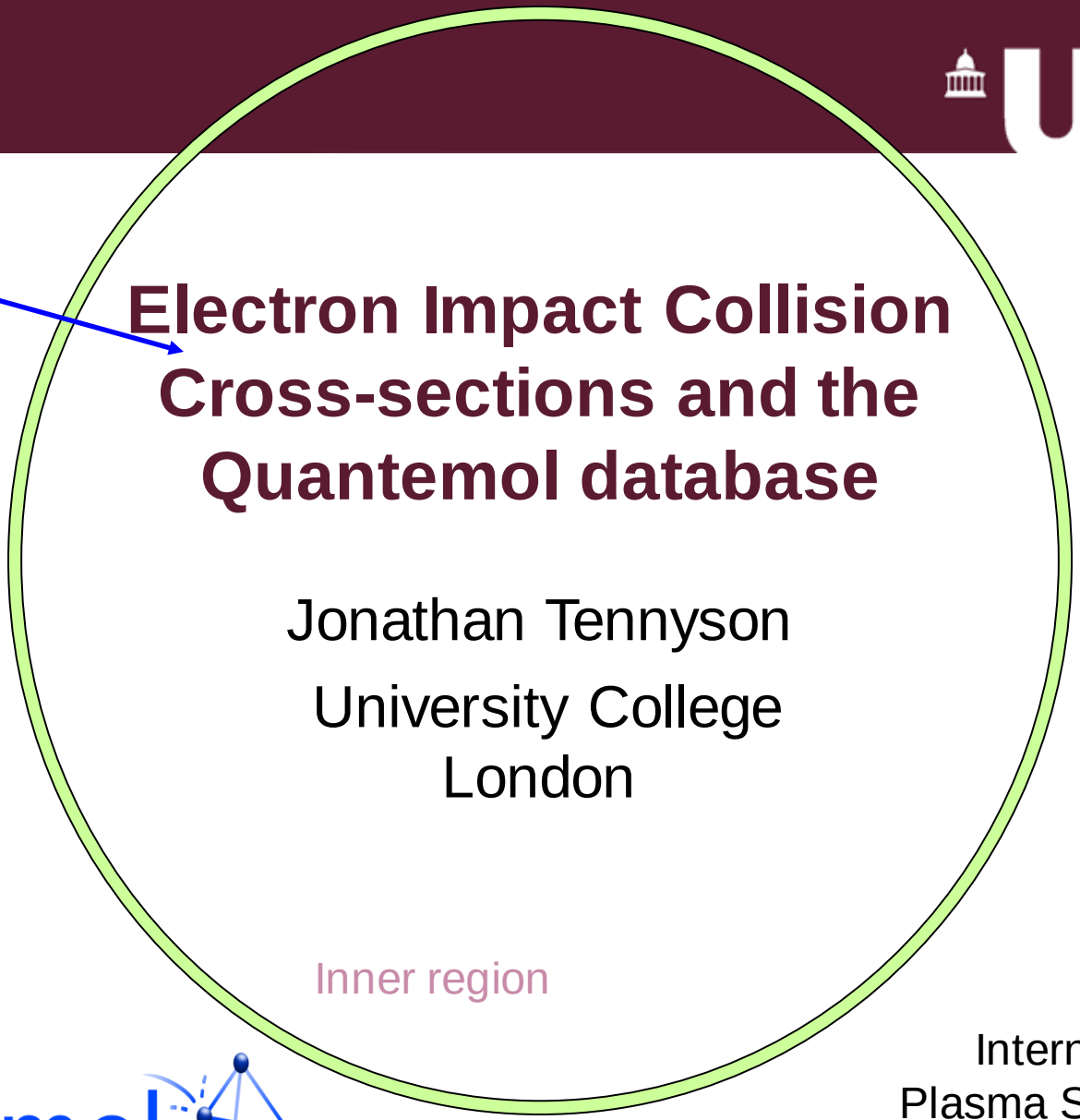


Electron Impact Collision Cross-sections and the Quantemol database

Jonathan Tennyson

University College London

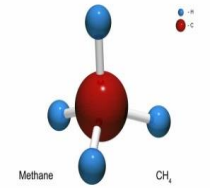
Quantemol

International Online Plasma Seminar (IOPS)
Oct 2021

About the Quantmol

Quantemol was founded in 2004 as a University College London spin-off providing user friendly interfaces for sophisticated academic codes. Company has expended to providing scientific consultancy services and in 2016 launched the QDB database. Has 3 main products:

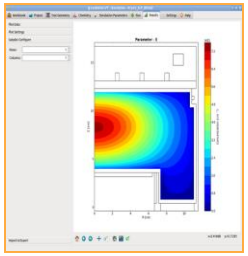
2019 QEC electron collisions



Quantum chemistry code based software to provide reaction rates

UKRmol+

2013 QVT Virtual Tool



Plasma modelling software to model plasma behaviour

Hybrid Equipment Plasma Model

2016 QDB plasma chemistry

Plasma chemistry database

Quantemol

Contents

1. Databases: QDB etc
2. Electron collision applications: process + calculations

   Fusion plasmas: BeH, H_2

   Technological plasmas

   Atmospheric: space craft re-entry

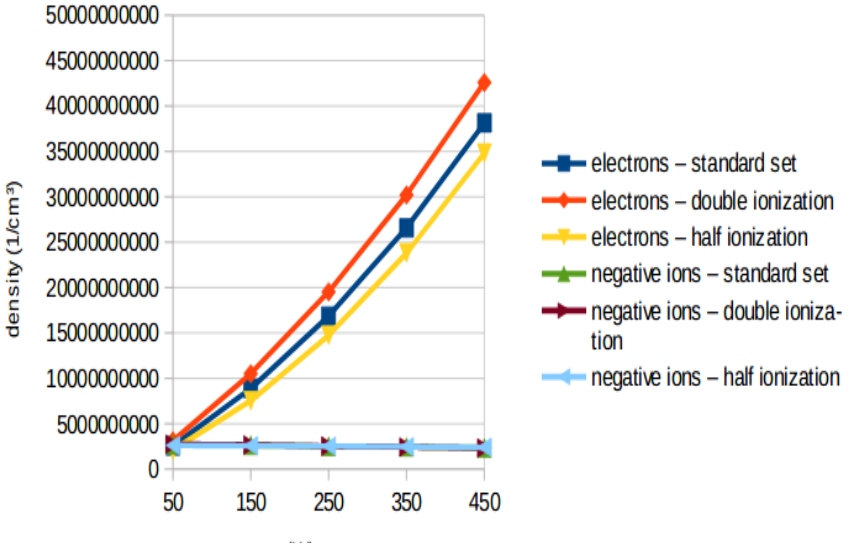
3. Future directions: photons

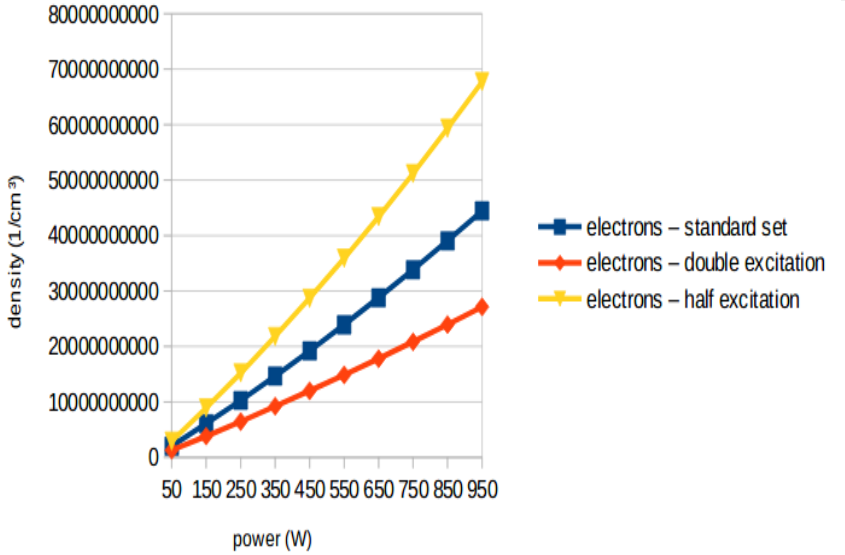
Plasma Modelling and Reaction data

A plasma model consists of two parts:

1. Physical model describing the particle motion
2. Chemical model which provides data for the physical model in the form of collision rates (ionization sources, collision frequency, diffusion coefficient).

Accuracy of the physical model depends strongly on the accuracy of the chemical model.





Which data are needed?

Gas Phase:

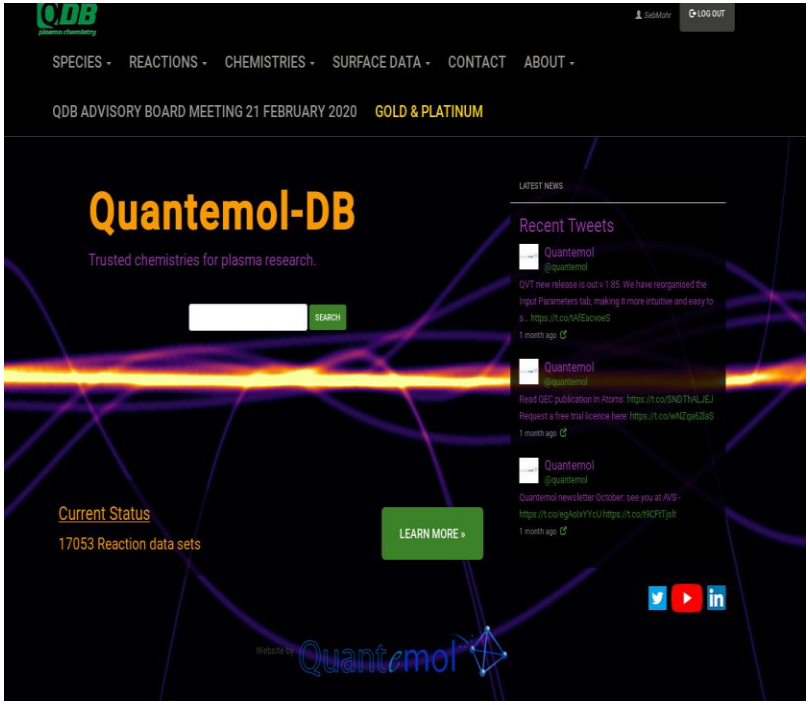
- Electron - heavy particle collisions: elastic, excitation, ionization, dissociation, attachment, recombination. Preferably as cross-sections, though some codes exclusively use rate coefficients.
- Heavy particle collisions: charge exchange, ion-ion recombination, chemical reactions, Penning ionization etc. Almost exclusively as rate coefficients

Classifications mainly important to correctly calculate energy losses/transfer.
For databases, classification allows search for specific reactions.

Active databases providing electron – molecule collision data

	Electron-collision data	Other data included
Astrophysics		
BASECOL	Rotational excitation	Heavy particle inelastic cross sections
KIDA	Dissociative recombination	Reaction rates
UDfA	Dissociative recombination	Reaction rates
Fusion		
NIFS	Excitation processes	Reactions rates
NFRI	Excitation processes	Reactions rates
ALADDIN	Excitation processes	Reactions rates
Atmospheric re-entry		
Phys4Entry	Vibrational excitation	Heavy particle inelastic cross sections
Plasma physics		
LXCat	Excitation processes	Atomic cross sections
Technological plasmas		
QDB	Excitation processes+	Reaction rates

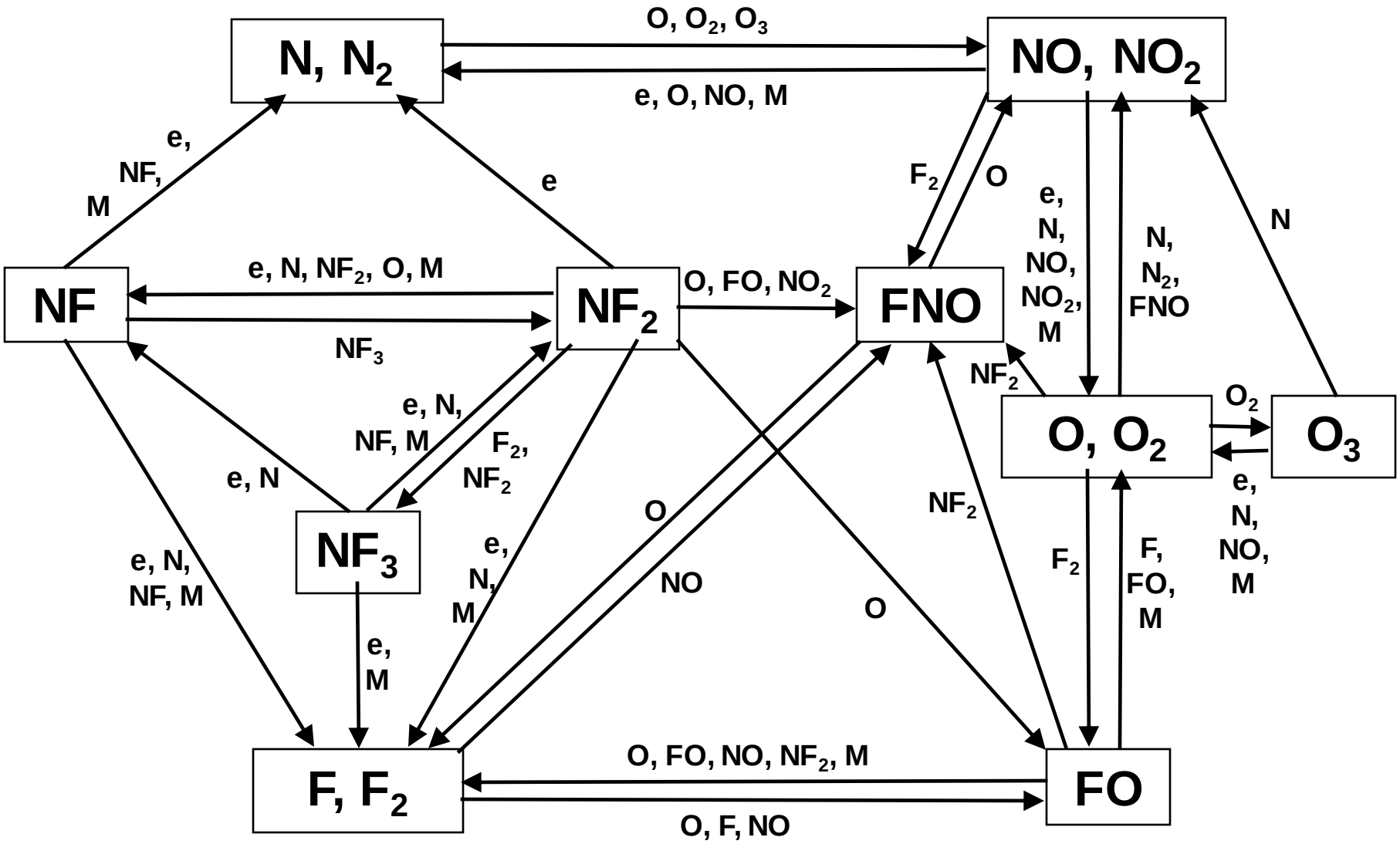
QDB: A species and reactions database for plasma applications aimed, mostly, at low-temperature plasmas



J. Tennyson et al, QDB: a new database of plasma chemistries and reactions, *Plasma Sources Sci. Technol.*, **26**, 055014 (2017).
5000 reactions, 29 complete chemistry sets

2021 release being finalised
30000 reactions, 38 complete chemistry sets + new functionality

REACTION MECHANISM: NF_3/O_2



M represents 3rd body.

