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Issues with CR- and plasma chemistry modelling for fusion boundary plasmas

Detlev Reiter

25th Technical Meeting of the International Atomic and Molecular Data Centre Network (DCN)

IAEA's Headquarters in Vienna, Austria, from 30 September to 2 October 2019

Detlev Reiter, personal notes:

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- Representing Forschungszentrum Jülich in DCN: 2011-2017
- March 2019: Retired from FZ Jülich
- From September 2019:

  Member of ISFN (ITER scientific fellowship network,

  representing : Heinrich Heine University Düsseldorf, Germany
- Email: reiterd@uni-duesseldorf.de

Tasks in ISFN related to AMS data:

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- Radiation transfer: photo-excitation, photo-ionization, photo-dissociation, line broadening bidirectional reflectance functions (BDRF)
- Chemical kinetics → physical kinetics, e.g. NH_x, BeH_x systems
- (p +e)+H_2: isotopic effects (H_2, D_2, T_2 HD, HT, DT, and their ions) ("on the fly" CR codes embedded in transport models)

ITER NEWSLINE - 24 Jun, 2019

ITER Director-General Bernard Bigot signs the IAEA-ITER Practical Arrangements in the presence of Mikhail Chudakov, IAEA Deputy Director General and Head of the Department of Nuclear Energy

IAEA and ITER

Even closer cooperation

Under Practical Arrangements signed in June, the International Atomic Energy Agency and the ITER Organization will be expanding and deepening a long history of cooperation.

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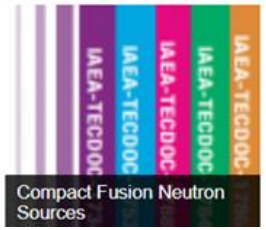
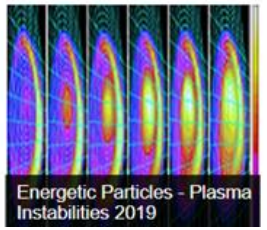
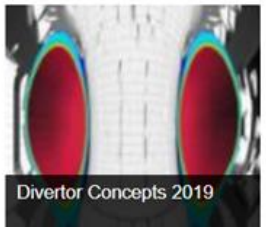
*The International Atomic Energy Agency (IAEA) fosters international collaboration and coordination to help close the existing gaps in physics, technology and regulation and move forward in developing the peaceful use of fusion energy. The IAEA's activities in this field cover, among others, plasma physics and fusion power, technologies and material, both for magnetic and inertial fusion. The Fusion Portal is dedicated to all these activities, ranging from **Conferences**, **Coordinated Research Projects**, **Meetings, Workshops and Schools**, to providing **News Media** and **Publications** related to these projects.*

News story

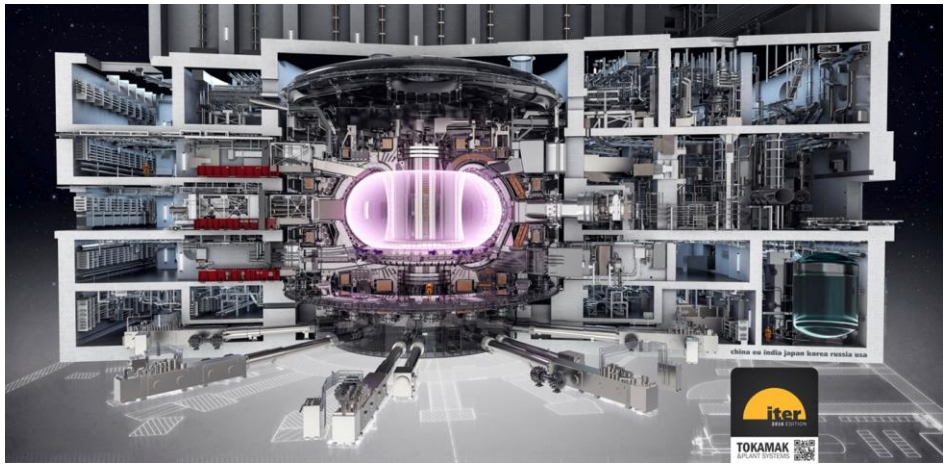
- **A history of fusion research and development: Part two**
- **Pathways to Energy from Inertial Fusion: Materials beyond Ignition – CRP F13016 Successfully Completed**

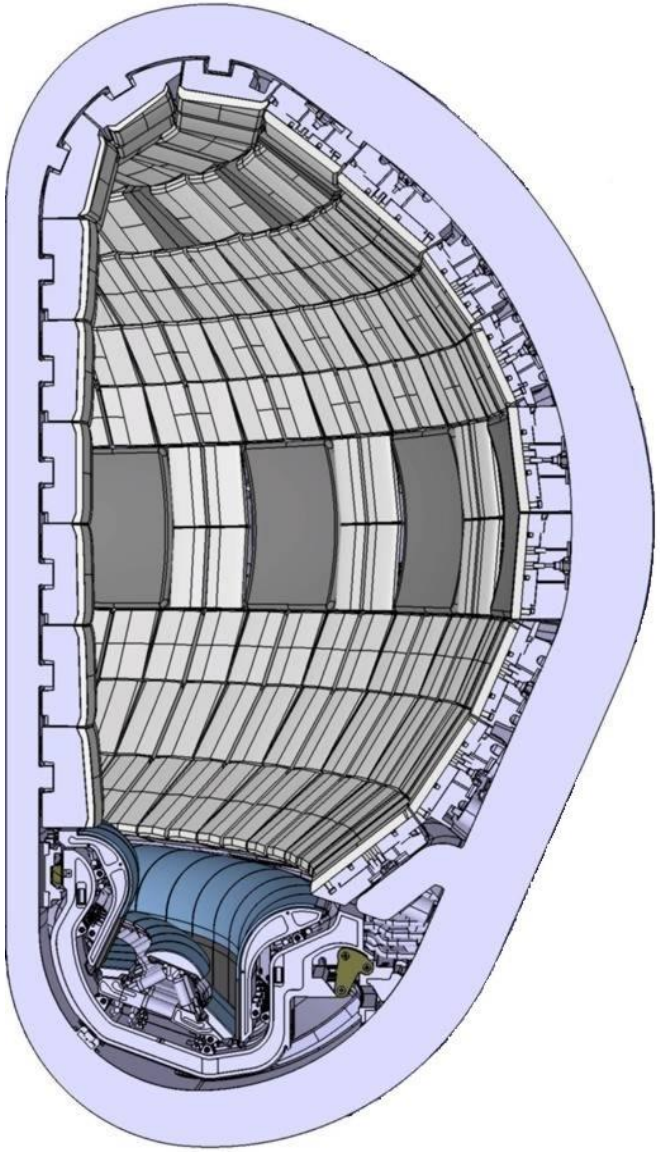






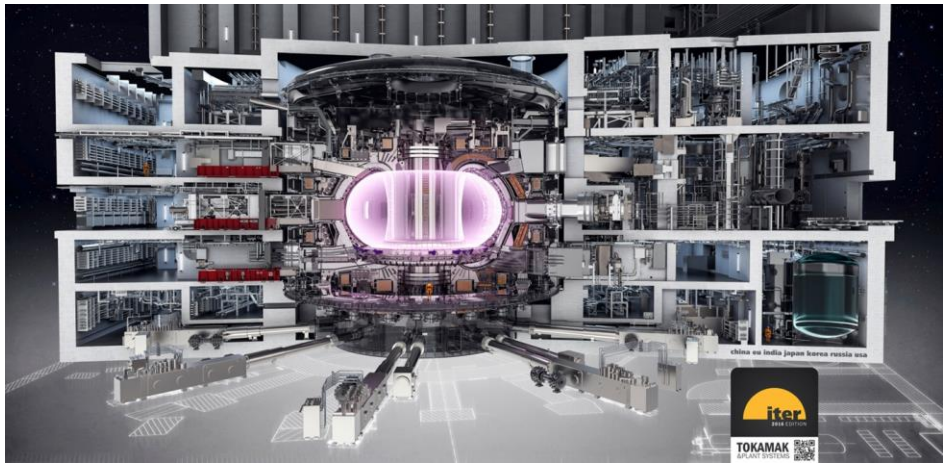
List of the main elements relevant to the ITER plasma

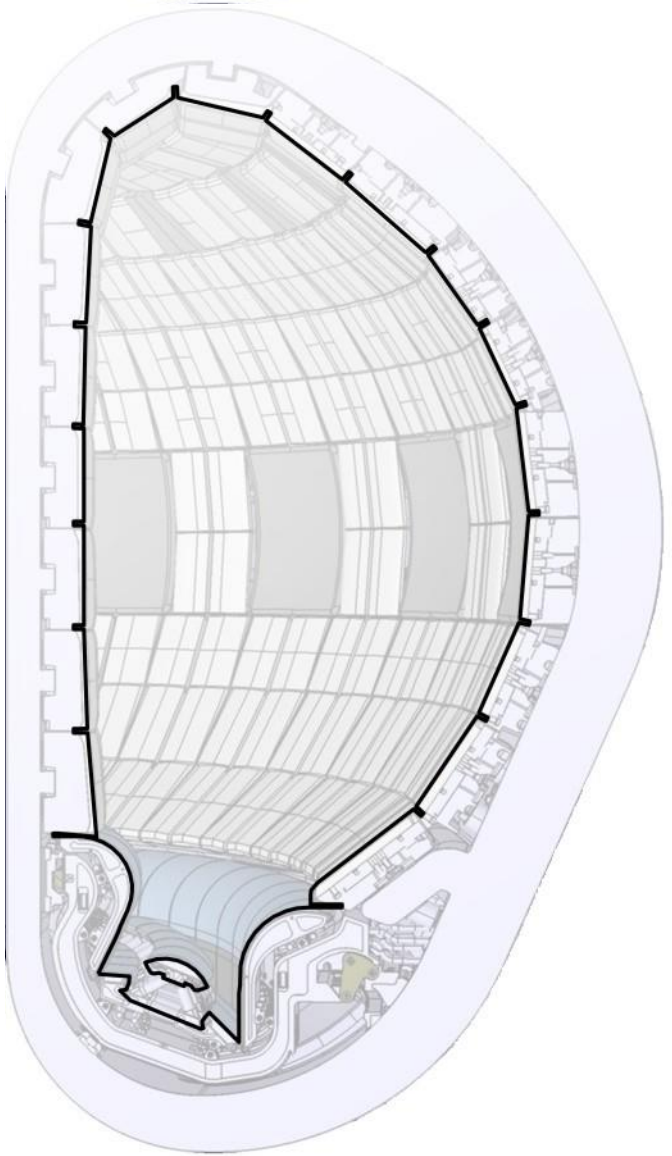




Courtesy: S. Lisgo, 2018

List of the main elements relevant to the ITER plasma





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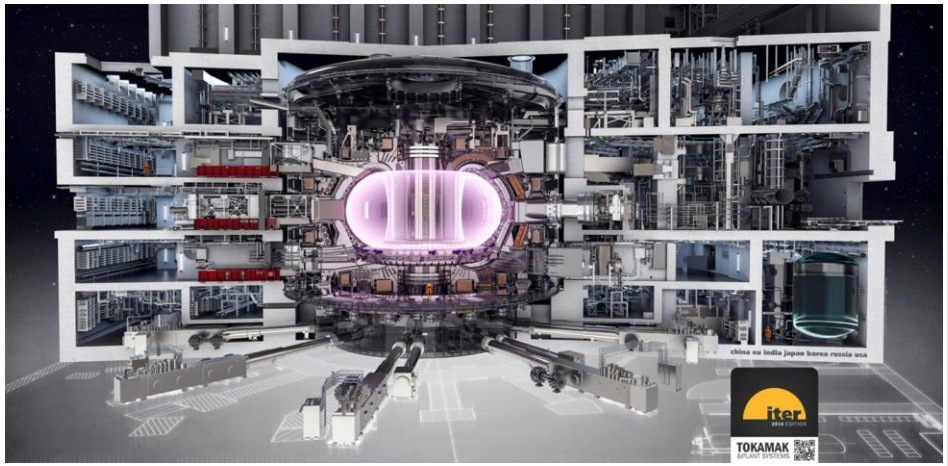

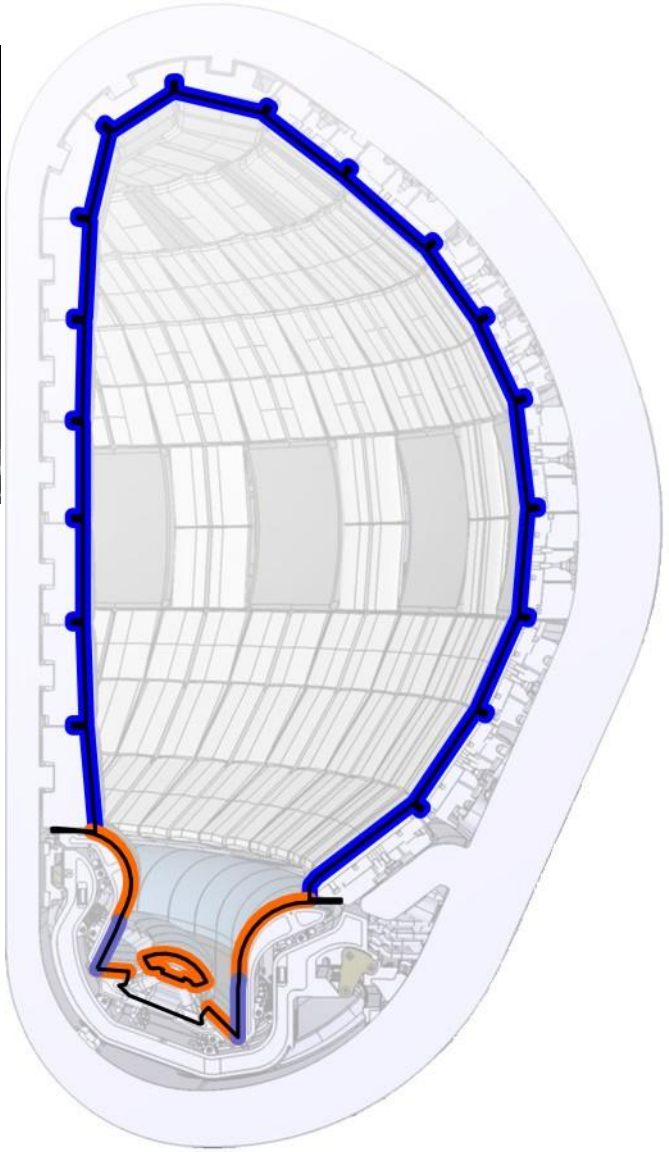

Courtesy: S. Lisgo, 2018

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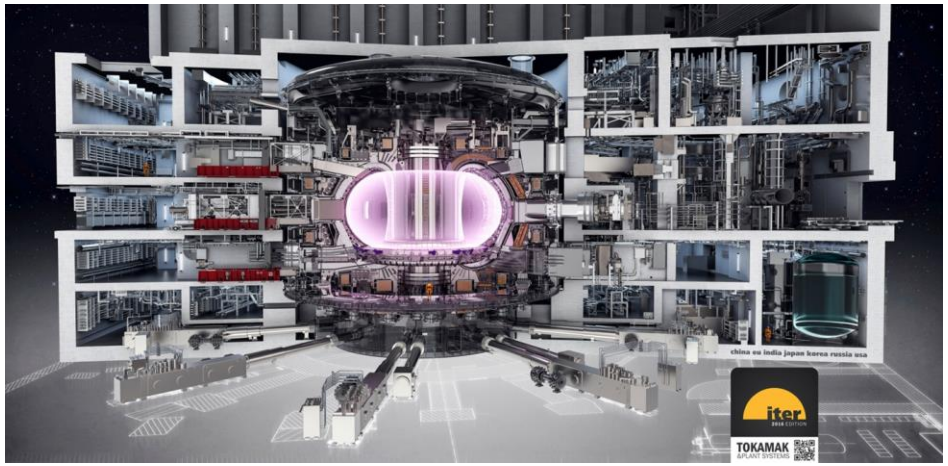

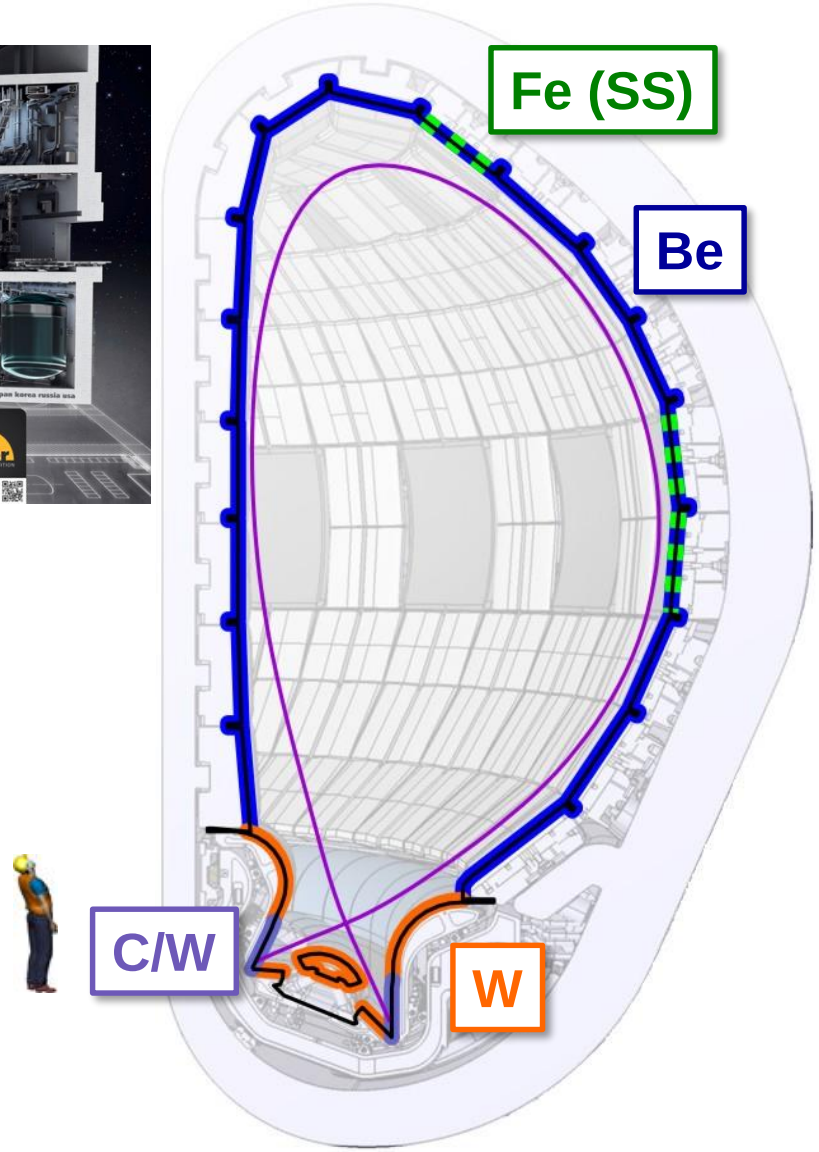

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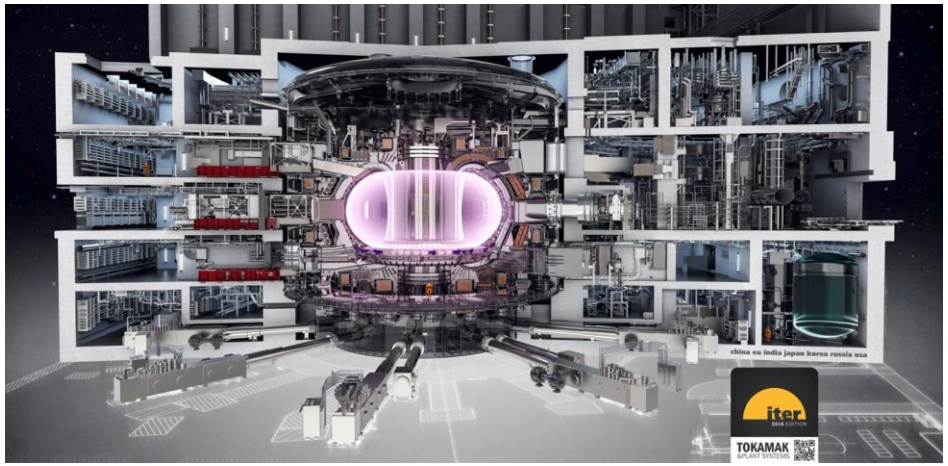

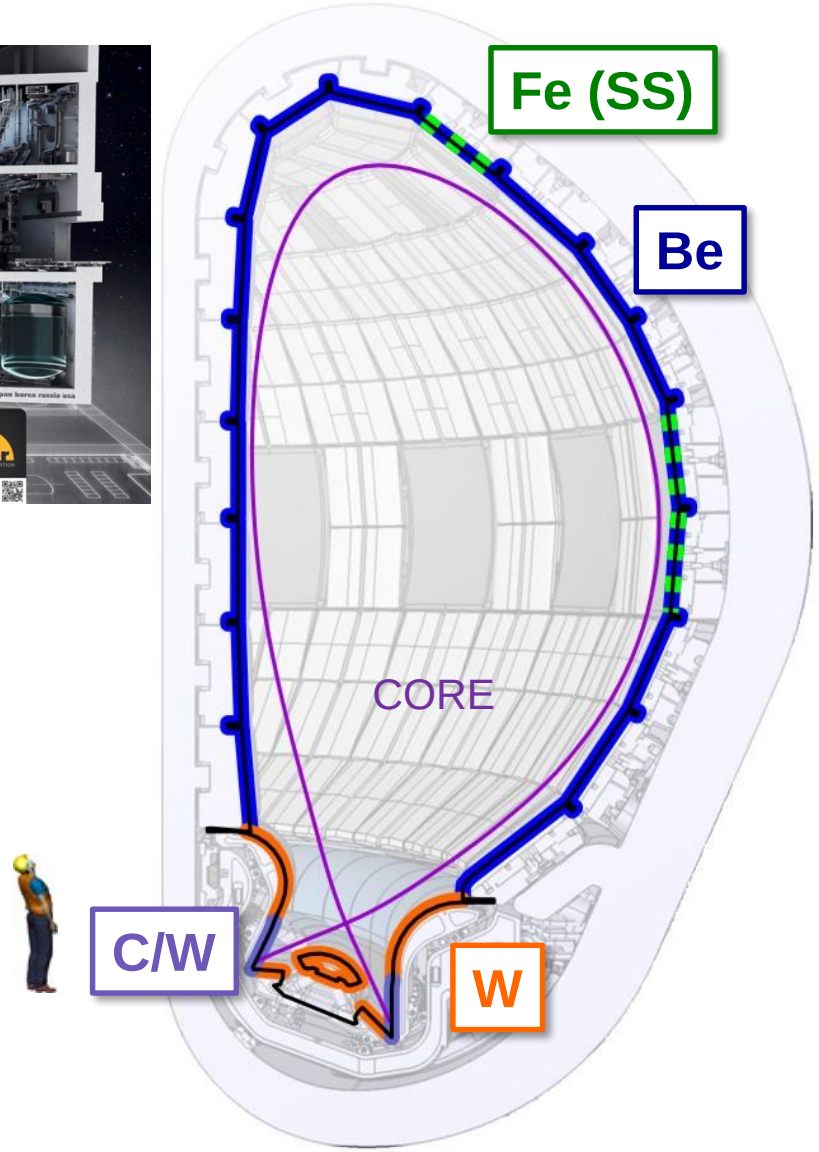

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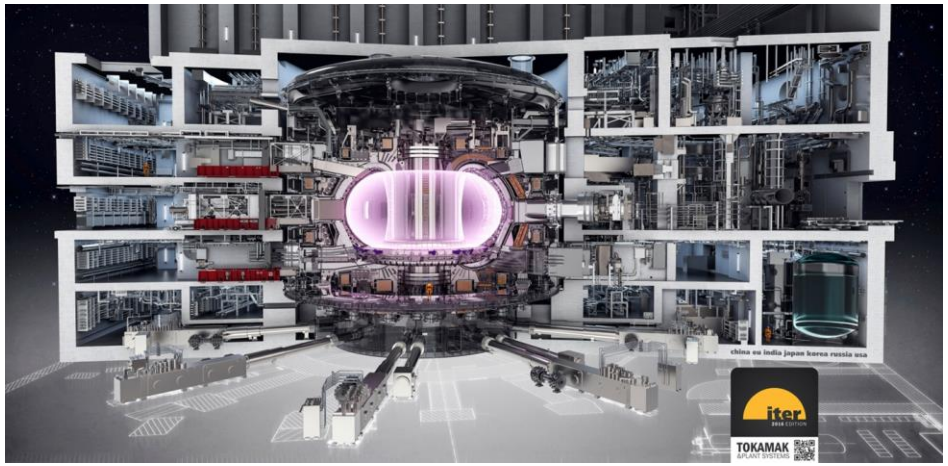

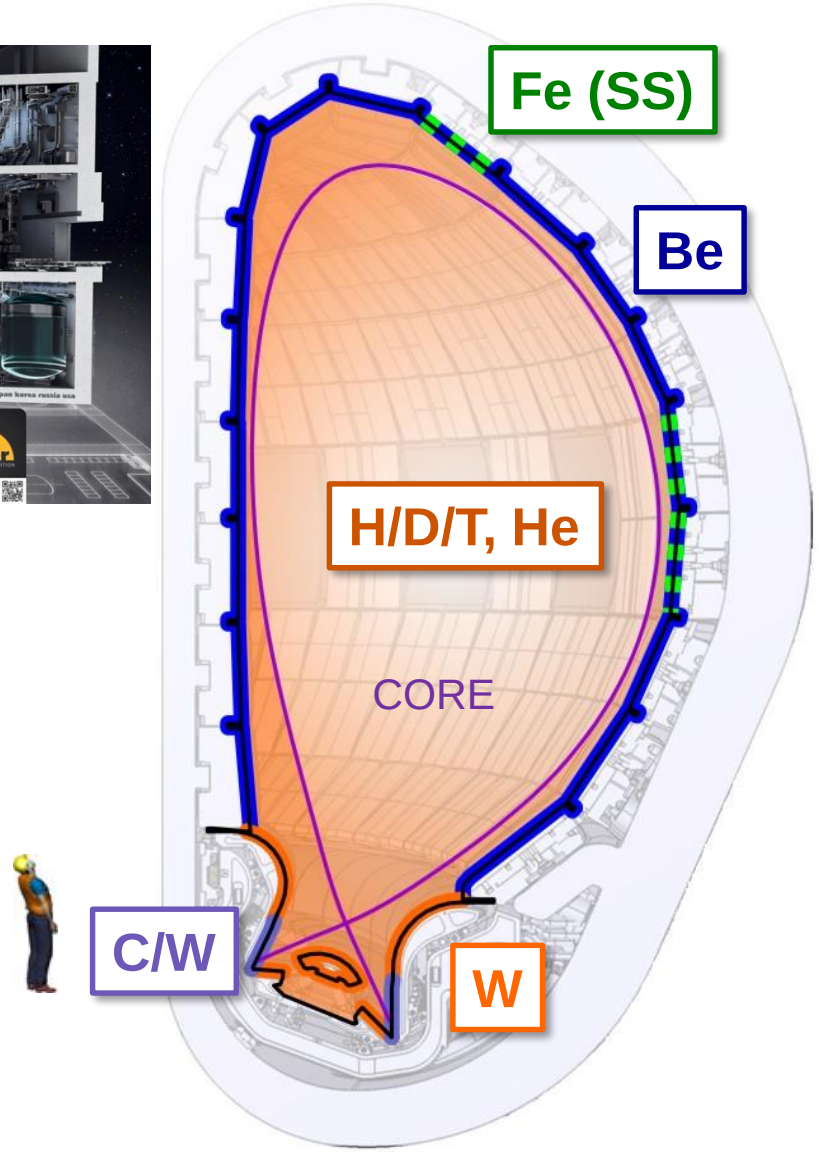

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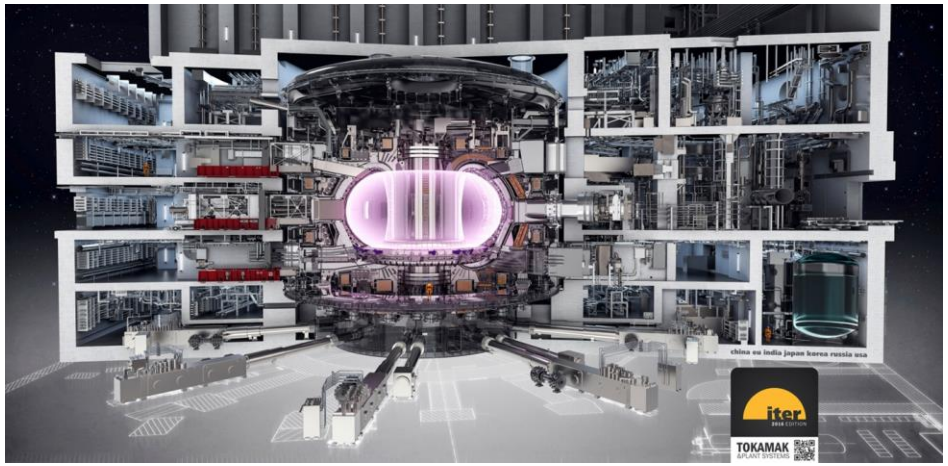
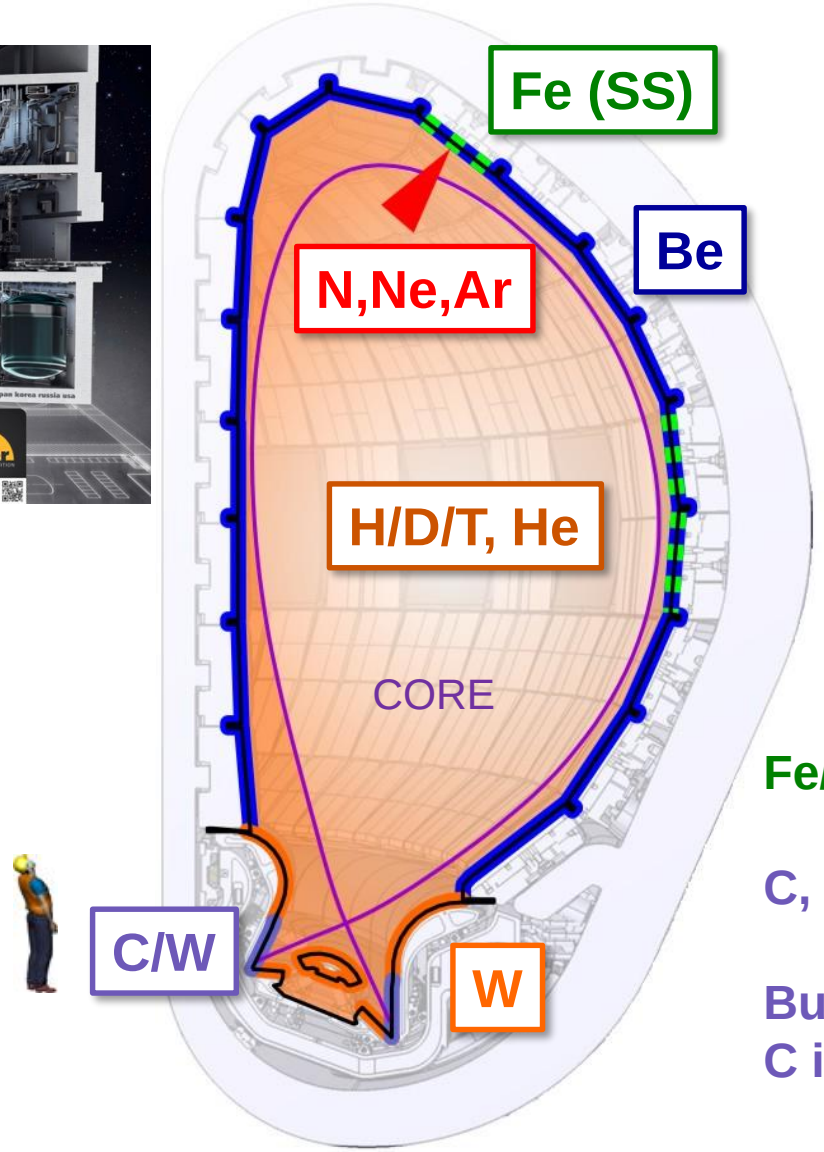




Fe/SS, 2011: armour at diagnostics port plugs

C, in 2013: replaced by all W divertor

But:

C in: W7X (2016), JT-60SA (2019),…

MOLECULAR PROCESSES CONSIDERED IN FUSION:

- $e,p + H_2(v_i) \rightarrow \ldots$, $e+H_2^+(v_i) \rightarrow H + H^*$ divertor detachment dynamics,

  www.amdis.iaea.org, data center network, Atoms 2016, D. Wuenderlich, U.Fantz, IPP Garching, K. Sawada, M.Goto, NIFS, and Fursa et al, PRL 2016

  $e+H2^+(v)$: Int. Conference series: Dissociative Recombination 1-9 (1988 -2012)

- $e,p + C_xH_y \rightarrow \ldots.$, $e+C_xH_y^+ \rightarrow \ldots.$ C erosion and migration, tritium retention,….

