Known and unknown in electron-atom and molecule scattering: review talk

Grzegorz P. Karwasz & Kamil Fedus
Institute of Physics
Faculty of Physics, Astronomy and Applied Informatics,
University Nicolaus Copernicus , 87100 Torun, Poland

Mi-Young Song
Plasma Technology Research Center, National Fusion Research Institute
814-2 Osikdo-dong, Gunsan-si, Jeonbuk, 573-540 Korea

International Atomic Energy Agency
Atomic Molecular Data Services
Provided by the Nuclear Data Section

IAEA Decenial Meeting,
Daejeon 15.12.2014

Outline:

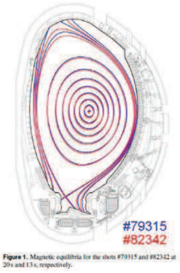
Rationale: edge and divertor plasma

Influence of atomic physics on EDGE2D-EIRENE simulations of JET divertor detachment with carbon and beryllium/tungsten plasma-facing components

Table 3. Atomic and molecular reactions included in the physics models used in EIRENE (also valid for D).

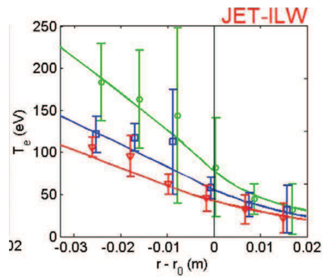
NIMBUS-like model	Kotov-2008 model
(1) $e + H^0 \to 2e + H^+$	Same reactions as default plus:
(2) $H^+ + H^0 \to H^0 + H^+$	(9) $H_2 + H^+ \to H^+ + H_2$
(3) $e + C^0 \to 2e + C^+$	(10) $H_2 + H^+ \to H_2^+ + H^0$
(4) $e + H_2 \to 3e + 2H^+$	(11) $e + H_2 \to 2e + H_2^+$
(5) $e + H_2 \to e + 2H^0$	(replacing (4))
(6) $e + H_2 \to 2e + H^+ + H^0$	(12) $e + H_2^+ \to e + H^0 + H^+$
(7) $e + H^+ \to H^0$	(13) $e + H_2^+ \to 2e + 2H^+$
(8) $2e + H^+ \to e + H^0$	(14) $e + H_2^+ \to 2H^0$
No CRM[a] for (4), (5) and (6)	CRM[a] for (11), (5) and (6)

[a] Collisional Radiative Model.



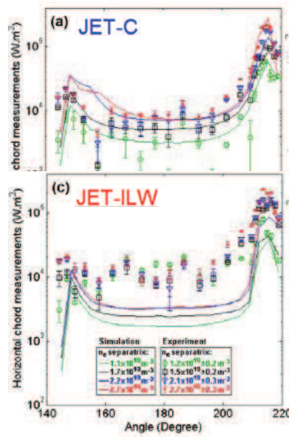
Guillemaut et al. Nucl.Fusion **54** (2014) 093012

Rationale: electron T and power irradiated



Electron temperature during three points of density ramp: good agreement

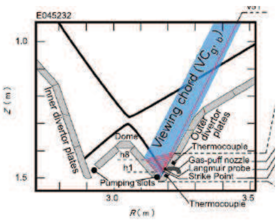
Guillemaut et al. Nucl.Fusion (2014)

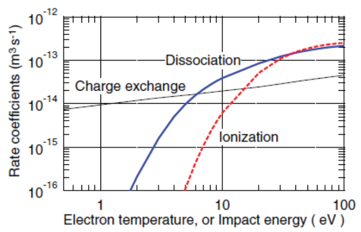


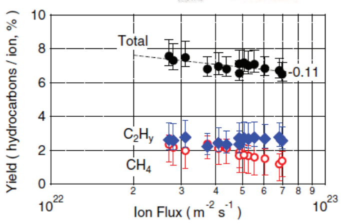
Power irradiated (0.5-1.5 MW) simulation:
JET-C <10%   JET-ILW factor 3!