Diagram ignores ions which are also important.

QDB species - Data Model

Fundamental species Object RP:

- Chemical formula (without states), i.e. CF4, Ar+, O-
- Mass
- Charge
- Thermodynamic properties
- States

State Object RP:

- Name (string)
- State type

State objects are connected to the RP objects. An RP can have multiple states and the same state can be attached to multiple RPs.

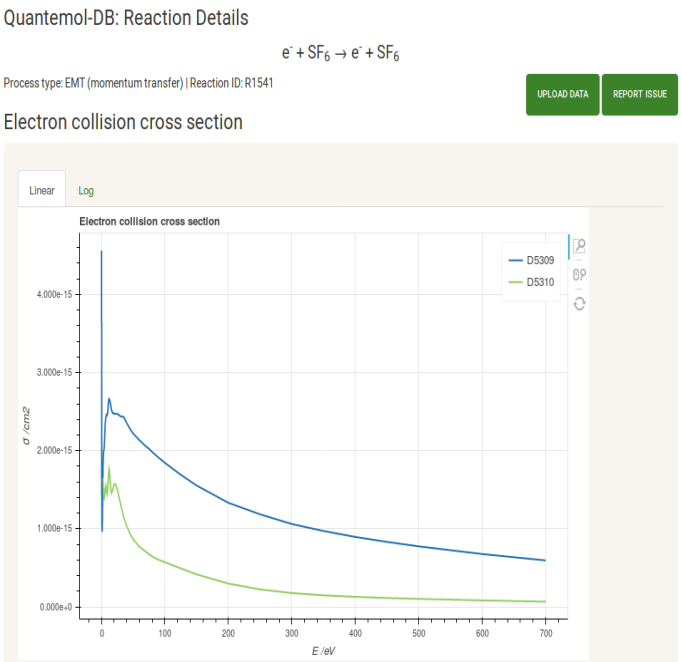
QDB states - Available states

State	Denomination
Atomic electronic excitation	Electronic Configuration: 1s2,1s2.2s2.2p6 Atomic Term Symbols: 3P, $^3P_{1/2}$
Molecular electronic excitation	Molecular Term Symbols: 3Π,X(3Π)
Rotational States	Total Rotational Quantum Number: J=0,J=3/2
Diatomic Vibrational States	Vibrational Quantum Number: v=0, v=1
Polyatomic Vibrational States	Normal Mode Formulation: v1, v1+v4, 3v2+v3
Generic/Pooled States	*,**,v=*,J=*

QDB - Reaction model

Reaction object stores:

- Reactants and Products (RPs)
- Type of reaction



ReactionDataSet object stores:

- Associated reaction
- Type: Cross section or coefficient
- Reference
- Energy-dependent cross section or
- Rate coefficient parameters A,n,E
- Uncertainties in cross section or rate coefficient parameters

Each dataset can only be attached to one reaction!

QDB - Chemistry Set Model

QDB provides pre-assembled chemistry sets for commonly used gas mixtures.

The chemistry object stores:

- The datasets used (not reactions)
- Child reactions to replace parent reactions
- Feed Gases

Other properties such as species are not stored but derived from the used datasets.

Rating	ID	Mixture	Reactions
★★★★☆	C3	N_2/H_2 chemistry	138
★★★★☆	C4	Ar/H_2 chemistry	64
★★★☆☆	C5	O_2/H_2 chemistry	115
★★★★☆	C6	SF_6/O_2 chemistry	147
★★★★☆	C7	CF_4/O_2 chemistry	169
★★★★☆	C8	SF_6 chemistry	57
★★★★☆	C9	CF_4 chemistry	79
★★★★☆	C10	$CF_4/O_2/H_2/N_2$ chemistry	299
★★★☆☆	C11	C_4F_8 chemistry	144
★★★☆☆	C13	SiH_4 chemistry	62
★★☆☆☆	C14	SiH_4/NH_3 chemistry	81
★★★★☆	C15	Ar/O_2 chemistry	51
★★★☆☆	C16	$Ar/O_2/C_4F_8$ chemistry	342
★★☆☆☆	C17	$SiH_4/Ar/O_2$ chemistry	178
★★☆☆☆	C18	Ar/Cu chemistry	26
★★★★☆	C19	$Cl_2/O_2/Ar$ chemistry	65
★★★★☆	C20	$Ar/BCl_3/Cl_2$ chemistry	59
★★★☆☆	C21	Ar/NH_3 chemistry	157
★★★★☆	C22	CH_4/H_2 chemistry	179
★★☆☆☆	C23	C_2H_2/H_2 chemistry	80
★★☆☆☆	C24	CH_4/NH_3 chemistry	262
★★☆☆☆	C25	C_2H_2/NH_3 chemistry	169
★★☆☆☆	C26	He/O_2 chemistry	83
★★★★☆	C27	$CF_4/CHF_3/H_2/Cl_2/O_2/HBr$ chemistry	568
★★★☆☆	C28	CH_4/N_2 chemistry	536
★★★★☆	C29	SF_6 / CF_4 / O_2 chemistry	293
★★☆☆☆	C30	Ar/Cu/He chemistry	24
★★★☆☆	C31	Ar/NF_3 chemistry	93
★★★☆☆	C32	$SF_6/CF_4/N_2/H_2$ chemistry	187
★★★★★	C33	$Ar/NF_3/O_2$ chemistry	310
★★★☆☆	C35	C_2F_6 / SiO_2(s) plasma etch	9
★★★☆☆	C36	CF_4 / SiO_2(s)	66
★★★☆☆	C37	He chemistry	16
★★★★★	C38	O_2 chemistry	50
★★★★☆	C39	Ar chemistry	18
★★★☆☆	C40	N_2 chemistry	27
★★★★★	C41	H_2 chemistry	27
★★★★★	C42	Reduced $CF_4/O_2/N_2/H_2$ Chemistry (1 - 30 mTorr)	83

QDB - Surface data - Coefficients

Sticking and return coefficients are used in plasma simulations to calculate particle losses and gains at surfaces. Example:

Oxygen atoms have (hypothetically) a sticking coefficient of 0.5 and return coefficient for O_2 of 0.1. Hence, half of the oxygen atoms hitting the surface will be lost and 10% will return as O_2.

Species	Surface	Formula	Parameters	Comment
O	Steel	p	p=1.0	Clean Surface
O	Steel	p	p=0.1	Saturated Surface

QDB - Surface data - Combined mechanisms

For complex surface reaction such as chemical etches, only sets of reactions have all the necessary information, i.e. the individual reactions on their own are stored in the database but only shown to the user in the context of a full set. The reactions itself are objects similar to surface reactions connected to reactants and products (gas phase and surface separately) and the coefficient parameters.

Reaction	Formula	Parameters	Comment
$F + Si\_S \rightarrow SiF\_S$	p	p=1.0	Implies activation by ions
$F + SiF\_S \rightarrow SiF_2\_S$	p	p=0.1	Implies activation by ions
$F + SiF_2\_S \rightarrow SiF_3\_S$	p	p=0.1	Implies activation by ions
$F + SiF_3\_S \rightarrow SiF_4$ (+ Si_S)	p	p=0.2	Implies activation by ions
$F^+ + SiF_2\_S \rightarrow SiF_2 + F$ (+ Si_S)	$p_0(\sqrt{E}-\sqrt{E_{th}})$	p=0.1, E_{th}= 5 eV	-

QDB - Services

Sebastian Mohr
Quantemol

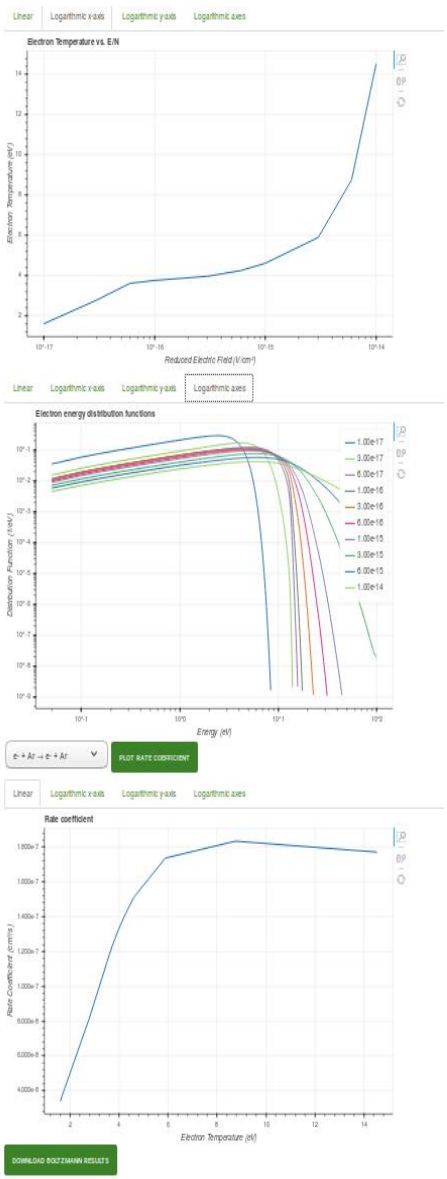
- Reaction sets
- Downloads of chemistry sets in ready to use format for commonly used software packages.
- A Dynamic Chemistry generator to assemble bespoke chemistry sets from reactions available on QDB.
- A Boltzmann-Solver to calculate rate coefficients for non-Maxwellian EEDFs.
- A 0D Model to calculate reactor-averaged particle densities.
- Chemistry Reduction service to optimize a set for specific process parameters, see:

M. Hanicinec, S. Mohr and J. Tennyson, Fast species ranking for iterative species-targeted skeletal reduction of reaction sets, *Plasma Sources Sci. Tech*., **29**, 125024 (2020)

QDB - Boltzmann - Solver

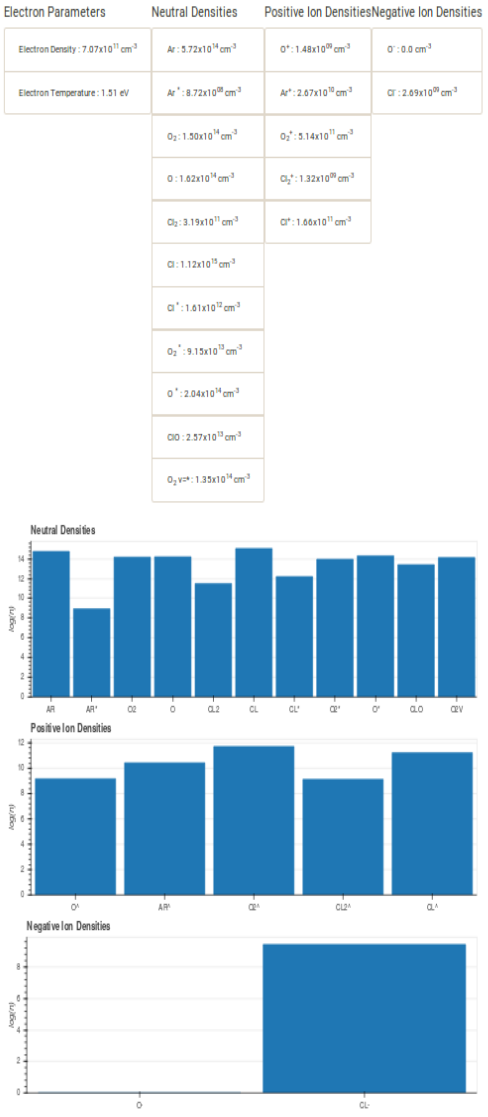
As the electron energy distribution function in a plasma is often non-Maxwellian, the rate coefficients need to be calculated for these. QDB has an online Boltzmann-Solver to calculate EEDFs and corresponding rate coefficients.

Defining relative densities of heavy particles and the gas temperature, it yields the EEDFs, electron temperature as function of the reduced electric field, and rate coefficients as function of temperature or reduced electric field.



QDB - 0D Model

QDB has an online global model which calculates particle densities and electron temperature for given process parameters such as pressure, power, and gas flows.



Low-energy electron collision processes

Elastic scattering

$AB + e \longrightarrow AB + e$

Rotational excitation

$AB(N'') + e \longrightarrow AB(N') + e$

Vibrational excitation

$AB(v''=0) + e \longrightarrow AB(v') + e$

Dissociative recombination/Dissociative attachment

$AB + e \longrightarrow A + B$

Electronic excitation

$AB + e \longrightarrow AB^* + e$

Impact dissociation

$AB + e \longrightarrow A + B + e$

Impact ionisation (e,2e)

$AB + e \longrightarrow AB^+ + e + e$

Increasing Energy

Electron-molecule collisions – Why theory?

