Atomic and Molecular data for collisional radiative modelling relevant to fusion

D. Wünderlich and U. Fantz

Atomic and Molecular Data for fusion: Outline of the talk.

- Collisional radiative modelling for fusion
- Atomic and molecular data for collisional radiative modelling
- Application of collisional radiative models

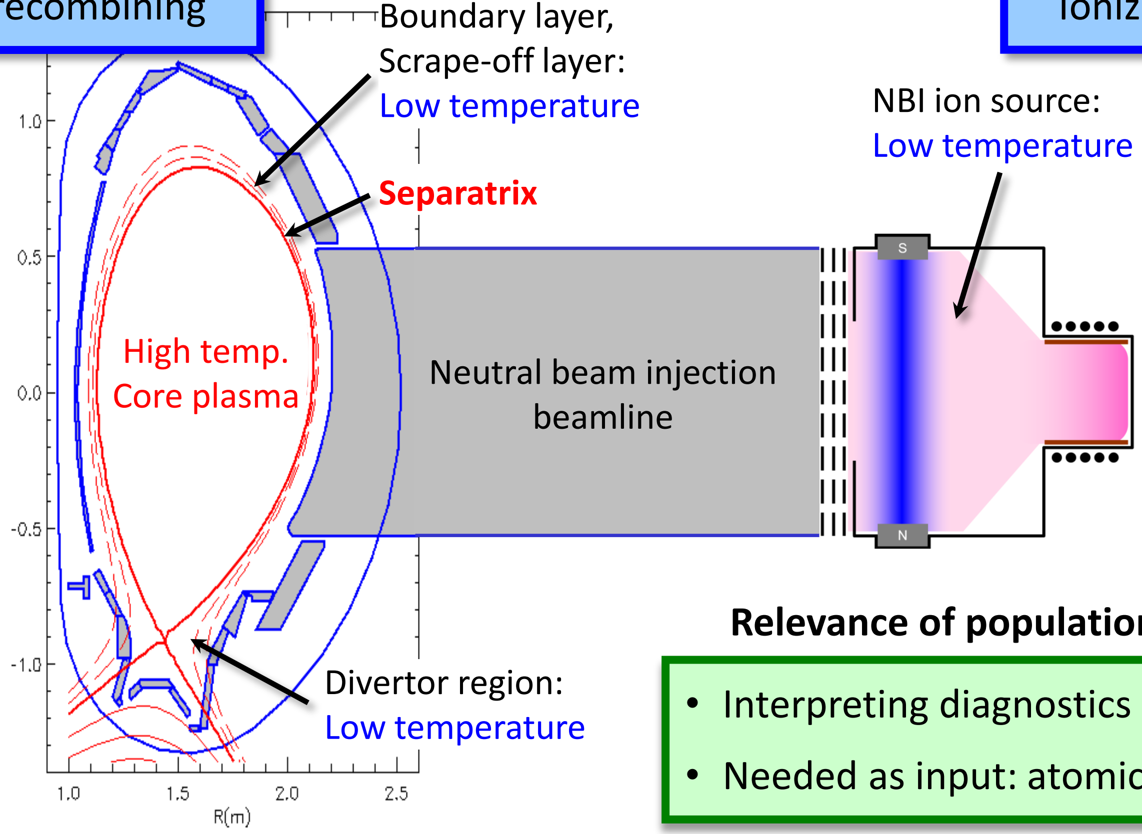
Population models for fusion plasmas: Overview.

Tokamak plasma edge

Wide parameter range
T_e=50 eV … below 1 eV
n_e=10^{18} m^{-3} … 10^{21} m^{-3}
Ionizing → recombining

NBI ion source plasma

Wide parameter range
T_e= ≈10 eV … ≈1 eV
n_e=10^{18} m^{-3} … 10^{17} m^{-3}
Ionizing → recombining



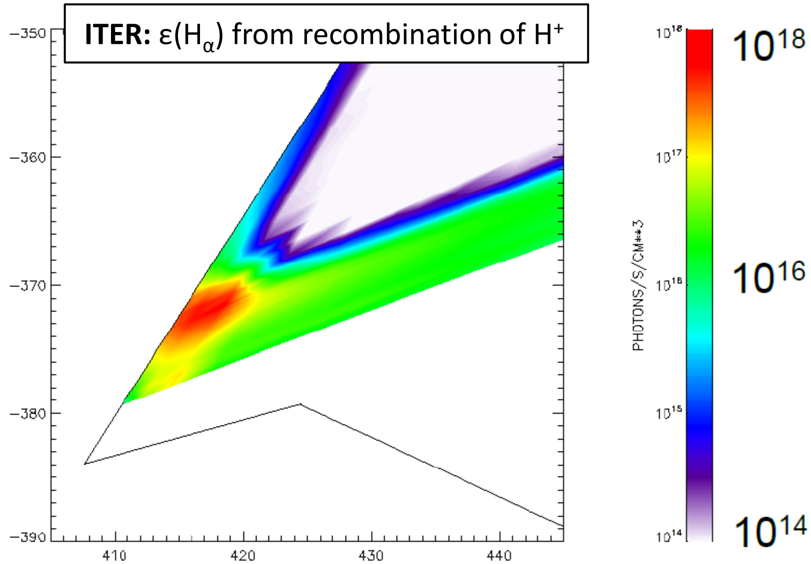
Relevance of population models:

- Interpreting diagnostics results.
- Needed as input: atomic and molecular data.

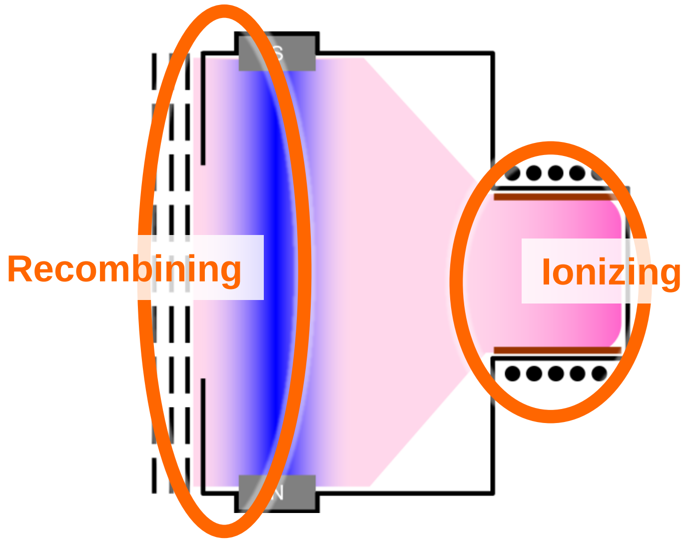
Population models for fusion plasmas: Motivation and relevant species.