  Excited states of products (CH(A→X)) ?

  R. Janev et al., Phys. Plasma (2002, 2004) 11, IAEA: www.amdis.iaea.org, APID Vol 16 (2012)

- $e+H_3^+(v3) \rightarrow \ldots.$, DR, DE,…. H_3^+ probably irrelevant in fusion plasmas

  M. Larsson et al., PRL (1993) 70, S. Datz et al., PRL (1995) 74, and: Conference series: DR 1-9

- $e+ BeH/BeH^+ \rightarrow \ldots.$ possible role on spectroscopy and on material migration:

  Formation rates ?? 10% of Be sputtering? Volumetric particle exchange reactions ?

  J.B. Roos et al. Phys. Rev A (2009) 80, IAEA Atomic Molec. data unit CRP 2012-2015

  Exp.: UC Louvain, Theory: I. Schneider et al., Univ. Du Havre, J. Tennyson et al. (Quantemol), R. Celiberto et al. (Bari)

  Multiple aspects solved, but data scattered in literature, not jet compiled into a single comprehensive database.

- $e+ N_2, N_2^+ \rightarrow \ldots.$ N_2-seeding, plasma cooling: Ammonia formation. So far mostly: only resulting atomic ions N, N^+, N^{++},…. but first plasma chemistry databases emerge

  See planetary atmospheric entries research, e.g. A. Bultel et al, Universite de Rouen, France

MOLECULAR PROCESSES CONSIDERED IN FUSION:

- $e,p + C_xH_y \rightarrow ....$, $e+C_xH_y^+ \rightarrow ....$ C erosion and migration, tritium retention,….

Excited states of products (CH(A→X)) ?

R. Janev et al., Phys. Plasma (2002, 2004) 11, IAEA: www.amdis.iaea.org, APID Vol 16 (2012)

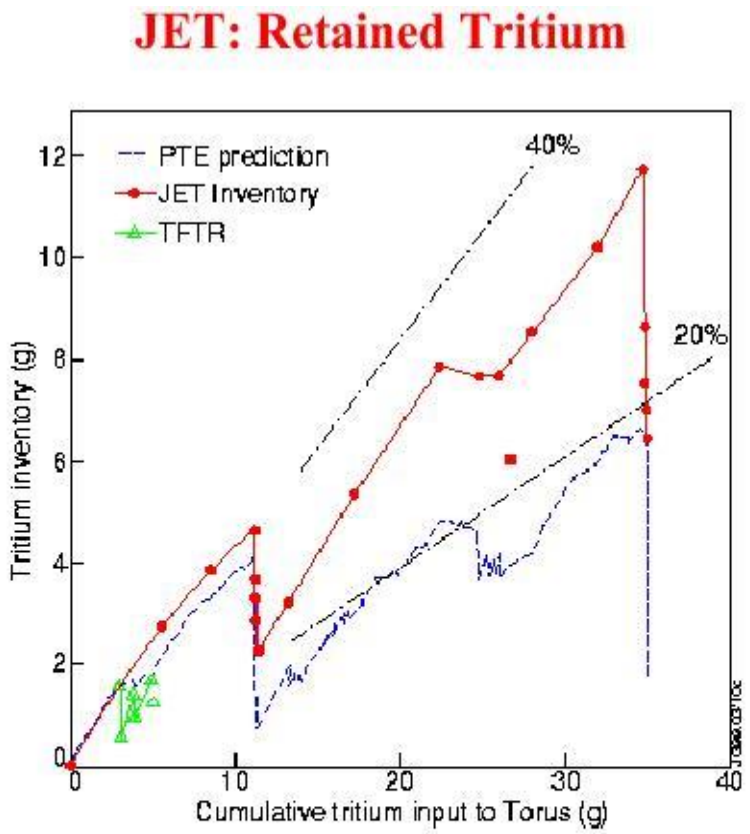
Fusion had not progressed very far until carbon based plasma facing components were used (mid eighties of last century).

Mostly studied then: atomic C spectroscopy and transport,
little interest in carbon containing molecules, initially.

This changed in the years following 1997: the tritium experiments at JET

The tritium retention issue:

On JET, operated with tritium (1997), the tritium inventory built up without saturation limit.

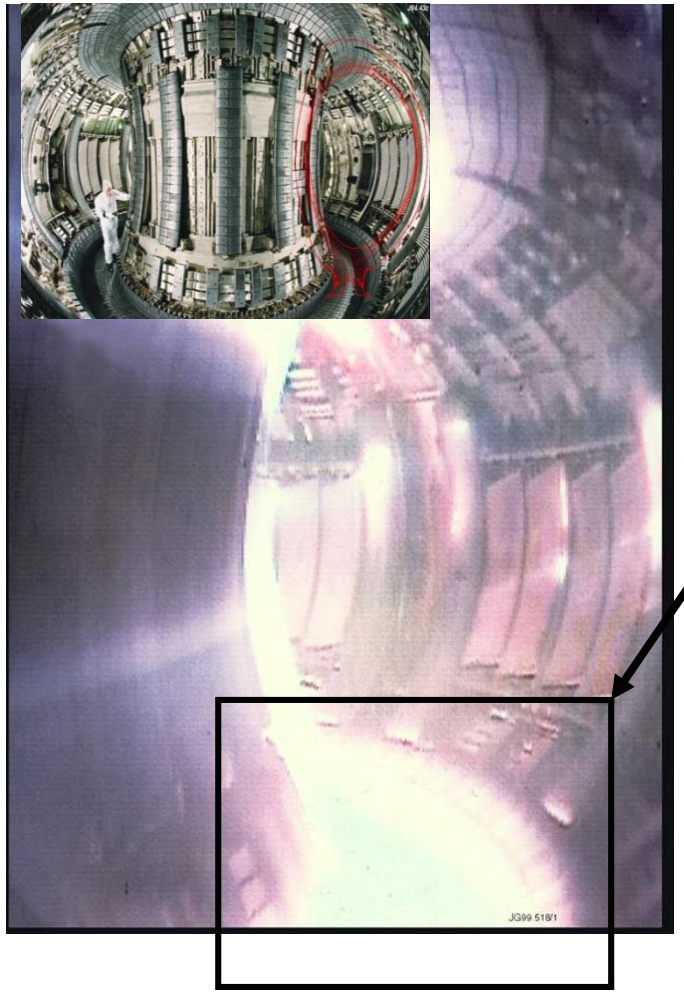


The rate of T retention in JET during DTE1 was 40% of input, reducible to 17% after cleanup in D, without sign of saturation.
P. Andrew, et al, FED 47 (1999) 233.

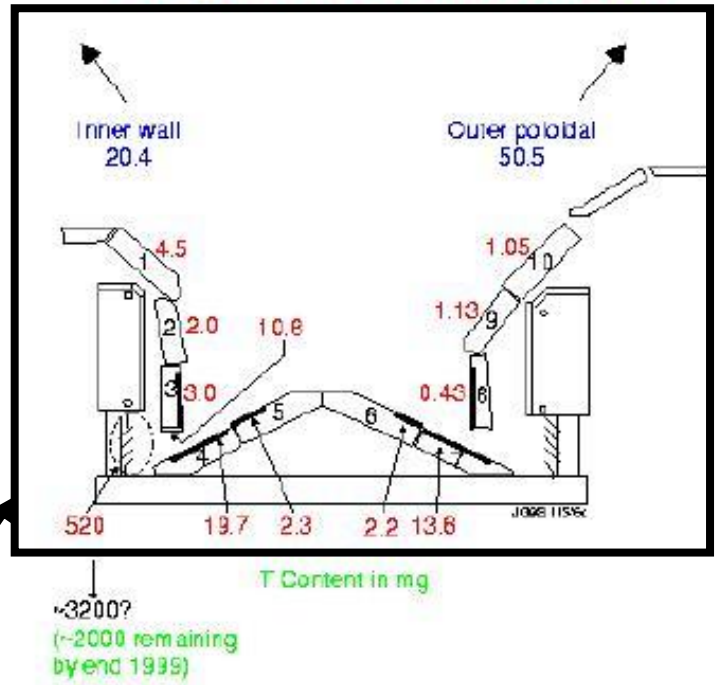
Extrapolation to ITER: the permitted in-vessel T inventory, 0.7 kg, could be reached in 100 shots

Carbon re-deposition, tritium co-deposition in JET

JET, Joint European Torus



Location of tritium in JET vessel during the post-DTE1 shutdown

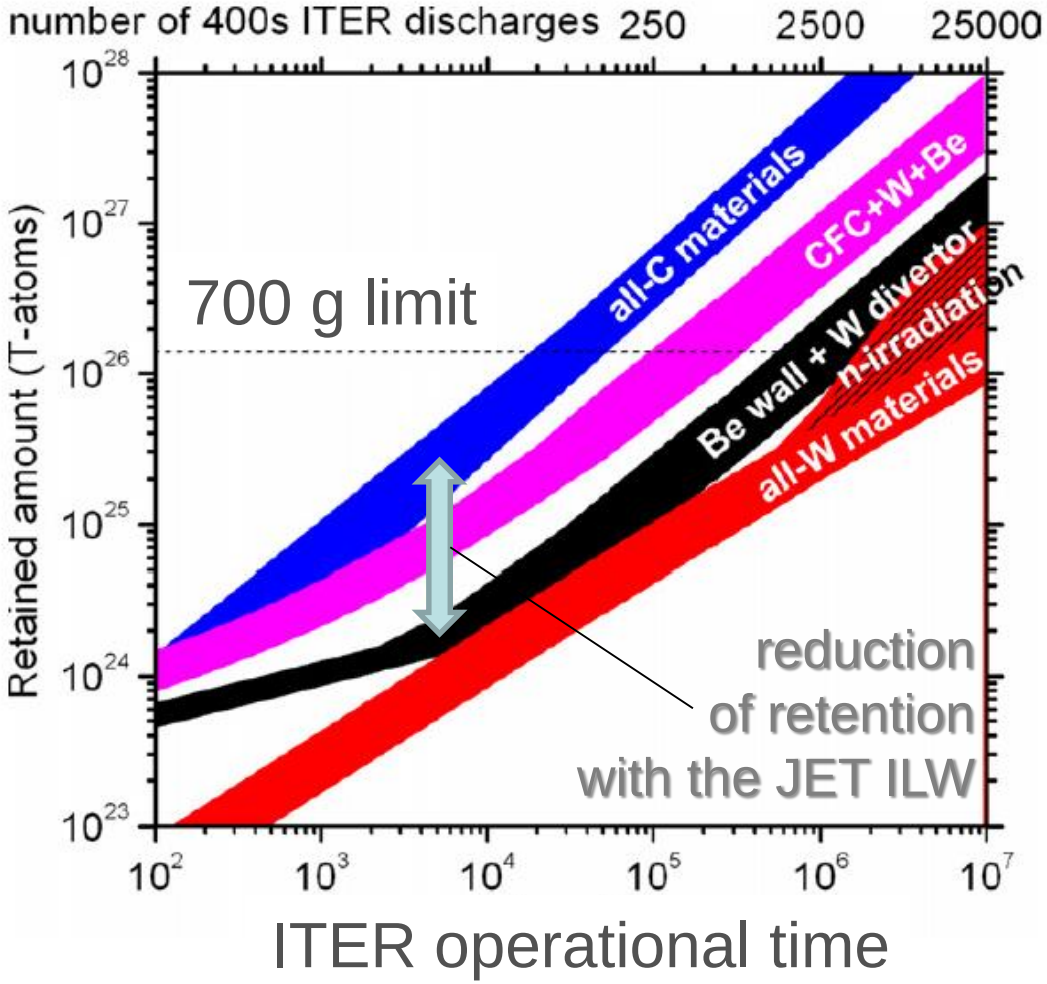


The location of the deposition is surprising: only a few mgs were found on typical tiles, but 520 mg were vacuumed up from the cooled, out-of-sight louvers, suggesting up to 3200 mg also that have fallen through to the vessel floor.

J.P. Coad, et al, J Nucl Mater 290-293 (2001) 224.

Predictions of fuel retention in ITER

fuel retention in C versus W



J. Roth et al., Plasma Phys. Cont. Fus. 50 (2008)

Data derived from empirical results obtained at **AUG, JET** and **PISCES** and modelling of erosion & re-deposition

Conclusion:

Fuel retention with carbon divertor is unacceptably large

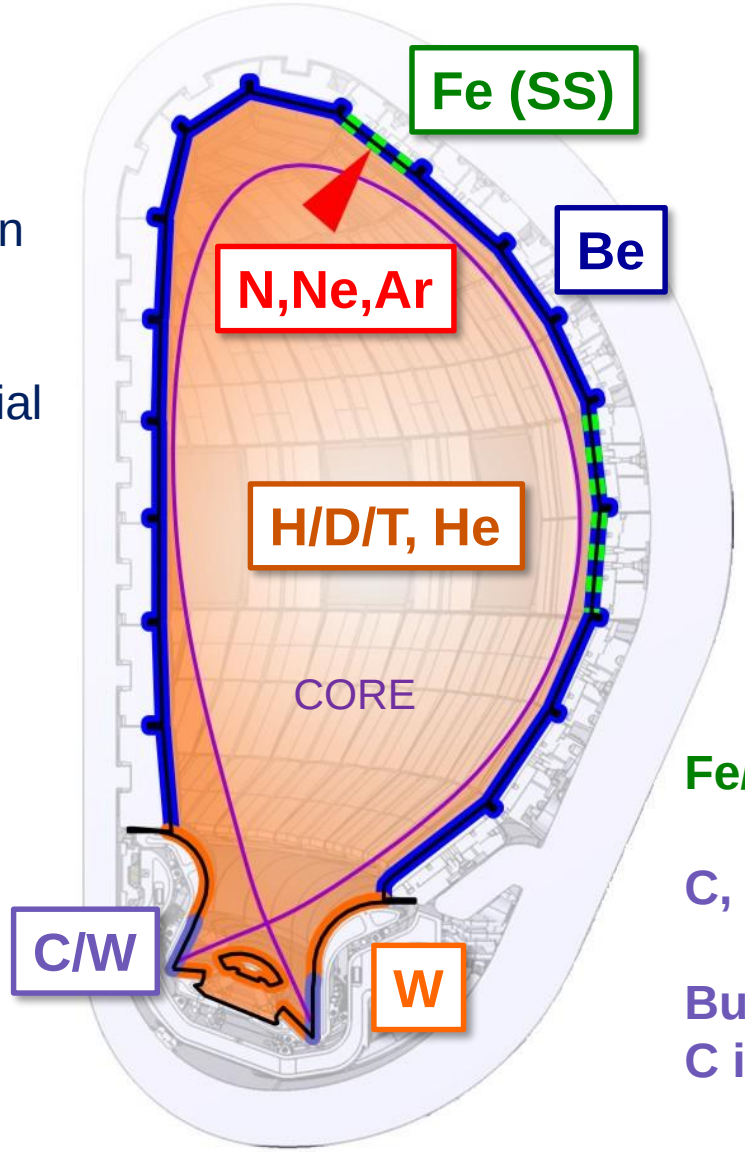
List of the main elements relevant to the ITER plasma

Because of T-retention and migration Carbon was removed from ITER design in 2013.
I.e. the material we knew most about in fusion, and the most forgiving material too (does not melt), was removed.

This puts BeH, BeH_2 into focus, wrt. its tritium issues:

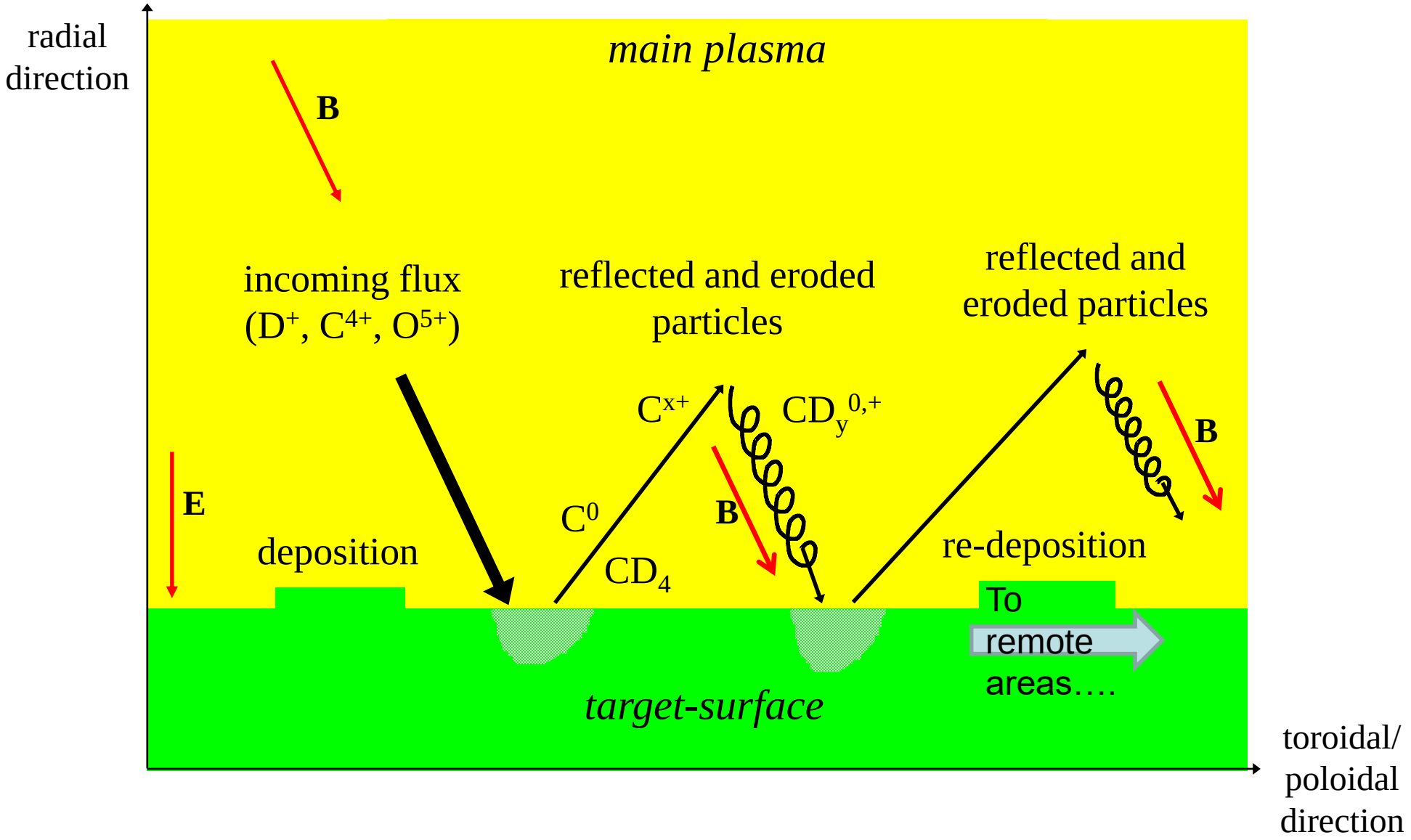
- Transport modelling of pathways
- spectroscopical wall erosion rate quantification

And: Ammonia (NHx) formation in remote subdivertor region, vacuum system, in case of divertor plasma N-cooling



Fe/SS, 2011: armour at diagnostics port plugs
C, in 2013: replaced by all W divertor → N, Ne, Ar cooling?
But:
C in: W7X (2016), JT-60SA (2019),…

Release (chem. sputtering) and migration + fragmentation of hydrocarbons



Courtesy: A. Kirschner, FZ Jülich

PLASMA CHEMISTRY DATABASES: FAR SOL, SUB-DIVERTOR

C_xH_y as a role model for other Hydrides (Be_xH_y, NH_x, HeH^+,….systems?)

- Already done SiH_y: Janev, Reiter, Contr. Plasma Physics, 2003,43,401-417

Chemistry | Physics

Extensions, evaluations, new exp. and theor. results →

1987 | 2002-2004 | 2012

Plasma chemical rate constants (Arrhenius form) for well stirred, equilibrium, low T conditions

A.B. Ehrhardt, W. D. Langer, Report PPPL-2477, Princeton (1987).

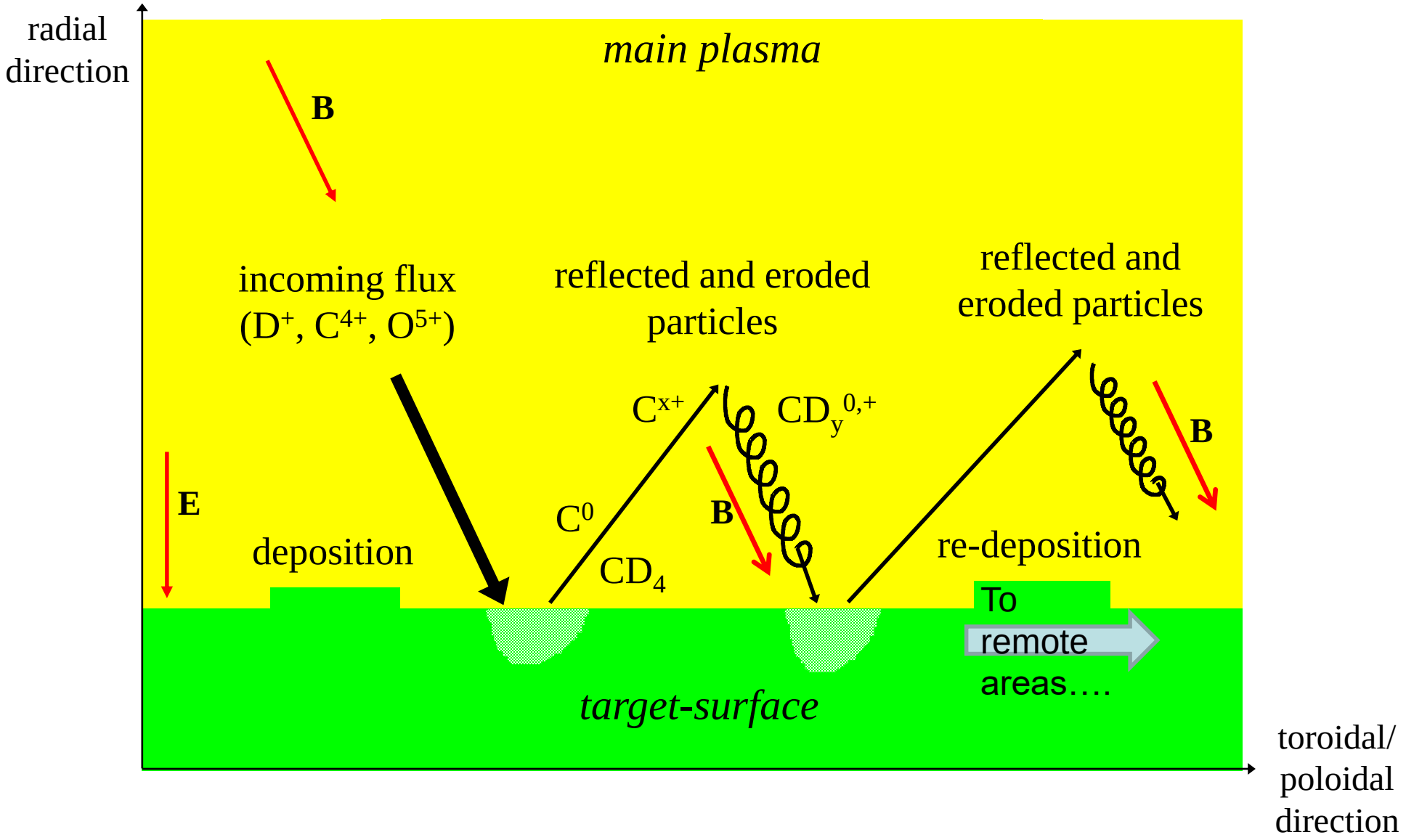
Comprehensive set.
Cross sections already, but universal fit expression for all types of processes
→ poor asymptotic behaviour

R.K. Janev, D. Reiter
Phys. Plasmas, Vol 9, 9, (2002) 4071
Phys. Plasmas, Vol 11,2, (2004) 780

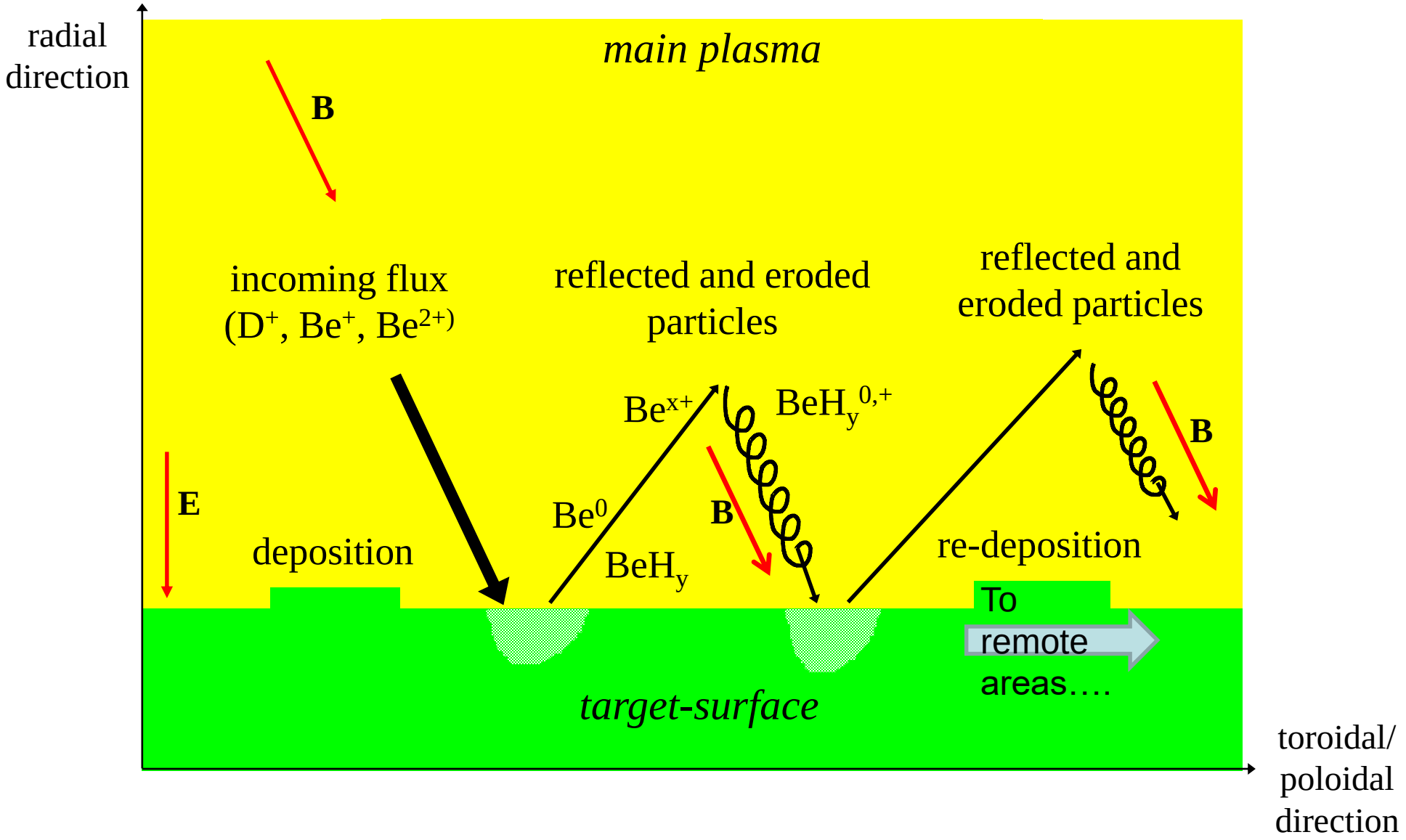
Classification of processes,
Asympt. correct fits,
separate form for each category of reactions

APID 16, IAEA AMD unit

Release (chem. sputtering) and migration + fragmentation of hydro**carbons**



Release (sputtering, volumetric formation/fragementation) and migration + fragmentation of **beryllium** hydrides



MOLECULAR PROCESSES CONSIDERED IN FUSION:

- e+ BeH/BeH^+ → …. possible role on spectroscopy and on material migration:

Formation rates ?? 10% of Be sputtering? Volumetric particle exchange reactions ?