- Need for complete datasets
- Experiment slow and expensive: best for benchmarking
- (Almost) impossible to study radicals experimentally
- (Almost) impossible to study excited states experimentally

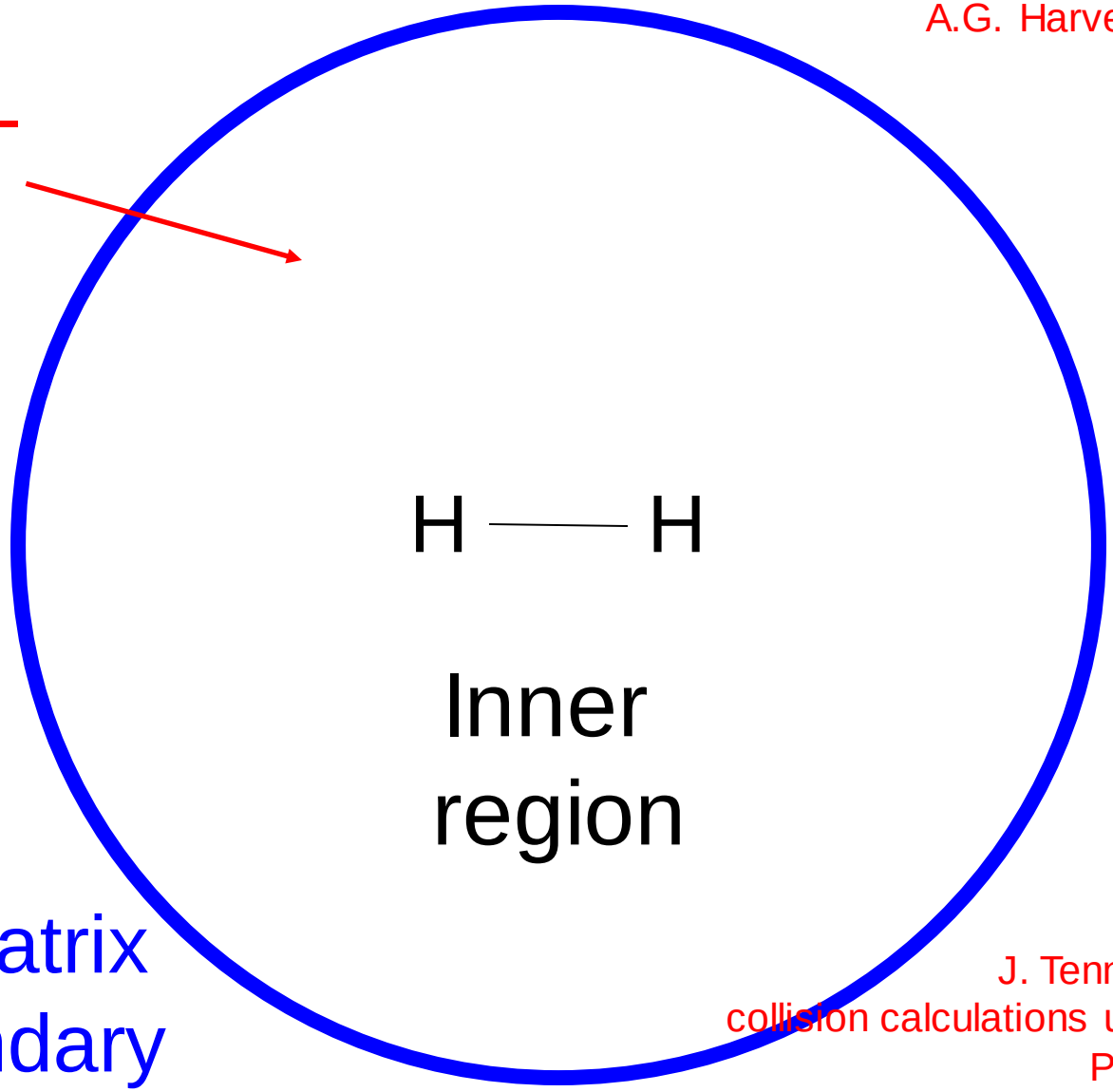
K. Bartschat and M.J. Kushner,
Electron collisions with atoms, ions, molecules, and surfaces:
Fundamental science empowering advances in technology,
Proc. Nat. Acad. Sci., **113**, 7026 (2016).

The R-matrix method:

UKRmol+

Z. Masin, J Benda, J.D. Gorfinkiel, A.G. Harvery, J. Tennyson, UKRMol+ Computer Phys. Comms., 249, 107092 (2020)

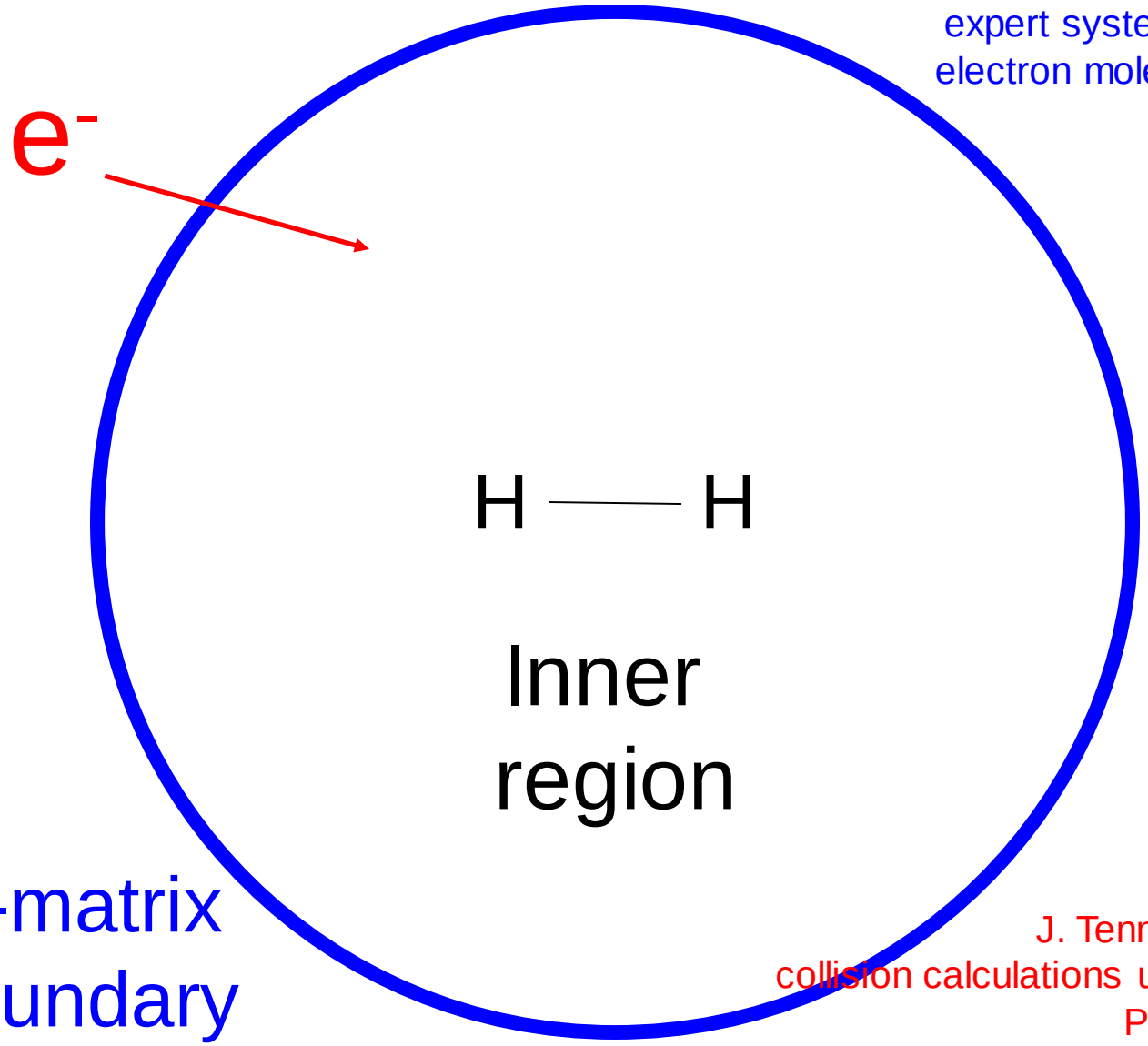
B-Splines
Large R-matrices



J. Tennyson, Electron – molecule collision calculations using the R-matrix method, Phys. Rep., 491, 29 (2010).

The R-matrix method:

Cooper et al., Quantemol Electron Collision: an expert system for performing UKRmol+ electron molecule collision calculations, Atoms, **74**, 97 (2019)



J. Tennyson, Electron – molecule collision calculations using the R-matrix method, Phys. Rep., 491, 29 (2010).

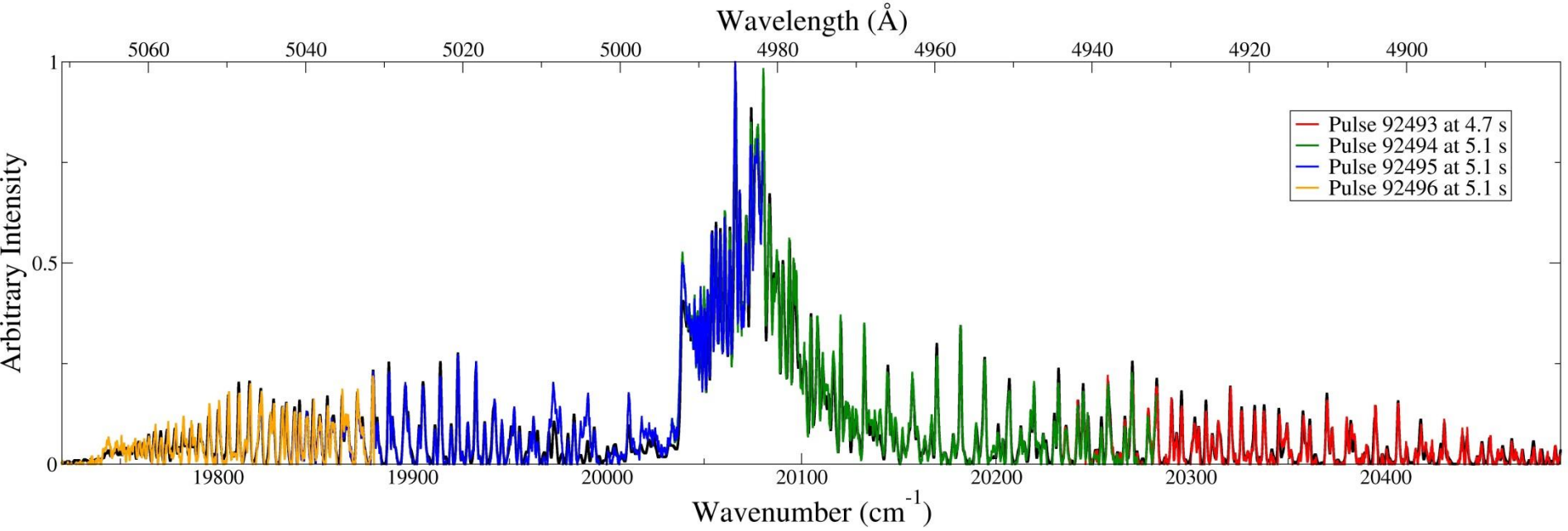
Fusion appications: BeH / BeD / BeT

- Be coating of walls at JET (ITER)
- BeD observed product
- Monitor Be erosion

Daniel Darby-Lewis

In collaboration with Kerry Lawson (CCFE)

BeD spectra measured in JET



Red, green, blue and orange regions are different pulses.

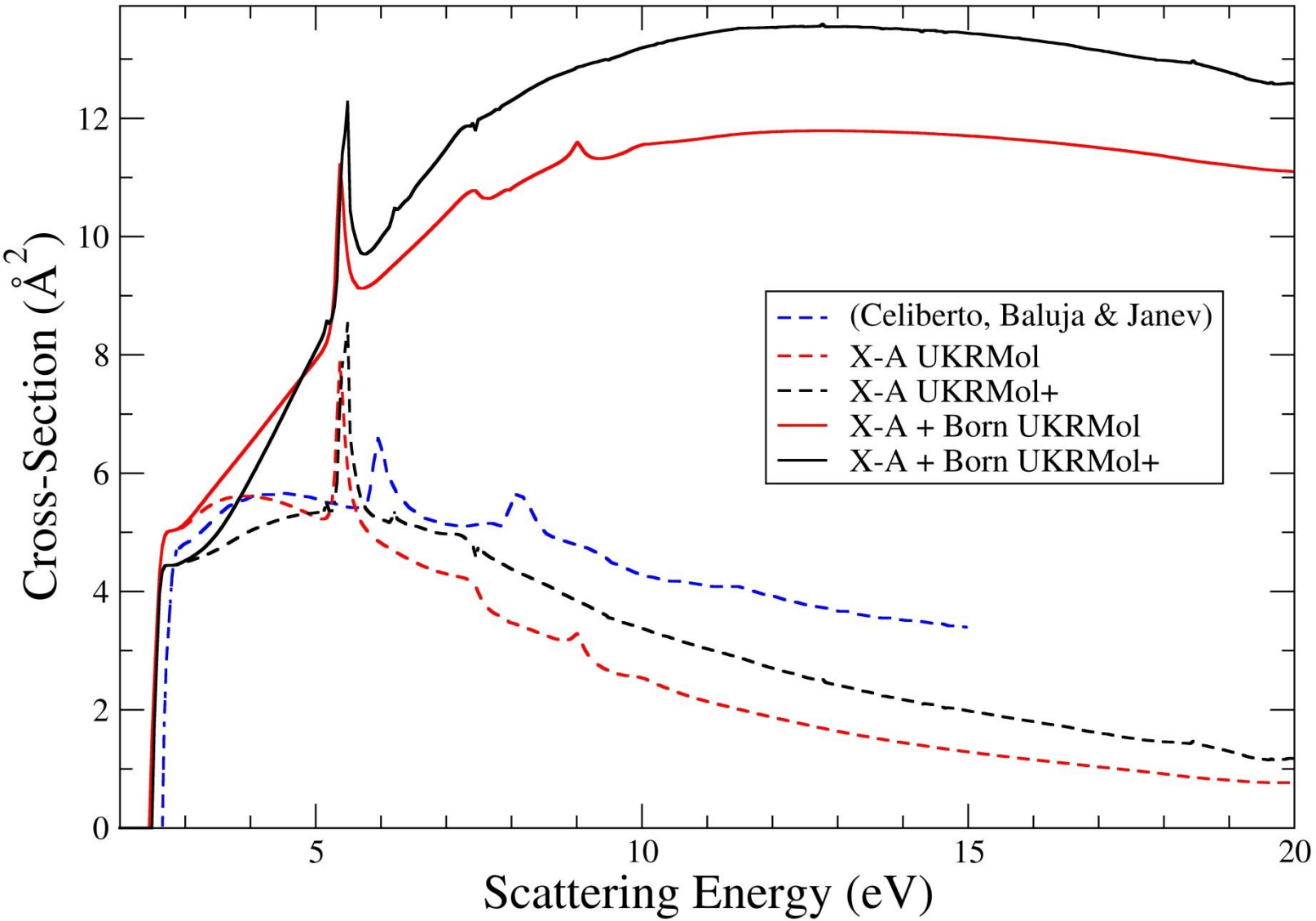
D. Darby-Lewis, J. Tennyson, K.D. Lawson, S.N. Yurchenko, M.F. Stamp, A. Shaw, S. Brezinsek and JET Contributor, Synthetic spectra of BeH, BeD and BeT for emission modelling in JET plasmas, *J. Phys. B: At. Mol. Opt. Phys.*, 51, 185701 (2018)