Low-temperature regions of tokamak plasma

- Operated in H_2, D_2 and/or T_2.
- High relevance of atomic and also molecular processes, especially in the detached case.
- Molecular assisted recombination.
- Impurity seeding (N_2, Ar, …) $\Rightarrow$ enhanced radiation losses.
- Optical thickness.



Picture by courtesy of D. Reiter, FZ Jülich



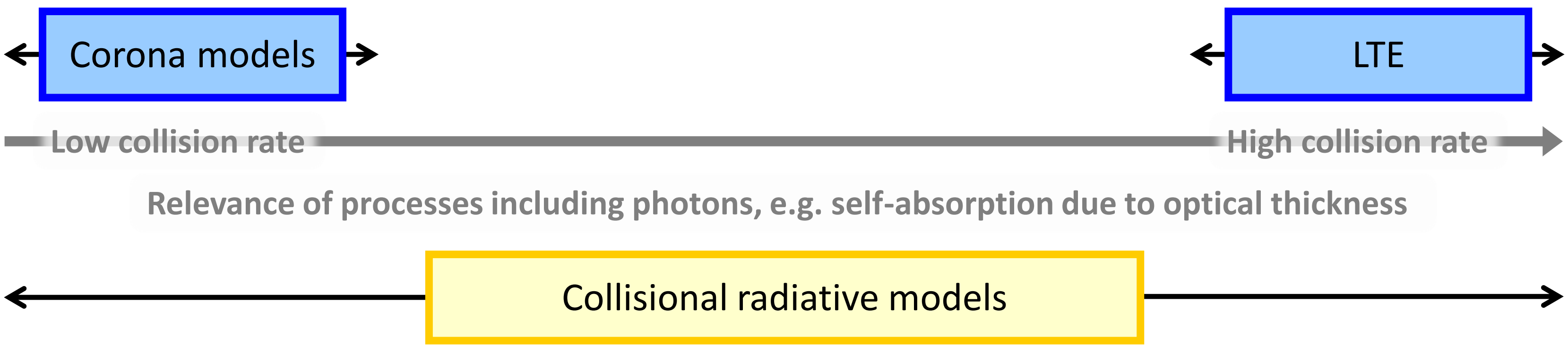
Ion source for neutral beam injection

- Operated in hydrogen or deuterium.
- Presence of caesium.
- Well defined transition ionizing-recombining plasma (created by a magnetic filter field).
- Optical thickness.

Population models for fusion plasmas: Collisional Radiative models.

Population models

- Predict population densities in dependence of plasma parameters (T_e, n_e, ground state densities).
- Main field of application: plasma diagnostics.



Collisional radiative models

Balance all relevant exciting and de-exciting reactions.

⇒ Needed: extensive data base of reaction probabilities.

⇒ Drastically increased complexity for molecules (vibrational and rotational excitation).

Error bar of model results directly correlates with the quality of the used input data.

Population models for fusion plasmas: Yacora and available Collisional Radiative models.

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

- Used and improved for more than 16 years.
- Almost all available CR models are relevant for application in plasmas used for fusion:

CR model for…		# states	Comment
H_2	Electronic states only	33	Issues with some cross sections, well benchmarked
	Some vibrational states	214	Issues with some cross sections, well benchmarked
	Vib-rot resolved	>626	Ext. Corona models for different transitions
H		44	Coupling to H^+, H_2^+, H_3^+, H^-, very well benchmarked
He		19	Very well benchmarked
Ar		16	Well benchmarked
Ar^+		84	Only a collection of input data, not benchmarked
N_2	Electronic states only	6	Includes energy transfer to metastable Ar
C_2	Vibrationally resolved	80	
CH	Vibrationally resolved	29	
Cs		11	Includes MN H^- with Cs^+, well benchmarked

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

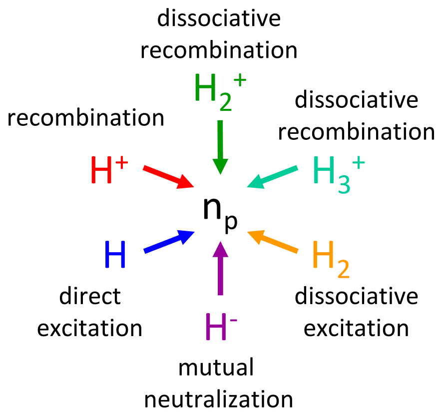
- Collisional radiative modelling for fusion
- Atomic and molecular data for collisional radiative modelling
- Application of collisional radiative models

Atomic data in Collisional Radiative models: Situation for light atoms.

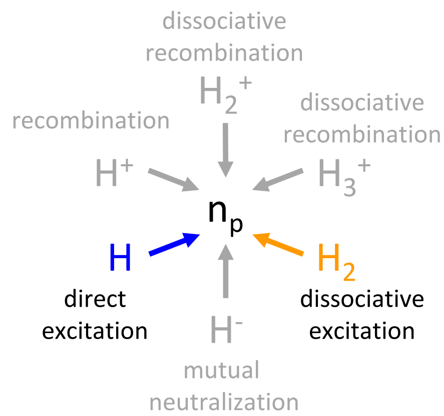
Collisional radiative modelling for light atoms:

- Very good completeness and quality of the available input data (for direct excitation).
- Some small adjustments were performed in the last years. Example: hydrogen.

