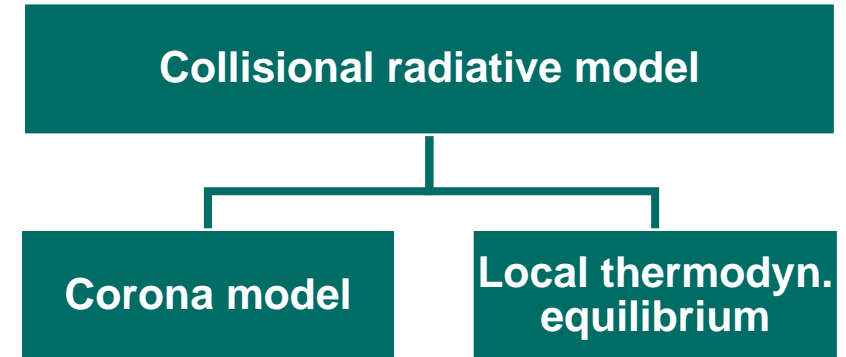
D. Wunderlich et al, Atoms 4, 2016, 26

Yacora is a flexible (0D)-solver for CR models:

- Used and improved for more than 20 years
- Many CR models built on that solver, focus here: H and H₂

CR model for...	# states	Comment	
H ₂	Electronic states only	33	Well benchmarked
	Some vibrational states	214	Well benchmarked
	Vib-rot resolved	>626	Extended Corona models
H	44	Coupling to H⁺, H₂⁺, H₃⁺, H⁻, very well benchmarked	
He	19	Very well benchmarked	
Ar		Well benchmarked	

Additionally available are: Ar⁺, Cs, N₂, C₂, CH in different status,



- Extensive data base of reaction probabilities
- Drastically increased complexity for molecules
- Data for H based on ADAS and ...
- Data for H₂ based on MCCC data and ...

L. Scarlett et al, ADNDT 137, 2021, 101361

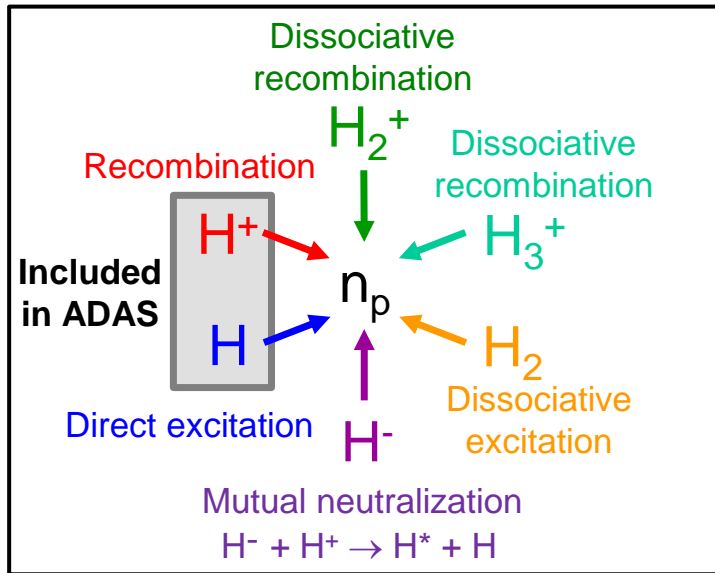
- Dedicated PhD thesis, present status in