Interpretation requires collisional-radiative model

Step 1 e + BeH ($X\ ^2\Sigma^+$) → e + BeH ($A\ ^2\Pi$)

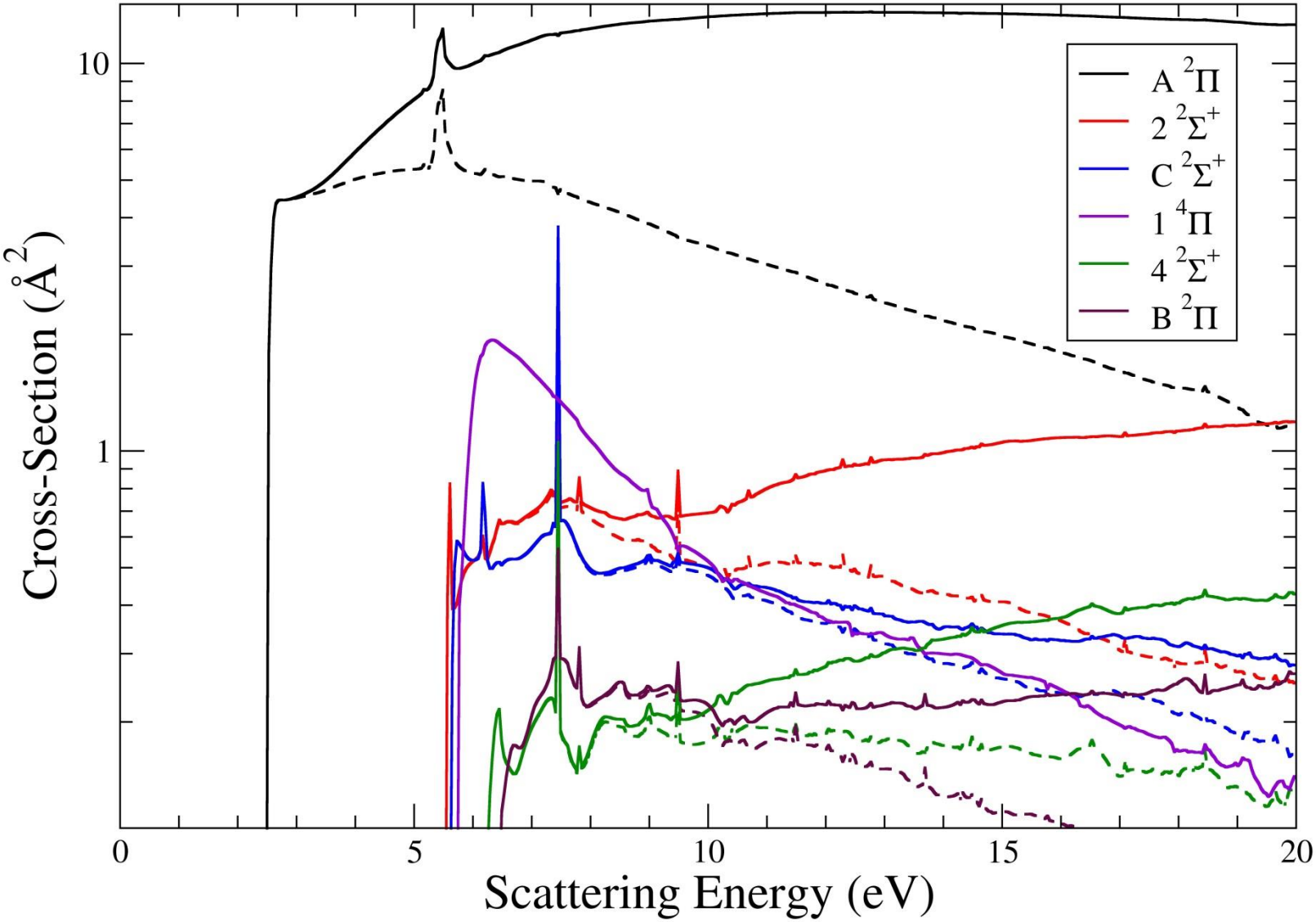
Step 2 BeH ($A\ ^2\Pi$, v',J') → BeH ($X\ ^2\Sigma^+$,v'',J'') + hν

e + BeH ($X\ ^2\Sigma^+$) → e + BeH ($A\ ^2\Pi$)



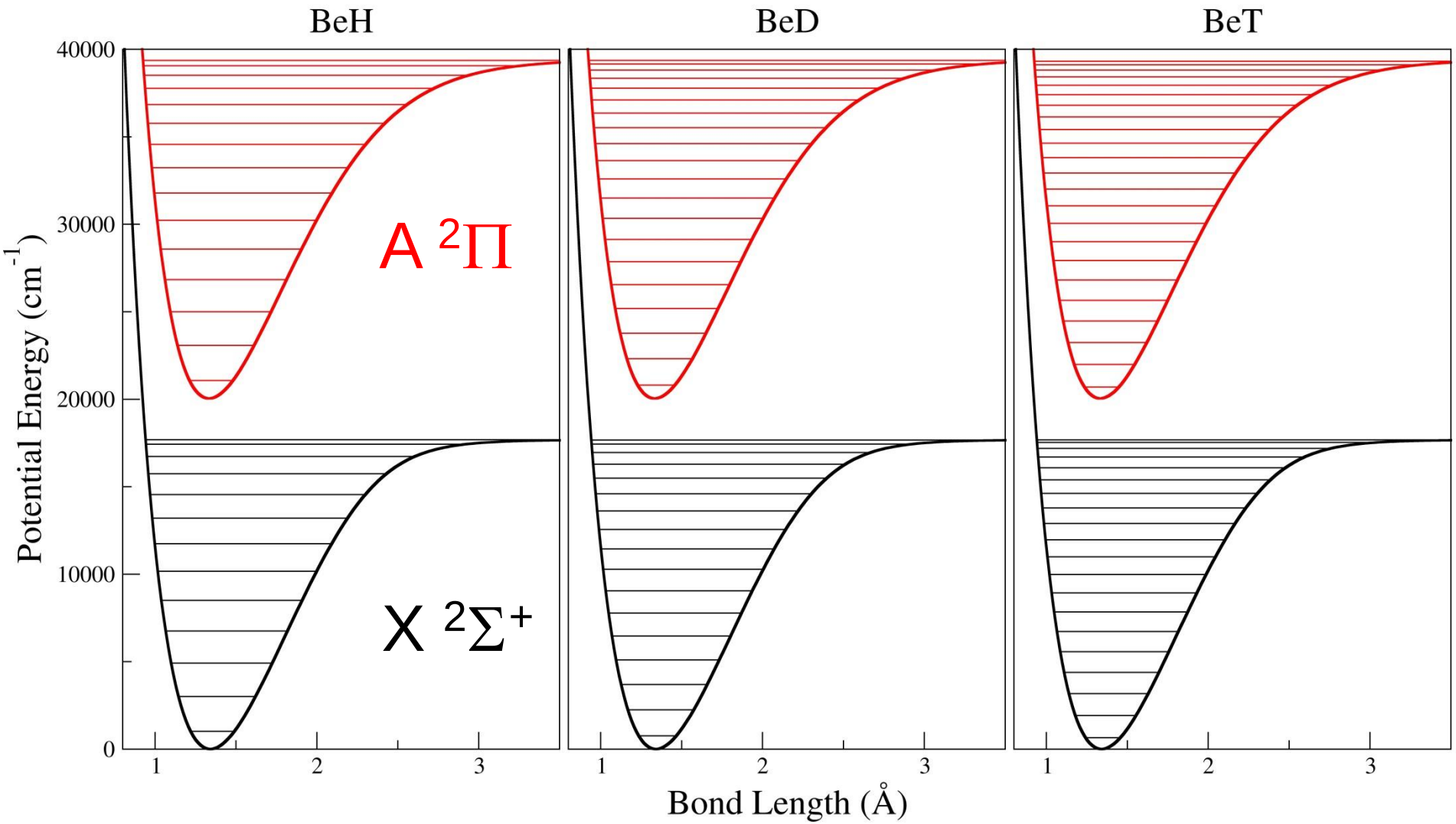
D. Darby-Lewis, Z. Masin & J. Tennyson, *J. Phys. B: At. Mol. Opt. Phys*, **50**, 175201 (2017).

Electron impact electronic excitation of the BeH (BeD)



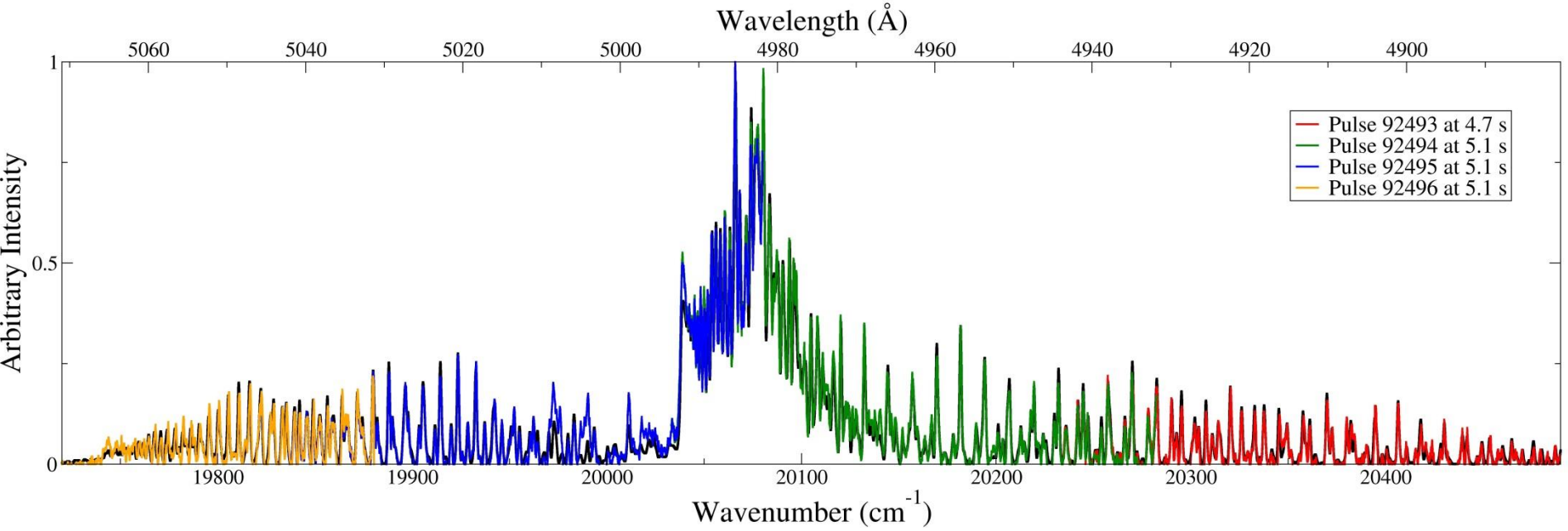
D. Darby-Lewis, Z. Masin & J. Tennyson, *J. Phys. B: At. Mol. Opt. Phys*, **50**, 175201 (2017).

Spectroscopic model for BeH/BeD/BeT



D. Darby-Lewis, J. Tennyson, K.D. Lawson, S.N. Yurchenko, M.F. Stamp, A. Shaw, S. Brezinsek and JET Contributor, Synthetic spectra of BeH, BeD and BeT for emission modelling in JET plasmas, *J. Phys. B: At. Mol. Opt. Phys.*, **51**, 185701 (2018)

BeD spectra measured in JET

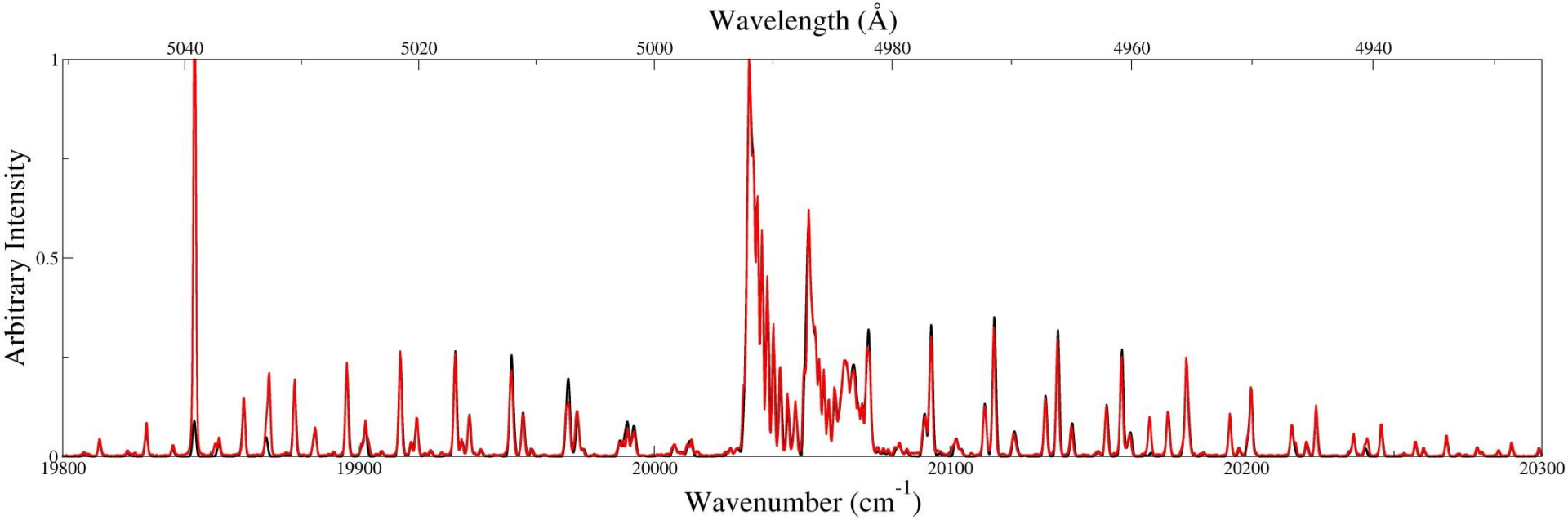


Red, green, blue and orange regions are different pulses.