Excitation of atomic hydrogen…

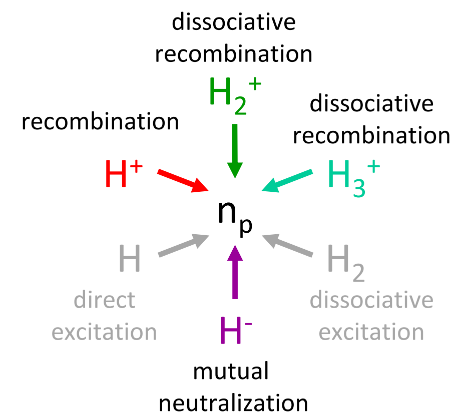


…in ionizing…



- **Attached divertor plasma**
- **Driver region of NBI sources**

…and recombining plasmas



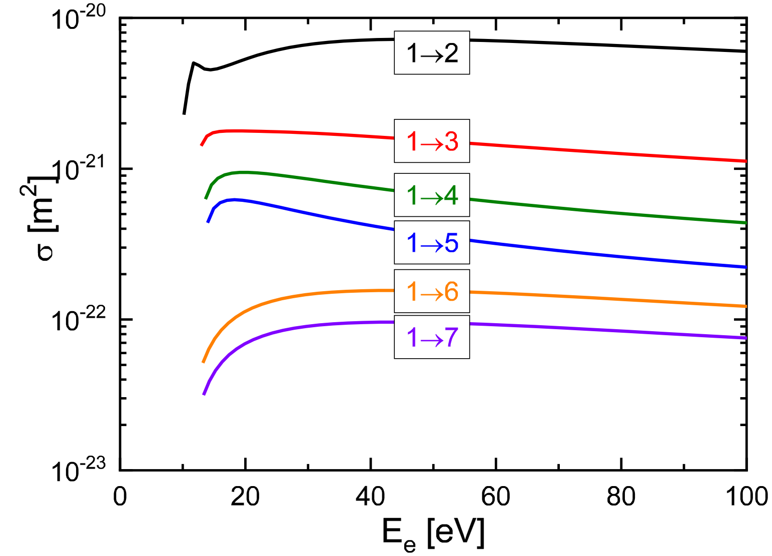
- **Detached divertor plasma**
- **Expansion region of NBI sources**

Huge number of free parameters ⇒ Evaluation needs a lot of time and experience

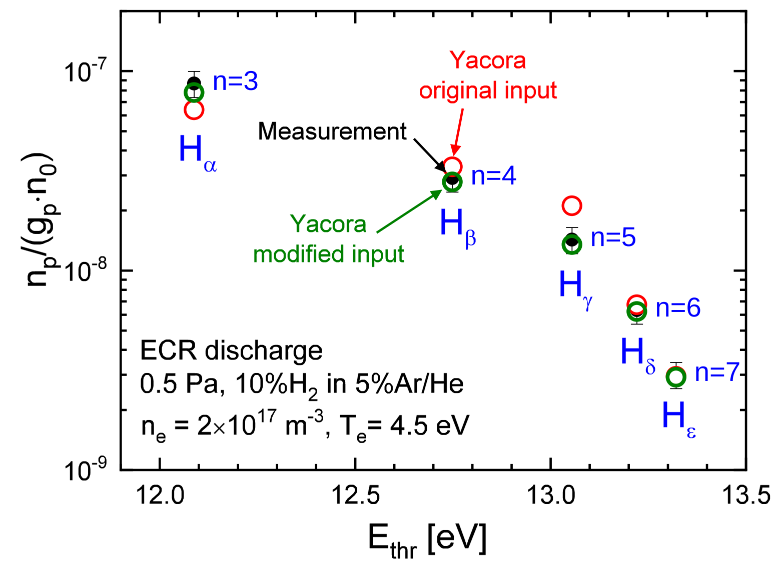
Atomic data in Collisional Radiative models: Correction of literature data for the hydrogen atom.

Data by Janev et al:

- Compilation of recent calculations and measurements
- Low energies (E_e<40 eV): discontinuity between cross sections for 1→5 and 1→6
  - Reason: different primary data sources (R-Matrix, semi empirical modification of Born-Bethe)
  - Solution: fit of rate coefficients
  - Result: excellent agreement of measurement and model for ionizing plasma with known T_e and n_e ✔



Benchmarked set of rate coefficients for direct excitation



R. Janev et al, JÜL-4105, Forschungszentrum Jülich, 2003
D. Wünderlich et al, JQSRT 110, 2009, 62

Molecular data in Collisional Radiative models: Franck-Condon factors and Transition probabilities for H_2.

Prepare extension of cross section database

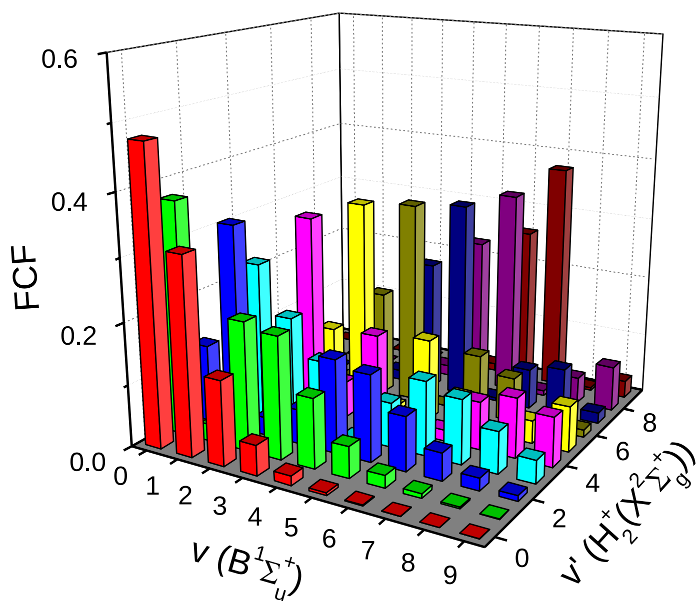
Collect and prepare eigenvalues of electronic wave functions (=potential energy curves)