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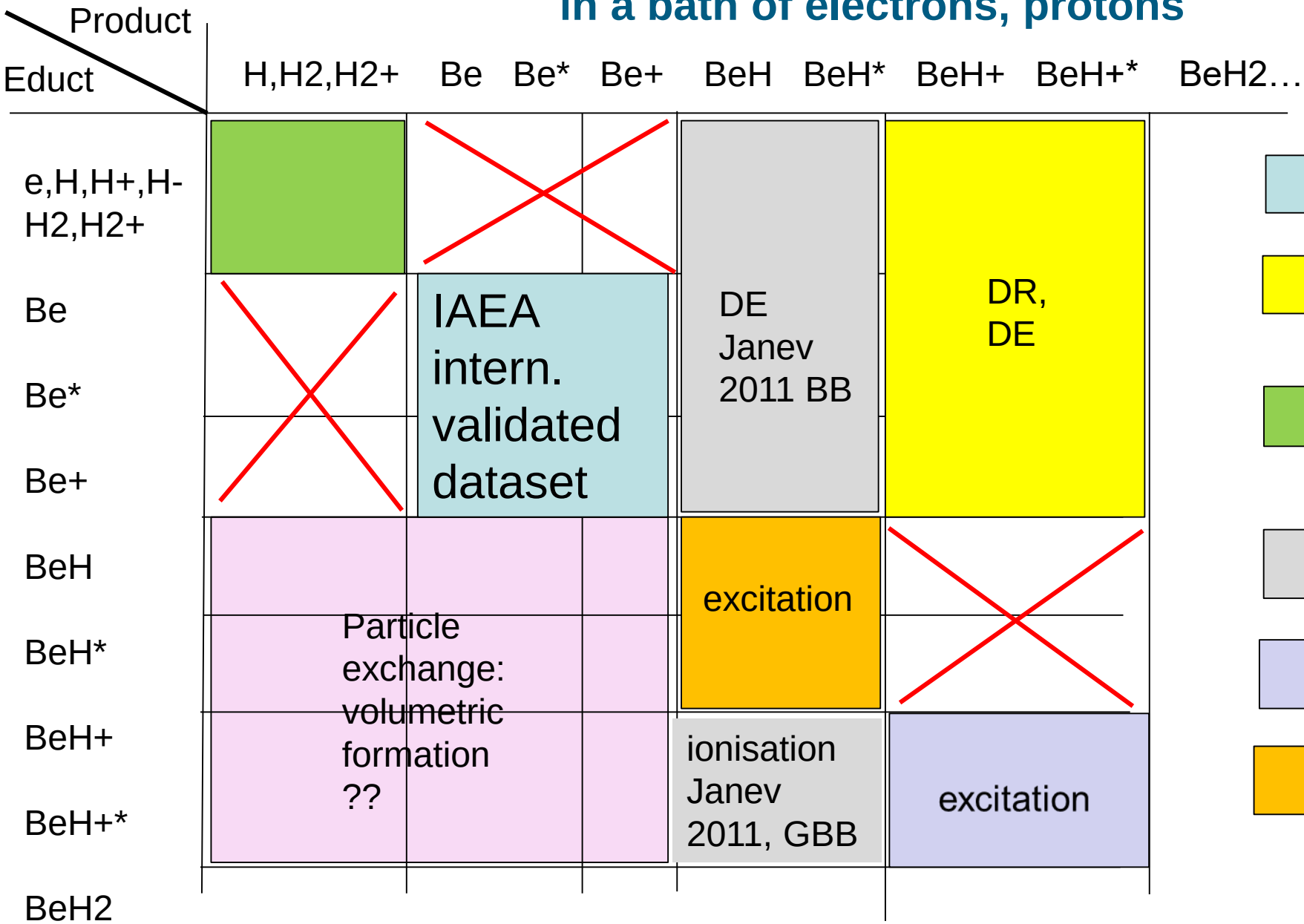
Multiple aspects solved, but data scattered in literature, not jet compiled into a single comprehensive database.

IAEA Consultancy Meeting, June 2019: review of data status

Available (2019): CR matrix for the Be – BeH_y system

in a bath of electrons, protons



[7] Ballance 2003; and Bartschat 2016; and Dipti, 2018, ADNDT

[5] Schneider 2017, 2018
[4] Ross 2009
[6] Laporta 2017

Sawada 2016
Wünderlich 2016
Janev-Reiter 2013

Janev 2011, GBB, BB
„if you must guess“,
www.hydkin.de

[8] Celiberto 2012; and Tennyson 2012

Janev 2011, BB
[9] Celiberto 2013
[10]Tennyson 2017

Issues:

Many individual data now, spread all over the place.

- Overlapping energy range, temperature range ?
- Resolution wrt. vibr., rot., electr. states within each block ?
- Detailed balance ?
- Near threshold and asymptotic behaviour of cross sections, and rate coefficients ?
- Reaction kinetics (KER: kinetic energy releases), branching ratios?
- Heavy particle collisions: particle exchange – charge exchange
- Surface processes: formation of BeH_y ?

Experiments (fusion relevant)

[1] Nishijima D, Doerner R P, Baldwin M J, De Temmerman G and Hollmann E M
2008 Plasma Phys. Control. Fusion 50 125007 (PISCES Be, BeH, exp.)

[2] Brezinsek S, Stamp M F et al., 2014, Nucl. Fusion 54 103001 (11pp) and:
Brezinsek S, Widdowson A et al., 2015 Nucl. Fusion 55 063021 (JET, Be wall: exp.)

Codes (fusion relevant)

www.hydkin.de (2011 -2017) and:
[3] Björkas C,…Janev R K et al,
2013 Journal of Nuclear Materials 438 (2013) S276–S279 (ERO code BeH, BeH+)

Collision data

[4] Roos J B, Larsson M, Larson A and Orel A E
2009 Phys. Rev. A 80 012501 (BeH+, DR)

[5] Niyonzima S, …, Schneider I et al 2017 At. Data Nucl. Data Tables 115–116 287–308 (BeH+, calc.) and:
Niyonzima S, …, Schneider I et al 2018 Plasma Sources Science and Technology (BeD+, calc.)

[6] Laporta V et al
2017 Plasma Phys. Control. Fusion 59 045008 (BeH+, calc.)

[7] Ballance C P et al, 2003 Phys Rev A 68 062705 ;
and: Zatsarinny, O, Bartschat K et al, 2016, Journal of Physics B: Atomic, Molecular and Optical Physics; 49 235701
and: Dipti, T,…, Ralchenko Y, et al 2019 Atomic Data and Nuclear Data Tables, 127–128, https://doi.org/10.1016/j.adt.2018.11.001. (Be, Be*, Be+, calc.)

[8] Celiberto R, Janev R and Reiter D, 2012 Plasma Phys. Control. Fusion 54 035012 and:
Chakrabarti K, Tennyson J 2012 Eur. Phys. J.D 66, 31 (BeH+, X to A,B; calc.)

[9] Celiberto R, Baluja K L and Janev R K
2013 Plasma Sources Sci. Technol. 22 015008 (BeH, X to A, calc.)

[10] Darby-Lewis D, Mašín Z and Tennyson J
2017 J. Phys. B: At. Mol. Opt. Phys. 50 175201 (BeH, excit, calc.)

Data usage in fusion is now far behind the data availability

Next steps:
- Data processing
- Data evaluation
- Data implementation

Collision data, cont.

T Maihom, I Sukuba, R Janev,…T Märk,… 2013 Eur. Phys. J. D (2013) 67: 2 (DM: BeH→ BeH+)

….. and more ?

Spectroscopic data preliminary, not nearly complete….: tbd (DR)

Machado F B C, Ornellas F R, 1991, J. Chem. Phys., Vol. 94, No. 11,1 7237 (BeH+)

D Darby-Lewis, J Tennyson, K D Lawson, et al, 2018 J. Phys. B: At. Mol. Opt. Phys. 51 185701
(BeH, BeD, BeT: A→ X)

J. Pitarch-Ruiz, J. Sánchez-Marin, 2008 J. Chem. Phys. 129, 054310

B. Yadin, T. Veness, P. Conti, Ch. Hill, S. N. Yurchenko and J Tennyson 2012 Mon. Not. R. Astron. Soc. 000, 1 14 (ExoMol, ro-vib BeH)

G Duxbury et al 1998 Plasma Phys. Control. Fusion 40 361
http://dx.doi.org/10.1088/0741-3335/40/3/002 (BeD)

John A. Coxon, R. Colin, Journal of Molecular Spectroscopy, Vol. 181, No. 1. (January 1997), pp. 215-223
http://dx.doi.org/10.1006/jmsp.1996.7153 (BeH+)

….. and more ?

The computational plasma boundary science challenge

SEPARATING KNOWN FROM UNKNOWN: COMPUTATIONALLY

In most applications of A&M data in low temperature plasma chemistry:

$$\frac{\partial}{\partial t} n_i + \vec{\nabla} \cdot \left(n_i \vec{V}_i \right) \approx \frac{n_i}{\tau} = S_{n_i}$$

Plasma transport: known

A&M unknown

Well stirred conditions,
Near equilibrium, homogeneous,
isotropy

In magnetically confined fusion plasmas:

$$\frac{\partial}{\partial t} n_i + \vec{\nabla} \cdot \left(n_i \vec{V}_i \right) = S_{n_i}$$

Plasma transport: unknown

known

Anomalous transport
Drifts, electrical currents,
Kinetic corrections

"If we are confident in a plasma state, then we can quantify A&M processes in it".

Plasma boundary equations: ("transport approx.")

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Particle conservation:

$$\frac{\partial n_i}{\partial t}+\nabla\cdot\left(n_i\mathbf{V}_i^{eff}\right)=S_i^n \quad \text{where} \quad \mathbf{V}_i^{eff}=V_{i\|}\mathbf{b}+\frac{c}{B}\mathbf{b}\times\nabla\varphi+\frac{cT_i}{Z_i e}\nabla\times\left(\frac{\mathbf{b}}{B}\right)-\frac{D_{an}}{n_i}\nabla_\perp n_i$$

Parallel momentum conservation:

$$m_i\frac{\partial n_i V_{i\|}}{\partial t}+\nabla\cdot\left(m_i n_i\mathbf{V}_i^{eff}V_{i\|}\right)=-\mathbf{b}\cdot\nabla p_i+Z_i e n_i\mathbf{b}\cdot\nabla\varphi-\mathbf{b}\cdot\nabla\Pi_{i\|}+\frac{3}{2}\frac{(\mathbf{b}\cdot\nabla B)}{B}\Pi_{i\|}+\nabla\cdot\left(\eta_2\nabla V_{i\|}\right)+S_{i\|}^m+F_{ie\|}$$

Charge conservation:

$$\nabla\cdot\left(\mathbf{J}^{eff}\right)=0 \quad \text{where} \quad \mathbf{J}^{eff}=J_\|\mathbf{b}+cp\nabla\times\left(\frac{\mathbf{b}}{B}\right)+\mathbf{J}_\perp^{vis+in+s}-\sigma_{an}\nabla\varphi$$

$$\mathbf{J}_\|=\sigma_\|\left[\frac{1}{e}\left(\frac{1}{n_e}\nabla_\| p_e+\frac{\kappa_{12}}{\kappa_{11}}\nabla_\| T_e\right)-\nabla_\|\varphi\right]$$

Energy conservation:

$$\frac{3}{2}\frac{\partial p_i}{\partial t}+\nabla\cdot\mathbf{q}_i^{eff}=\mathbf{V}_i\cdot\nabla p_i-\boldsymbol{\Pi}_i:\nabla\mathbf{V}_i+Q_i, \quad \text{where } \mathbf{q}_i^{eff}=-\kappa_\|^i\nabla_\| T_i-\kappa_\perp^i\nabla_\perp T_i-\chi_{an}n_i\nabla T_i+\frac{5}{2}p_i\mathbf{V}_i^{eff}$$

$$\frac{3}{2}\frac{\partial p_e}{\partial t}+\nabla\cdot\mathbf{q}_e^{eff}=\mathbf{V}_e\cdot\nabla p_e+Q_e, \quad \text{where } \mathbf{q}_e^{eff}=\frac{\kappa_{12}}{\kappa_{11}}\frac{T_e}{e}J_\|\mathbf{b}-\kappa_\|^e\nabla_\| T_e-\kappa_\perp^e\nabla_\perp T_e-\chi_{an}n_e\nabla T_e+\frac{3}{2}\frac{T_e}{m_e\Omega_e^2\tau_e}\nabla_\perp p+\frac{5}{2}p_e\mathbf{V}_e^{eff}$$

The generic equation, for all A&M effects „S“ in plasma (or in any other given inhomogeneous medium): „Boltzmann (linear) transport equation“, solved with conventional Monte Carlo transport codes. In fusion: e.g. EIRENE code, DEGAS-2, NEUT2,etc

$$\frac{1}{v}\frac{\partial\phi(\mathbf{r},\Omega,E,t)}{\partial t}+\Omega\cdot\nabla\phi(\mathbf{r},\Omega,E,t)+\Sigma(\mathbf{r},E,t)\phi(\mathbf{r},\Omega,E,t)$$
$$=\int\int\Sigma(\mathbf{r}',\Omega',E'\rightarrow\mathbf{r},\Omega,E)\phi(\mathbf{r}',\Omega',E',t)d\Omega'dE'+Q,$$

Neutrons: nuclear science and engieering → linear, or nonlinear: MC - T- H **(e.g.: MCNP)**
Radiation: astro and laser physics → linear, or nonlinear: MC – temp. fields
Neutrinos:
Electrons: solid state physics applications
Neutral atoms/molecules: magnetic fusion → linear, or nonlinear: MC – plasma (transport) dynamics

And many more….

Here go the data (e.g. nuclear data)
In fusion: AM&S data

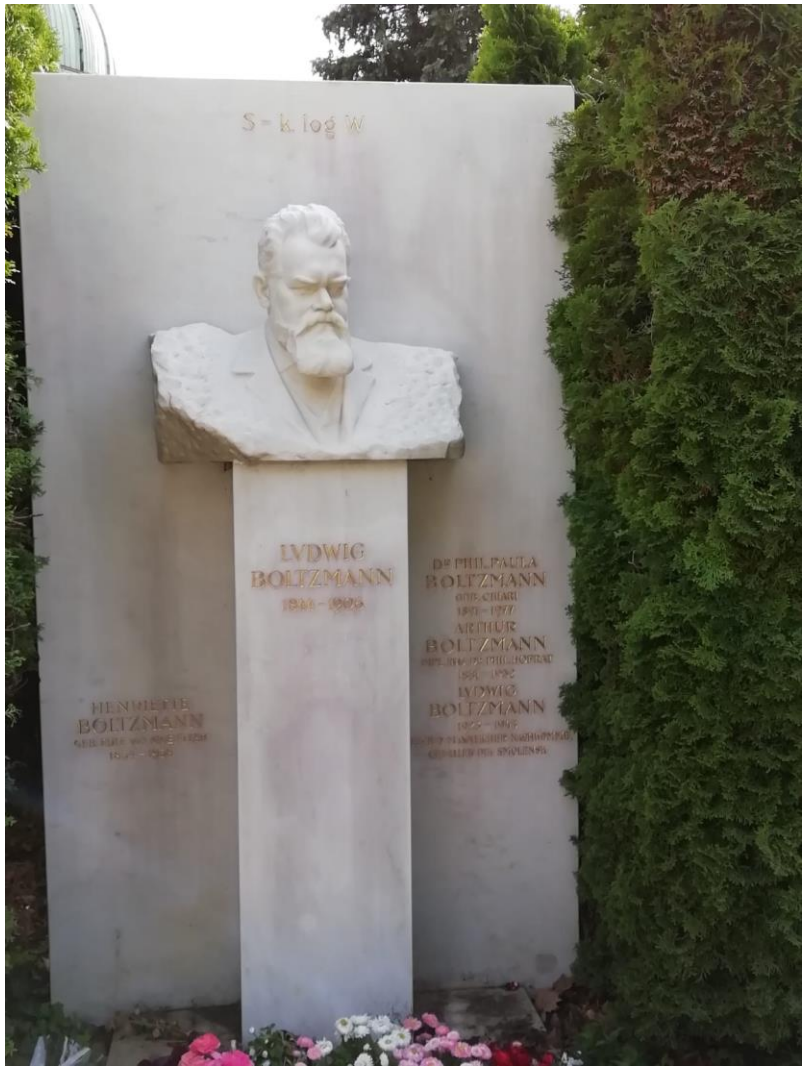
→ requires: balanced, internally consistent, complete, convenient,…A&M data sets

$$\frac{1}{v}\frac{\partial\phi(\mathbf{r},\Omega,E,t)}{\partial t}+\Omega\nabla\phi(\mathbf{r},\Omega,E,t)+\Sigma(\mathbf{r},E,t)\phi(\mathbf{r},\Omega,E,t)$$
$$=\int\int\Sigma(\mathbf{r}',\Omega',E'\rightarrow\mathbf{r},\Omega,E)\phi(\mathbf{r}',\Omega',E',t)d\Omega'dE'+Q,$$

Neutrons: nuclear science and engineering → linear, or nonlinear: MC - T- H
Radiation: astro and laser physics → linear, or nonlinear: MC – temp. fields
Neutrinos:
Electrons: solid state physics applications
Neutral atoms/molecules: magnetic fusion → linear, or nonlinear: MC – plasma (transport) dynamics

And many more….

Ludwig Boltzmann: S=k log W



Vienna Central Cemetery, May 2019

Starting from Boltzmann:
Constructing transport models for gases and plasmas
(classical Chapman-Enskog-method, Grad-method, 1930 - 1960 both: series expansions near a Maxwellian distribution)

For a given collision process, cross section σ(E)

Find „collision integrals“

$$Q^l(T) = \int_{E_{th}}^{\infty} dE\sigma(E)E^l f_{maxw}(E,T), \quad l \geq 1$$

From those: transport coefficients (viscosity, thermal conductivity)
or source rates S, Q from particles, momentum and energy

e.g. *l*=1: (Maxw. reaction rate coefficient k(T))

PLASMA CHEMISTRY DATABASES: FAR SOL, SUB-DIVERTOR

C_xH_y as a role model for other Hydrides (Be_xH_y, NH_x, HeH^+,….systems?)

- Already done SiH_y: Janev, Reiter, Contr. Plasma Physics, 2003,43,401-417

Chemistry | Physics

Extensions, evaluations, new exp. and theor. results →

1987 | 2002-2004 | 2012

Plasma chemical rate constants (Arrhenius form) for well stirred, equilibrium, low T conditions

A.B. Ehrhardt, W. D. Langer, Report PPPL-2477, Princeton (1987).

Comprehensive set.
Cross sections already, but universal fit expression for all types of processes
→ poor asymptotic behaviour

R.K. Janev, D. Reiter
Phys. Plasmas, Vol 9, 9, (2002) 4071
Phys. Plasmas, Vol 11,2, (2004) 780

Classification of processes,
Asympt. correct fits,
separate form for each category of reactions

APID 16, IAEA AMD unit

PLASMA CHEMISTRY DATABASES (RATE CONSTANTS)

- **N_xH_y (Nitrogen, Ammonia)**

Chemistry | Physics

2017 — 2018 — ?? — ??

Plasma chemical rate constants (Arrhenius) for well stirred, equilibrium, low T conditions

ITER database, distributed with SOLPS
S. Touchard et al. Nuclear Materials and Energy 18 (2019) 12-17

T. Body et al. Plasma Phys. Control. Fusion 60 (2018) 075011 (16pp)
0D plasma chemical model, Incl. experimental tests, at MAGPIE plasma device, conclusions also about surface mechanisms

R. Perillo et al. Plasma Phys. Control. Fusion 60 (2018) 105004 (18pp)

If upgrading from 0D reaction kinetics → 2D or 3D transport formulations needed ??:

Turn this info into comprehensive cross section database, e.g. as in 2002-2004 hydrocarbon database

Evaluation, Recommended data set APID xxx ??, IAEA AMD unit

Transport collision integrals for Arrhenius rates:

HEINRICH HEINE
UNIVERSITÄT DÜSSELDORF

- Rate coeff.: $K(T) = k'T^{\alpha}e^{-E_{th}/kT} = k_0\beta^{-\alpha}e^{-E_{th}\beta}$

  Well stirred, low T, near equilibrium **(not in fusion plasmas)**

- Reconstructing cross section from it:

$$\alpha = -3/2: \quad \sigma(E) = k_0\sqrt{\pi\mu/8}\cdot\frac{\delta(E-E_{th})}{E}$$

$$\alpha > -3/2: \quad \sigma(E) = k_0\sqrt{\pi\mu/8}\,\frac{1}{\Gamma(\alpha+3/2}\cdot\frac{(E-E_{th})^{\alpha+1/2}}{E}$$

$$\Rightarrow Q^l(T) = \int_{E_{th}}^{\infty} dE\sigma(E)E^l f_{maxw}(E,T), \quad l \geq 1$$

→ consistent transport model

E: COM collision energy, μ: reduced mass

MOLECULAR PROCESSES CONSIDERED IN FUSION:

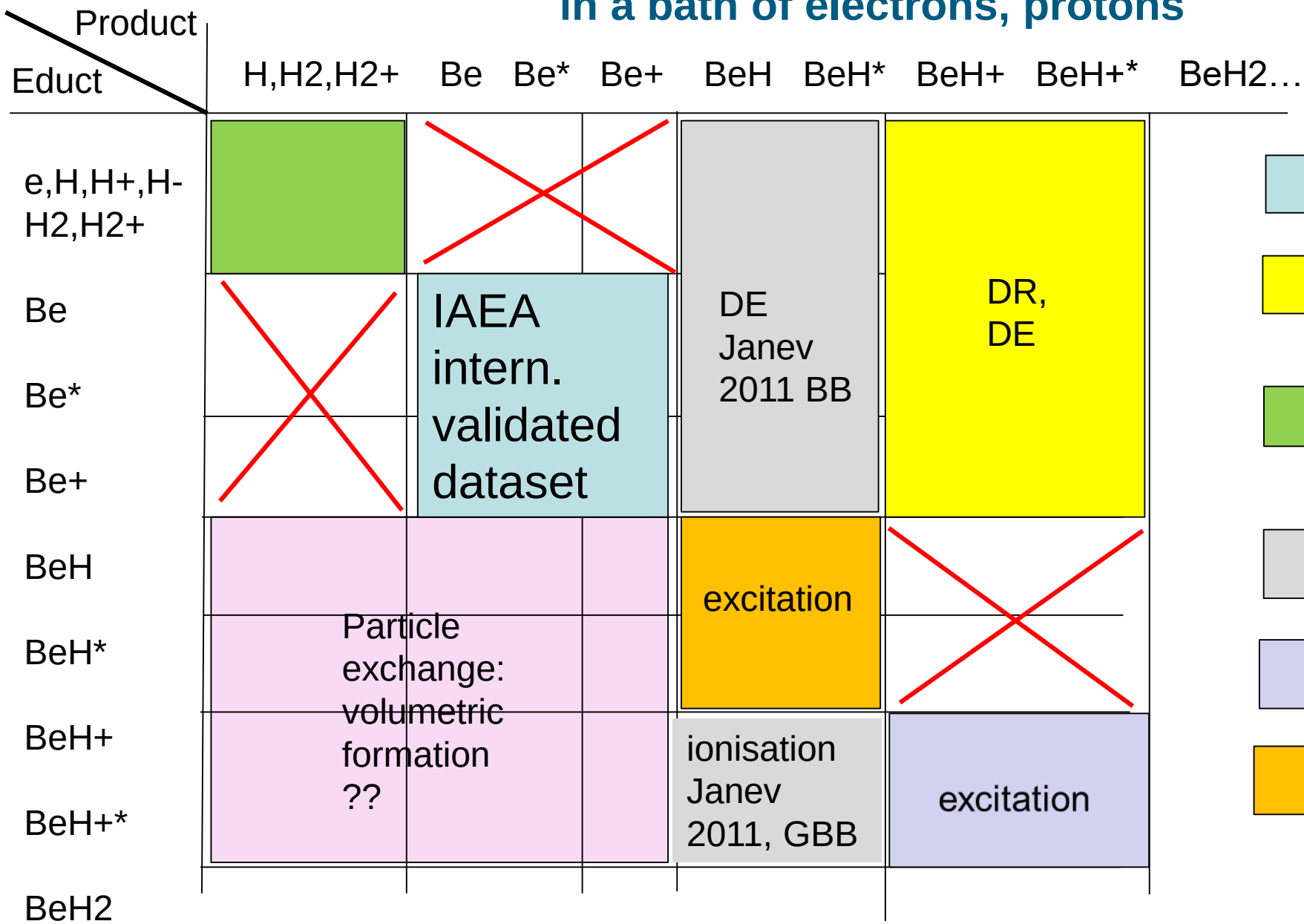
- $e,p + H_2(v_i) \rightarrow \ldots$, $e+H_2^+(v_i) \rightarrow H + H^*$ divertor detachment dynamics,

www.amdis.iaea.org, data center network, Atoms 2016, D. Wuenderlich, U.Fantz, IPP Garching, K. Sawada, M.Goto, NIFS, and Fursa et al, PRL 2016

$e+H2^+(v)$: Int. Conference series: Dissociative Recombination 1-9 (1988 -2012)

Available (2019): CR matrix for the Be – BeH_y system

in a bath of electrons, protons



[7] Ballance 2003; and Bartschat 2016; and Dipti, 2018, ADNDT

[5] Schneider 2017, 2018
[4] Ross 2009
[6] Laporta 2017

Sawada 2016
Wünderlich 2016
Janev-Reiter 2013

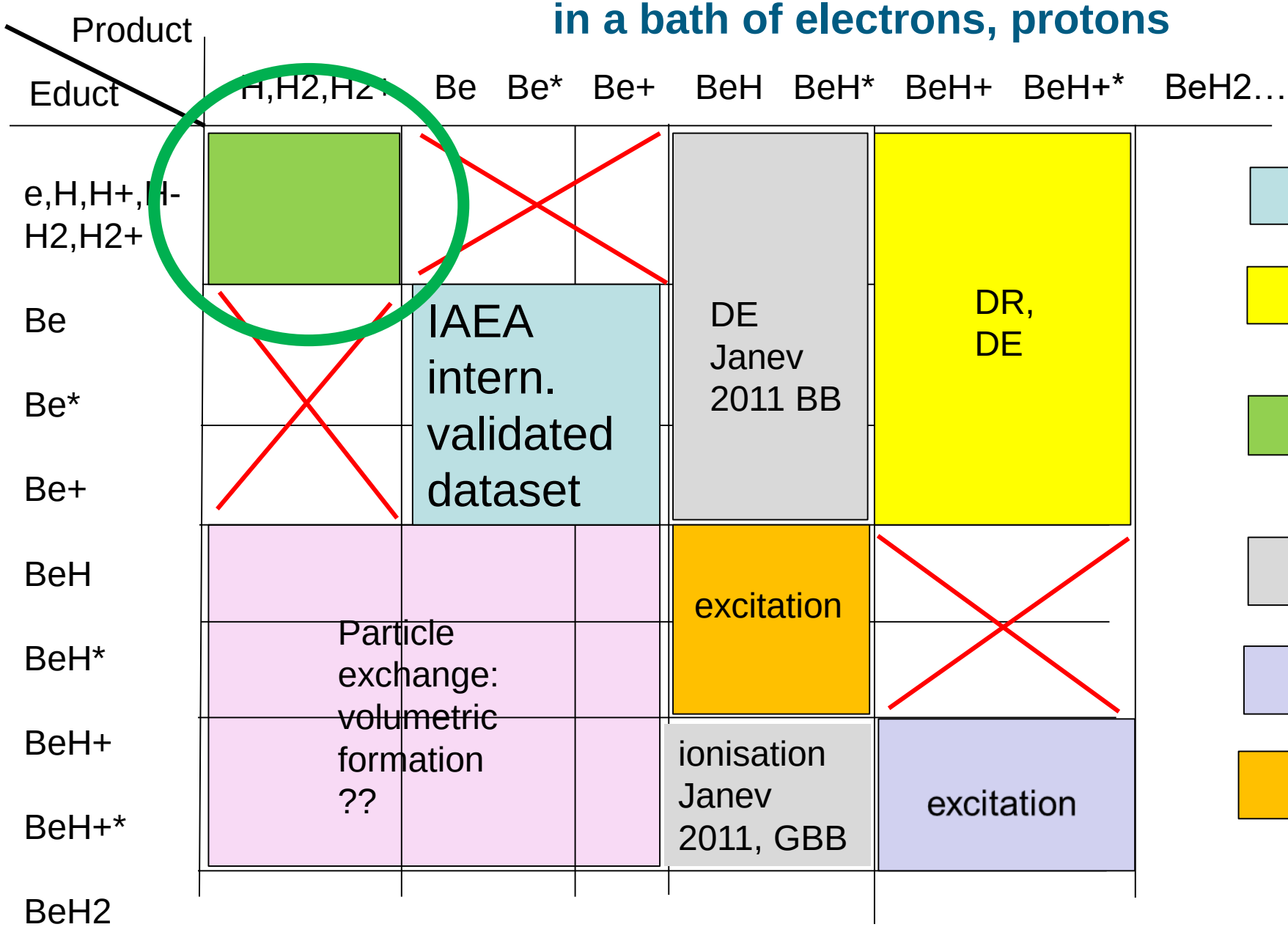
Janev 2011, GBB, BB
„if you must guess“,
www.hydkin.de