Spectral fit: black lines. Gives: T_{rot} = 3800 K, T_{vib} = 4700 K

D. Darby-Lewis, J. Tennyson, K.D. Lawson, S.N. Yurchenko, M.F. Stamp, A. Shaw, S. Brezinsek and JET Contributor, Synthetic spectra of BeH, BeD and BeT for emission modelling in JET plasmas, *J. Phys. B: At. Mol. Opt. Phys.*, 51, 185701 (2018)

BeH spectra measured in Julich



Spectrum from a H doped lamp with a Be target: Measured red. Black synthetic generated at T_{rot} = 540 K and T_{vib} = 3440 K

Interpretation requires collisional-radiative model

Step 1 e + BeH ($X\ ^2\Sigma^+, v', J'$) → e + BeH ($A\ ^2\Pi, v'', J''$)

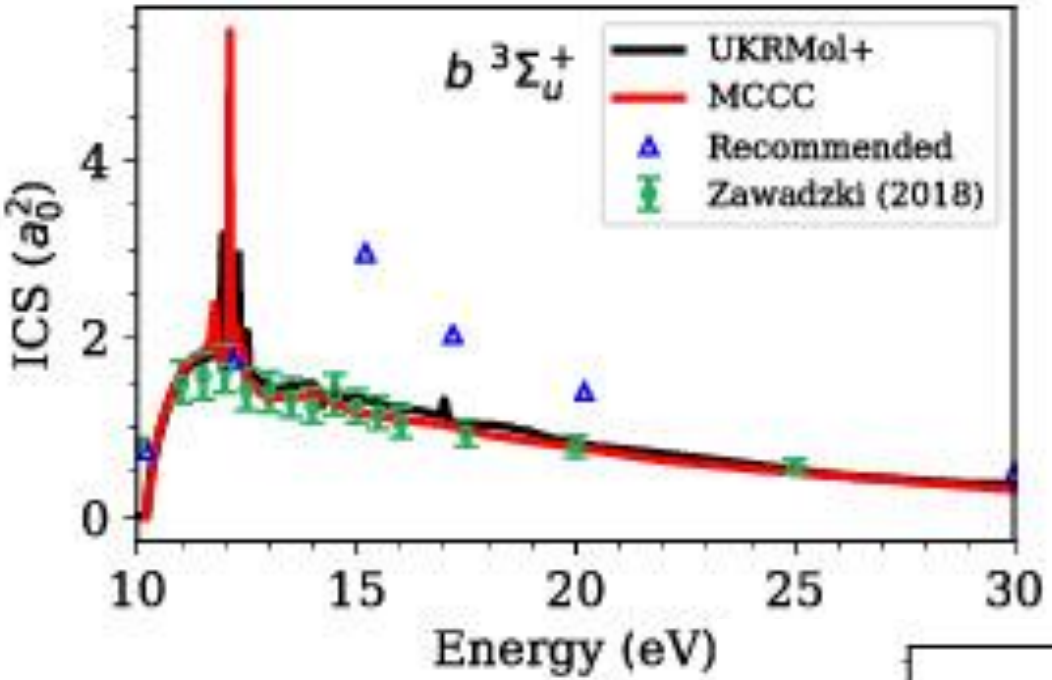
Step 2 BeH ($A\ ^2\Pi$, v', J') → BeH ($X\ ^2\Sigma^+, v'', J''$) + $h\nu$

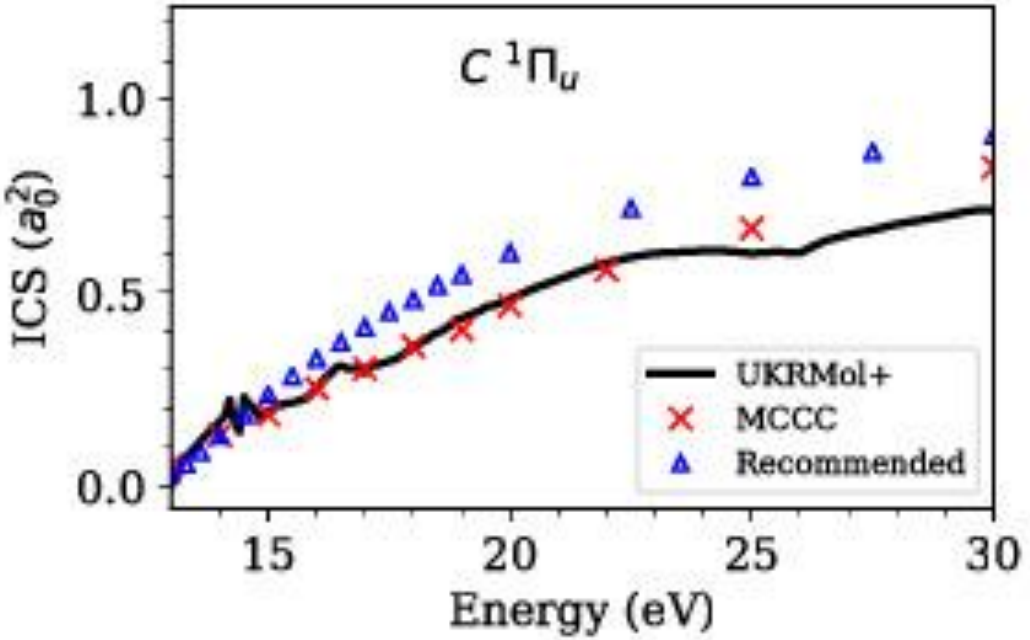
Fusion appications?: H_2/ D_2 /T_2 etc

- New UKRmol+ allows study of diffuse targets
- Considering collisions going up H(n=3) states
- R-matrix sphere with a = 100 a.u. !
- Consider collisions from excited states

Tom Meltzer

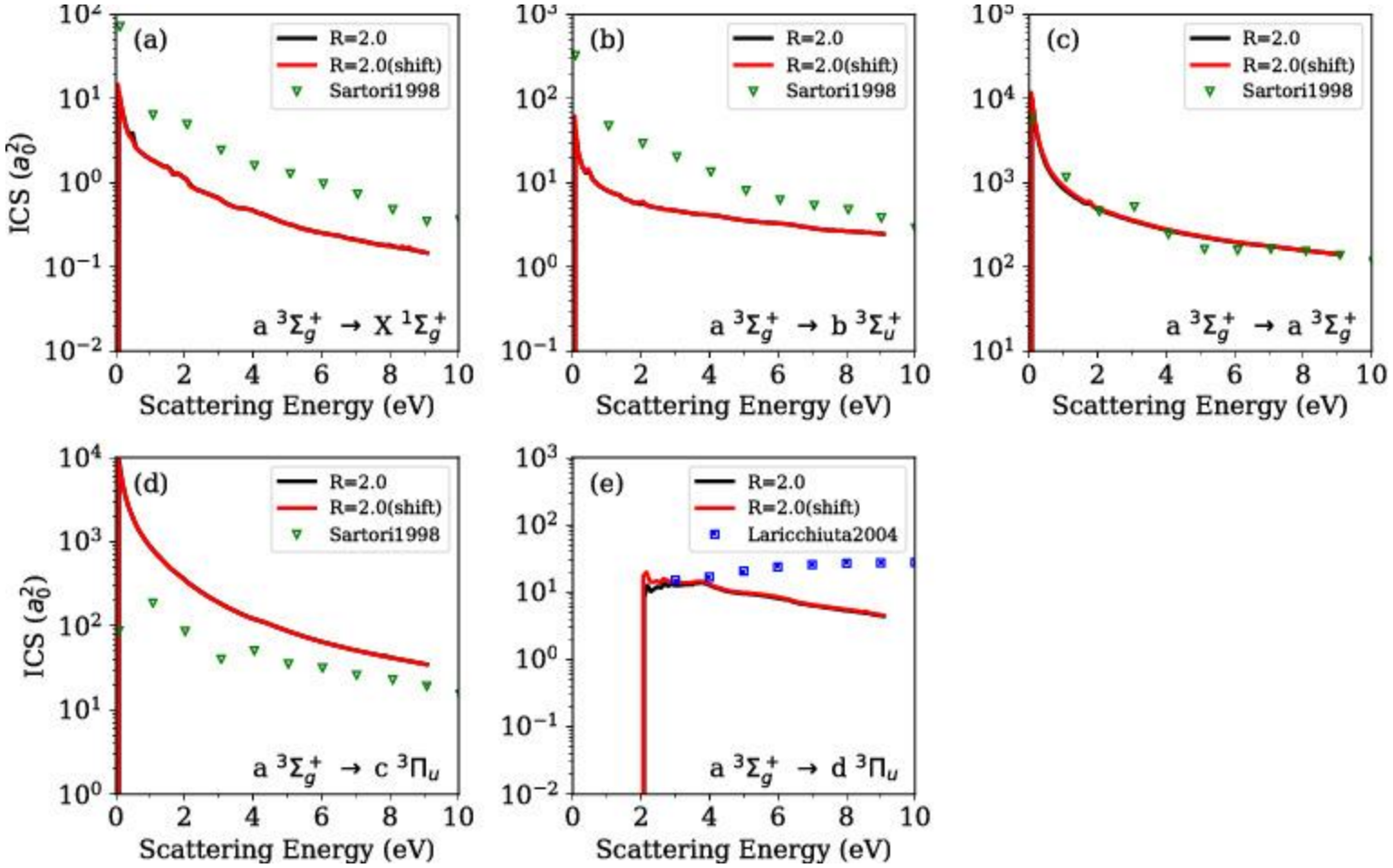
H_2 electronic excitation cross sections from X state





T. Meltzer et al. Benchmark Calculations of Electron Impact Electronic Excitation of the Hydrogen Molecule, *J. Phys. B: At. Mol. Opt. Phys.*, **53**, 145204 (2020).

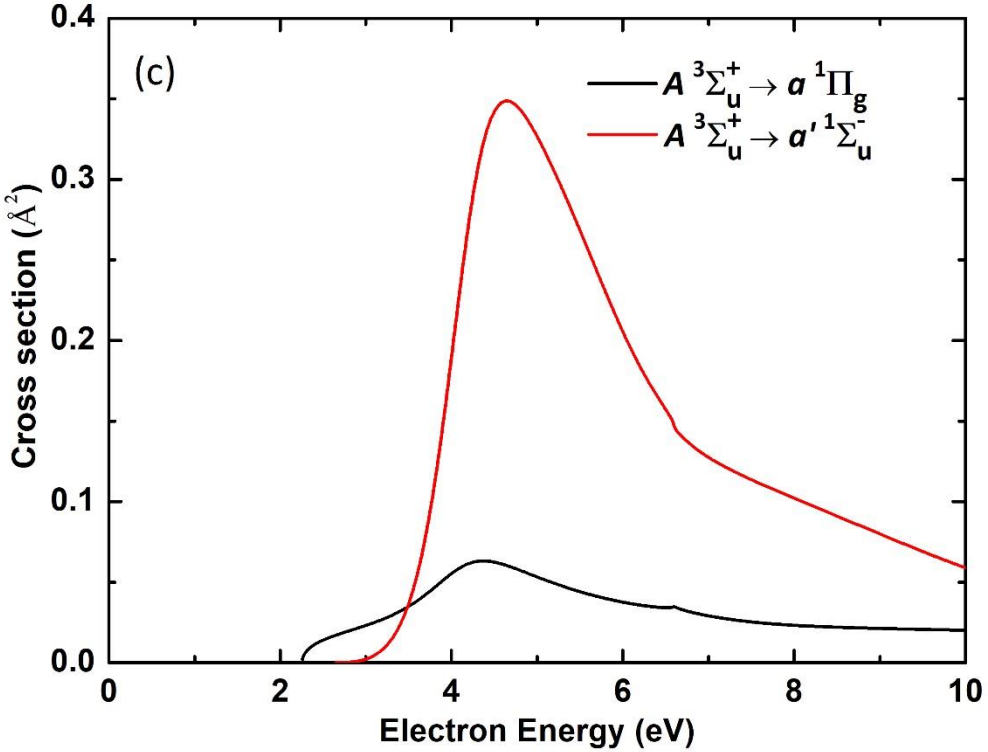
H_2 electronic excitation from excited states

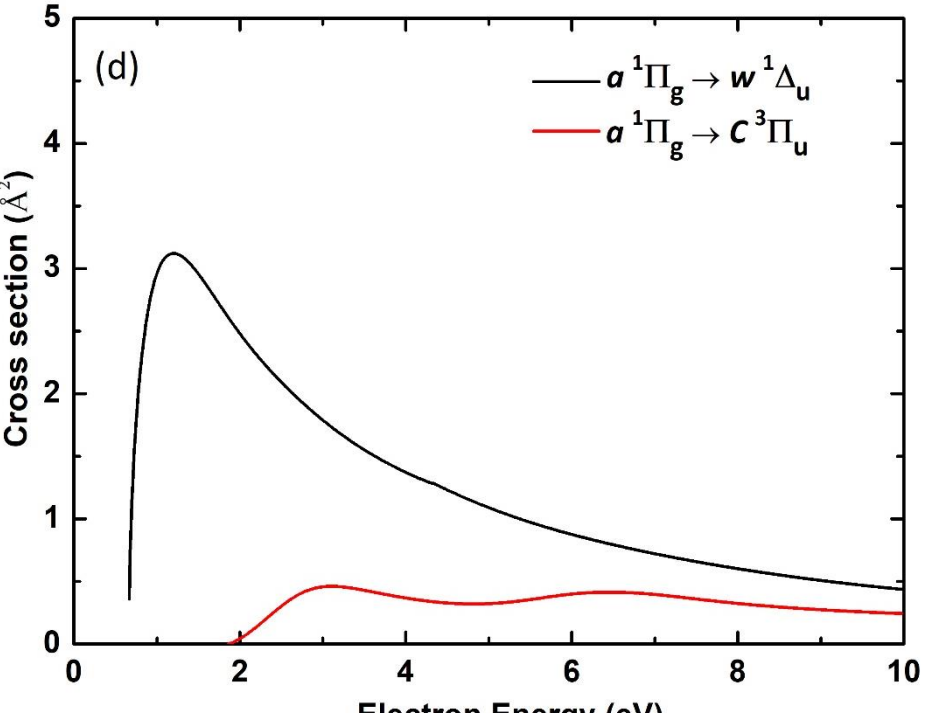


T. Meltzer and J. Tennyson, Electron Collisions with Molecular Hydrogen from Electronically Excited States Using the R-matrix Method, *J. Phys. B: At. Mol. Opt. Phys.*, **53**, 245203 (2020).