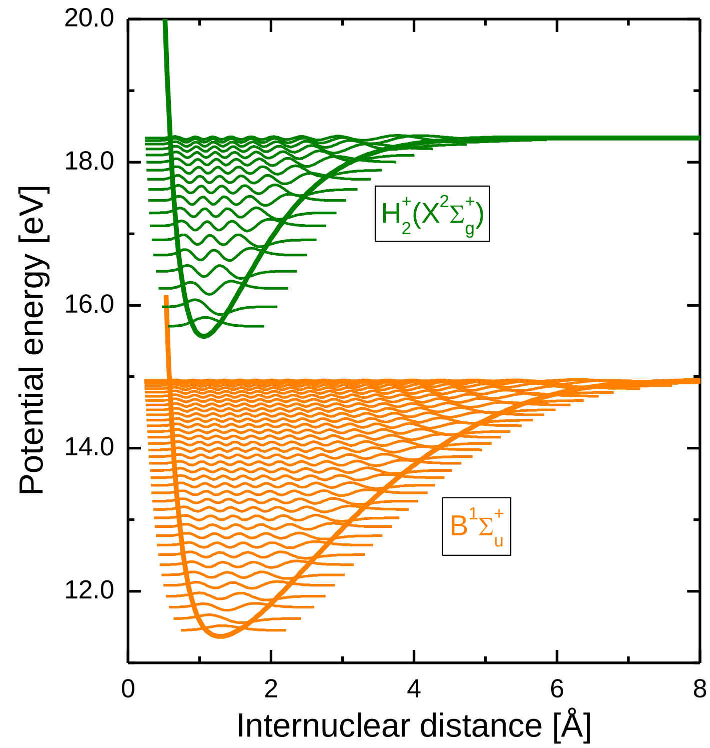
$\Rightarrow$ Vibrational eigenvalues

$\Rightarrow$ Vibrational wave functions

$\Rightarrow$ Franck Condon Factors

… for H_2 and H_2^+ (and its isotopomeres)





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
…					

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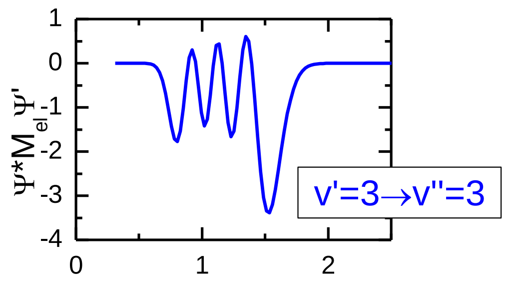
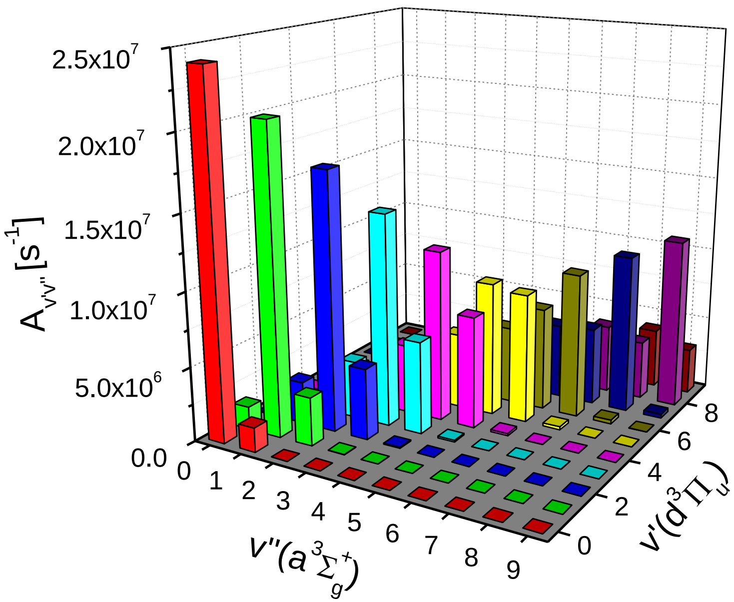
… for H_2 and H_2^+ (and its isotopomeres)

Collect and prepare dipole transition matrix elements

$\Rightarrow$ Einstein coefficients





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
…					

U. Fantz, ADNDT 92, 2006, 853
D. Wünderlich, ADNDT 97, 2011, 152

Molecular data in Collisional Radiative models: State-resolved ionization cross sections for H_2.

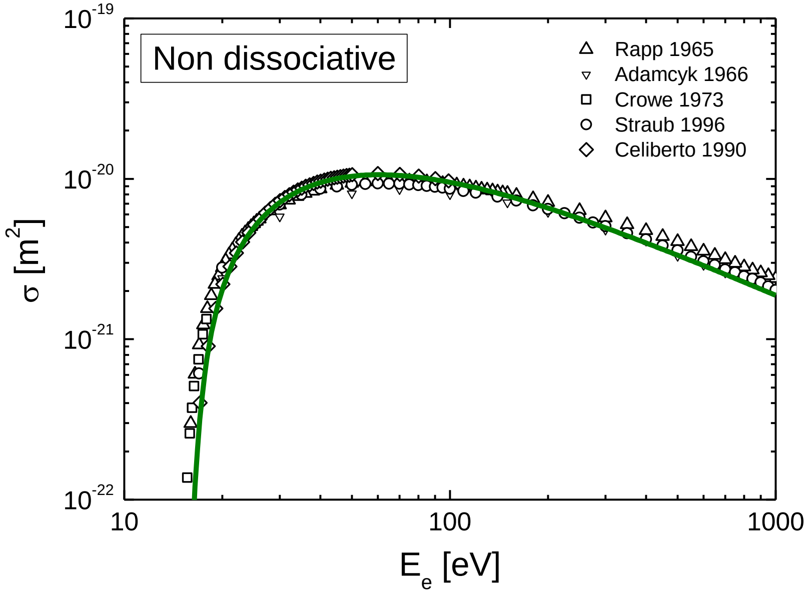
Literature: virtually no data for ionization of excited states in H_2