R. Bergmayr et al, Eur. Phys. J. D 77, 2023, 302

D₂ in preparation



Atomic and molecular hydrogen models



- Ionizing and recombining plasmas
- Opacity is an option

Electron ion recombination

Molecular assisted recombination

EIR

MAR

Ionization

$T_e < .5 \text{ eV}, n_e = 10^{21} \text{ m}^{-3}$

$T_e \sim 2-5 \text{ eV}, n_e = 10^{19}-10^{21} \text{ m}^{-3}$

$T_e > 10 \text{ eV}$

H₂ models for different purposes

Electronic states

Population factors,
Effective rate coefficients

For full analysis:
coupling of H and H₂

Vibrationally resolved

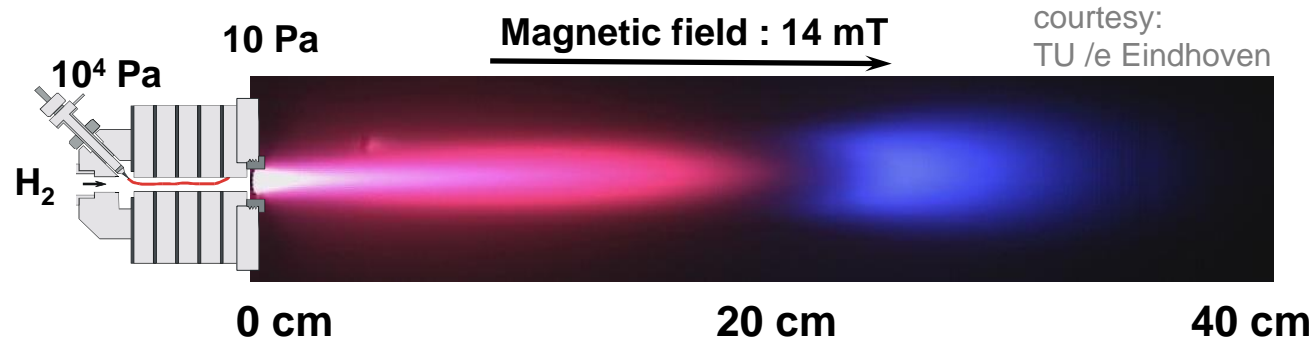
Vibrational population
H₂(v)

Ro-vib, resolved
Corona

Simulation of spectra

Example for analysing recombining and ionizing plasmas

Linear plasma device: cascaded arc at TU/e Eindhoven

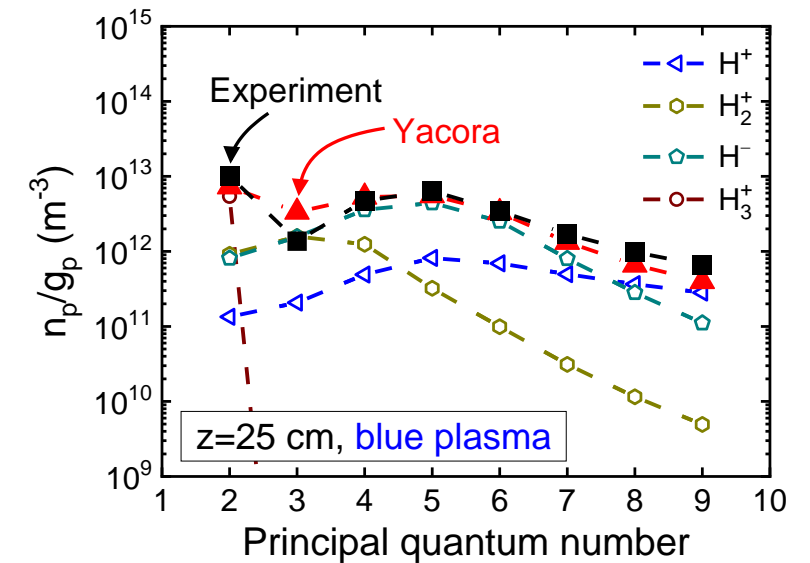
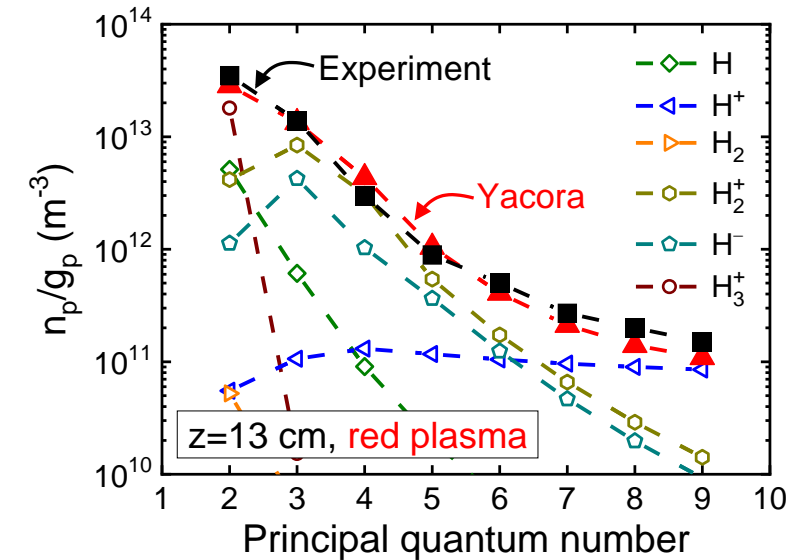