[8] Celiberto 2012; and Tennyson 2012

Janev 2011, BB
[9] Celiberto 2013
[10]Tennyson 2017

Available (2019): CR matrix for the Be – BeH_y system

in a bath of electrons, protons



[7] Ballance 2003; and Bartschat 2016; and Dipti, 2018, ADNDT

[5] Schneider 2017, 2018
[4] Ross 2009
[6] Laporta 2017

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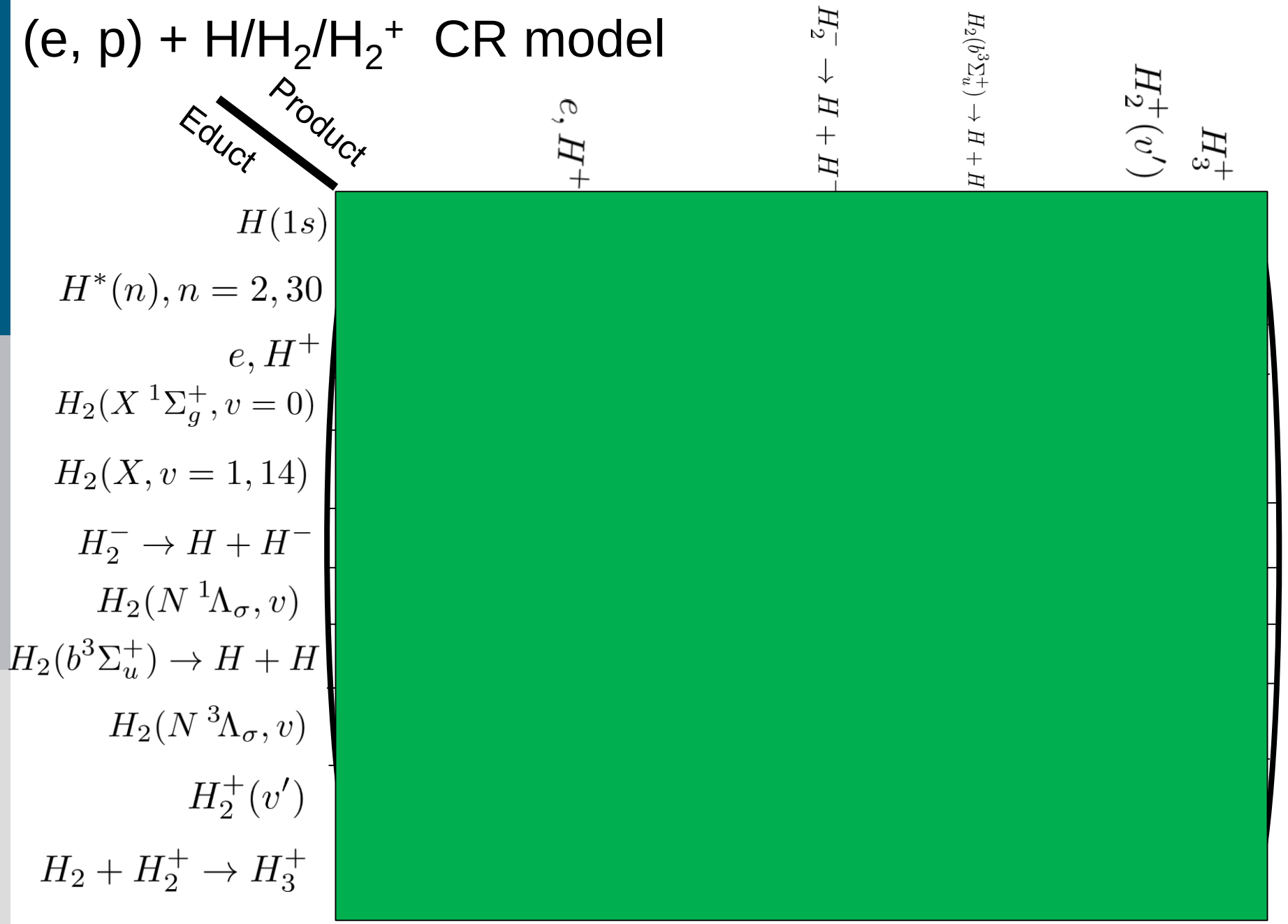
Janev 2011, GBB, BB
„if you must guess“,
www.hydkin.de

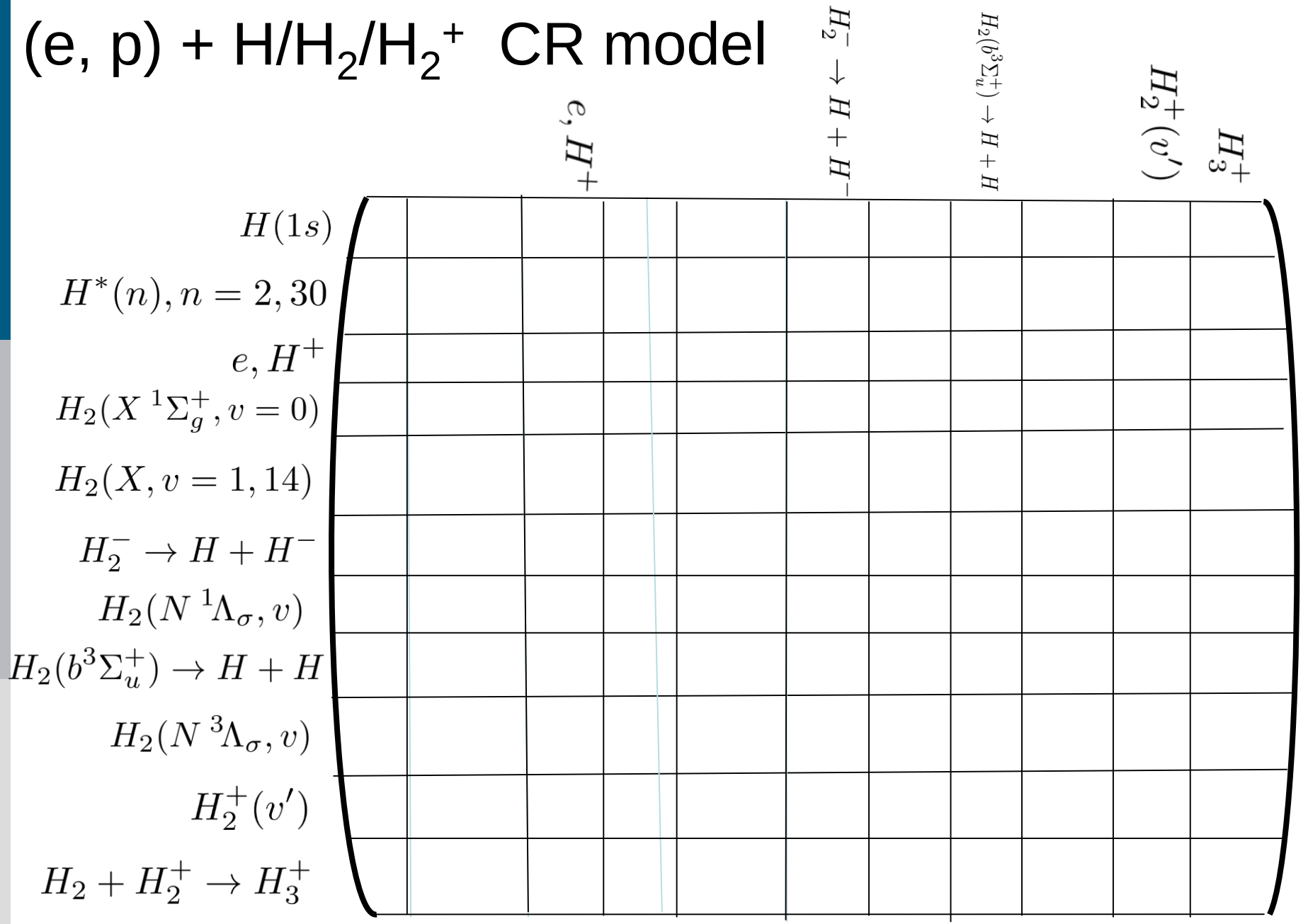
[8] Celiberto 2012; and Tennyson 2012

Janev 2011, BB
[9] Celiberto 2013
[10]Tennyson 2017

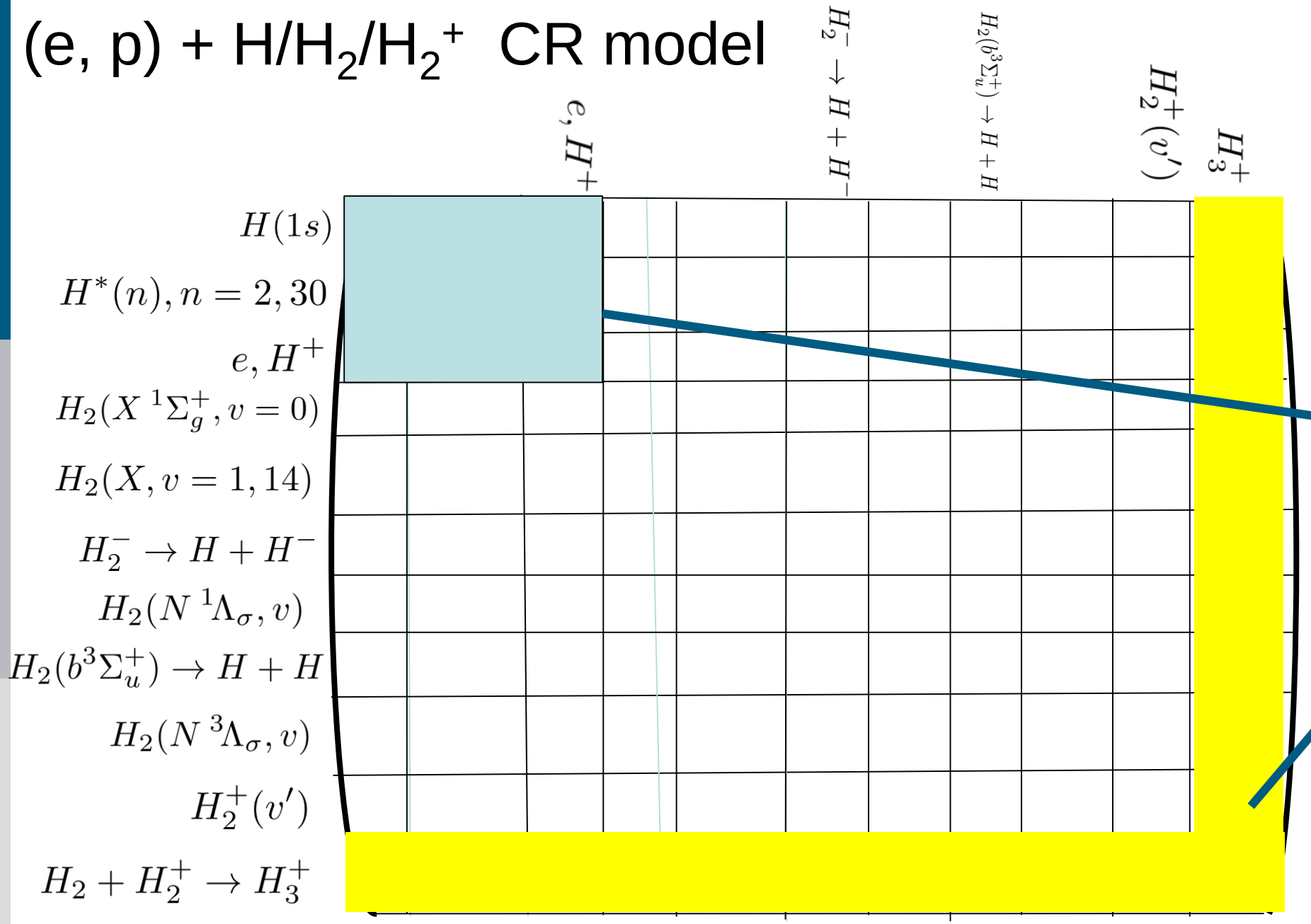
(e, p) + $H/H_2/H_2^+$ CR model



(e, p) + H/H_2/H_2^+ CR model



(e, p) + H/H_2/H_2^+ CR model



H - atom CR Codes Since 1960th, Johnson-Hinnow

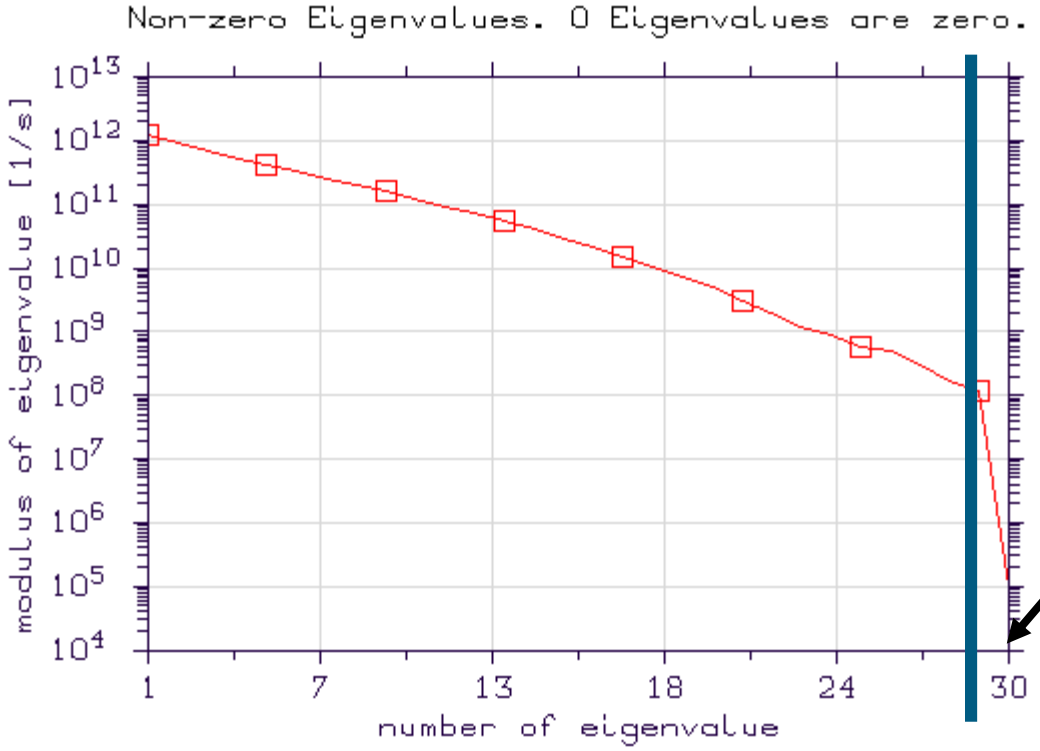
H_3^+: non-linear part. Probably not needed in fusion plasmas (but: in small technical plasma devices)

HYDKIN: spectral analysis for reaction kinetics

Warm up: H-atom, CR model: H(1),H*(2),….,H*(30),H^+

(i,k-excitation, i-ionization A_ik, and k,i de-excitation

Eigenvalues of Hydrogen CR Rate Matrix @ Te = 10 eV, ne = 1e13



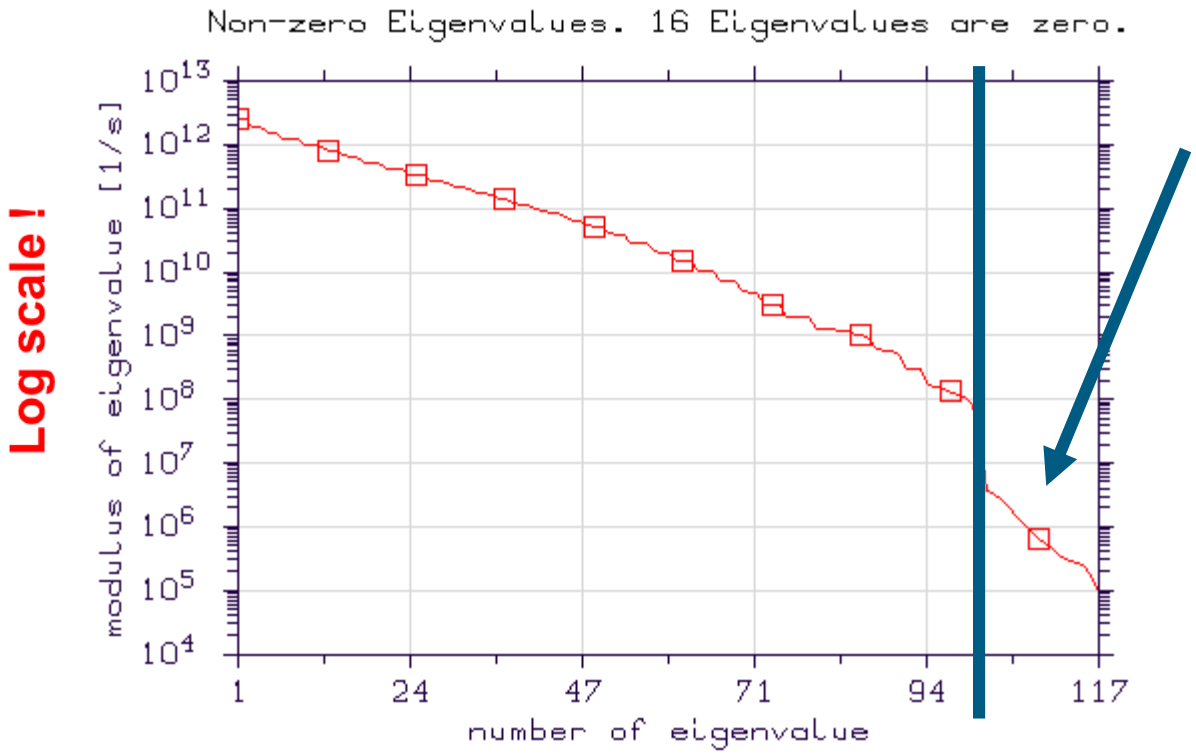
Log scale !

One, out of the 30 eigenvalues of H-CR Matrix, is order of magnitudes smaller than the others. Ground state H(1s)

Very disparate time scales → Model reduction possible
→ Use effective CR rates, with only H and H^+ kept separate in transport equations.

HYDKIN: spectral analysis for reaction kinetics

Coupled H-H^+-H_2-H_2^+ CR model, @ 10 eV, 1e13 cm-3
134 species/states, 16 final states, 117 non-zero eigenvalues



16 eigenvalues are orders of magnitude smaller than all the others.

These correspond to H(1s) and the H2(v, v=0,14) vibr. states in electronic ground state

→ 16 (“metastables”), 16 coupled transport (Boltzmann) eqs. for them.

All the other ≈100 states can be condensed, in effective CR rates and hence be removed from transport problem.

The curse of dimensionality:

eff. Rates(Te, ne, Ti, ni, E, opacity, loss times), → multidim. tables?

Solution: brute force computing power: solve CR models “on the fly”, rather than lookup in precomputed tables (done in EIRENE code for H (2001), He (2018) , next: H_2, Be,….

Synthetic helium beam diagnostic and underlying atomic data

W. Zholobenko[1,2], M. Rack[1,3], D. Reiter[1], M. Goto[4], Y. Feng[2], B. Küppers[1] and I

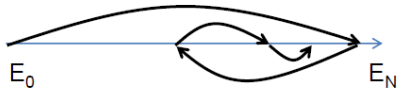
Published 20 September 2018 • © EURATOM 2018
Nuclear Fusion, Volume 58, Number 12

Same trend in fission (neutronics):
Massive distributed computing vs. complex

MC Neutron : Cross Sections

- Take up 80% of overall computing time :

This time is mostly spent in the **Binary Search** to locate **E** in the energy grid :



Bouncing binary search → 65% LLC misses

(Ref : John R Tramm and Andrew R Siegel. “Memory bottlenecks and memory contention in multi-core monte carlo transport codes”. Annals of Nuclear Energy, 82:195–202, 2015)

- Analysis shows that:
  - The energy grid is **accessed randomly**
  - The floating point unit is mostly idle because of **cache misses**
  - The vector unit does **nothing**

Y. WANG, C. CALVIN – CEA/DRF – Maison de la Simulation
E. BRUN, F. MALVAGI – CEA/DEN

The addressed problems

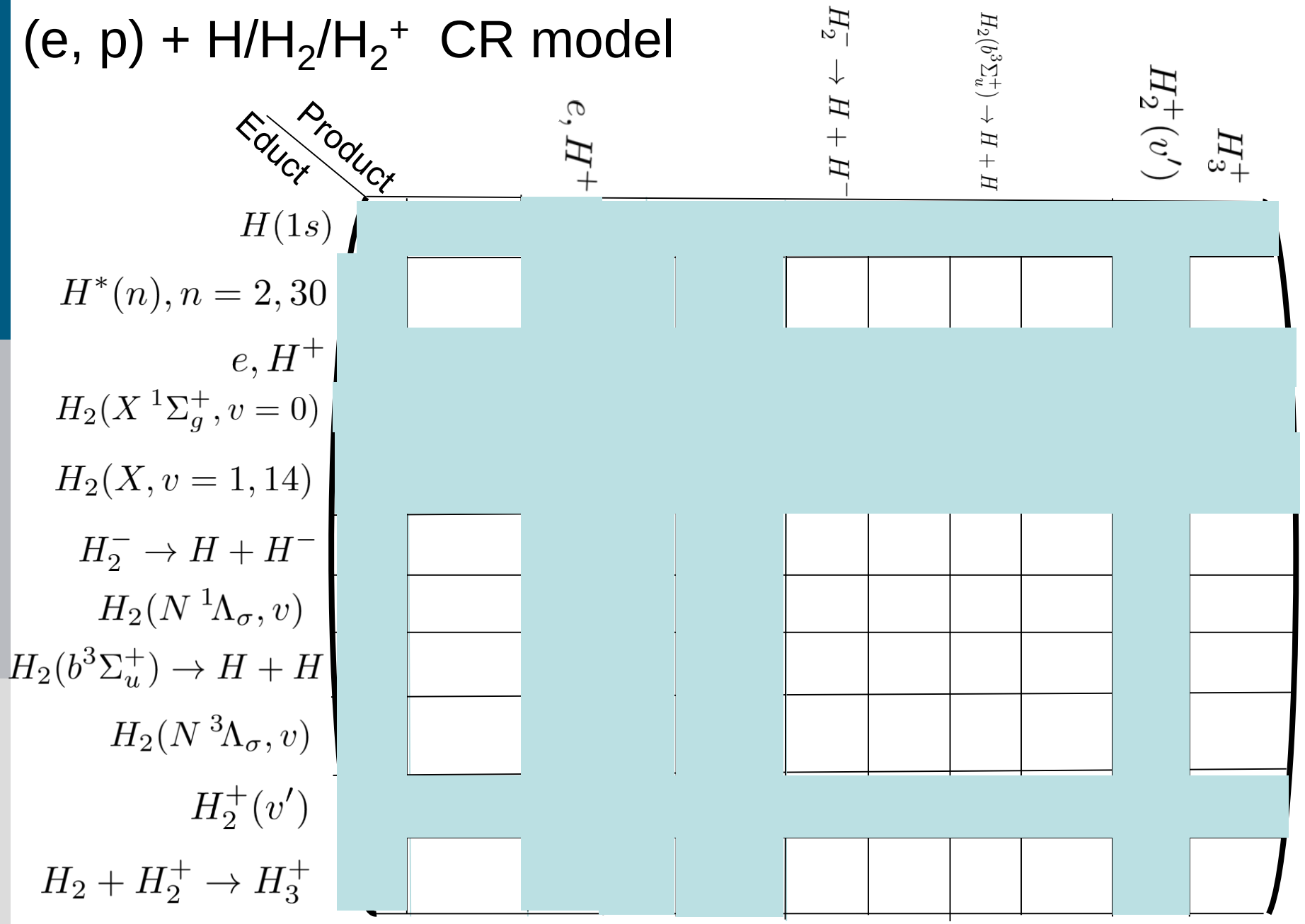
Optimization of the cross-section lookup:

- Both in terms of CPU performances and memory footprint
- We focus on many core architecture (multilevel parallelism and vectorization)
- Try to find efficient approaches for many core architecture: from memory bound problem → CPU-bound problem

2 approaches:

- Classical one: cross-sections are pre-computed and stored into memory – Find an optimal energy lookup algorithm
- One-the-fly cross sections calculations: minimize memory footprint – But what about performances ?

(e, p) + $H/H_2/H_2^+$ CR model



Remove species, for which we solve transport equations. (here: 18)
Solve for CR Population of the rest, taking the former as Known (here: 120)

Rapid progress in molecular H_2 data, often tested against experimental results in small (linear) plasma devices

Recommended entry point to the data-bases used here (and in other edge codes):
3 recent reviews (2016) from an IAEA “coordinated research project” (CRP) 2011-2016

atoms MDPI www.mdpi.com/journal/atoms

Dirk Wünderlich and Ursel Fantz

Atoms 2016,4,26;doi:10.3390/atoms4040026

Keiji Sawada and Motoshi Goto

Atoms 2016,4,29;doi:10.3390/atoms4040029

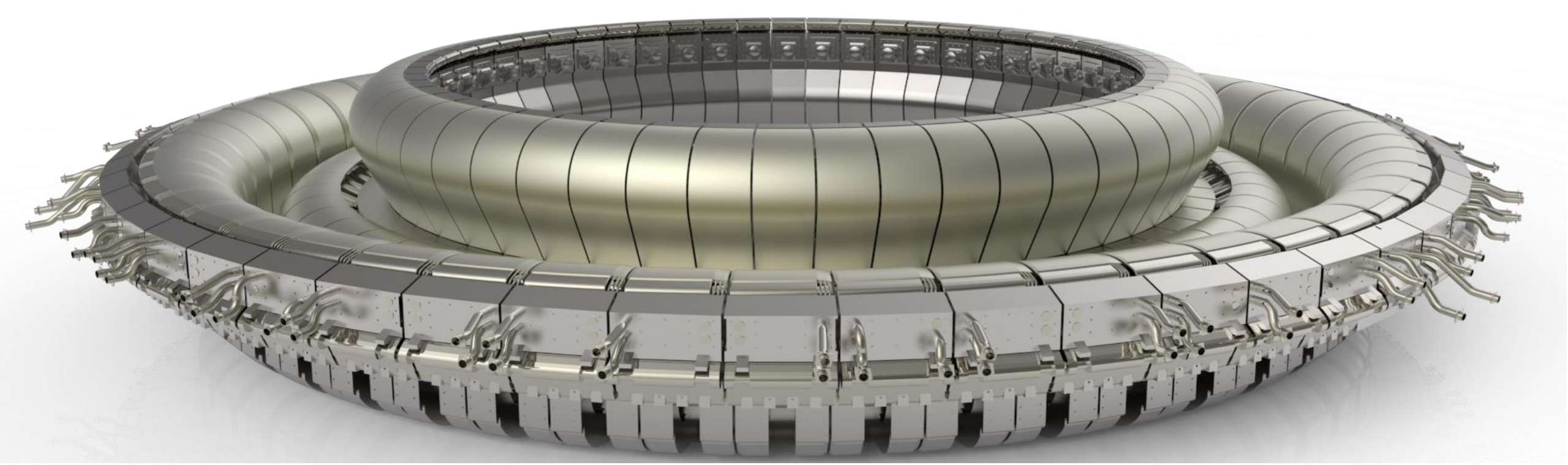
Roberto Celiberto, Mario Capitelli et al.