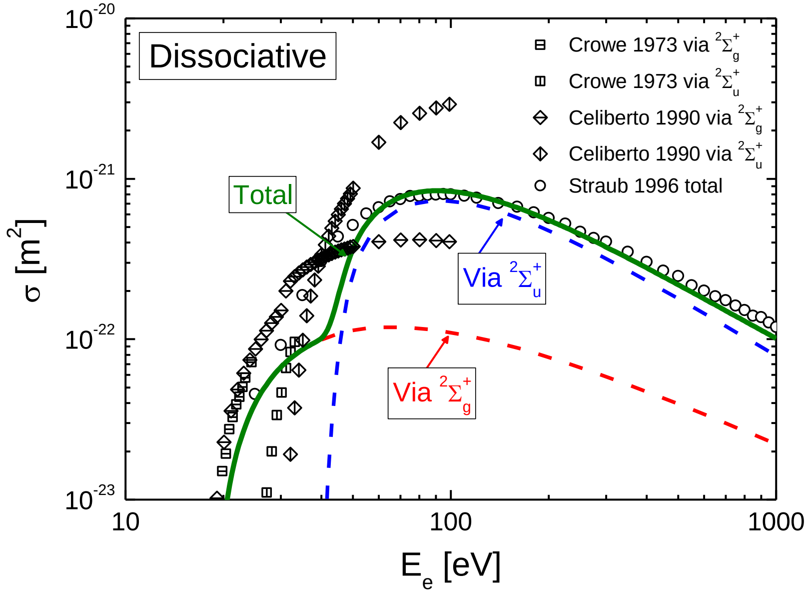
- Performed calculations based on the Gryzinski method.
- Dissociative and non-dissociative channel.

$H_2(X^1)$: Comparison with existing data (experimental and theoretical)

- Perfect agreement for non-dissociative and dissociative ionization. ✔
- Reason: removing one electron easy to be described by simplified methods.

D. Wünderlich, Chem. Phys. 390, 2011, 75

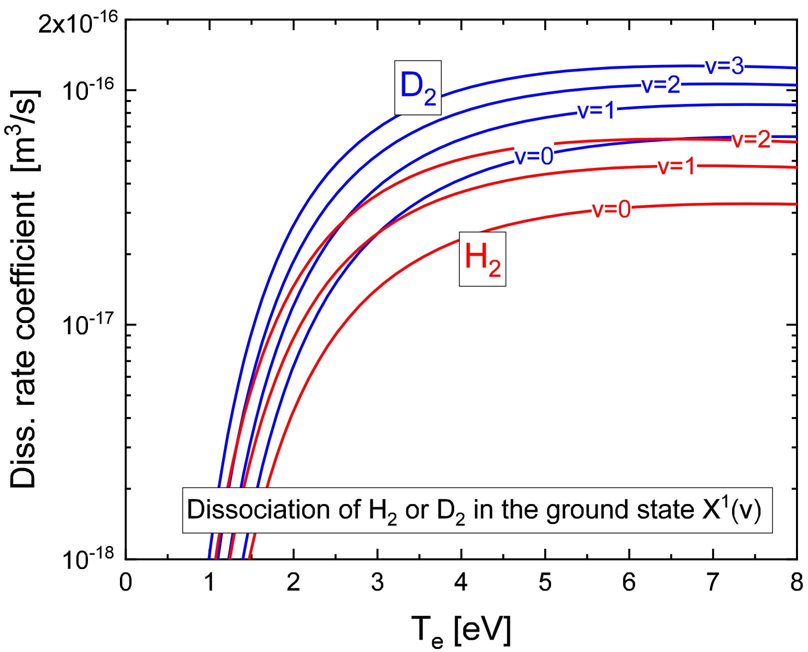


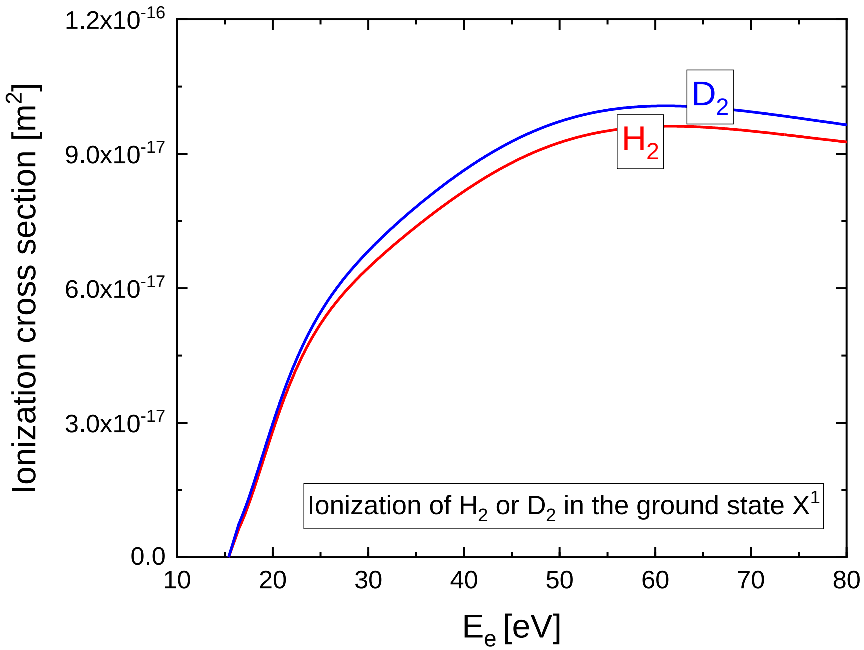


Molecular data in Collisional Radiative models: Relevance of the isotope effect.

Isotope effect mainly caused by:

- More tight vibrational and rotational energy level spacing in D_2.
- Impact on wave functions and threshold energies.





C.S. Trevisan et al, Plasma Phys. Control. Fusion 44, 2002, 1263.
C.S. Trevisan et al, Plasma Phys. Control. Fusion 44, 2002, 2217.