Plasma parameters from Thomson scattering, probes, OES, ...

W.E.N. van Harskamp, Phys. Rev. E 83, 2011, 036412

Excellent agreement experiment ↔ Yacora for red and blue plasma

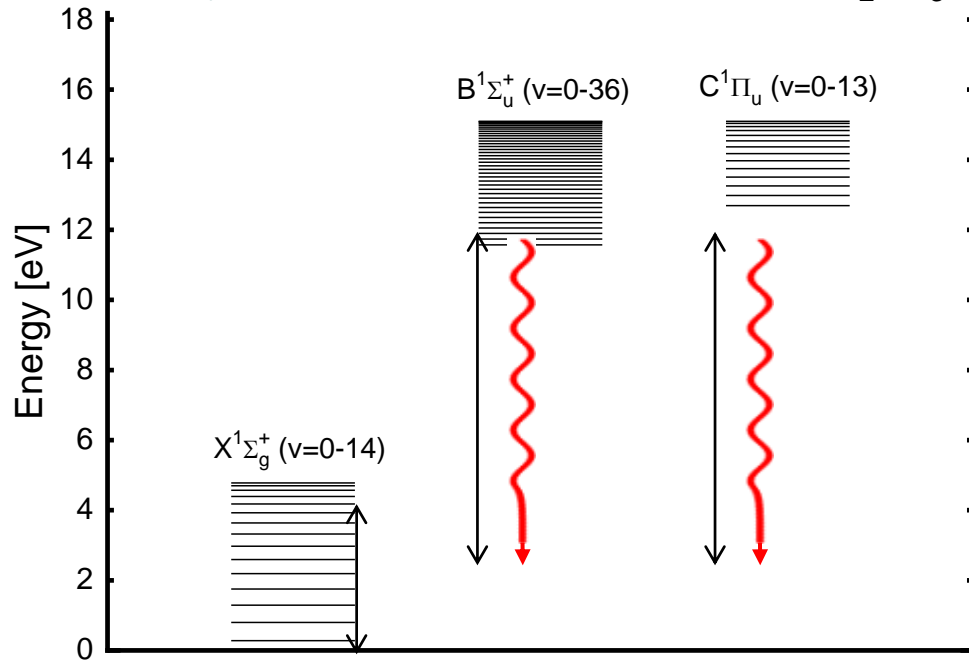
- Atomic and molecular excitation channels play a role
- **Correct prediction of overpopulation of n=4,5 and 6**