N_2 electronic excitation from excited states

He Su

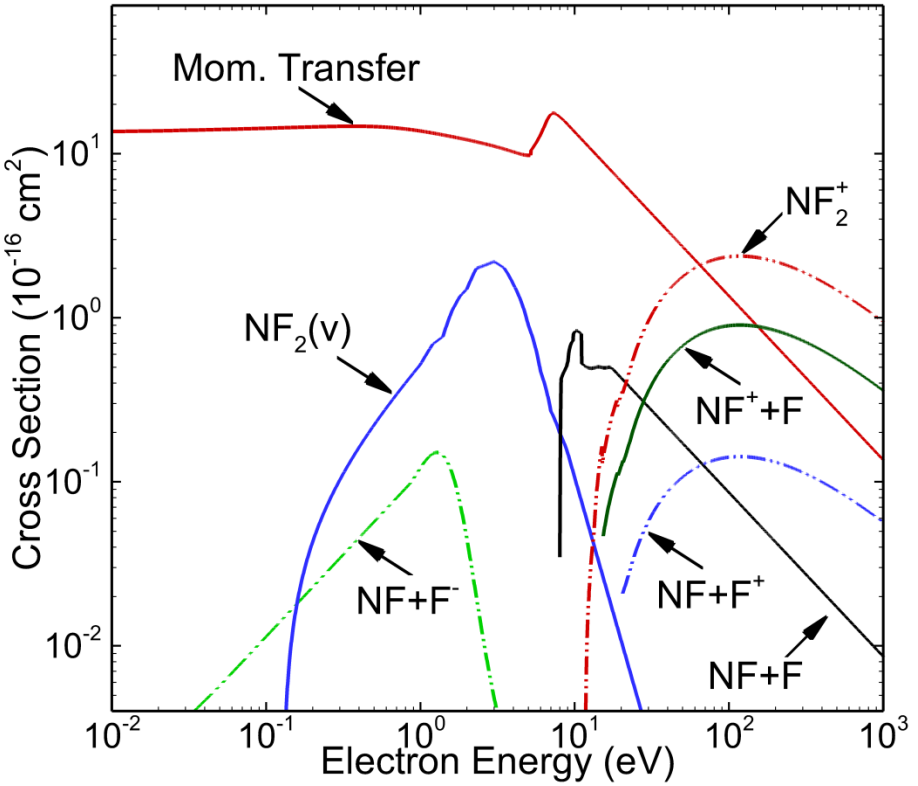




He Su, X. Cheng, H. Zhang & J. Tennyson, J. Phys. B: At. Mol. Opt. Phys., 54, 115203 (2021)

ELECTRON IMPACT NF_x CROSS SECTIONS

- **Electron impact cross sections for NF_x not well known.**
- **Few direct measurements of NF_3 cross sections – mostly derived from swarm data.**
- **No direct (or swarm) measurements for NF_2, NF.**
- ***Ab initio* R-matrix method used to computationally generate self-consistent set of electron impact cross sections for NF_3, NF_2, NF.**



NF_2 cross sections obtained using R-matrix method.

James Hamilton

J.R. Hamilton, J. Tennyson, S. Huang and M.J. Kushner, Calculated cross sections for electron collisions with NF_3, NF_2 and NF, Plasma Sources Sci. Technol, 26, 065010 (2017).

Plasma chemistries:

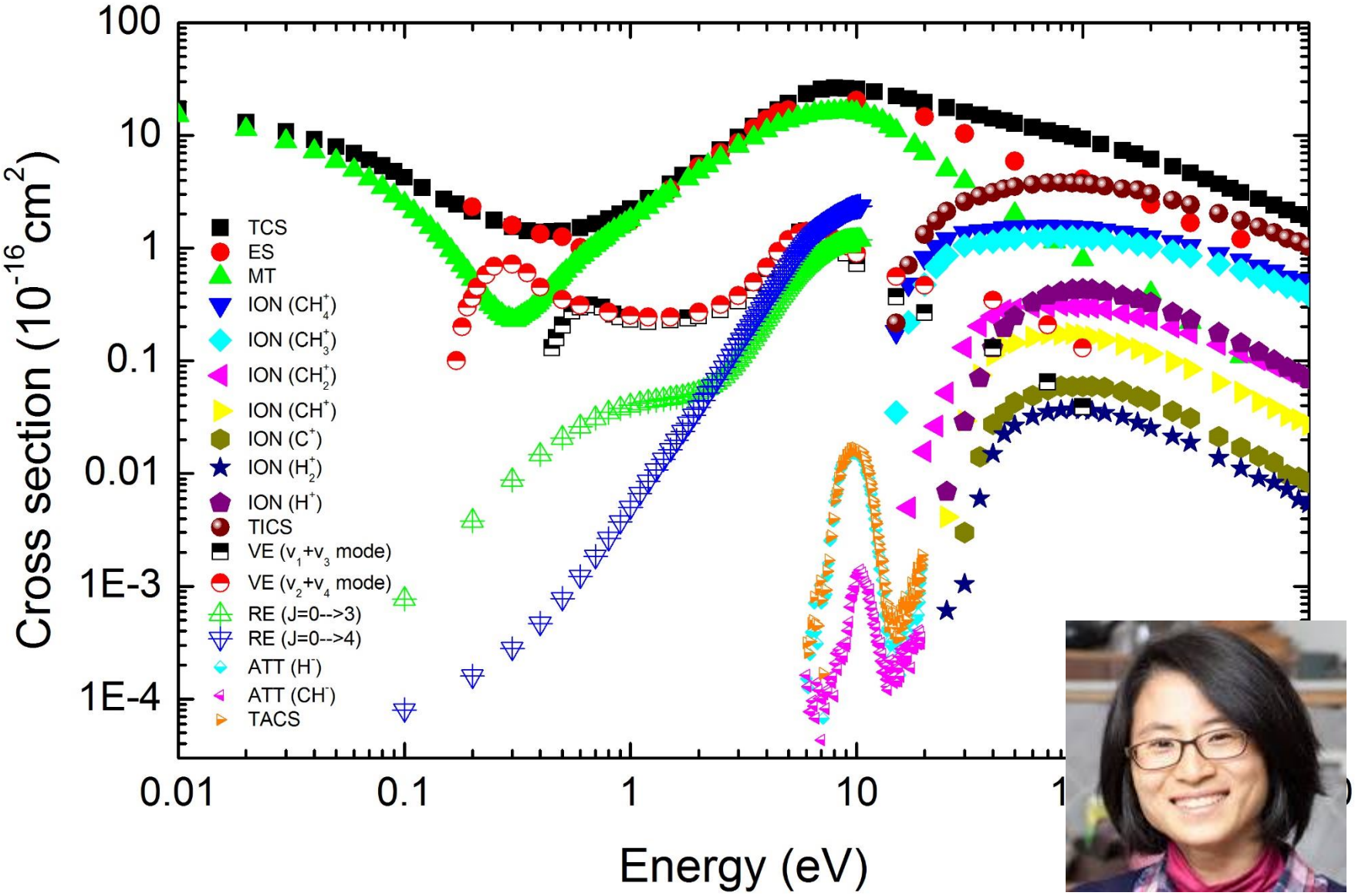
Driven by a whole variety of
e – molecules
Heavy particle reactions

Eg NF_3/O_2 mixture

S. Huang, V. Volynets, J.R. Hamilton, S. Lee, I.-C. Song, S. Lu, J. Tennyson & M.J. Kushner, Insights to Scaling Remote Plasma Sources Sustained in NF_3 Mixtures, *J. Vac. Sci. Technol. A*, **35**, 031302 (2017)

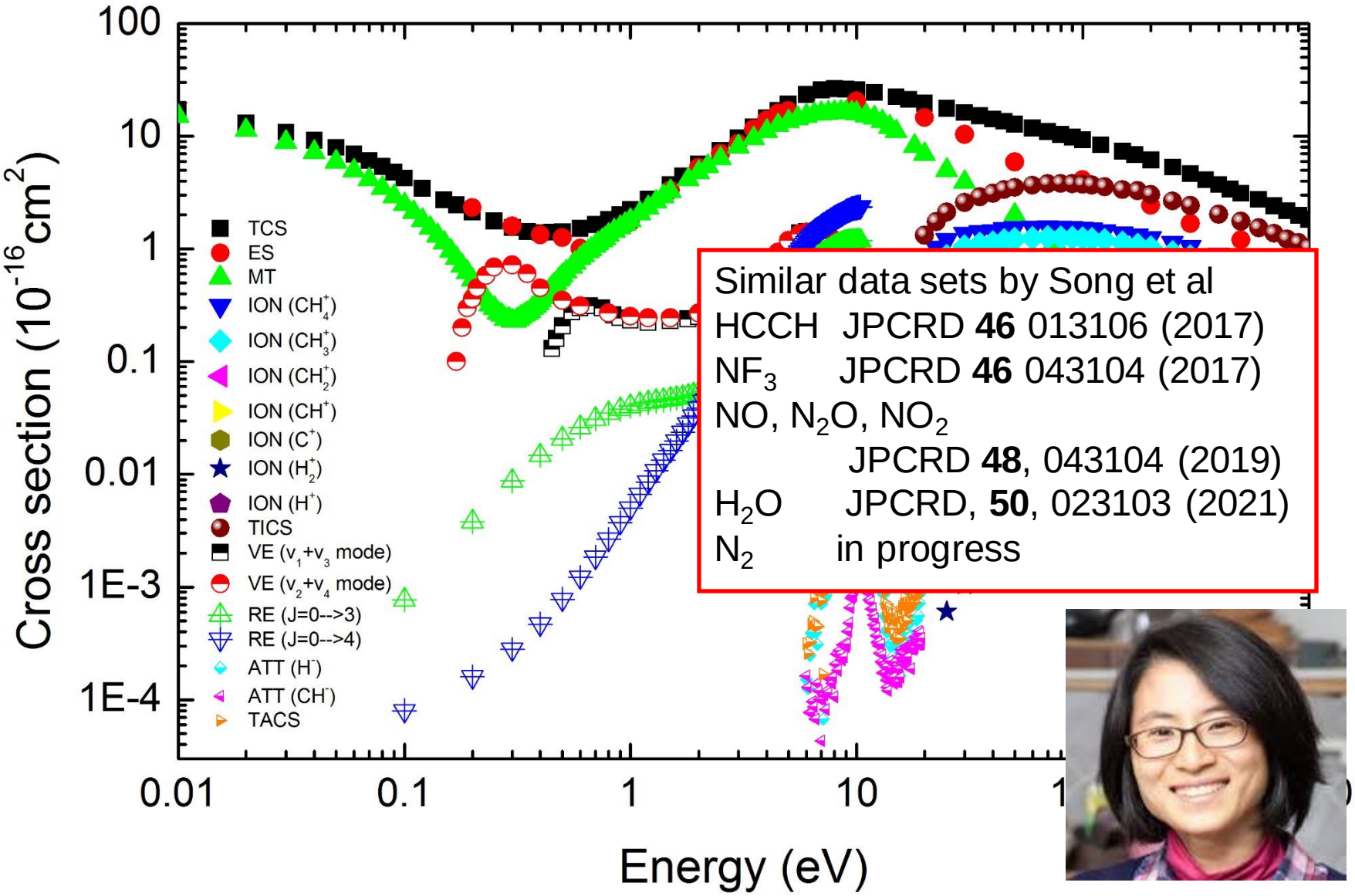
Process	Rate Coefficient[b)]	Reference	ΔH (eV)[b)]
Electron Impact NF_x			
$e + NF_3 \rightarrow NF_3 + e$	c)	[17]	d)
$e + NF_3 \rightarrow NF_2 + F^-$	c), e)	[17]	-1.0
$e + NF_3 \rightarrow NF_3(v) + e$	c), f)	[17]	
$e + NF_3 \rightarrow NF_2 + F + e$	c)	[17]	-5.8
$e + NF_3 \rightarrow NF + F + F + e$	c)	[17]	-6.1
$e + NF_3 \rightarrow NF_3^+ + e + e$	c)	[17]	
$e + NF_3 \rightarrow NF_2^+ + F + e + e$	c)	[17]	-0.5
$e + NF_3 \rightarrow NF^+ + F + F + e + e$	c)	[17]	-4.2
$e + NF_3 \rightarrow F^+ + NF_2 + e + e$	c)	[17]	-1.1[g)]
$e + NF_2 \rightarrow NF_2 + e$	c)	[18]	
$e + NF_2 \rightarrow NF + F^-$	c)	[18]	-0.5
$e + NF_2 \rightarrow NF_2(v) + e$	c), f)	[18]	
$e + NF_2 \rightarrow NF + F + e$	c)	[18]	-5.1
$e + NF_2 \rightarrow NF_2^+ + e + e$	c)	[18]	
$e + NF_2 \rightarrow NF^+ + F + e + e$	c)	[18]	
$e + NF_2 \rightarrow F^+ + NF + e + e$	c)	[18]	
$e + NF \rightarrow NF + e$	c)	[18]	
$e + NF \rightarrow N + F^-$	c)	[18]	-0.6
$e + NF \rightarrow NF(v) + e$	c), f)	[18]	
$e + NF \rightarrow NF(^1\Delta) + e$	c), f)	[18]	
$e + NF \rightarrow NF(^1\sum^+) + e$	c), f)	[18]	
$e + NF \rightarrow N + F + e$	c)	[18]	-4.0
$e + NF \rightarrow NF^+ + e + e$	c)	[18]	
$e + NF \rightarrow N^+ + F + e + e$	c)	[18]	
$e + NF \rightarrow F^+ + N + e + e$	c)	[18]	
$e + NF_3^+ \rightarrow NF_2 + F$	1×10^{-7}	est. [29], h)	-11.1
$e + NF_2^+ \rightarrow NF + F$	1×10^{-7}	est. [29]	-6.3[g)]
$e + NF^+ \rightarrow N^* + F$	1×10^{-7}	est. [29]	-7.1
Electron Impact F_2/F			
$e + F_2 \rightarrow F_2 + e$	c)	[30]	
$e + F_2 \rightarrow F^- + F$	c)	[30]	-1.8
$e + F_2 \rightarrow F + F + e$	c)	[30]	-1.6
$e + F_2 \rightarrow F_2^* + e$	c)	[30]	
$e + F_2 \rightarrow F_2^+ + e + e$	c)	[30]	
$e + F_2^+ \rightarrow F + F^*$	1×10^{-7}	est. [29]	-0.6
$e + F \rightarrow F + e$	c)	[31]	
$e + F \rightarrow F^* + e$	c)	[31]	
$e + F \rightarrow F^+ + e + e$	c)	[31]	
$e + F^* \rightarrow F^+ + e + e$	c)	[31]	
$e + F^+ \rightarrow F^*$	$5.3 \times 10^{-12}\ T_e^{-0.5}$	est. [32]	
$e + e + F^+ \rightarrow F^* + e$	$5.12 \times 10^{-27}\ T_e^{-4.5}$	est. [32]	
Electron Impact N_xO_y			
$e + NO \rightarrow NO + e$	c)	[33]	