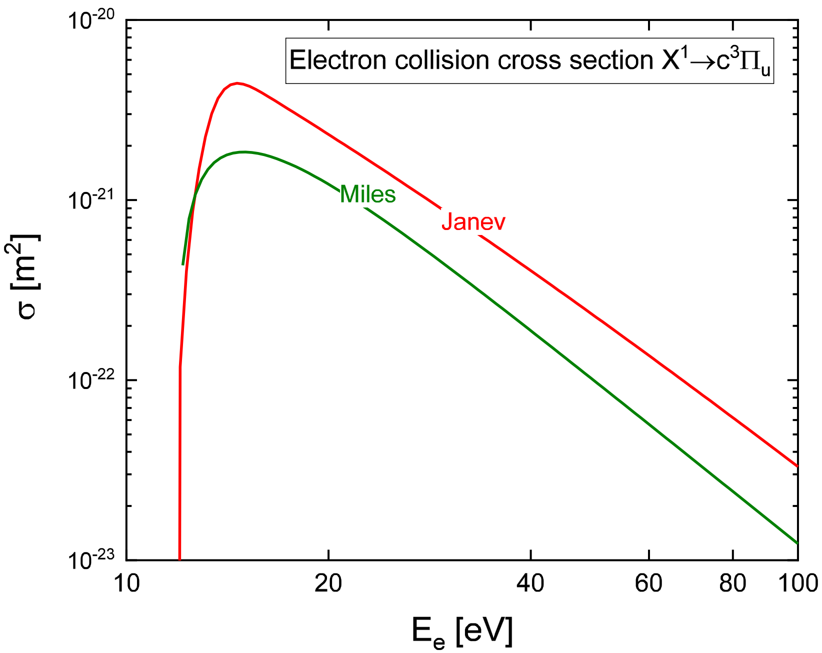
J.S. Yoon et al, J. Phys. Chem. Ref. Data 37, 2008, 913
J.S. Yoon et al, Rep. Prog. Phys. 73, 2010, 116401

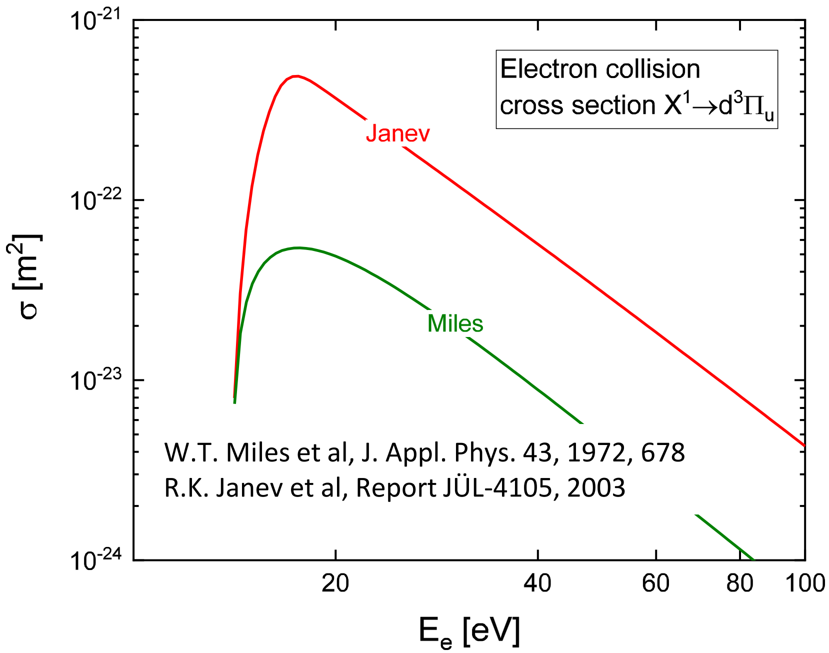
Molecular data in Collisional Radiative models: Excitation cross sections: lack of data for H_2 (and its isotopes!).

Excitation processes in the H_2 molecule:

- Data collections by Tabata (2000) and Yoon (2008): only a few reactions.
- Calculations by Celiberto (2001): only a few transitions, but isotope effect.
- Miles: semi empiric cross sections, 1972.
- Janev: summary of recent measurements and calculations, 2003.

Significant inconsistencies





T. Tabata et al, ADNDT 76, 2000,1 J.S. Yoon et al, J. Phys. Chem. Ref. Data 37, 2008, 913 R. Celiberto et al, ADNDT 77, 2001, 161

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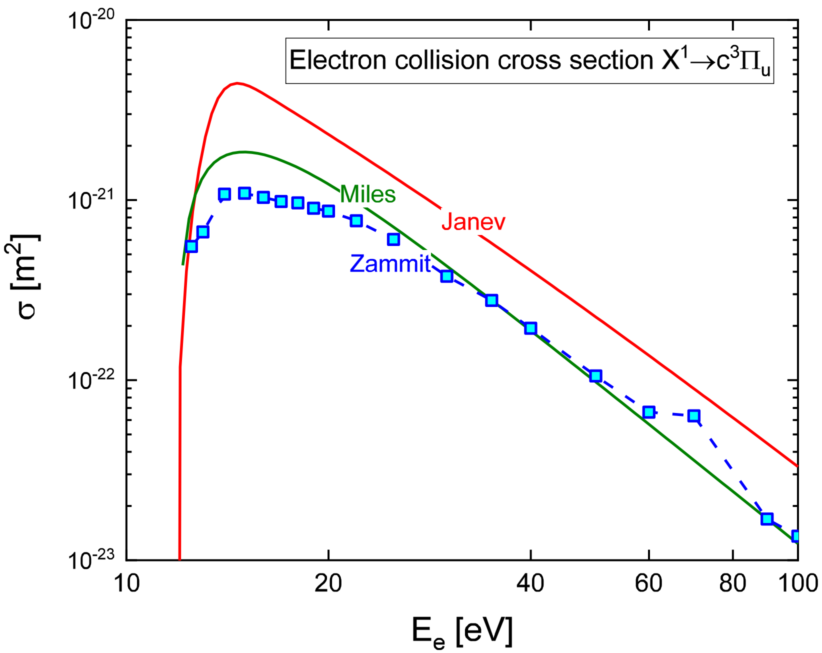
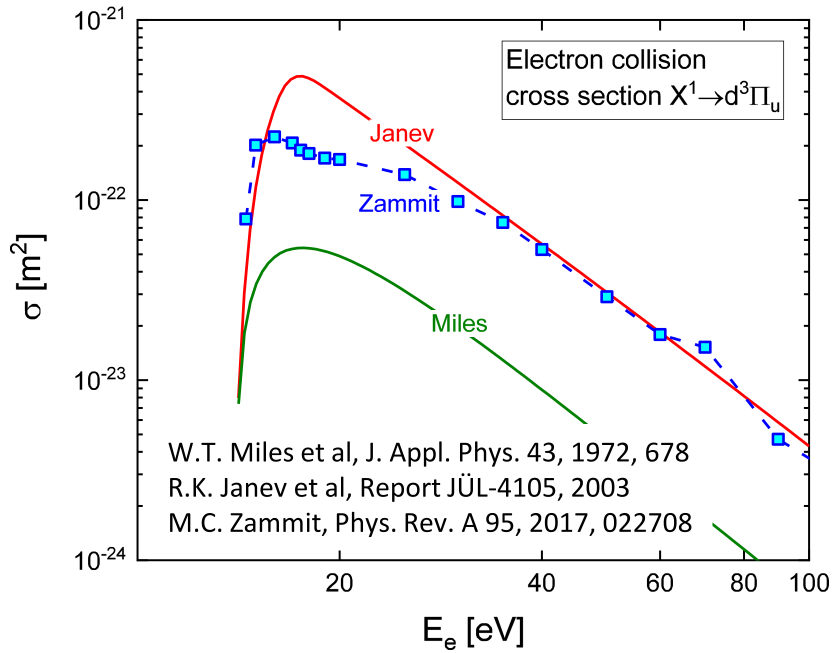
$\Big\}$ Significant inconsistencies