Vibrationally resolved CR model, $H_2(v)$ population

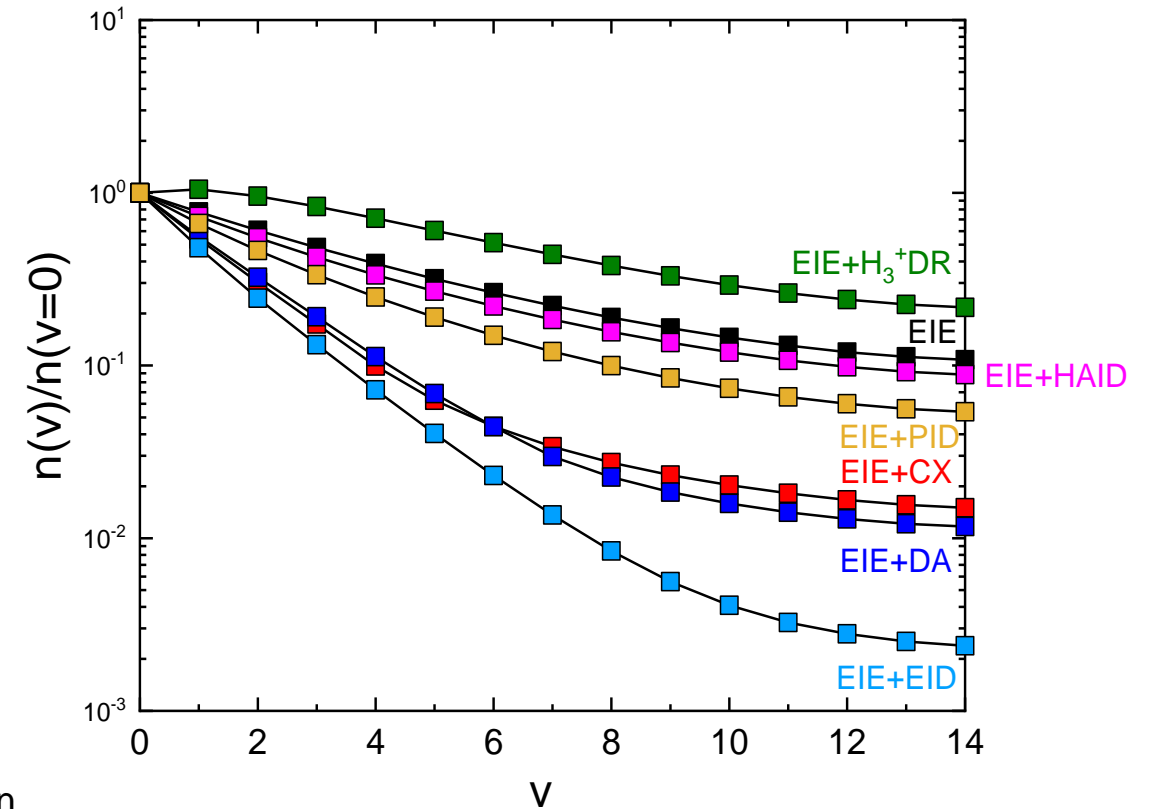
Electron collisions, spontaneous emission,
including B^1 and C^1 states
Heavy Particle Collisions (H, H^+, H^-, H_2, H_3^+),



- EIE: Electron impact Excitation
- EID: Electron Impact Dissociation
- H3+DR: Diss. recombination H_3^+
- DA: Dissociative Attachment
- CX: Charge Exchange
- HAID: H Impact Dissociation
- PID: Proton Impact Dissociation

Divertor plasma conditions

$T_e = T_H = T_{H^+} =$	$n_e = 10^{20} \text{ m}^{-3}$	$n_{H^+} = 4 \cdot 10^{19} \text{ m}^{-3}$
$= T_{H_2^+} = T_{H_3^+} = 2 \text{ eV}$	$n_{H_2} = 5 \cdot 10^{19} \text{ m}^{-3}$	$n_{H_2^+} = 4 \cdot 10^{19} \text{ m}^{-3}$
$T_{H_2} = 2/3 \text{ eV}$	$n_H = 5 \cdot 10^{18} \text{ m}^{-3}$	$n_{H_3^+} = 2 \cdot 10^{19} \text{ m}^{-3}$