Atoms 2017,5,18;doi:10.3390/atoms5020018

Data usage in fusion is now far behind the data availability

First ab initio electron-molecule CCC calculations now become available (one of the golden standards for electron collision processes in small systems) for the e+H_2 and e+H_2^+ systems: Curtin Univ. Perth, Australia
Zammit, Savage, Fursa & Bray, Phys. Rev. Lett. 16 (2016) 233201 and Phys. Rev. A 90,022711 (2014), and Phys. Rev. A 95,022708(2017)

The ITER tungsten divertor

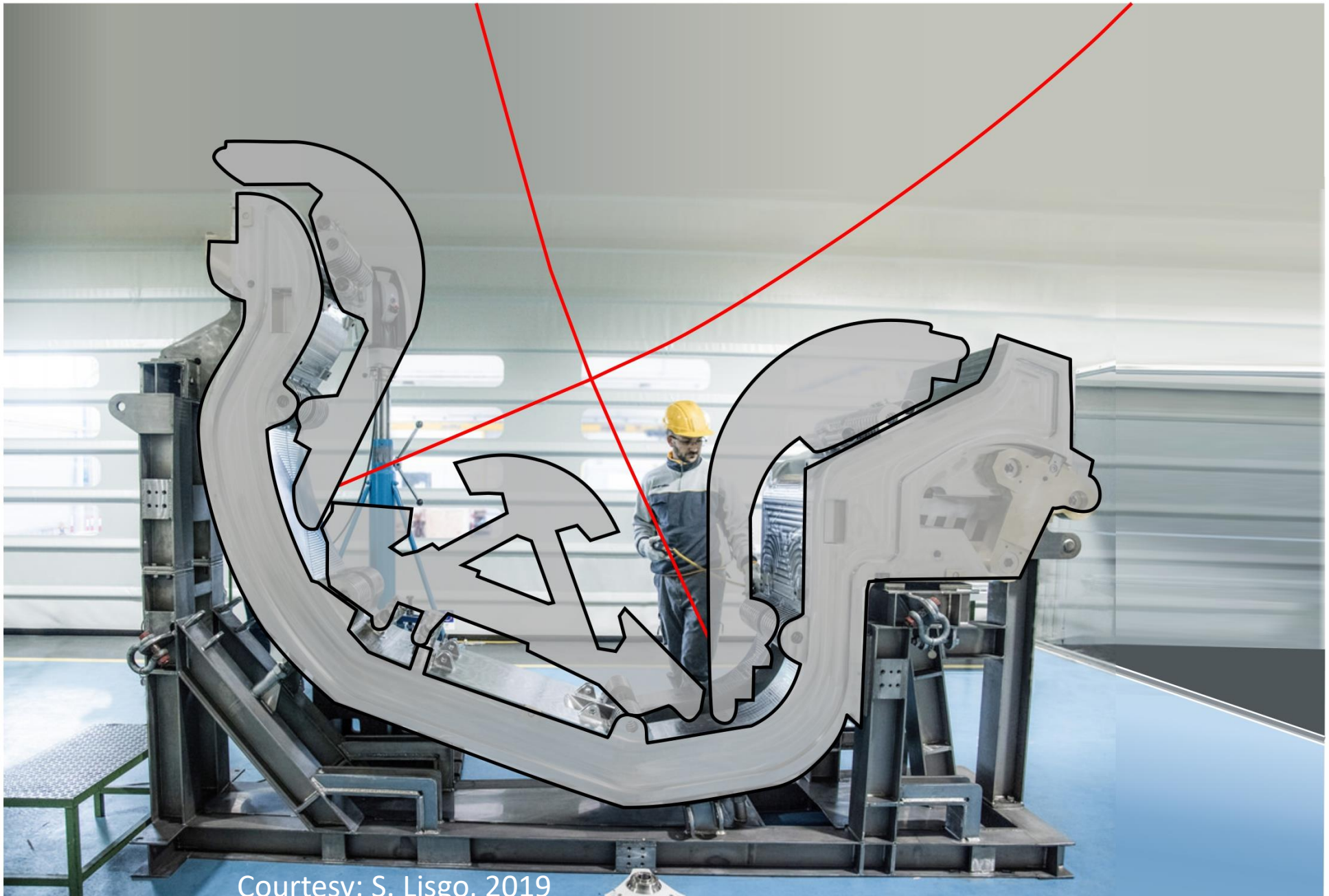


- The most sophisticated tokamak divertor ever built
  - 54 individual cassettes, fully water cooled, designed to handle up to ~100 MW in steady state
  - Now entering the procurement phase → design essentially complete

The ITER divertor

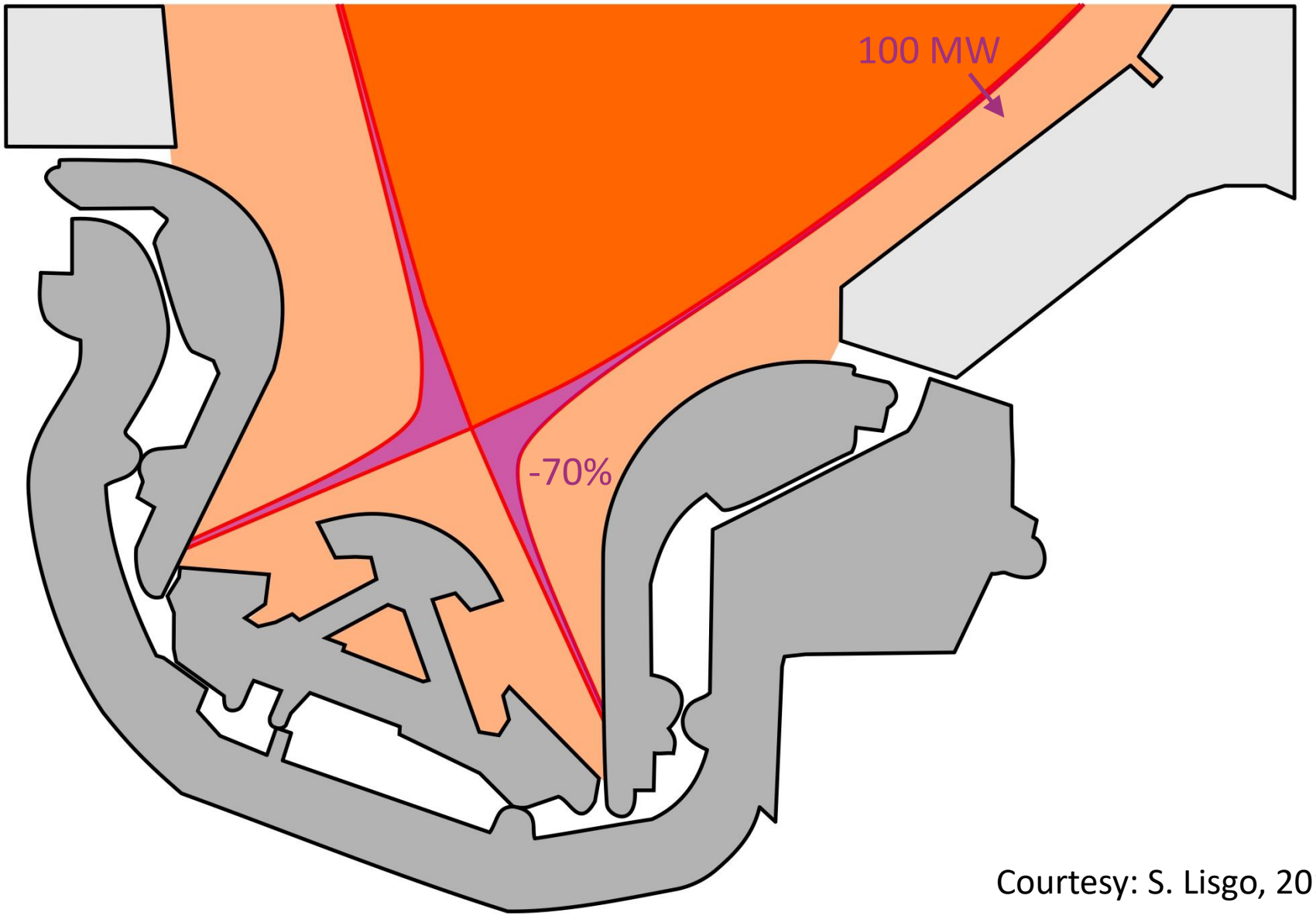
Courtesy: S. Lisgo, 2019

The ITER divertor



Courtesy: S. Lisgo, 2019

The ITER divertor

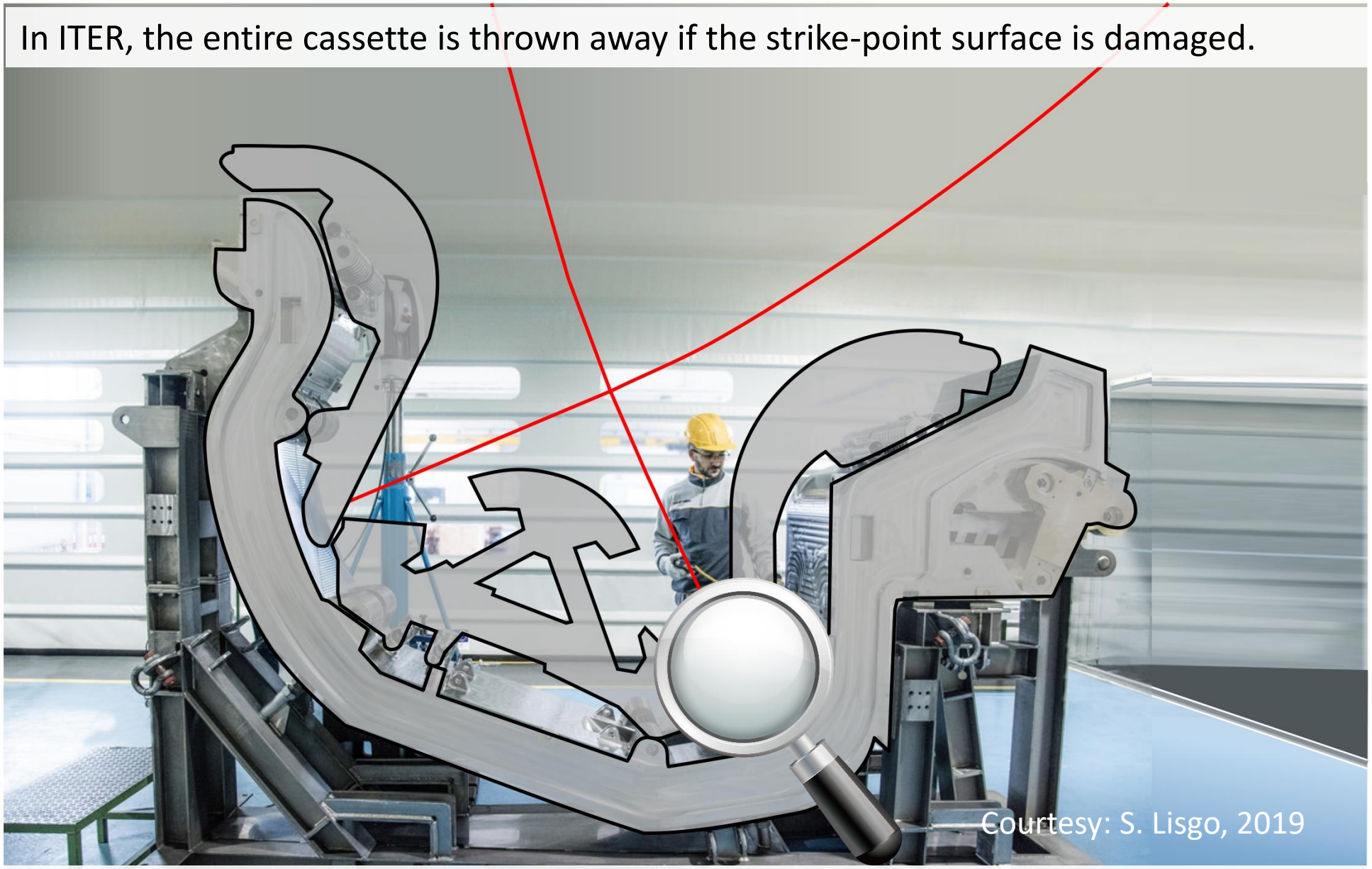


Courtesy: S. Lisgo, 2019

Recall: a 5 mm λ_q at the outer mid-plane is assumed for the **power channel**.

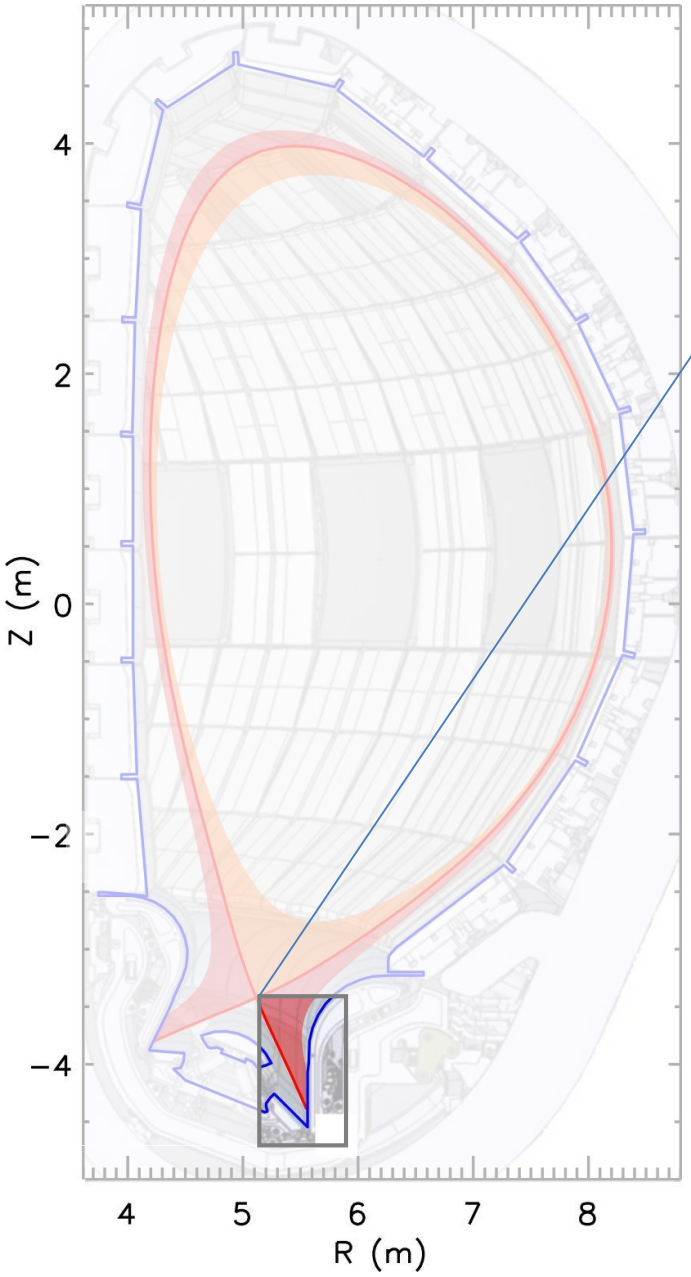
Also, the current DEMO reference involves large modular components

In ITER, the entire cassette is thrown away if the strike-point surface is damaged.

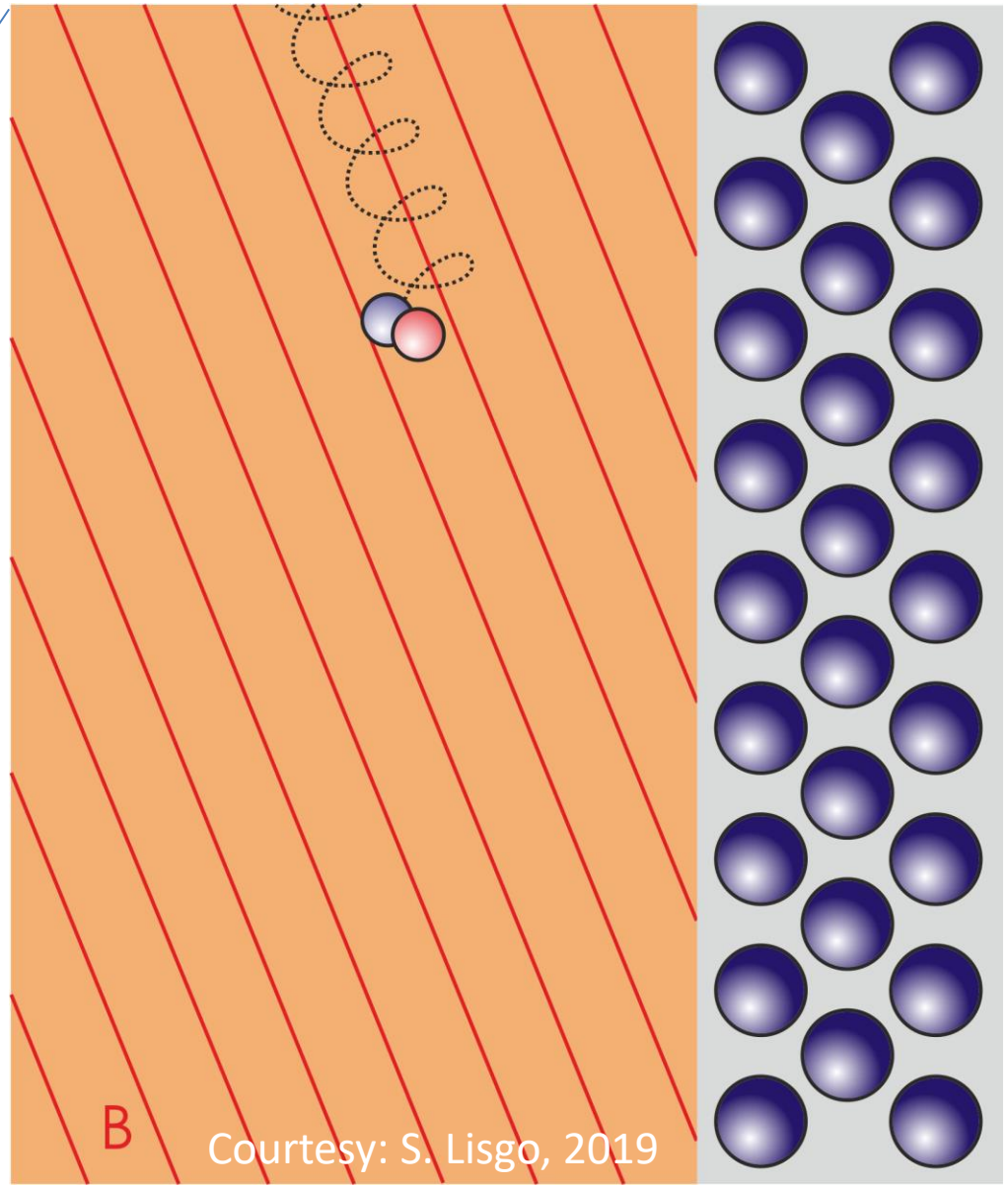


(Replacement time of 6 months, and only 4 spare cassettes. 5 years to make new ones.)

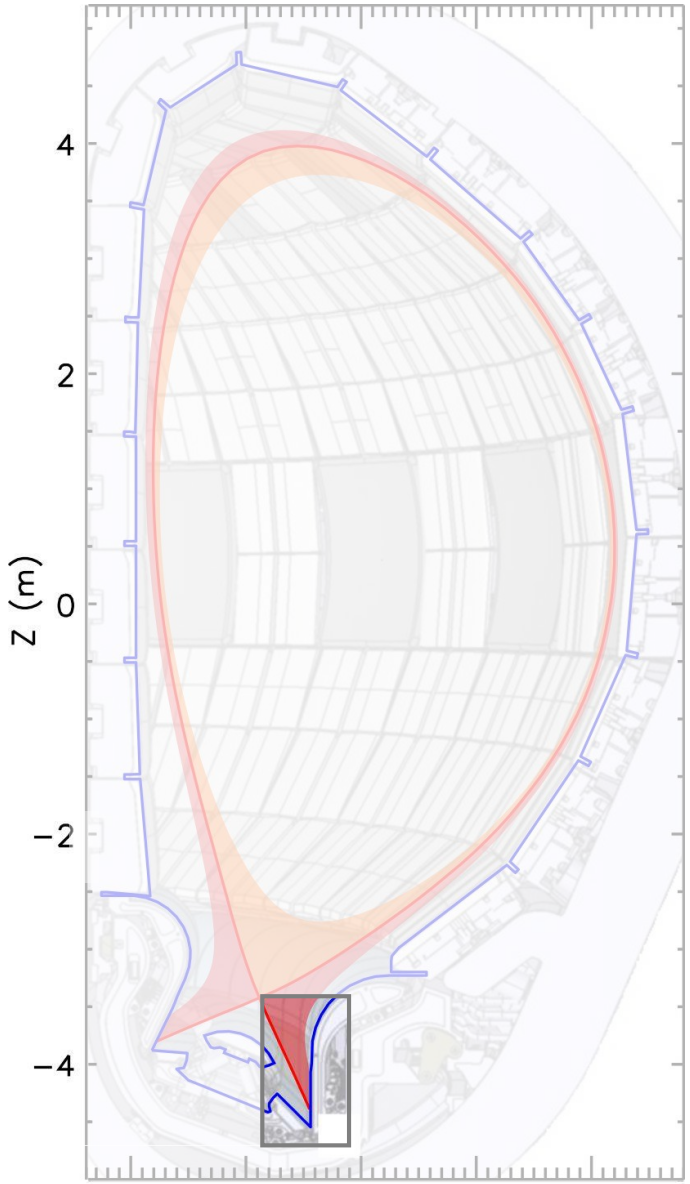
Dissipation – Divertor detachment



ION STREAMING TO SURFACE

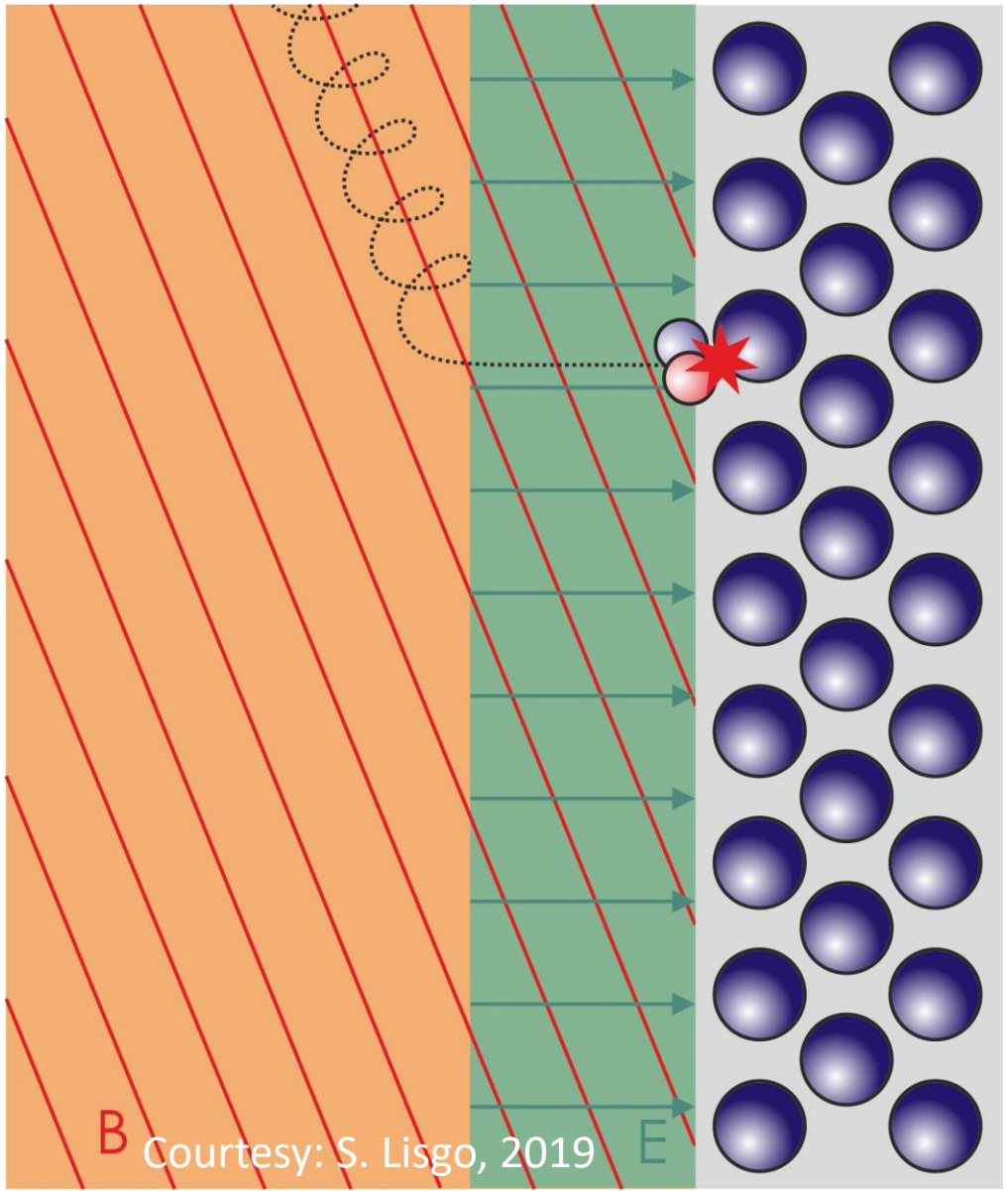


Dissipation – Divertor detachment



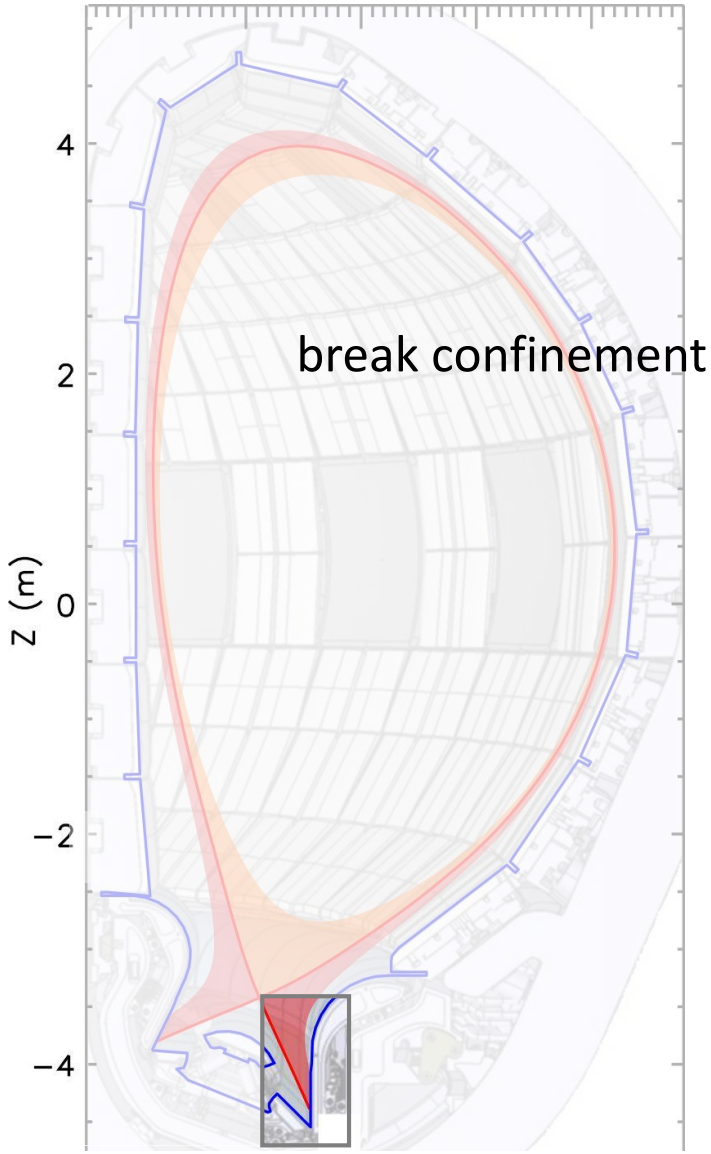
[Stangeby …]

SHEATH ACCELERATION TO THE TARGET



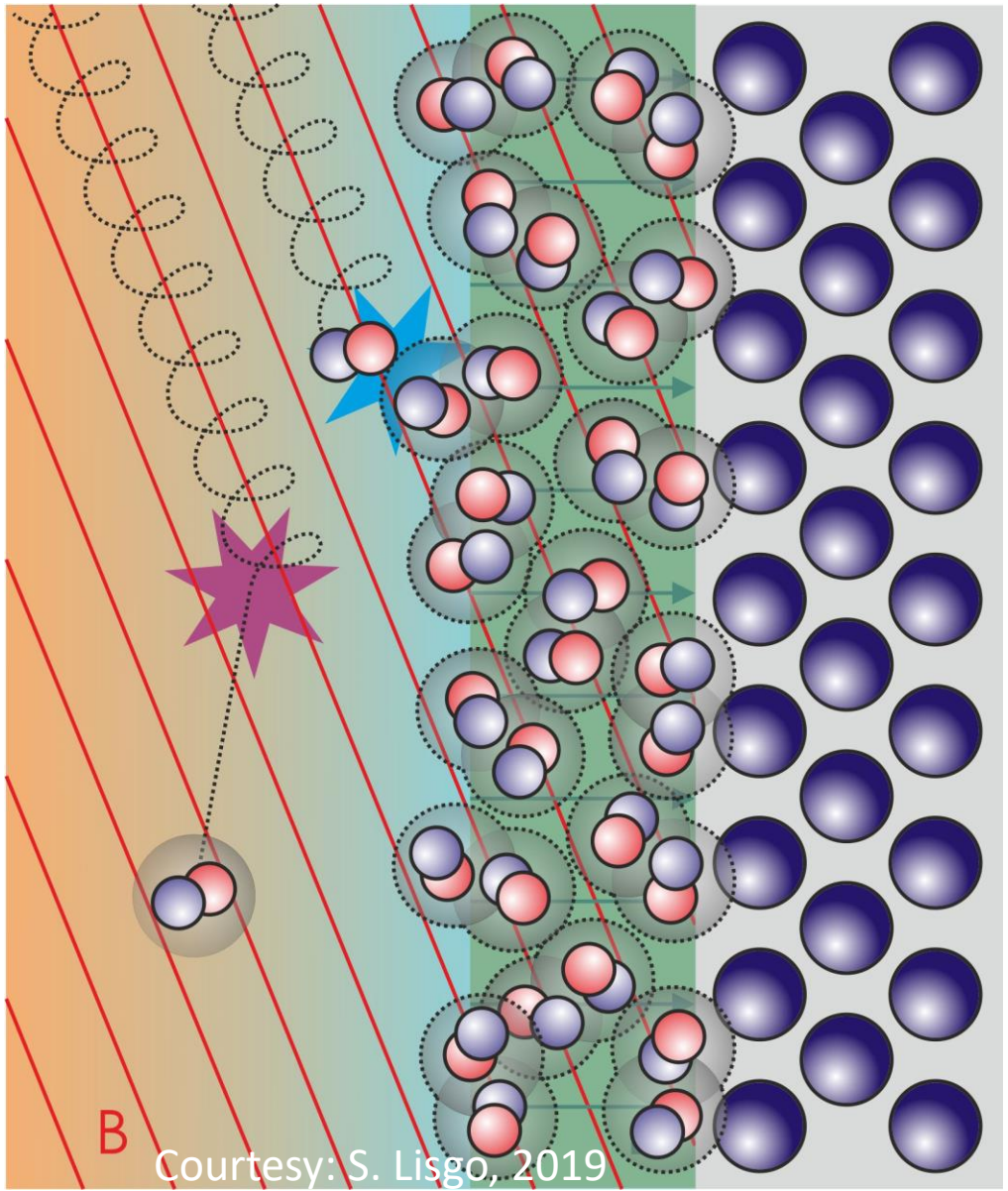
Courtesy: S. Lisgo, 2019

Dissipation – Divertor detachment : Stability and control issues?