- New consistent data set: CCC (Convergent Close-Coupling), 2017 and ongoing.





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Molecular data in Collisional Radiative models: Example: Determine the ratio n(H)/n(H_2).

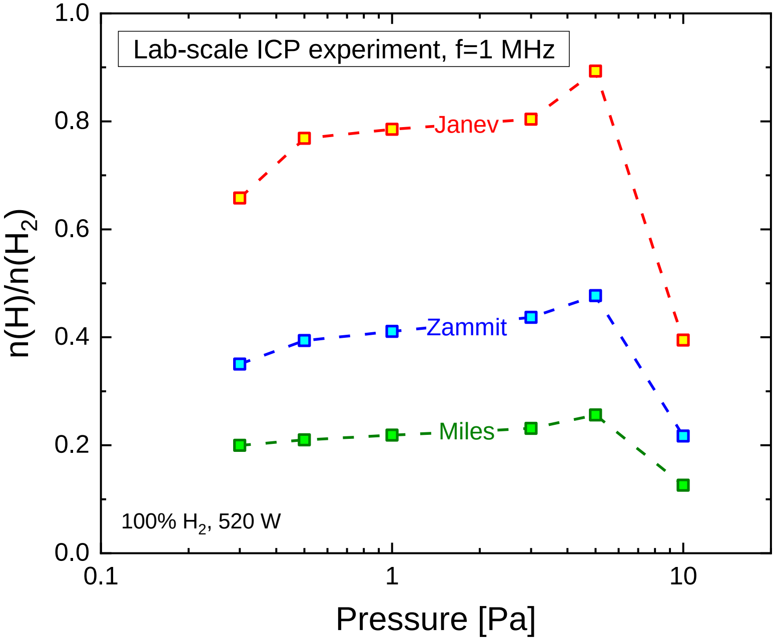
Models using Miles, Janev and CCC data:

- Differences in population densities directly mapped onto diagnostics results
- Up to now: model almost non-usable due to inconsistencies in the input data.
- CCC cross sections in between results based on Janev than Miles.

New CCC data may enable performing dedicated extensions:

- Excited state-excited state reactions (high relevance in the triplet system).
- Isotope effect (H_2, D_2, T_2)

Significant step towards (finally) a correct description of emission from H_2



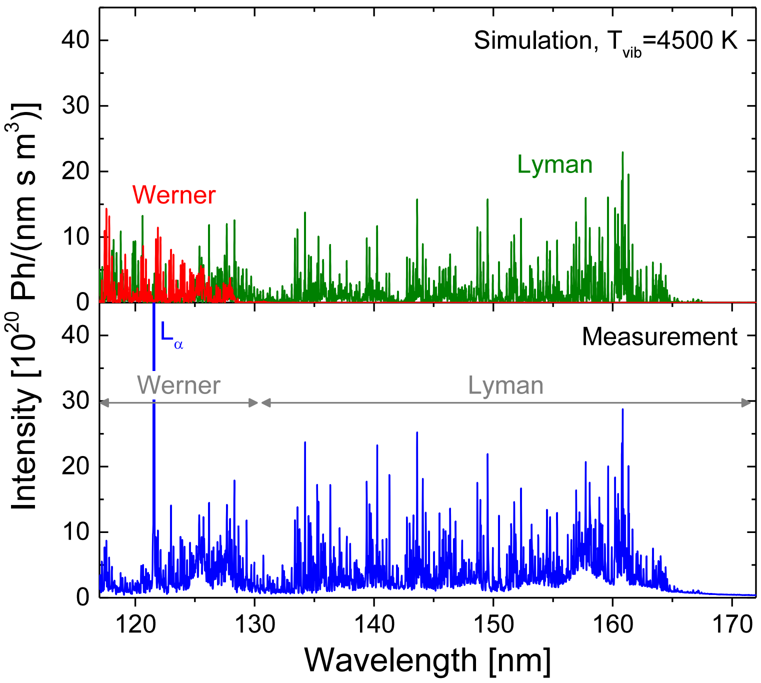
Outline of the talk.

- Collisional radiative modelling for fusion
- Atomic and molecular data for collisional radiative modelling
- Application of collisional radiative models

Application of population models: Vibrational-rotationally resolved corona model for H_2.

Werner ($C^1\Pi_u \rightarrow X^1\Sigma_g^+$) and Lyman ($B^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$) bands

- Resonant transitions in the VUV/UV
- Overlap between Werner and Lyman
  $\Rightarrow$ high relevance for the interpretation of measured spectra
  $\Rightarrow$ Important role of model (e.g. scaling measurment to the full band)
- Position of the lines and general structure well described by the model
- Next step: investigate influence of cascades on the vibrational and rotational population
  (steps toward a CR model needed?)