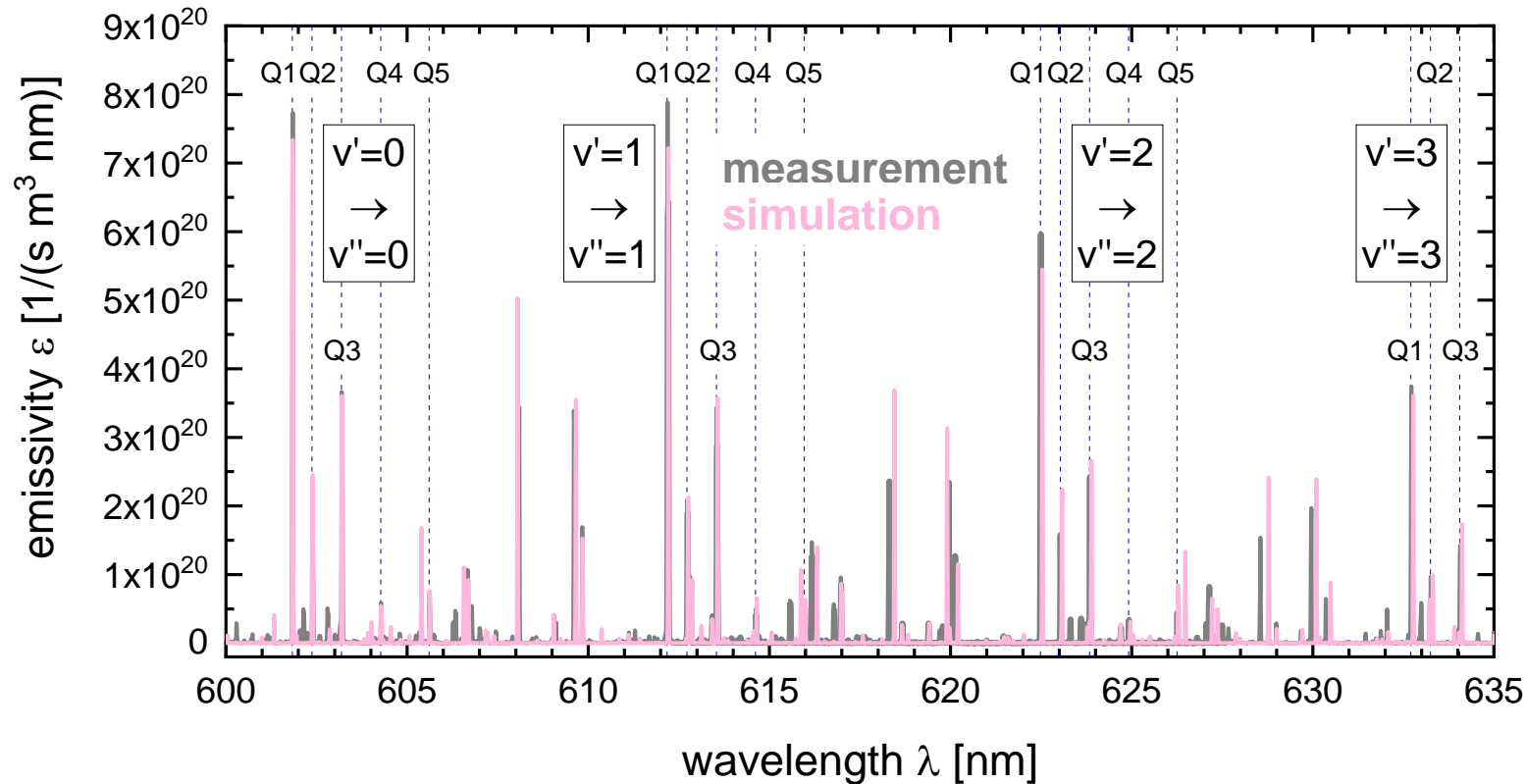
Ro-vibrationally resolved (corona) model

Simulation of spectra

Example: Fulcher transition in a low temperature ICP

$$T_e = 9 \text{ eV}$$

$$n_e = 2 \times 10^{16} \text{ m}^{-3}$$



$$T_{\text{rot},1} = 500 \text{ K}$$
$$T_{\text{rot},2} = 7500 \text{ K}$$
$$T_{\text{vib}} = 4200 \text{ K}$$

Closing remark

We look forward to analysing the Magnum PSI data and participating in the measurements.