Cross sections for electron collisions with methane



M.-Y. Song, J.S. Yoon, H. Cho, Y. Itikawa, G. Karwasz, V. Kokoouline, Y. Nakamura & J. Tennyson, J. Phys. Chem. Ref. Data, **44**, 023101 (2015)

Cross sections for electron collisions with methane



Similar data sets by Song et al

HCCH JPCRD **46** 013106 (2017)

NF_3 JPCRD **46** 043104 (2017)

NO, N_2O, NO_2 JPCRD **48**, 043104 (2019)

H_2O JPCRD, **50**, 023103 (2021)

N_2 in progress

M.-Y. Song, J.S. Yoon, H. Cho, Y. Itikawa, G. Karwasz, V. Kokoouline, Y. Nakamura & J. Tennyson, J. Phys. Chem. Ref. Data, **44**, 023101 (2015)

PHYS4ENTRY

PLANETARY ENTRY INTEGRATED MODELS

SEVENTH FRAMEWORK PROGRAMME

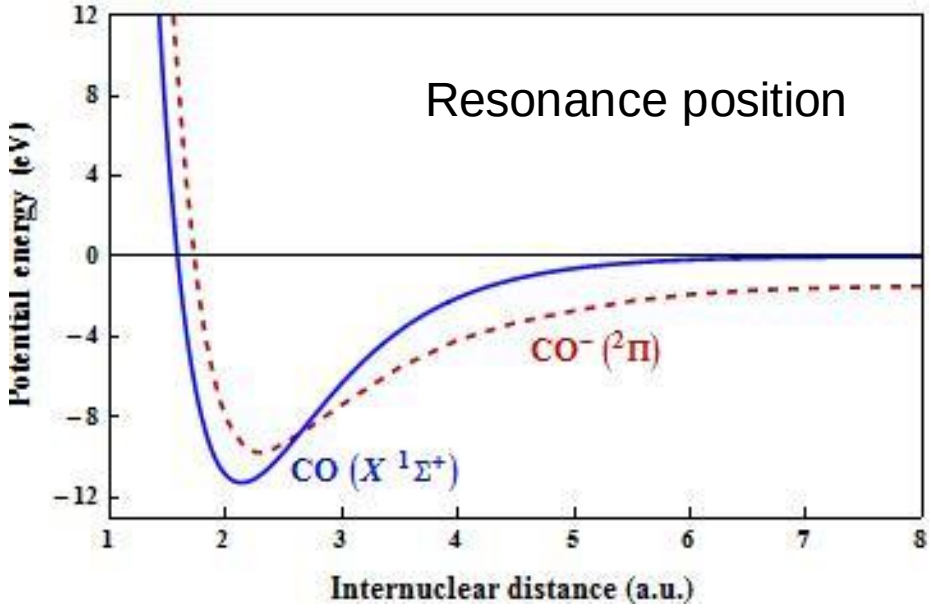
plasmas created on spacecraft (rocket) re-entry

Vibrational excitation of key molecule: Venus, Mars, Earth

Vincenzo Laporta

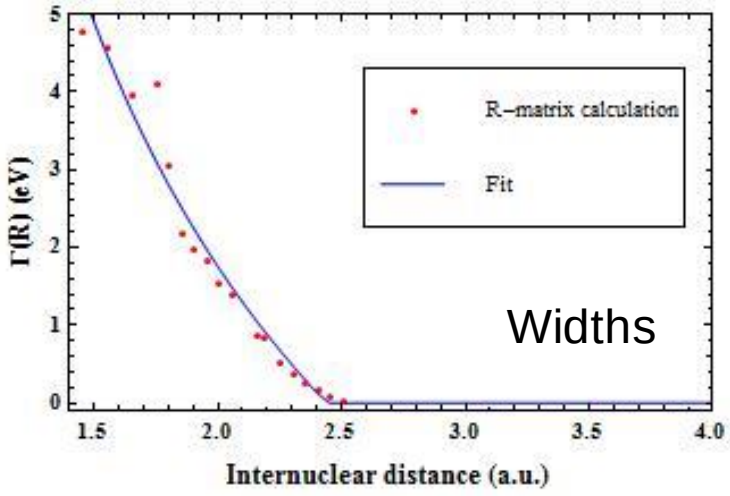
R. Celiberto et al,
Atomic & molecular data for spacecraft re-entry plasmas,
Plasma Sources Sci. Technol,
26, 033004 (2016).

Electron – CO: $^2\Pi$ resonance



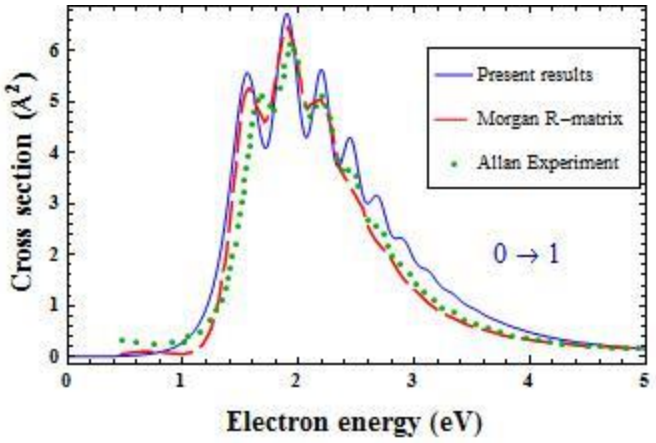
R-matrix resonance positions and widths

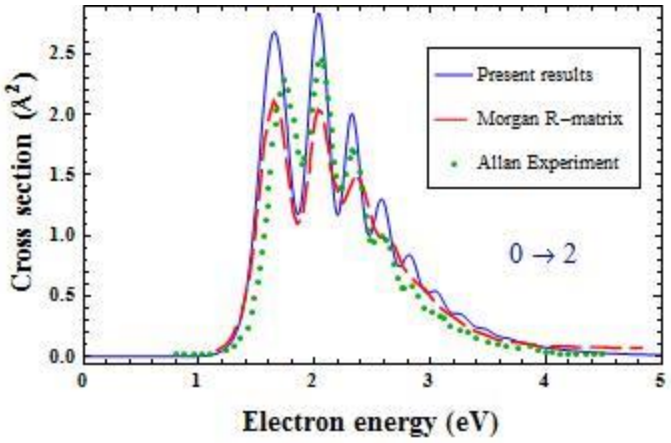
Static exchange plus polarisation (SEP) model

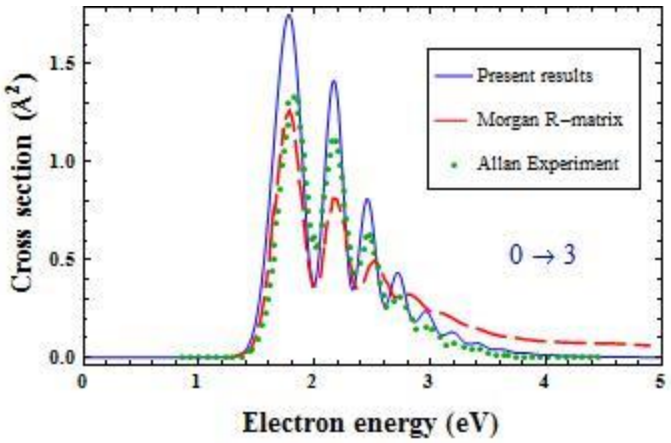


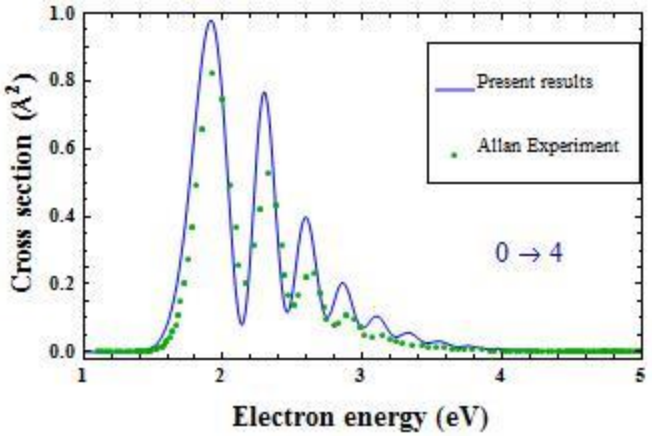
Electron – CO:

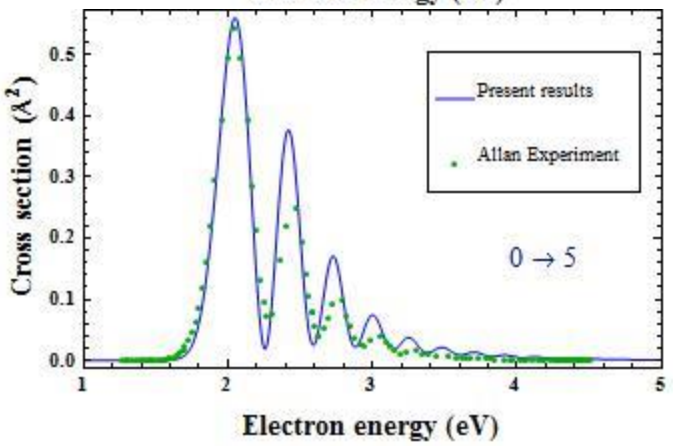
resonance enhanced vibrational excitation 0 → v'







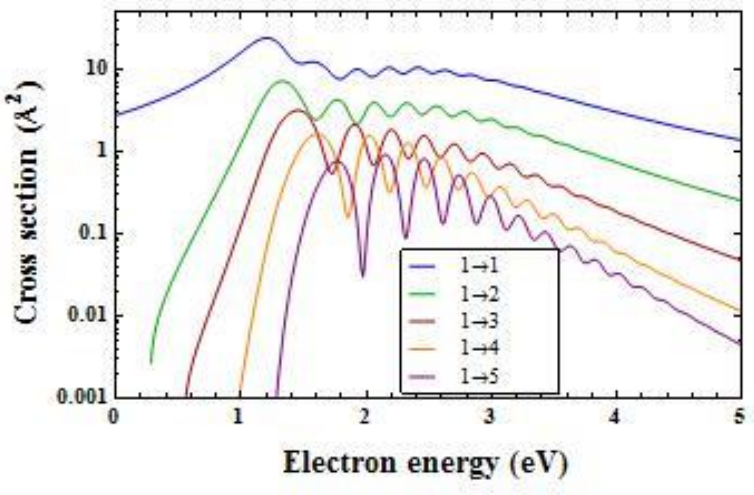


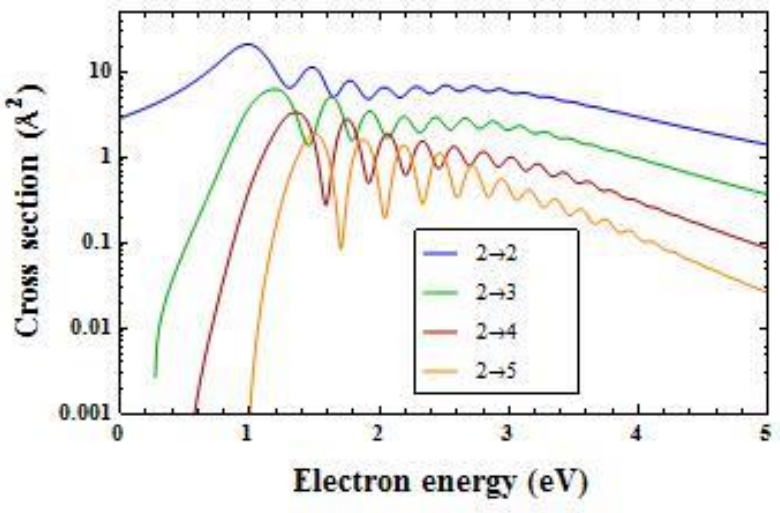


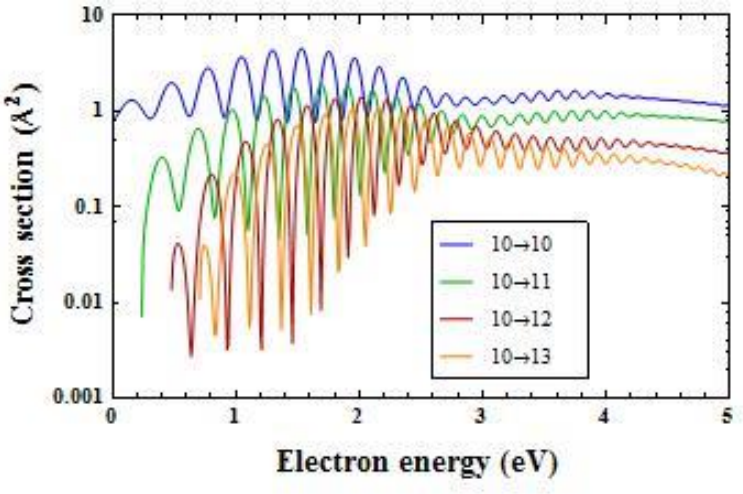
Electron – CO:

resonance enhanced vibrational excitation

High v' – v"(>0)