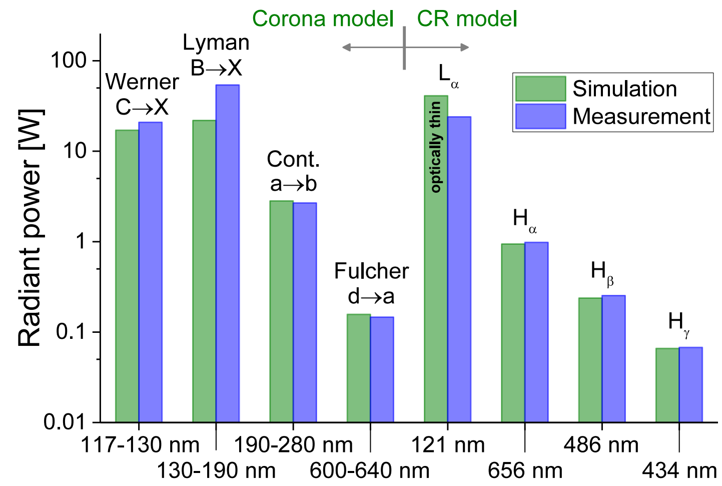
Very good results of ro-vibrational Corona models for Werner and Lyman H_2

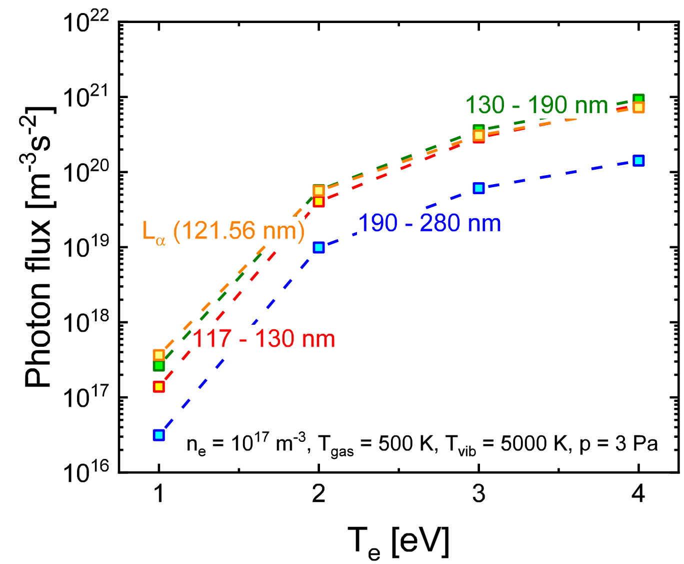
Application of population models: Vibrational-rotationally resolved corona model for H_2.

Determine power radiated by photons and ratio fluxes photons/atoms/ions

- ICP (f=13.56 MHz), P<600 W, p<10 Pa
- Plasma parameters from Balmer lines and CR model
- Emission from defined wavelengh windows:
  - Werner: 117-130 nm
  - Lyman: 130-190 nm
  - Fulcher: 600-640 nm (diagonal bands)

⇒ apply ro-vibrationally resolved corona models to deduce total emission or for predictive modelling



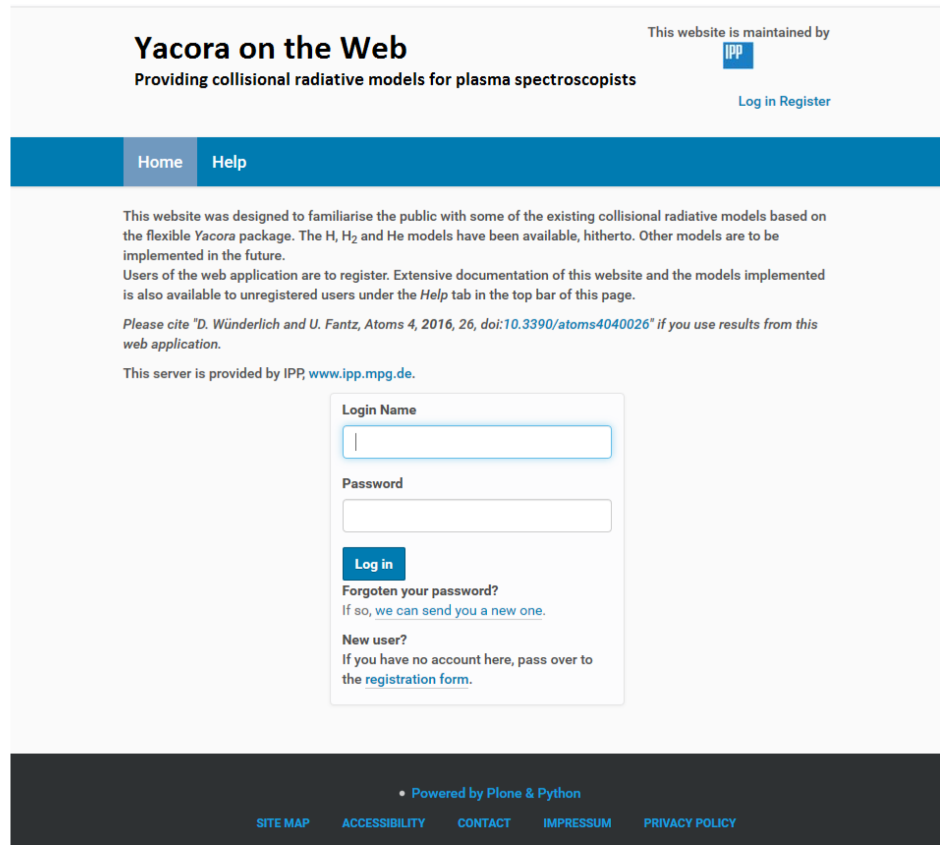


- Up to 21 % of P_{RF} measured as radiant power, mostly VUV/UV
- Photon fluxes ≈ ion fluxes, atomic fluxes much higher

Application of Collisional Radiative models: Yacora on the Web.

Yacora on the Web provides online access to selected Yacora CR models

www.yacora.de



Aims and features of Yacora on the Web

- Making public collisional radiative models based on Yacora in a user friendly environment.
- Available up to now: models for H, H_2 and He.
- Very simple registration (self registration).
- Extensive documentation available (also for anonymous users).
- Web application based on Plone and Python.

Conclusions

Input data set for population models of low-temperature plasmas

- Collected from different literature sources for different particle species.
- Extended and corrected where necessary and possible.

Yacora CR models for different particle species relevant for fusion

Relevance of processes including photons and the isotope effect $H_2 – D_2 – T_2$.

Thorough benchmark at different plasma experiments

- Low-temperature region (T_e<10eV) of fusion machines.
- Ion sources for NBI.
- Lab-scale experiments.