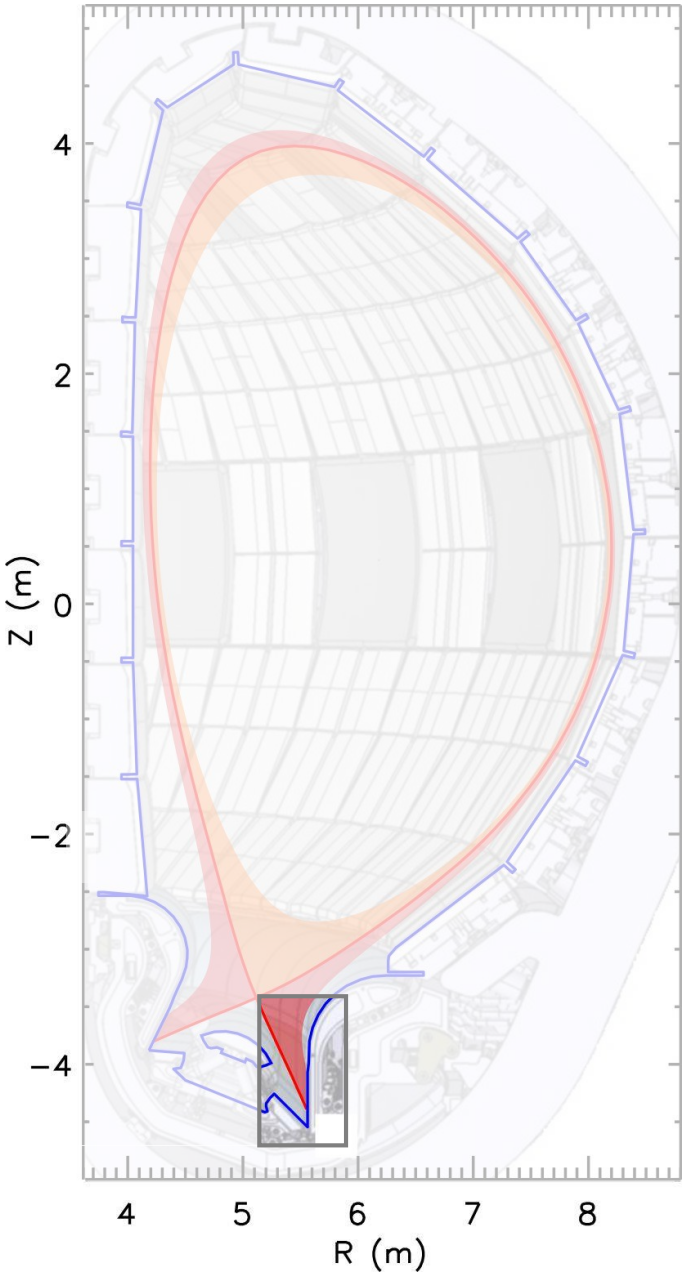


[LaBombard, McLean 2015, PPCF 2017, Krasheninnikov and Kukushkin 2017]

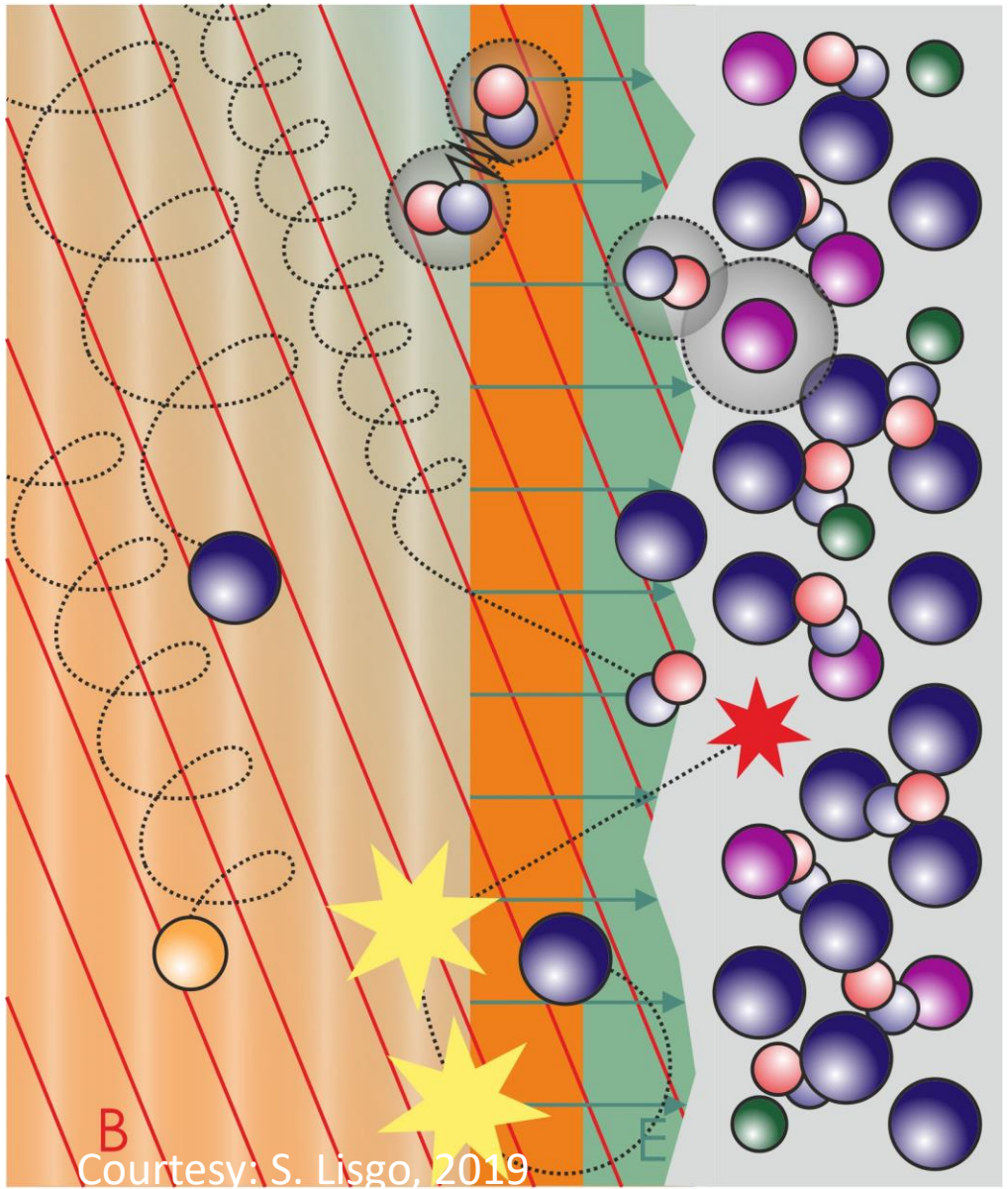
"GAS TARGET" FOR DETACHED PLASMA



Dissipation – Plasma-surface interaction can be a mess



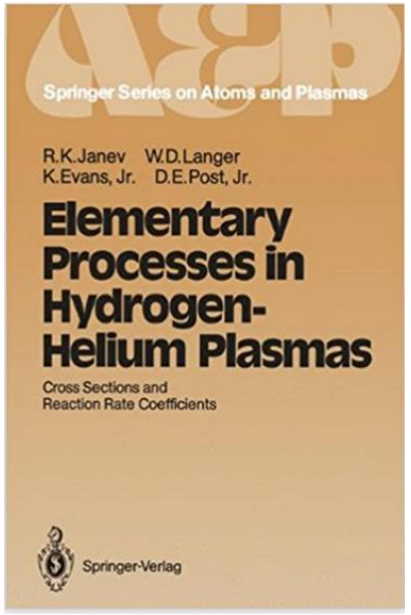
IMPURITY PRODUCTION (AND A LOT MORE…)



Courtesy: S. Lisgo, 2019

Most important molecular processes (reaction channels): attached plasmas

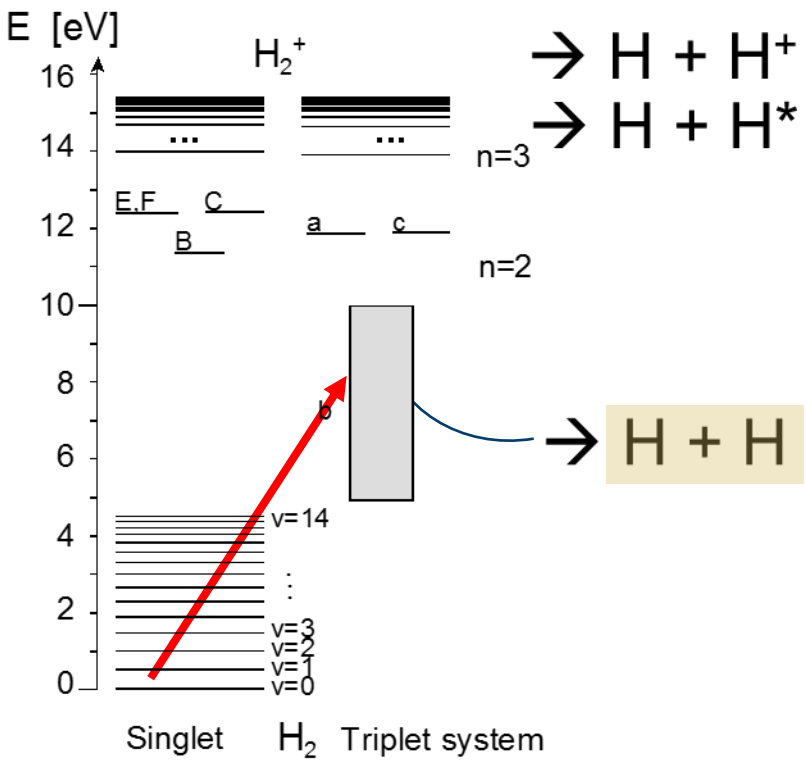
Janev et al., (1987)



Series: Springer Series on Atomic, Optical, and Plasma Physics (Book 4)
Hardcover: 326 pages
Publisher: Springer; 1 edition (November 18, 1987)
Language: English
ISBN-10: 3540175881
ISBN-13: 978-3540175889

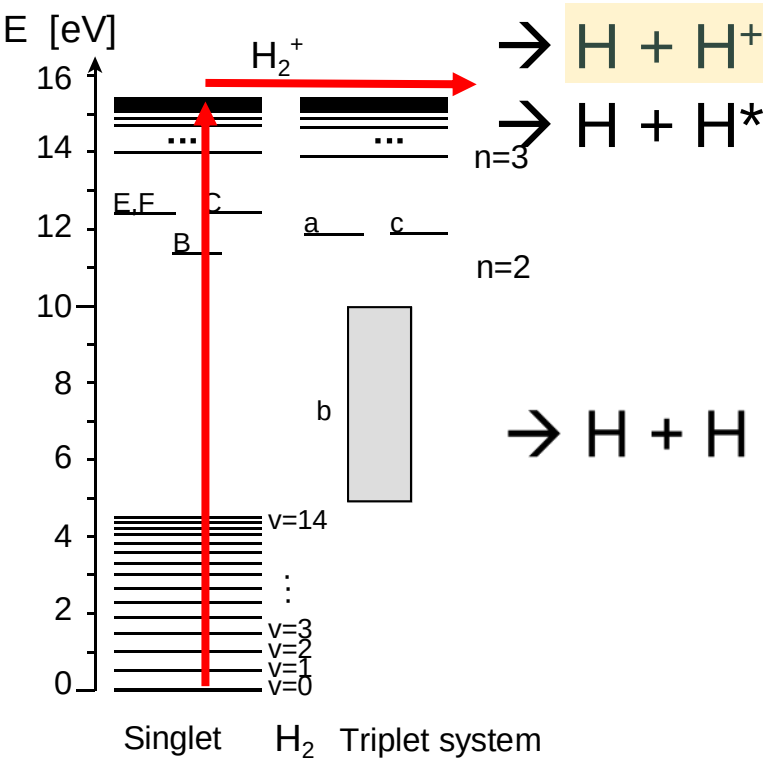
Attached, high recycling

Te ≈ 5 -10 eV



Attached, low recycling

Te ≥10 eV

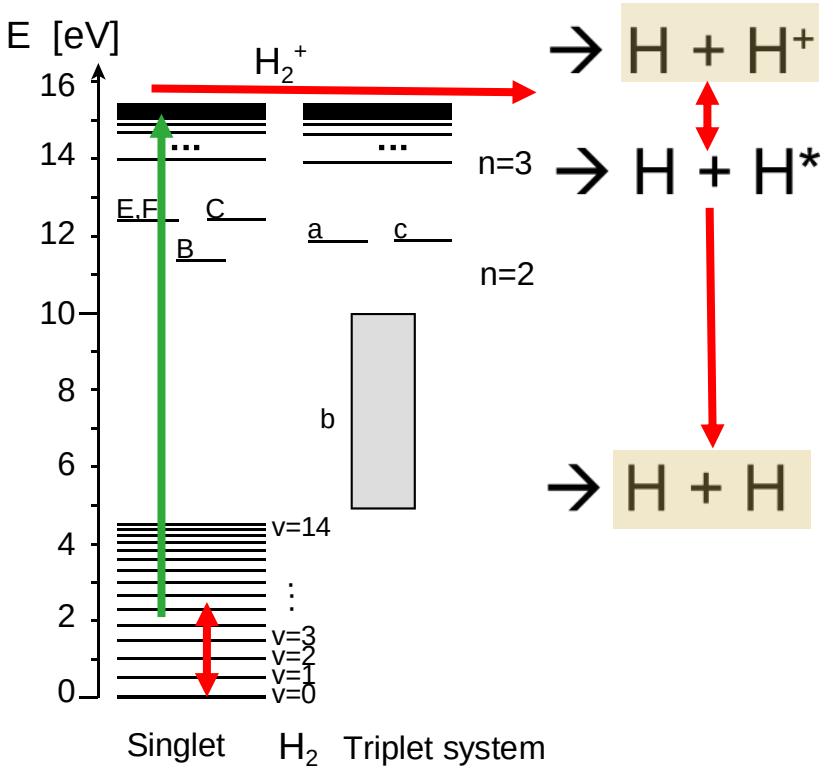


→ Electron collisions

Most important molecular processes (reaction channels)

Detached

Te ≈ 1 - 3 eV

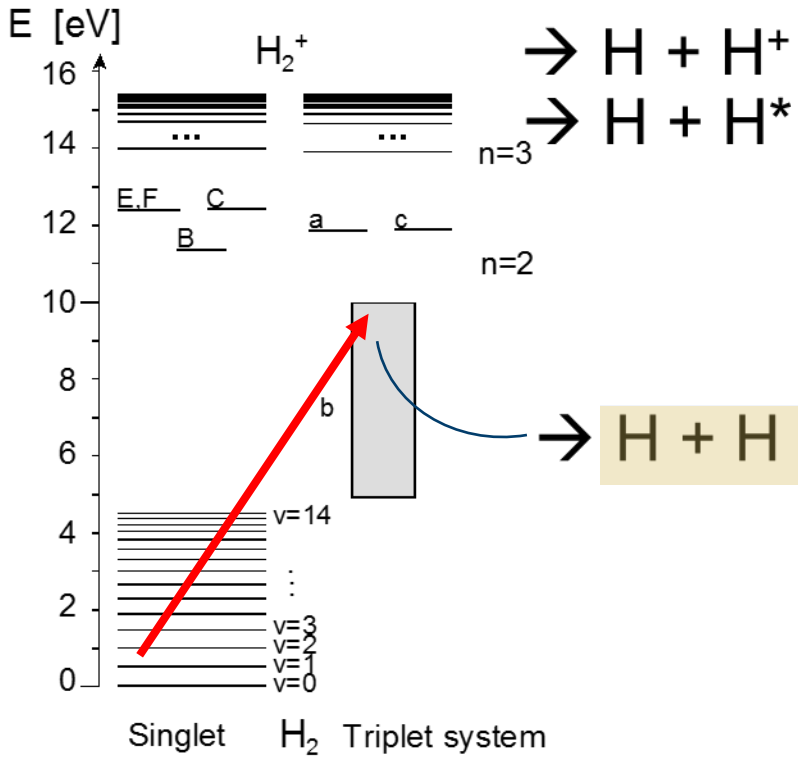


→ Electron collisions

→ Proton collisions

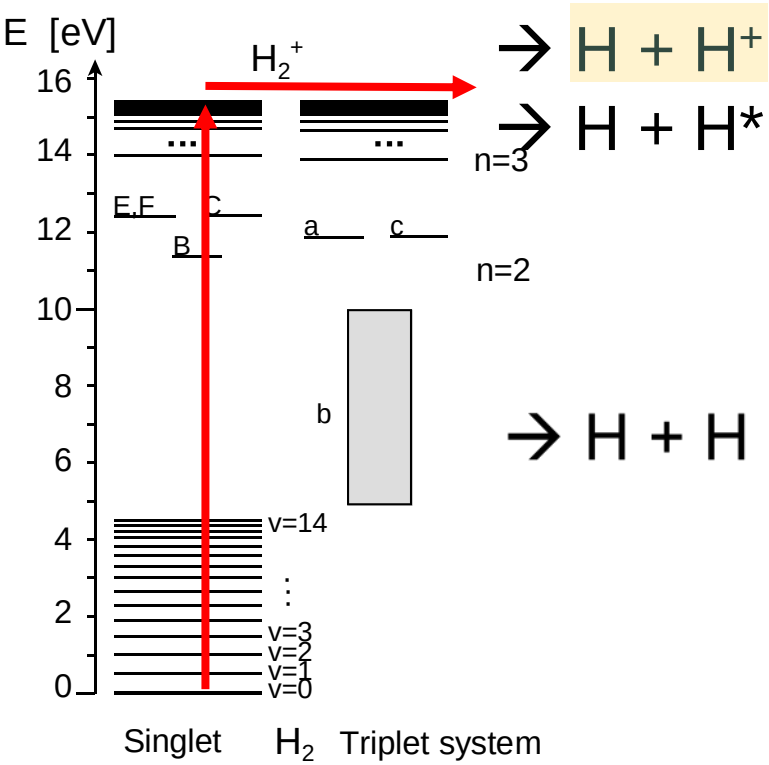
Attached, high recycling

Te ≈ 5 -10 eV



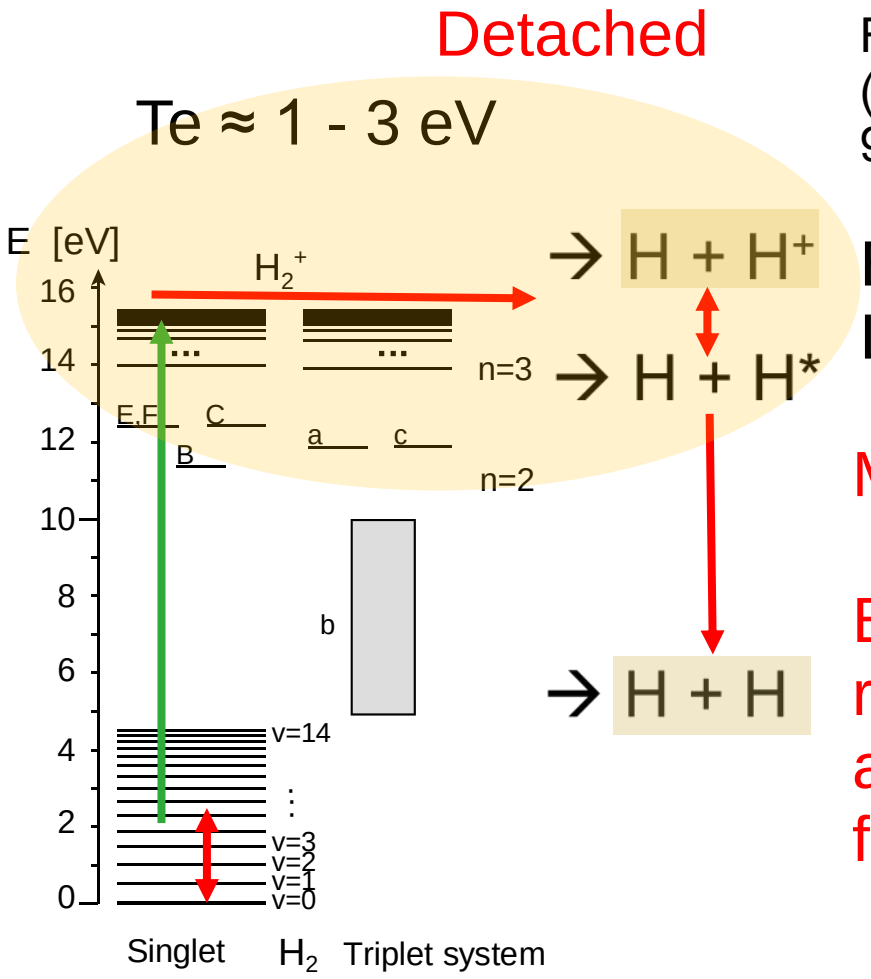
Attached, low recycling

Te ≥10 eV



JÜLICH Forschungszentrum

Most important molecular processes (reaction channels)



Realm for "dissociation recombination community",
(mostly: cosmology, astrophysics, ….applications)
9 International conferences "Dissociative recombination"
held (1988, Alberta, Canada -- 2012 Paris, France)

Bridgehead to fusion community:
Late Prof. Hidedazu Takagi, Kitasato Univ. Jp.

Multi step process:

But:
removes an ion-electron pair from the plasma flow
and replaces it by a thermal particle (atom or ion) taken
from former H_2

→ Relevance for particle balance: puff → divertor → pump
→ (density control, stability, ….)

ISOTOPE EFFECTS ? H → D → D/T

H2(v) vibrational kinetics is involved in a controlling way, resonance effects in ion conversion (IC)

Isotopomeres? D+ + HD(v) → … vs. $H^+ + D_2(v)$ → … ,

and DT, T_2, DT… ?

unknown territory (in fusion edge plasma science) ?

Collapsing isotopic effects

INSTITUTE OF PHYSICS PUBLISHING and INTERNATIONAL ATOMIC ENERGY AGENCY NUCLEAR FUSION

Nucl. Fusion **46** (2006) S260–S274 doi:10.1088/0029-5515/46/6/S06

Vibrational kinetics, electron dynamics and elementary processes in H_2 and D_2 plasmas for negative ion production: modelling aspects

M. Capitelli[1,2], M. Cacciatore[2], R. Celiberto[3], O. De Pascale[2], P. Diomede[1], F. Esposito[2], A. Gicquel[4], C. Gorse[1,2], K. Hassouni[4], A. Laricchiuta[2], S. Longo[1,2], D. Pagano[1] and M. Rutigliano[2]

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Online at stacks.iop.org/NF/46/S260

vibr. quantum number vs. vibrational eigenvalue

the behaviour of, respectively, the total and dissociative cross section for transitions to the members of the spectroscopic series $^1\Pi_u[np\pi]$, as a function of the principal quantum number n of the excited molecular state, for a given electron impact energy. The cross-sections decrease, due to increase in transition energy, scaling approximately with n as n^{-4}, a result which can be used in the improvement of the collisional radiative model for Rydberg states.

In [19] the dependence of the total excitation cross section on the molecular mass has been widely discussed. The observed shift to higher vibrational quantum numbers in the vibrational profile of heavier isotopes seems to be connected to the existence of an isotopic effect; however, this is only apparent and depends on the different level density in the same transition energy range for different isotopes; in fact the cross-sections collapse when plotted as a function of the vibrational eigenvalues. In the case of an e–V processes [20], plotting the monoquantic ($v_f = v_i + 1$) and biquantic ($v_f = v_i + 2$) resonant vibrational excitation cross sections, at a fixed incident energy, for H_2, D_2 and T_2 molecules, as a function of either the vibrational quantum number (figure 2(*a*)) or the corresponding vibrational eigenvalue, the same cross-section collapse has been observed, suggesting an energy-based scaling law.

The database reported in [18] has been enriched by the electron–molecule cross sections for transitions involving triplet states of H_2 molecule [21]:

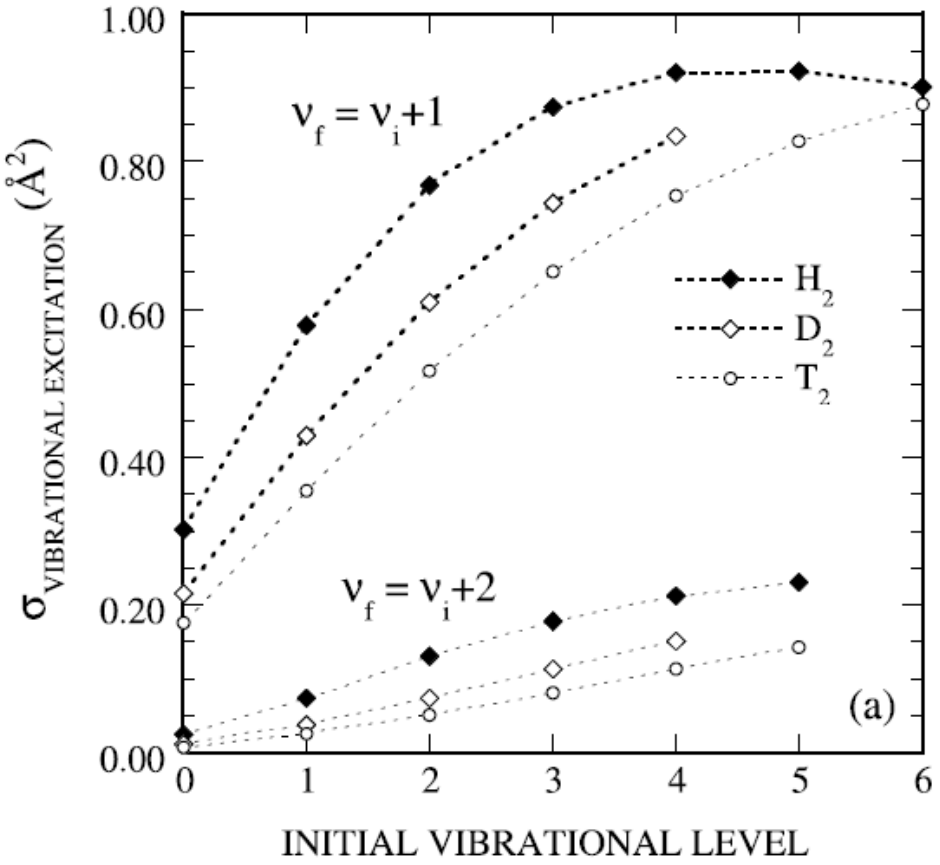
$$H_2(a\,^3\Sigma_g^+, v_i) + e \rightarrow H_2(d\,^3\Pi_u) + e, \quad (6)$$

$$H_2(c\,^3\Pi_u, v_i) + e \rightarrow H_2(g\,^3\Sigma_g^+) + e, \quad (7)$$

$$H_2(c\,^3\Pi_u, v_i) + e \rightarrow H_2(h\,^3\Sigma_g^+) + e, \quad (8)$$

in particular the *Fulcher band* has been considered; this system is important in spectroscopic diagnostic methods, providing information about the vibrational and translational temperatures of H_2 under non-equilibrium conditions [22].

e-V processes in $H_2(^1X_g;v)$



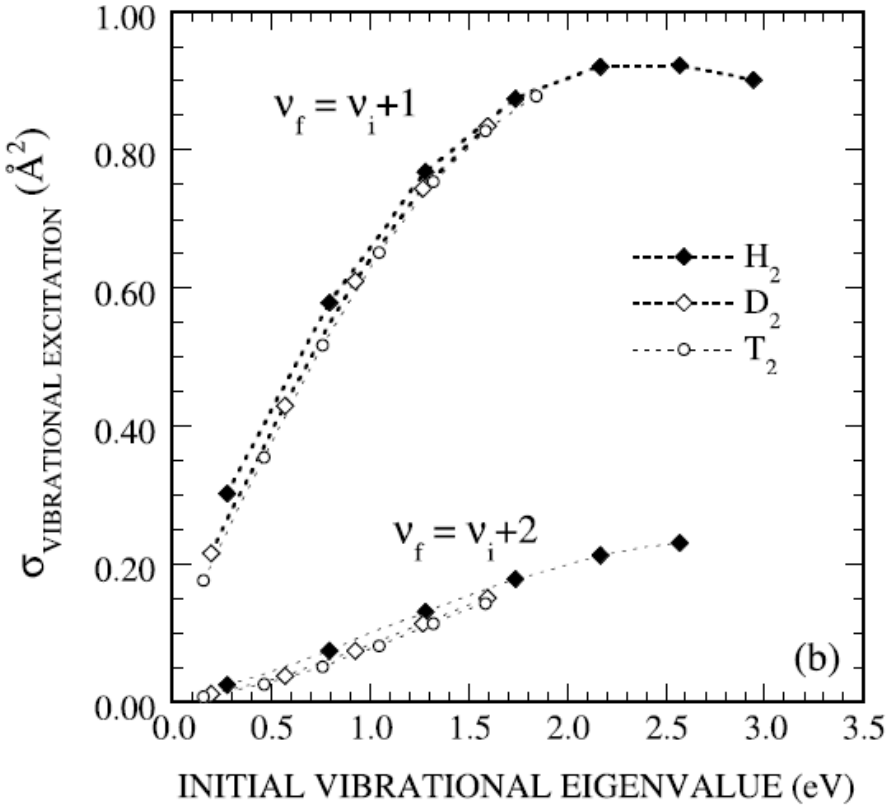


Figure 2. Cross section for the process $H_2(^1\Sigma_g^+, v_i) + e \rightarrow H_2^- \rightarrow H_2(^1\Sigma_g^+, v_f) + e$, for a fixed collision energy, $E = 5$ eV, as a function of (*a*) the vibrational quantum number v_i and (*b*) vibrational eigenvalue, for H_2 and its isotopic variants (close diamonds—H_2, open diamonds—D_2, open circles—T_2).

Also for other electron collision processes?

HEINRICH HEINE
UNIVERSITÄT DÜSSELDORF

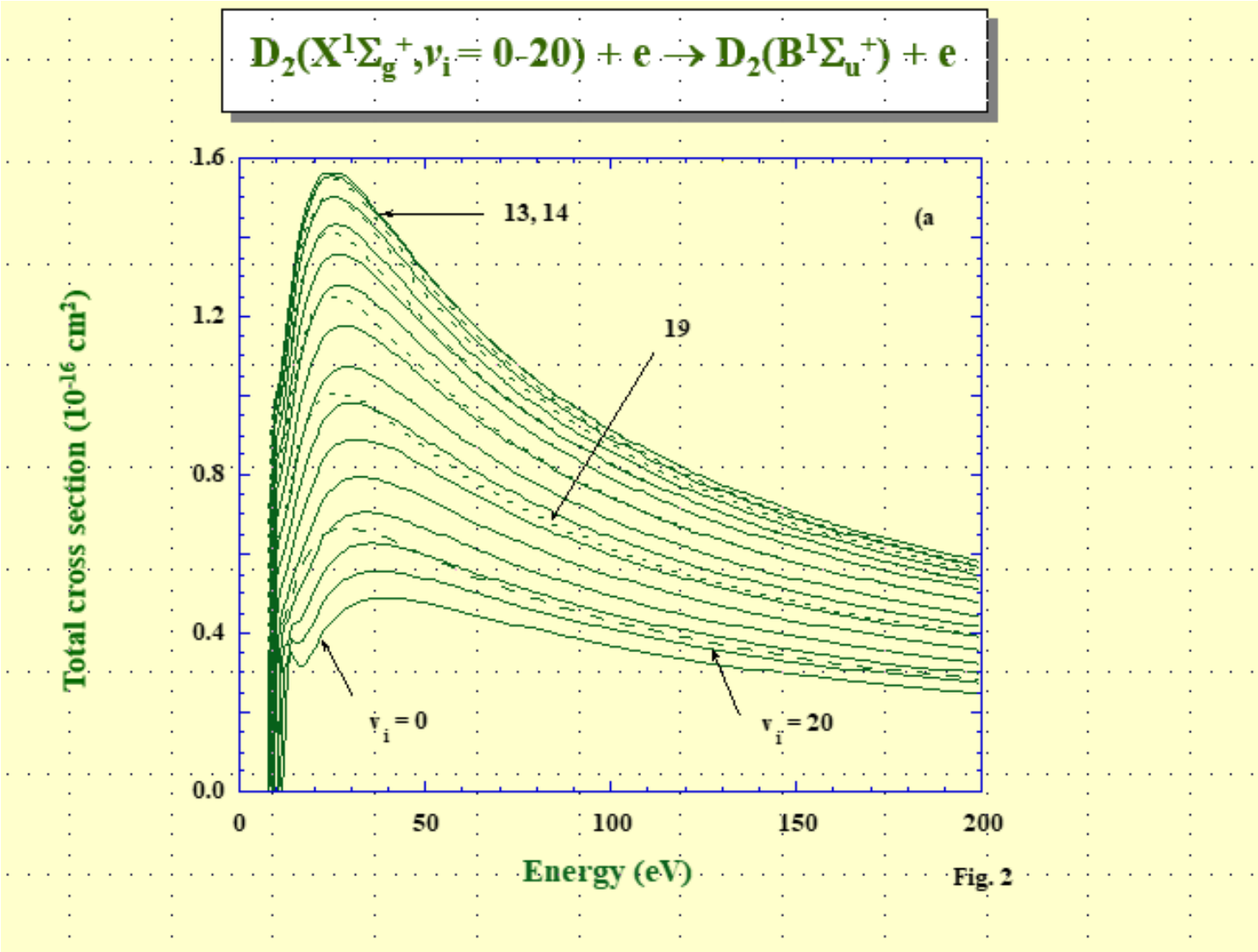
Presention by Roberto Celiberto,

at FZ-Juelich,

sometime in summer 2006

Talk starts: 30 pictures like this

- Audience getting tired….