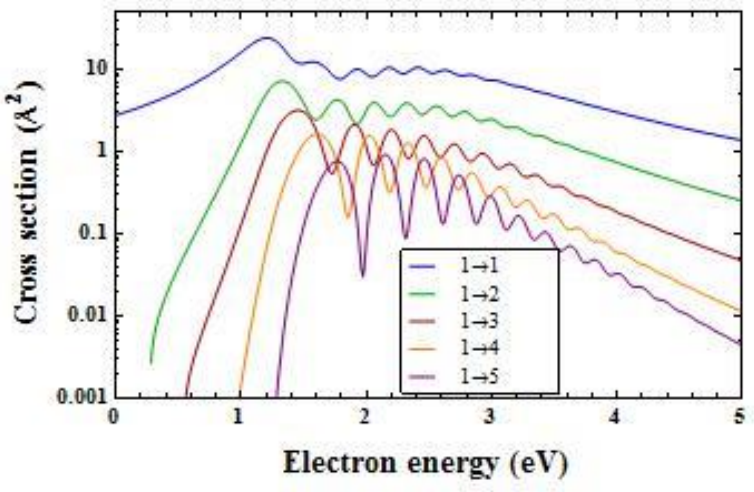
V Laporte, CM Cassidy, J Tennyson & R Celliberto,
Plasma Sources Sci. Technol. **21**, 045005 (2012)

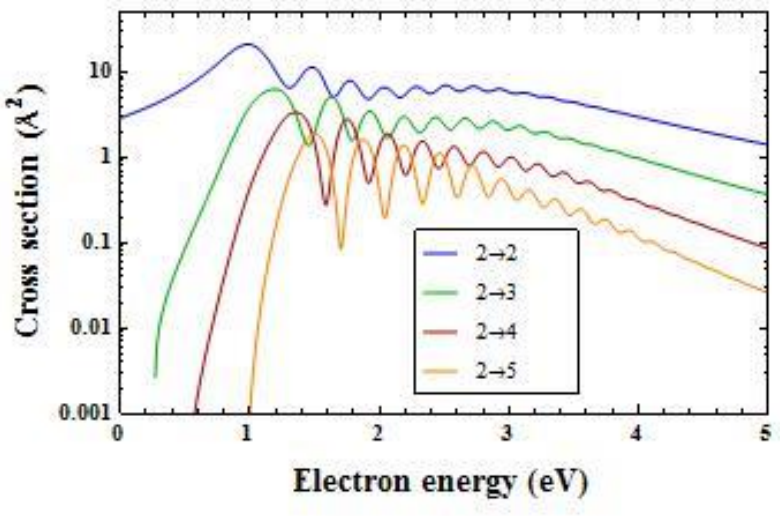
Electron – CO:

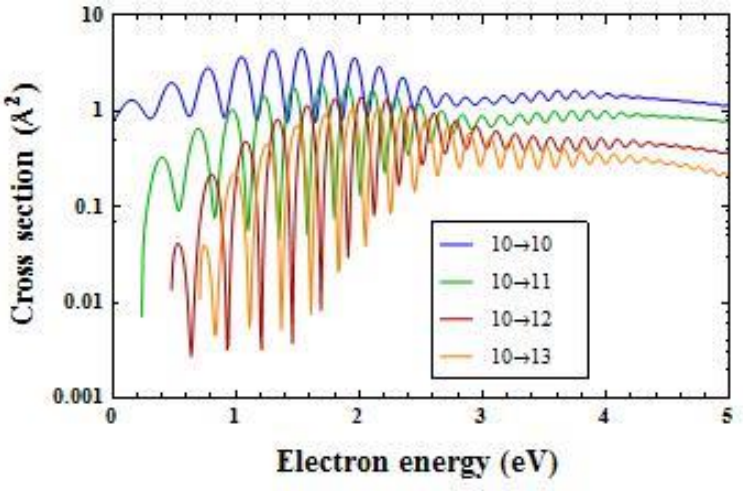
resonance enhanced vibrational excitation

High v' – v"(>0)

V Laporte, CM Cassidy, J Tennyson & R Celliberto, Plasma Sources Sci. Technol. **21**, 045005 (2012)







Dissociative attachment
+ impact dissociation of CO

V Laporte, J Tennyson & R Celliberto, Plasma Sources Sci. Technol., **25**, 01LT04 (2016).

Calculations extended to:

$e + NO(v'') \rightarrow e + NO(v')$

$e + NO(v'') \rightarrow N + O^-$

$e + O_2(v'') \rightarrow e + O_2(v')$

V. Laporta et al., PSST **22**, 025001 (2013) and **29**, 225293 (2020)

$e + O_2(v'') \rightarrow O + O^-$

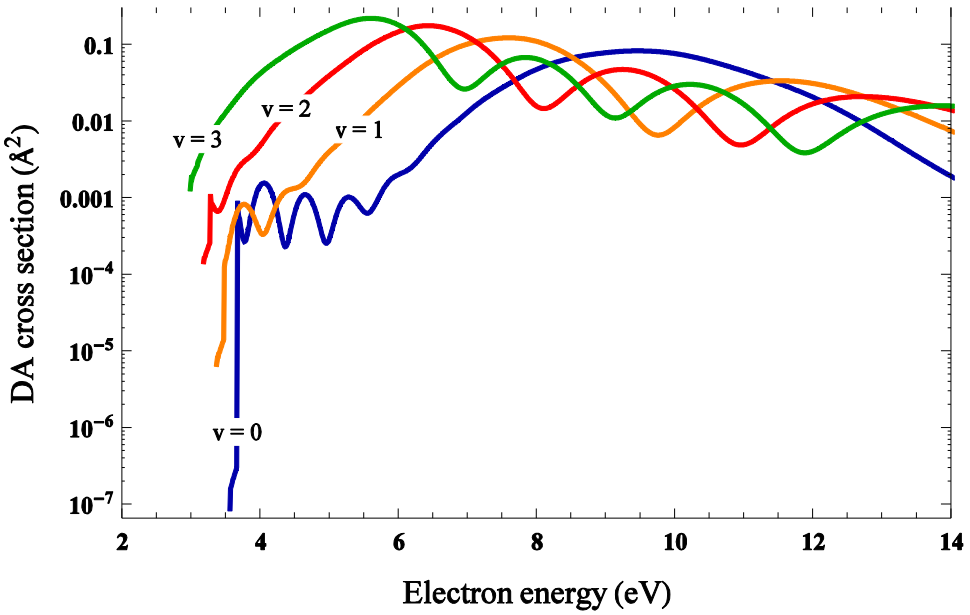
$e + N_2(v'') \rightarrow e + N_2(v')$

V. Laporta, D.A. Little, R. Celiberto & J. Tennyson, PSST, **23**, 065002 (2014)

$e + CO_2(v'') \rightarrow e + CO_2(v')$

V. Laporta, J. Tennyson & R. Celiberto, PSST, **25**, 06LT02 (2016).

Dissociative attachment of O_2



V. Laporta, R. Celiberto & J. Tennyson, Phys. Rev. A, **91**, 012701 (2015)

$e + OH(v'') \rightarrow e + O(^2P,^1D) + H$

And other cross sections

K. Chakrabarti et al., PSST **28**, 085013 (2019))

ExoMol

Hot line lists; Published in MNRAS

I. BeH, MgH, CaH
II. SiO
III. HCN/HNC
IV. CH_4
V. NaCl, KCl
VI.PN
VII. PH_3
VIII. H_2CO
IX. AlO
X. NaH
XI. HNO_3
XII. CS
XIII. CaO
XIV. SO_2
XV. HOOH
XVI. H_2S
XVII. SO_3
XVIII. VO
XIX. $H_2{}^{18}O$, $H_2{}^{17}O$
XX. H_3^+

XXI. NO
XXII. SiH_4
XXIII. PO, PS
XXIV. SiH
XXV. SiS
XXVI. SN, SH
XXVII. AlH
XXVIII. C_2H_4
XXIX. CH_3Cl
XXX. $H_2{}^{16}O$
XXXI. C_2
XXXII. TiO
XXXIII. MgO
XXXIV. PH
XXXV. NH_3
XXXVI SH (UV)
XXXVII HCCH
XXXVIII SiO_2
XXXIX CO_2
XL. H_3O^+

XLI: NaOH, KaOH
XLII: NO (UV)
XLIII: NaO
XLIV: SiO (UV)

In progress
D_3^+, D_2H^+ O_2, C_3, TiH, NaO, YO, SO, CaOH, AlF, AlCl, HCO^+

Formal data releases:
J. Tennyson *et al.*, J. Mol. Spectrosc. **373**, 73 (2016)
and JQSRT **255**, 107228 (2020)

ExoMol: 2011-16
ExomolHD: 2020-25

New: ELiDa: ExoMol Lifetimes Database

Martin Hanicinec and TianTian He

A data base of state lifefimes and branching ratios
- vibronic state resolved
- gives cascade through states by radiative decay

Plan:
- Couple with QDB
- Include radiative decay in the 0D model (PyGMolRT)
- Spectral modeling of the resultant plasma

Transitions from the state SiH B($^2\Sigma^+$); v=0

Transition	ΔE (eV)	Partial lifetime (s)	Branching ratio
SiH B($^2\Sigma^+$); v=0 → SiH X($^2\Pi$); v=3	0.170	6.24e-01	2.22e-01
SiH B($^2\Sigma^+$); v=0 → SiH X($^2\Pi$); v=2	0.150	7.09e-01	1.96e-01
SiH B($^2\Sigma^+$); v=0 → SiH X($^2\Pi$); v=4	0.182	7.95e-01	1.75e-01
SiH B($^2\Sigma^+$); v=0 → SiH X($^2\Pi$); v=1	0.124	9.85e-01	1.41e-01
SiH B($^2\Sigma^+$); v=0 → SiH X($^2\Pi$); v=5	0.183	1.14e+00	1.22e-01
SiH B($^2\Sigma^+$); v=0 → SiH X($^2\Pi$); v=6	0.193	1.99e+00	6.96e-02
SiH B($^2\Sigma^+$); v=0 → SiH X($^2\Pi$); v=7	0.205	3.83e+00	3.63e-02
SiH B($^2\Sigma^+$); v=0 → SiH X($^2\Pi$); v=8	0.226	8.87e+00	1.56e-02
SiH B($^2\Sigma^+$); v=0 → SiH X($^2\Pi$); v=0	0.111	9.61e+00	1.44e-02
SiH B($^2\Sigma^+$); v=0 → SiH X($^2\Pi$); v=9	0.260	2.30e+01	6.03e-03
SiH B($^2\Sigma^+$); v=0 → SiH X($^2\Pi$); v=10	0.265	6.32e+01	2.20e-03

Elida database is funded by STFC project ST/W000504/1.
It uses ExoMol data generated by ERC Advanced Investig

Elida Exomol lifetimes database
Data About API Contact

States of SiH

State	Energy (eV)	Lifetime (s)	Transitions from	Transitions to
SiH B($^2\Sigma^+$); v=12	0.196	3.04e-02	26	6
SiH B($^2\Sigma^+$); v=13	0.216	1.01e-01	26	
SiH B($^2\Sigma^+$); v=14	0.219	8.35e-03	22	
SiH B($^2\Sigma^+$); v=15	0.222	3.82e-02	25	1
SiH B($^2\Sigma^+$); v=16	0.226	7.80e-02	27	
SiH B($^2\Sigma^+$); v=17	0.233	6.79e-02	29	
SiH X($^2\Pi$); v=0	0.237	∞		23
SiH X($^2\Pi$); v=1	0.250	8.44e-03	1	29
SiH X($^2\Pi$); v=2	0.275	4.52e-03	2	34
SiH X($^2\Pi$); v=3	0.296	3.24e-03	2	39
SiH X($^2\Pi$); v=4	0.307	2.62e-03	2	41
SiH X($^2\Pi$); v=5	0.309	2.27e-03	3	41
SiH X($^2\Pi$); v=6	0.318	2.05e-03	3	44
SiH X($^2\Pi$); v=7	0.331	1.91e-03	3	40
SiH X($^2\Pi$); v=8	0.352	1.83e-03	3	37
SiH X($^2\Pi$); v=9	0.385	1.78e-03	3	38
SiH X($^2\Pi$); v=10	0.390	1.76e-03	4	37
SiH X($^2\Pi$); v=11	0.402	1.77e-03	4	36
SiH X($^2\Pi$); v=12	0.421	1.80e-03	4	39
SiH X($^2\Pi$); v=13	0.431	1.85e-03	4	36

«« « 1 2 3 4 » »»

Elida database is funded by STFC project ST/W000504/1.
It uses ExoMol data generated by ERC Advanced Investigator Projects 267219 and 883830.

Conclusions

1. Theory can provide a wealth of data important for plasma models;
2. Particular important for where experiment can't reach:
    a. Radicals and transient species;
    b. Excited states (and high temperatures)
    c. Isotopologues (ie isotopic substitution)
3. Uncertainty quantification: work in progress

4. Results should be available from databases!