Slide 31: collapsing isotopic effect

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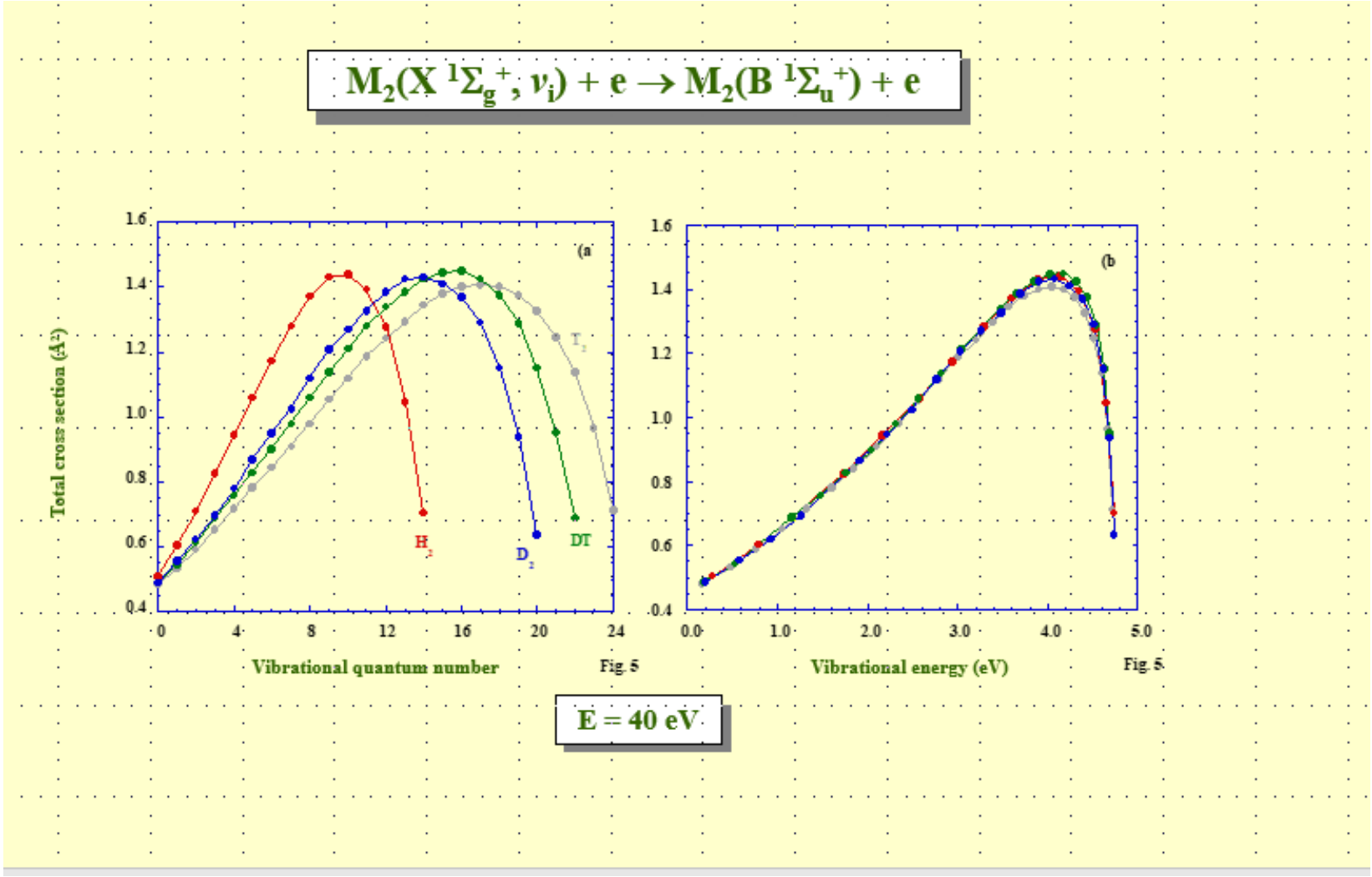
Wow !

That, if not an artifact of the computational method used, would be of key importance for data implementation



Talk continues with 25 pictures like this……

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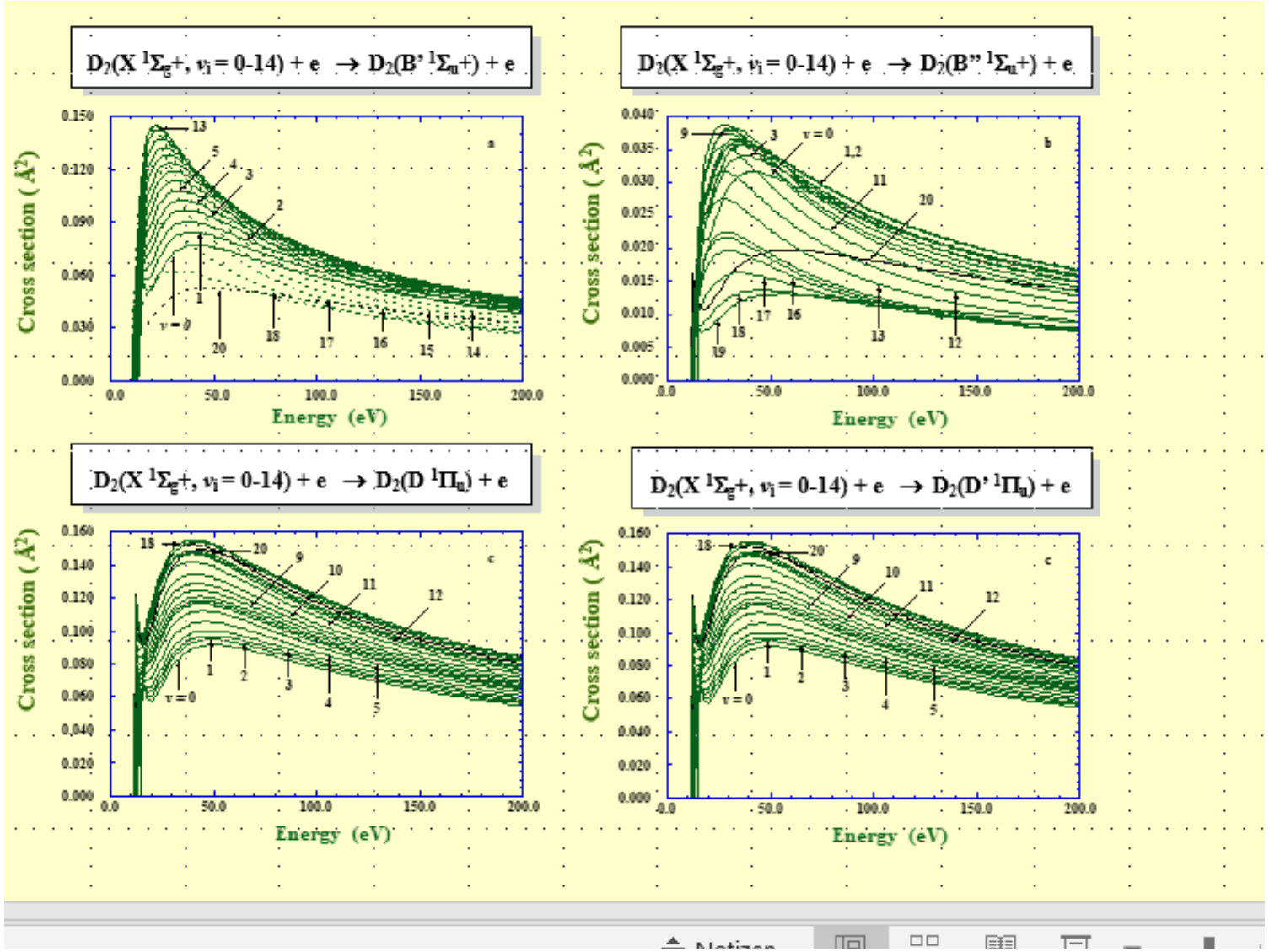
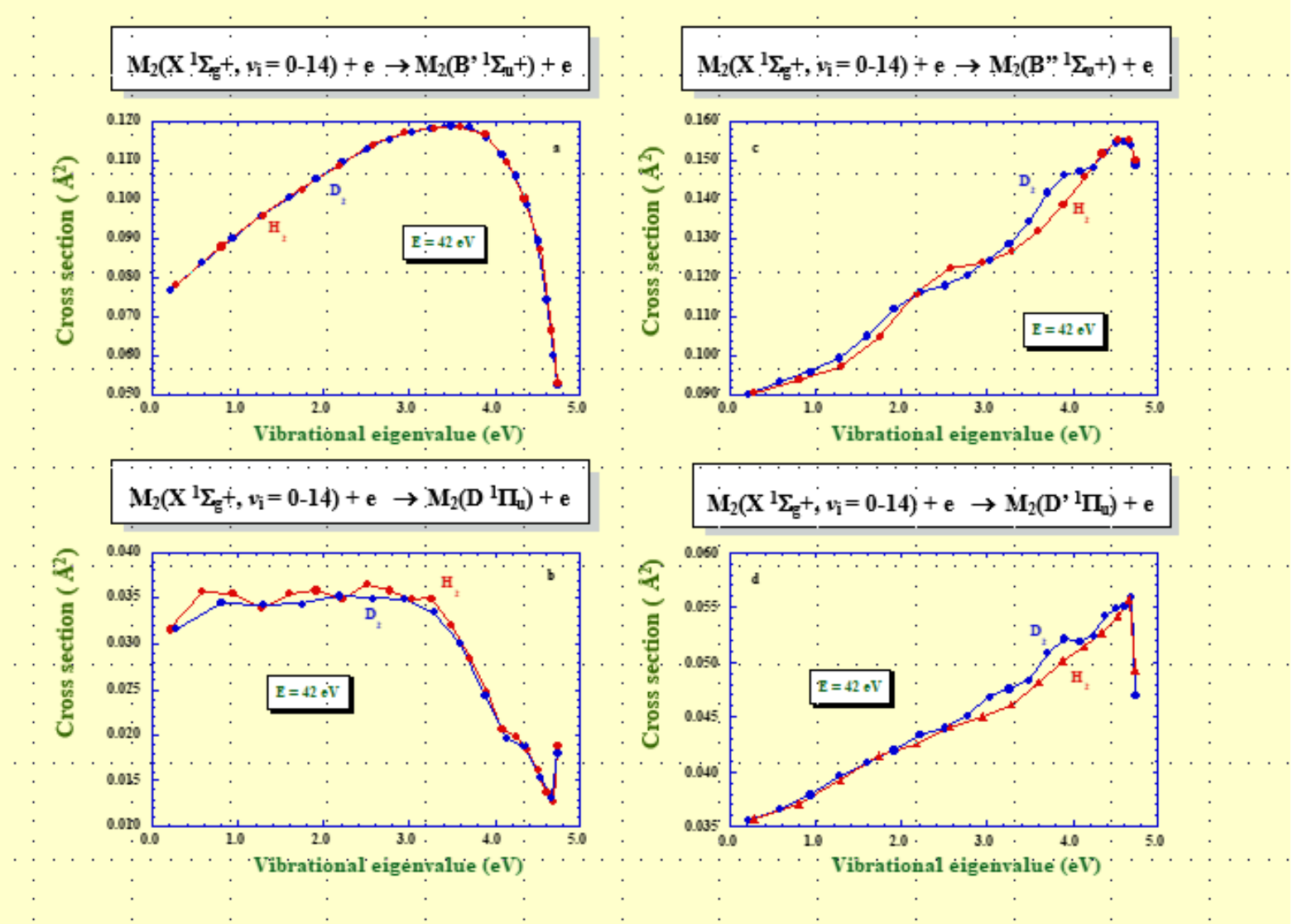
Almost falling asleep again….



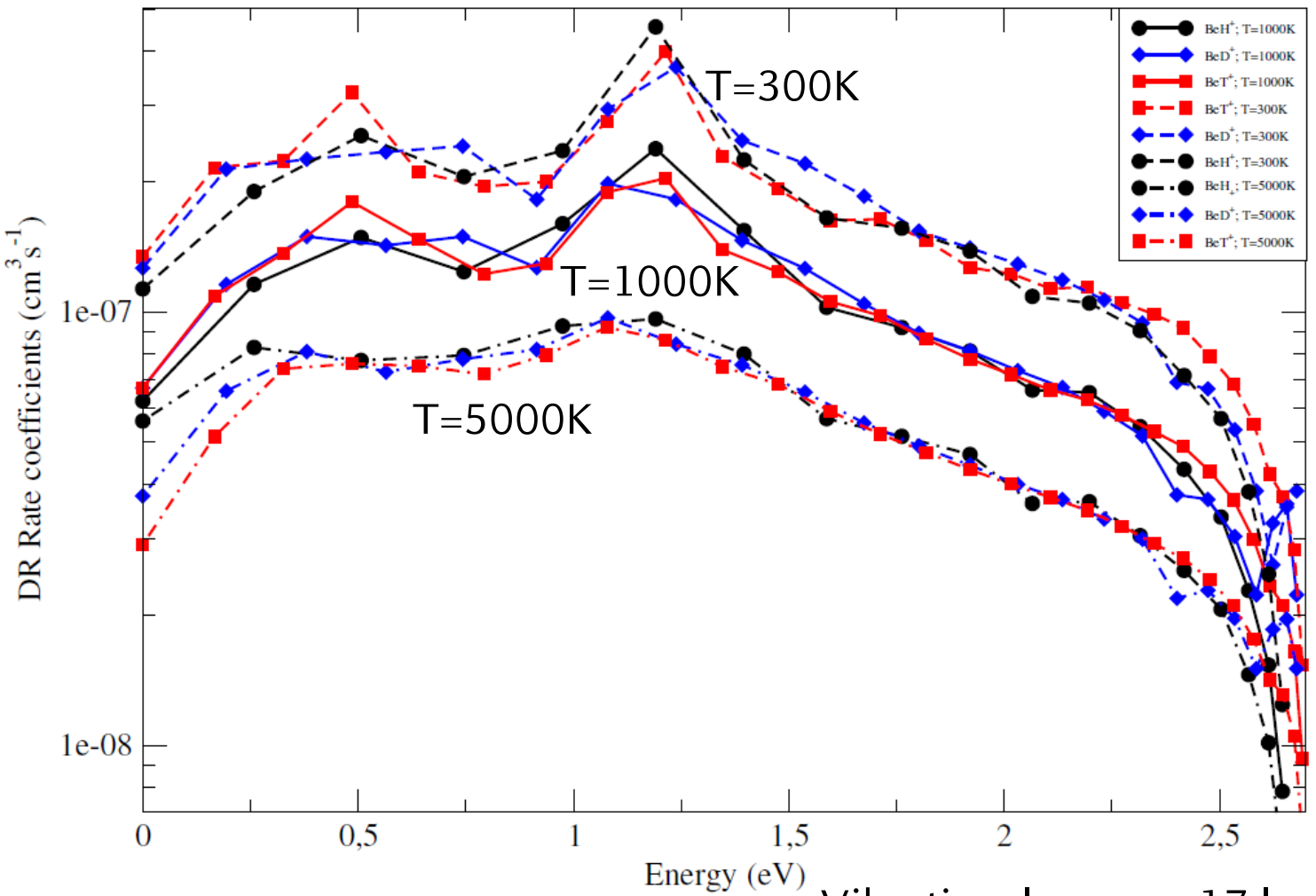
Slide 59: again: collapsing isotopic effects

Slide 59: the key result, again....

This was for electron impact excitation on H2, D2, T2, HD, HT, DT



Collapsing isotopic effects: BeH^+, BeD^+, BeT^+, DR



Priv. comm. Aug. 2019:

Ioan Schneider,

Université du Havre,

(follow up discussions from AMD unit CM meeting in June 2019)

Vibrational energy, 17 lowest levels of BeH^+, fake continuum

ISOTOPE EFFECTS ? H → D → D/T

M. Capitelli et al., Nucl Fus. 46 (2006)

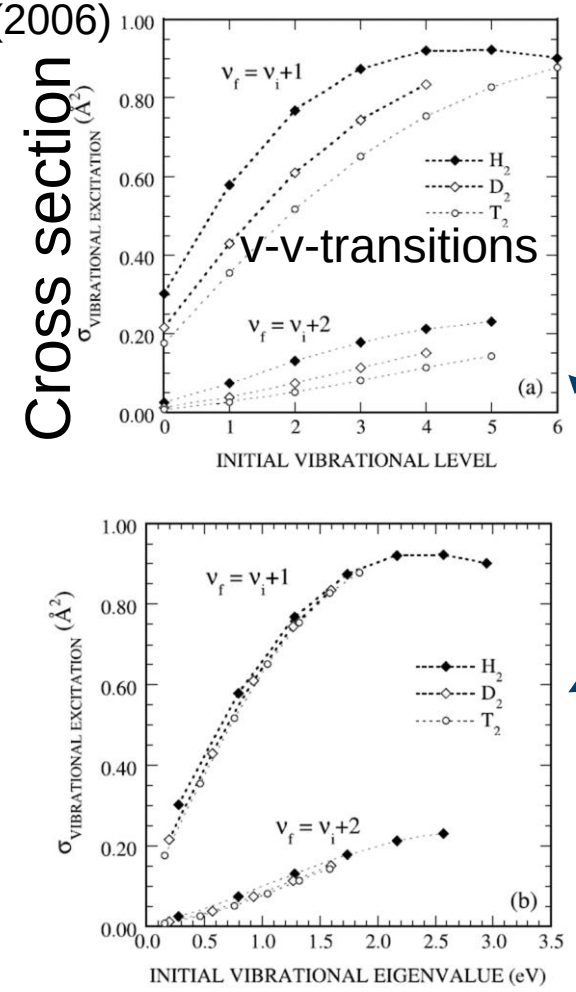


Figure 2. Cross section for the process $H_2(^1\Sigma_g^+, v_i) + e \rightarrow H_2^- \rightarrow H_2(^1\Sigma_g^+, v_f) + e$, for a fixed collision energy, $E = 5$ eV, as a function of (*a*) the vibrational quantum number v_i and (*b*) vibrational eigenvalue, for H_2 and its isotopic variants (close diamonds—H_2, open diamonds—D_2, open circles—T_2).

H2(v) vibrational kinetics is involved in a controlling way, resonance effects in ion conversion (IC)

Isotopomeres? D+ + HD(v) → … vs. H^+ + D_2(v)→ … , and DT, T_2, DT… ?

unknown territory (in fusion edge plasma science) ?

Currently:

Electron collisions: use vibrational energy, rather than vibrational quantum number (for H_2(v), D_2(v), T_2(v),….)

→ collapse to a single set (of isotope independent) rates.

Heavy particle collisions: scaling of cross sections to same collision velocity, rather than collision energy

→ collapse to a single set (of isotope independent) rates (as we have already seen in resonant charge exchange).

Collapsing isotopic effects

- When can we always rely on such simplifications?

- Not always.....

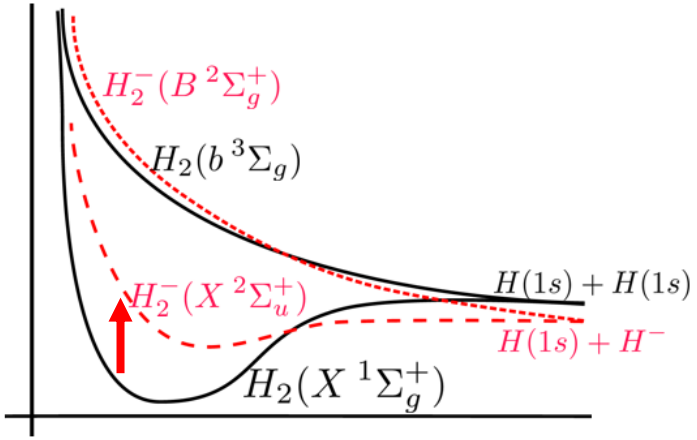
Isotope effects ? H_2^+ or H^- mitigated recombination channel:

From various code - experiment comparisons:

Looking for further (collisional) channels that might enhance cross field plasma losses (such as MAR). A. Kukushkin, …, D. Reiter 22nd PSI (Rome), NME 2017

Other channels with similar effects ?

e + H2(v) → H + H^-



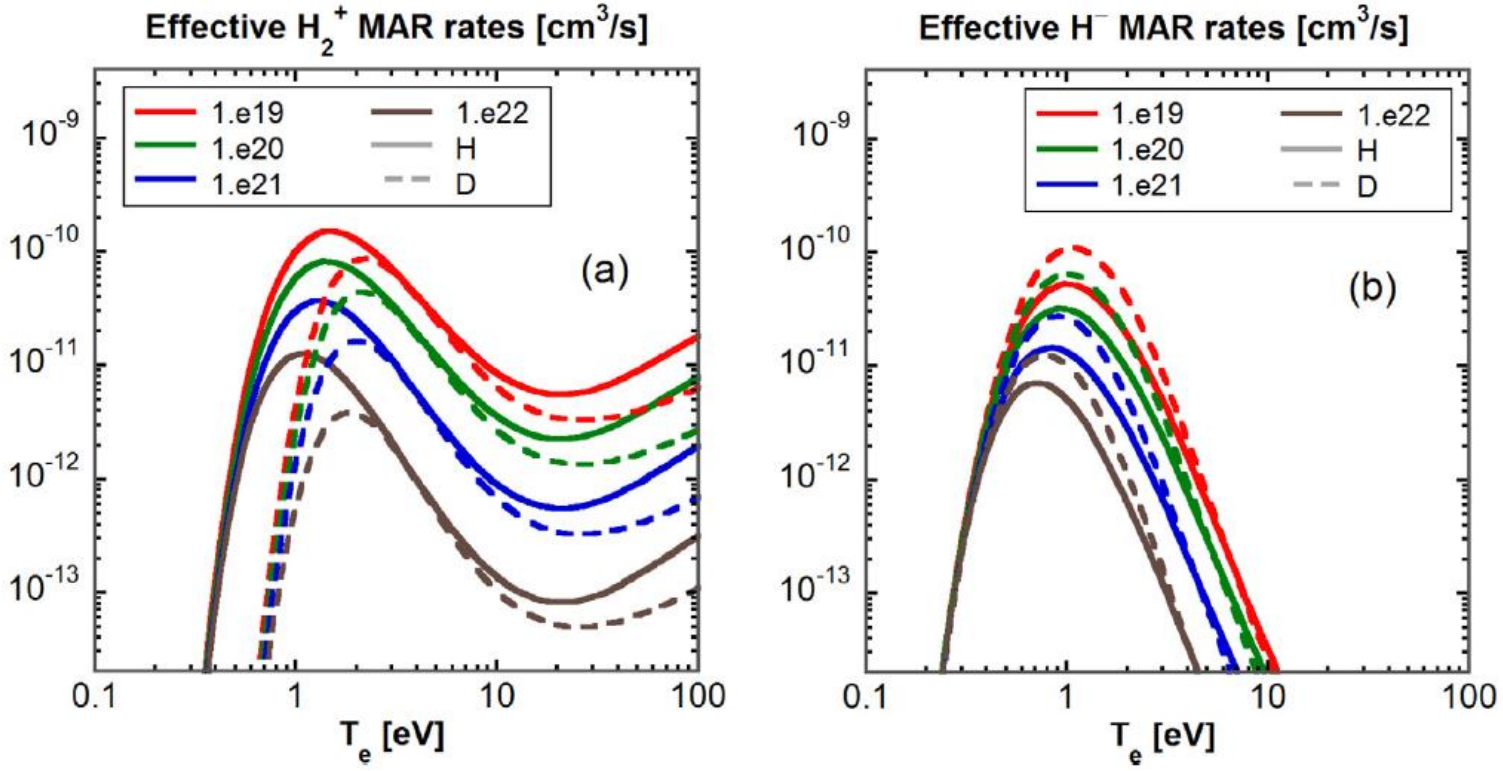


Fig. 2. Effective MAR rates for the H_2^+ (a) and H^- (b) branches, H (solid lines) and D (dashed lines) plasma, for different plasma density.

Enhanced D^- MAR over H^- MAR (loc cit.)? This was the wrong conclusion

A “true” isotope effect in dissociative attachment (caused by nuclear motion in molecule)

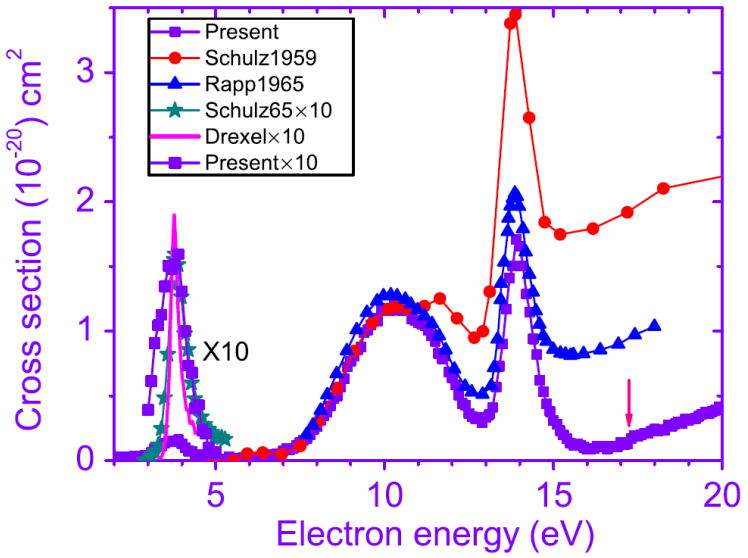
Dissociative attachment in D_2 is strongly reduced, compared to H_2

D.Rapp and D.D.Briglia, J.Chem.Phys.43,1480 (1965).

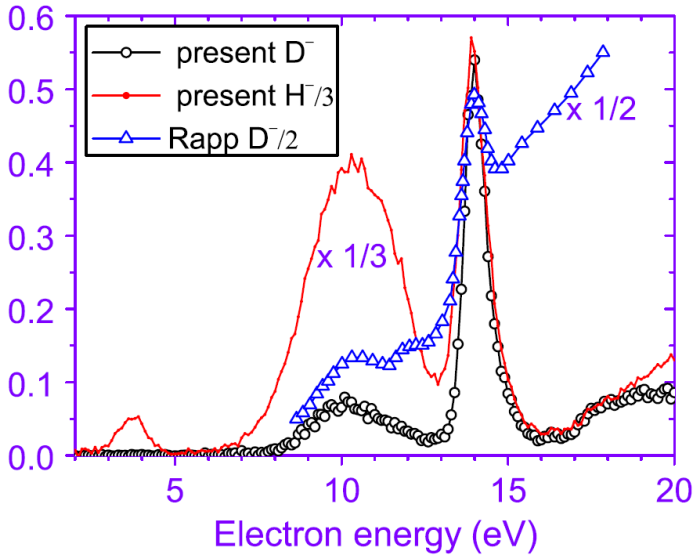
→ many theoretical and exp. confirmations since…, latest:

E.Krishnakumar,S. Denifl, I.Cadez et al.

PRL **106,** 243201 (2011)



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



$e + D_2(v) \rightarrow D + D^-$

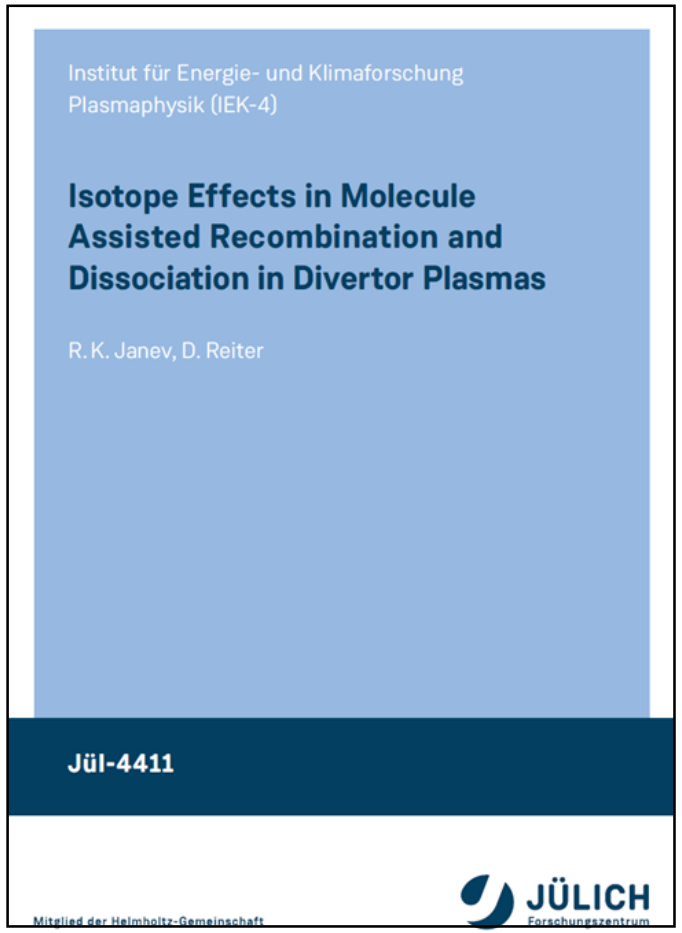
A “true” isotope effect in dissociative attachment

Wrapping this up: a plasma chemical approach (0D, rate constants,…loss times,..)

A. Negative Ion MAR/MAD	B. Ion-conversion MAR/MAD
1. $e+H_2 \rightarrow H^- + \underset{\sim}{H}$	14. $H^+ + H_2 \rightarrow \underset{\sim}{H} + H_2^+$
2. $H^+ + H^- \rightarrow H + H^*(n)$	15. $e + H_2^+ \rightarrow H + H^*(n)$
3. $e + D_2 \rightarrow D^- + \underset{\sim}{D}$	16. $D^+ + D_2 \rightarrow \underset{\sim}{D} + D_2^+$
4. $D^+ + D^- \rightarrow D + D^*(n)$	17. $e + D_2^+ \rightarrow D + D^*(n)$
5. $H^+ + D^- \rightarrow H^*(n) + D$	18. $H^+ + D_2 \rightarrow \underset{\sim}{H} + D_2^+$
6. $D^+ + H^- \rightarrow D^*(n) + H$	19. $D^+ + H_2 \rightarrow \underset{\sim}{D} + H_2^+$
7. $e + H^*(n) \rightarrow e + H^+ + e$	20. $H^+ + D_2 \rightarrow HD + D^+$
8. $e + D^*(n) \rightarrow e + D^+ + e$	21. $H^+ + D_2 \rightarrow HD^+ + D$
9. $H^+ + D^*(n) \rightarrow H^*(n' \neq n) + D^+$	22. $D^+ + H_2 \rightarrow HD + H^+$
10. $D^+ + H^*(n) \rightarrow D^*(n' \neq n) + H^+$	23. $D^+ + H_2 \rightarrow HD^+ + H$
11. $e + H^- \rightarrow e + \underset{\sim}{H} + e$	24. $H^+ + HD \rightarrow \underset{\sim}{H} + HD^+$
12. $e + D^- \rightarrow e + \underset{\sim}{D} + e$	25. $D^+ + HD \rightarrow \underset{\sim}{D} + HD^+$
13a. $e + HD \rightarrow H^- + \underset{\sim}{D}$	26a. $e + HD^+ \rightarrow H^*(n) + D$
13b. $e + HD \rightarrow D^- + \underset{\sim}{H}$	26b. $e + HD^+ \rightarrow D^*(n) + H$
	27. $e + H_2^+ \rightarrow e + H^+ + \underset{\sim}{H}$
C. Common Reactions	28. $e + D_2^+ \rightarrow e + D^+ + \underset{\sim}{D}$
34. $H^*(n) \rightarrow H^*(n' < n) + h\nu$	29a. $e + HD^+ \rightarrow e + H^+ + \underset{\sim}{D}$
35. $D^*(n) \rightarrow D^*(n' < n) + h\nu$	29b. $e + HD^+ \rightarrow e + D^+ + \underset{\sim}{H}$
36. $e + H^*(n) \rightarrow e + H^*(n' \neq n)$	30. $H^+ + HD \rightarrow H_2 + D^+$
37. $e + D^*(n) \rightarrow e + D^*(n' \neq n)$	31. $H^+ + HD \rightarrow H_2^+ + D$
38. $e + \underset{\sim}{H} \rightarrow e + H^+ + e$	32. $D^+ + HD \rightarrow D_2 + H^+$
39. $e + \underset{\sim}{D} \rightarrow e + D^+ + e$	33. $D^+ + HD \rightarrow D_2^+ + H$

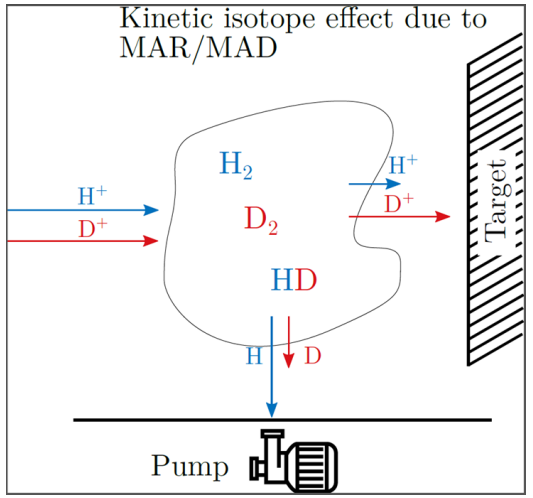
Table 1: Reaction in H_2/D_2 MAR and MAD kinetics

Long list of reactions → … estimate isotopically correct MAR rates, etc…



Report: JUEL 4411, June 2018

No enhanced “MAR”, but isotope separation in molecular cloud



Lighter isotope enhanced in neutralized channel (→ pump) (same trend in D-T mixture)

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Thank you for your attention!

Preface: A little bit of history….

1990: R.A. Hulse: ALADDIN atomic physics database system → IAEA AM data unit

THE ALADDIN ATOMIC PHYSICS DATABASE SYSTEM

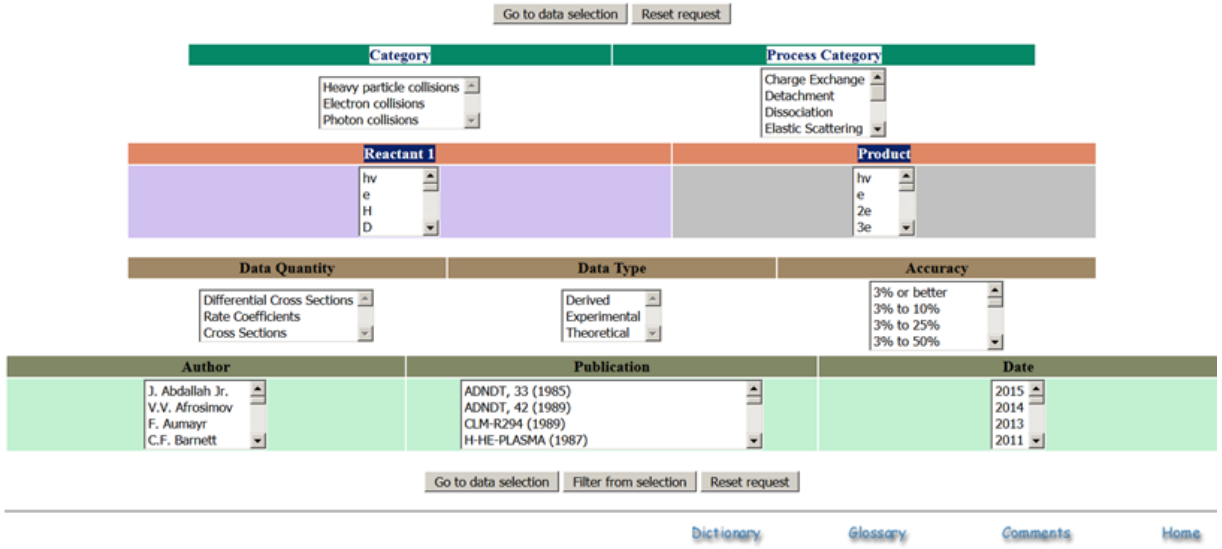
Russell A. Hulse
Princeton University, Plasma Physics Laboratory, Princeton, NJ 08543

ABSTRACT

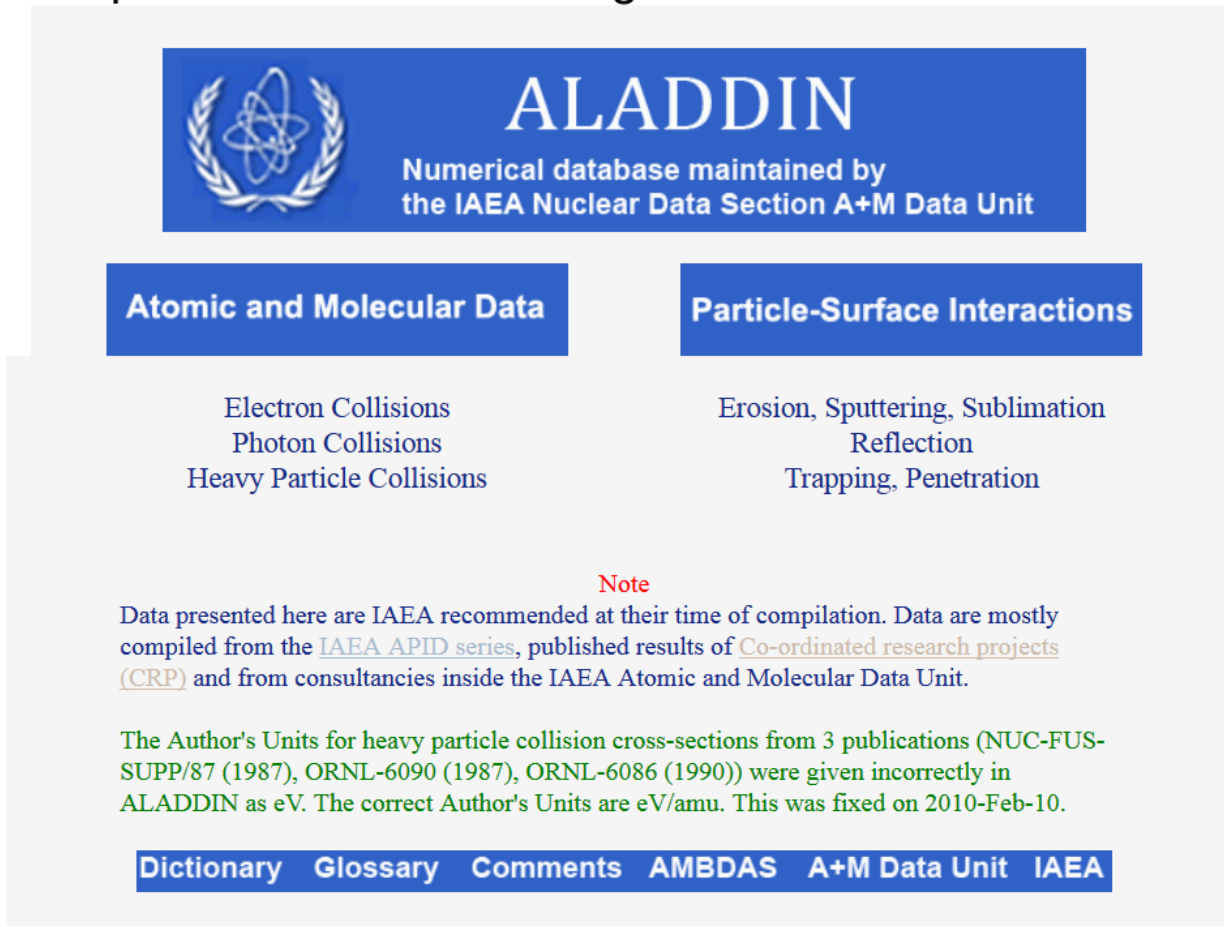
ALADDIN is an atomic physics database system which has been developed in order to provide a broadly-based standard medium for the exchange and management of atomic data. ALADDIN consists of a data format definition together with supporting software for both interactive searches as well as for access to the data by plasma modeling and other codes.

"Atomic Processes in Plasmas", Gaithersburg, MD, USA 1989
AIP Conference Proceedings 206

Primary source for data used in this talk



https://www-amdis.iaea.org/ Accessed: June 2018



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HOW SENSITIVE IS A RESULT TO PARTICULAR PROCESS REACTION RATES (OR TRANSPORT LOSSES) ?

Define sensitivity Z of density n_j wrt. reaction rate R_k
as logarithmic derivative:

$$Z = d(\ln n_j) / d(\ln R_k)$$

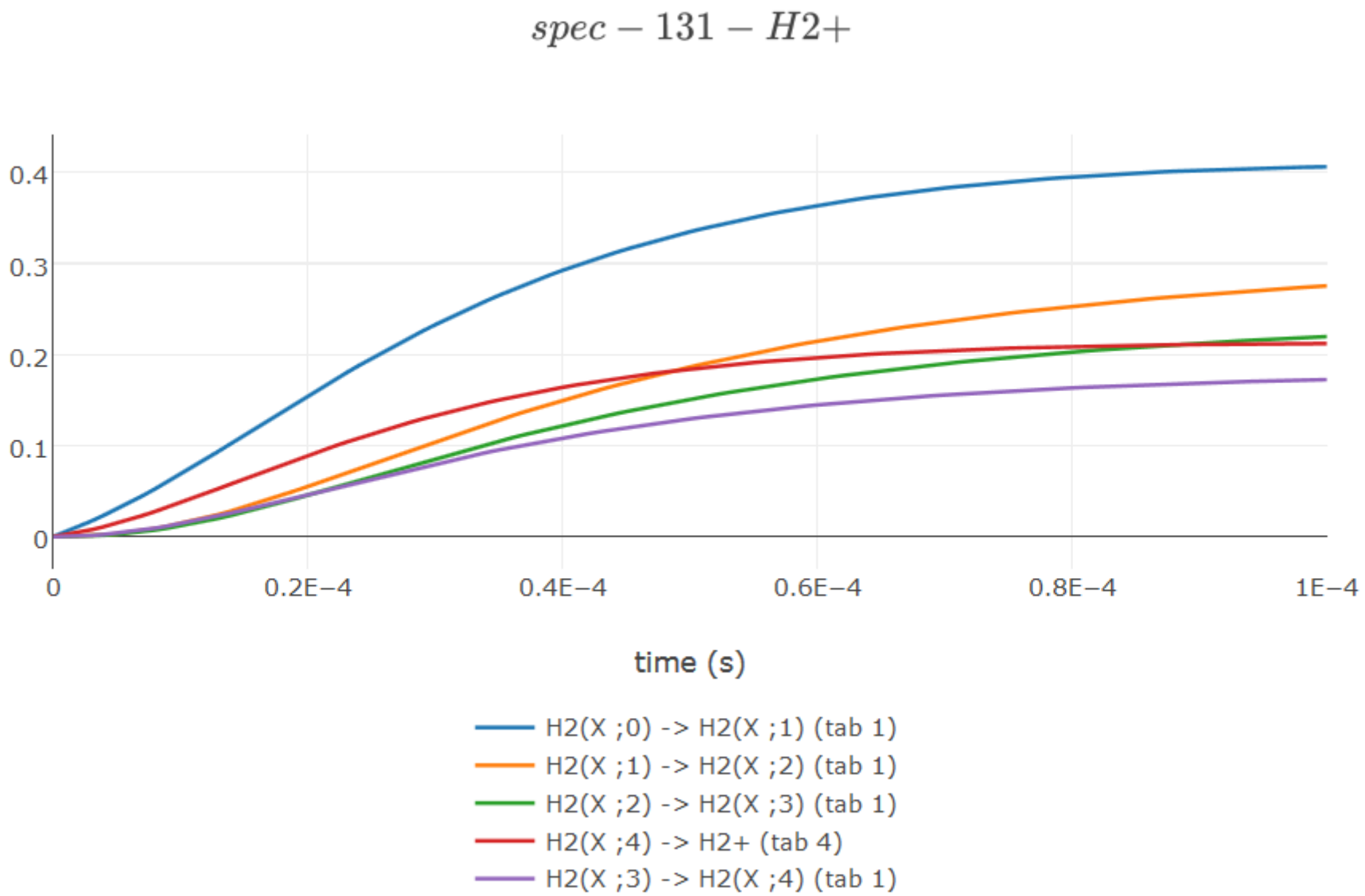
For n species in the system, and m different processes active,
there are n x m such sensitivity functions.

Fortunately: the system of DGL for these Z has the same form as
that for the densities n, and can also be solved in closed form
using the known eigenvalues and eigenvectors.

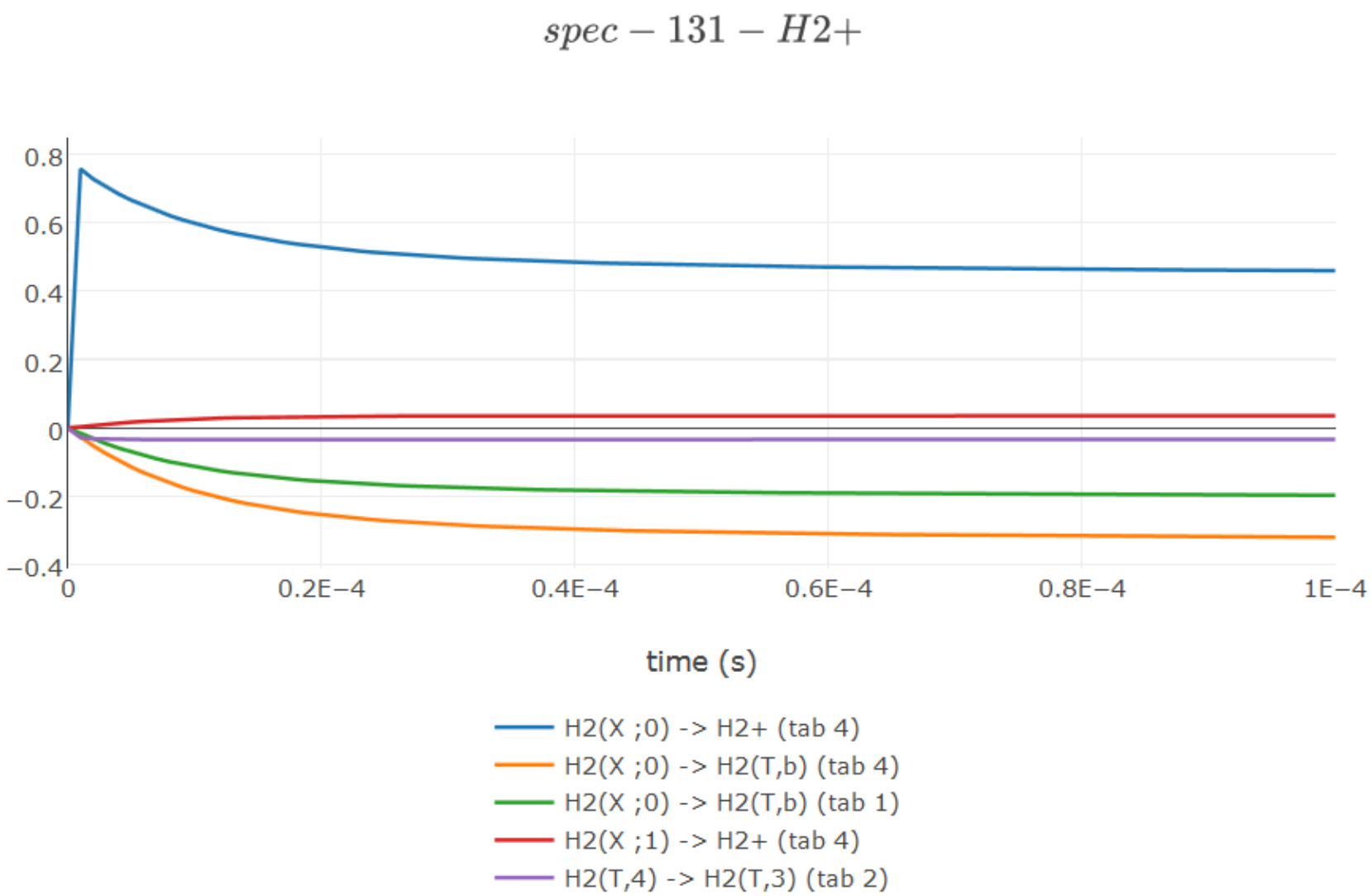
If this option is activated, HYKIN prints and plots the s (input)
largest (at $t=t_{max}$) such sensitivity functions

D. Reiter, Phys. Scr. **T138** (2009) 014014

Sensitivity study: H-H2-H2+ CR model: @1 eV



Sensitivity study: H-H2-H2+ CR model: @10 eV



CR Models in transport studies

$$\frac{\mathrm{d}n(p)}{\mathrm{d}t} = -\left\{\sum_{q\neq p} C(p,q)n_\mathrm{e} + \sum_{q<p} A(p,q) + S(p)n_\mathrm{e}\right\} n(p)$$
$$+ \sum_{q\neq p} \{C(q,p)n_\mathrm{e} + A(q,p)\}\, n(q) + \{\alpha(p)n_\mathrm{e} + \beta(p) + \beta_\mathrm{d}(p)\}\, n_\mathrm{i}n_\mathrm{e}.$$

$$\dot{\mathbf{n}} = \mathbf{M}(T_\mathrm{e}, n_\mathrm{e}) \cdot \mathbf{n} + \Gamma(T_\mathrm{e}, n_\mathrm{e}, n_\mathrm{i}), \quad \text{where}$$

$$\mathbf{M}_{pq} = \begin{cases} C(q,p)n_\mathrm{e} + A(q,p) & , \text{ if } p \neq q \\ -\sum_{j\neq p} C(p,j)n_\mathrm{e} - \sum_{j<p} A(p,j) - S(p)n_\mathrm{e} & , \text{ if } p = q \end{cases}$$

and $\Gamma_p = [\alpha(p)n_\mathrm{e} + \beta(p) + \beta_\mathrm{d}(p)]\, n_\mathrm{i}n_\mathrm{e}.$

2.1 Reducing the dimensionality

Equation (3) can be solved via e.g. eigenvalue decomposition or Laplace transformation. But in practice, the computational effort can be drastically reduced since the timescales for the development of different atomic states are very different. So, if diagnostics with finite temporal resolution are used, and no processes other than those in (1) are relevant on faster time scales, some of the states can be assumed stationary. The vector space of $\mathbf{n}$ can then be split in three,

$$\begin{pmatrix} \dot{\mathbf{n}}_P \\ \dot{\mathbf{n}}_Q \\ \dot{\mathbf{n}}_S \end{pmatrix} = \begin{pmatrix} \mathbf{M}_P & \mathbf{M}_{PQ} & \mathbf{M}_{PS} \\ \mathbf{M}_{QP} & \mathbf{M}_Q & \mathbf{M}_{QS} \\ \mathbf{M}_{SP} & \mathbf{M}_{SQ} & \mathbf{M}_S \end{pmatrix} \cdot \begin{pmatrix} \mathbf{n}_P \\ \mathbf{n}_Q \\ \mathbf{n}_S \end{pmatrix} + \begin{pmatrix} \Gamma_P \\ \Gamma_Q \\ \Gamma_S \end{pmatrix}, \tag{4}$$

where $\mathbf{n}_S$ is given by (2) and hence $\dot{\mathbf{n}}_S = 0$. We assume $\dot{\mathbf{n}}_Q = 0$ and immediately derive

$$\mathbf{n}_Q = -\mathbf{M}_Q^{-1}\left(\mathbf{M}_{QP}\mathbf{n}_P + \mathbf{M}_{QS}\mathbf{n}_S + \Gamma_Q\right), \tag{5}$$

$$\begin{aligned} \dot{\mathbf{n}}_P &= (\mathbf{M}_P - \mathbf{M}_{PQ}\mathbf{M}_Q^{-1}\mathbf{M}_{QP})\mathbf{n}_P + (\mathbf{M}_{PS} - \mathbf{M}_{PQ}\mathbf{M}_Q^{-1}\mathbf{M}_{QS})\mathbf{n}_S + \Gamma_P - \mathbf{M}_{PQ}\mathbf{M}_Q^{-1}\Gamma_Q \\ &= \mathbf{M}_{\text{eff}}\mathbf{n}_P + \Gamma_{\text{eff}}, \end{aligned} \tag{6}$$

which reduces the dimension of the ODE system to the dimension of the P space. In the last step we have used that both Γ and $\mathbf{n}_S$ are proportional to n_i and hence represent a source.

2.2 Formulation I ("meta-stable resolved")

Taking only the ground and the two meta-stable states into the P space, hence assuming $\dot{n} = 0$ for all the other states, eq. (5) can be written for a state q as

$$\mathbf{n}_Q|_q = n(q) = r_0(q) n_\mathrm{e} n_\mathrm{i} + r_1(q) n_\mathrm{e} n(1^1S) + r_2(q) n_\mathrm{e} n(2^1S) + r_3(q) n_\mathrm{e} n(2^3S). \tag{7}$$

$r_j(q)$ are called population coefficients and depend on T_e and n_e. The subscripts $j \in \{0,1,2,3\}$ stand for the ion, the ground state 1^1S, and the meta-stable 2^1S and 2^3S states, respectively. For the P space, hence $p \in \{1,2,3\}$, eq. (6) becomes

$$\dot{\mathbf{n}}_P|_p = \frac{\mathrm{d}}{\mathrm{d}t} n(p) = \sum_{j \neq p, j \neq 0} k_{jp} n(j) n_\mathrm{e} - k_p n(p) n_\mathrm{e} + k_{0p} n_\mathrm{i} n_\mathrm{e}. \tag{8}$$

Notice that the constraint on ion density n_i in [1, eq. (25)] is only valid in a closed system. In EIRENE, it is usually additionally modified by plasma transport (on larger time scales) and other collision terms.

The k's are the CR coupling coefficients and are given explicitly in terms of the population coefficients in [1]. From (6) we see that $(\mathbf{M}_\mathrm{eff})_{pp} = -k_p n_\mathrm{e}$, $(\mathbf{M}_\mathrm{eff})_{pj} = k_{jp} n_\mathrm{e}$ and $\Gamma_\mathrm{eff}|_p = k_{0p} n_\mathrm{i} n_\mathrm{e}$.

2.3 Formulation II ("meta-stable unresolved")

If the quasi-steady-state (QSS) assumption also holds for the meta-stable states, they may be also moved into the Q space. The P space becomes one dimensional - it is the most simple choice. The excited level population is then given by

$$\mathbf{n}_Q|_q = n(q) = R_0(q) n_\mathrm{e} n_\mathrm{i} + R_1(q) n_\mathrm{e} n(1^1S). \tag{9}$$

$R_0(q)$ and $R_1(q)$ are also called population coefficients. They are associated with the recombining and the ionizing plasma component, respectively. The time evolution of the ground state is written in the reduced form as

$$\dot{\mathbf{n}}_P = \frac{\mathrm{d}}{\mathrm{d}t} n(1^1S) = -\frac{\mathrm{d}}{\mathrm{d}t} n_\mathrm{i} = -S_\mathrm{CR} n(1^1S) n_\mathrm{e} + \alpha_\mathrm{CR} n_\mathrm{i} n_\mathrm{e}. \tag{10}$$

S_CR and $\alpha_\mathrm{CR}{}^\dagger$ are the CR ionization and recombination rate coefficients, respectively. S_CR, α_CR, $R_0(q)$ and $R_1(q)$ can be obtained directly from (5) and (6) or from k's and r's according to expressions given in [1, eq. (31-38)]. They are therefore functions of T_e and n_e.

6 Electron cooling rates

Often, EIRENE [7] is coupled to a plasma fluid code like B2 [9] or EMC3 (edge Monte Carlo 3D) [10] to describe the coupling of the plasma to neutrals. It acts then as a source (and sink) of the fluid due to neutrals, e.g. due to ionization (and recombination) - calculated with a CR model.

It also provides a source (and sink) for the fluid energy and momentum due to the exchange with neutrals. Here, only electron collisions are considered for helium: since $m_e \ll m_i$, momentum exchange can be neglected. The change in energy is expressed with the electron cooling rate density

$$W = \sum_p \Big\{ \chi(p) S(p) n_e n(p) + \sum_{q \neq p} [\chi(q) - \chi(p)] C(q,p) n_e n(q) - \chi(p) \alpha(p) n_e^2 n_i + W_\beta(p) n_e n_i + W_{\beta_d}(p) n_e n_i \Big\}. \quad (46)$$

It has the dimension "energy per time and volume". p and q are hereby energy states of the helium atom as in (1) and χ the ionization potential. $W_\beta(p)$ and $W_{\beta_d}(p)$ are the rate coefficients associated with the radiative and dielectronic recombination into state p.

6.2.1 Derivation

Having the expression in (46) fully defined, we notice that it depends on the helium population (and ion) density. Hence, a solution for the rate equation (1) is required. Naturally, we want to use the approximate solutions from formulation I or II: we insert (2) for $n \geq 21$ (Saha states), for $n < 21$ and $q \notin \{1^1S, 2^1S, 2^3S\}$ we use (7) in form. I or (9) for $q \neq 1^1S$ in form. II. We obtain

$$W = W_0^{\mathrm{I}} n_e n_i + W_1^{\mathrm{I}} n_e n(1^1S) + W_2^{\mathrm{I}} n_e n(2^1S) + W_3^{\mathrm{I}} n_e n(2^3S) \tag{56}$$

in formulation I and

$$W = W_0^{\mathrm{II}} n_e n_i + W_1^{\mathrm{II}} n_e n(1^1S) \tag{57}$$

in formulation II.

Explicitly, in form. I the cooling rate coefficients are

$$W_j^{\mathrm{I}} = \sum_p \left\{ \chi(p) S(p) n_e r_j(p) + \sum_{\substack{q \neq p \\ n<21}} [\chi(q) - \chi(p)] C(q,p) n_e r_j(p) \right\} \text{ for } j \in \{1,2,3\}, \tag{58}$$

$$\text{and } W_0^{\mathrm{I}} = \sum_p \left\{ \chi(p) S(p) n_e r_0(p) + \sum_{\substack{q \neq p \\ n<21}} [\chi(q) - \chi(p)] C(q,p) n_e r_0(p) \right.$$

$$\left. - \chi(p) \alpha(p) n_e + W_\beta(p) + W_{\beta_d}(p) + \sum_{\substack{q \neq p \\ n \geq 21}} [\chi(q) - \chi(p)] C(q,p) n_e Z(q) \right\}. \tag{59}$$

In form. II, $W_0^{\mathrm{II}} \mathrel{\hat{=}} W_0^{\mathrm{I}}$ with $R_0(p)$ instead of $r_0(p)$, and $W_1^{\mathrm{II}} \mathrel{\hat{=}} W_j^{\mathrm{I}}$ with $R_1(p)$ instead of $r_j(p)$.

6.3 Radiative loss rates

Similarly to the cooling rate, we can define the radiative loss rate

$$W_{\text{rad}} = \sum_p \left\{ \sum_{q>p} [\chi(q) - \chi(p)] A(q,p) n(q) - \left\langle (\frac{1}{2} m_e v^2 + \chi(p))(\sigma_\beta + \sigma_{\beta_d}) v \right\rangle \right\}. \tag{60}$$

$q > p$ means that state q lies energetically higher than state p. The second term accounts for the photons mentioned in chapter 6.1. Note: $W_{\text{rad}} < 0$. Like the cooling rate, it can be computed using formulation I or II, hence

$$W_{\text{rad}} = W^{\text{I}}_{\text{rad}_0} n_e n_i + W^{\text{I}}_{\text{rad}_1} n_e n(1^1S) + W^{\text{I}}_{\text{rad}_2} n_e n(2^1S) + W^{\text{I}}_{\text{rad}_3} n_e n(2^3S) \tag{61}$$

and

$$W_{\text{rad}} = W^{\text{II}}_{\text{rad}_0} n_e n_i + W^{\text{II}}_{\text{rad}_1} n_e n(1^1S). \tag{62}$$

Due to energy conservation, the plasma's thermal energy change (cooling/heating) must be balanced by change of the internal state (atomic level transition) and radiation. This also holds in the reduced formulations, hence

$$W_i = \sum_{j \neq i} [\chi(i) - \chi(j)] k_{ij} - W_{\text{rad}_i}. \tag{63}$$