Carbon sputtering by CH_4 and C_2H_y ions

The emission rates of CH, CD and C_2 spectral bands and a re-evaluation of th chemical sputtering yield of the JT-60U carbon divertor plates







Nakano et al. Nucl.Fusion **54** (2014) 043004

Data needed:
I Neutrals (H, C, C_2, Be, BeH_2, CH_4)

1. Total cross section
2. Partial cross sections:

elastic scattering   e+A → e+A
  rotational excitation   e+CH_4 (J=0) → e+CH_4 (J=2)
  vibrational excitation   e+AB(v=0) → e+AB(v>0)
electron attachment (dissociative)   e+AB → A^- + B
electronic excitation   e+A → e+A^*
  emission lines: A^* → A + $h\nu$
neutral dissociation   e+AB → A + B + e
  emisison from dissociation e + AB → A^* + B + e + $h\nu$
ionization   e+A → A^++2e
  dissociative ionization   e+AB → A + B^+ + 2°
  ionization into excited states e + A → $(A^+)^*$ + 2e

Data needed: II Positive ions (BeH^+)

1.Recombination: A^+ + e → A

1a. dissociative recombination: AB^+ + e → A^* + B

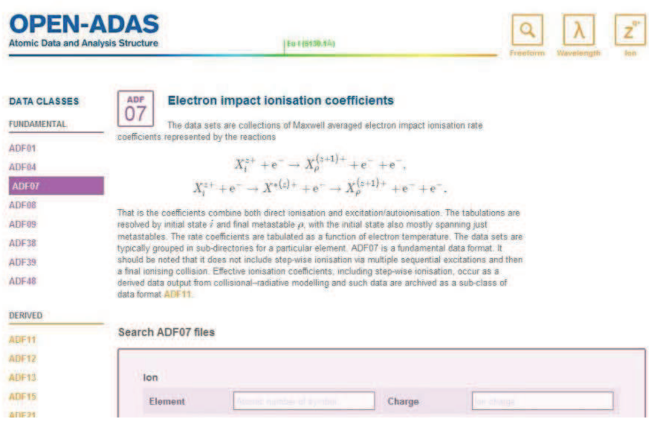
2. Partial cross sections:

vibrational excitation   e+AB(v=0) → e+AB(v>0)

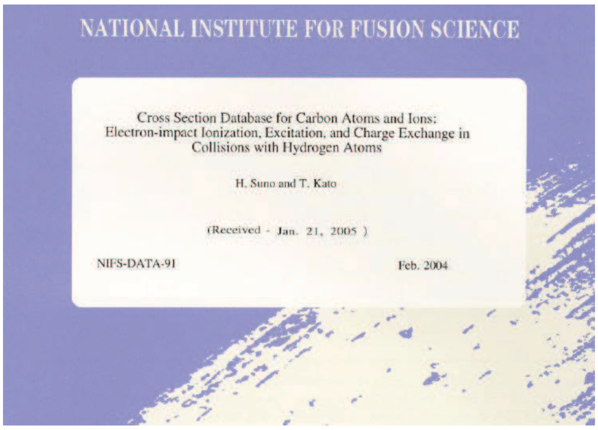
electronic excitation   e+A^+ → e + A^{+*}

double ionization   e+A^+ → A^{2+} + 2e

Databases



Databases


NATIONAL INSTITUTE FOR FUSION SCIENCE

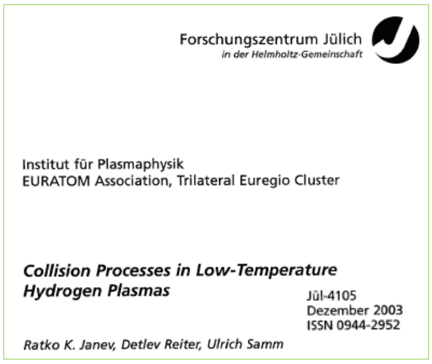
Cross Section Database for Carbon Atoms and Ions: Electron-impact Ionization, Excitation, and Charge Exchange in Collisions with Hydrogen Atoms

H. Suno and T. Kato

(Received - Jan. 21, 2005)

NIFS-DATA-91 Feb. 2004

Databases

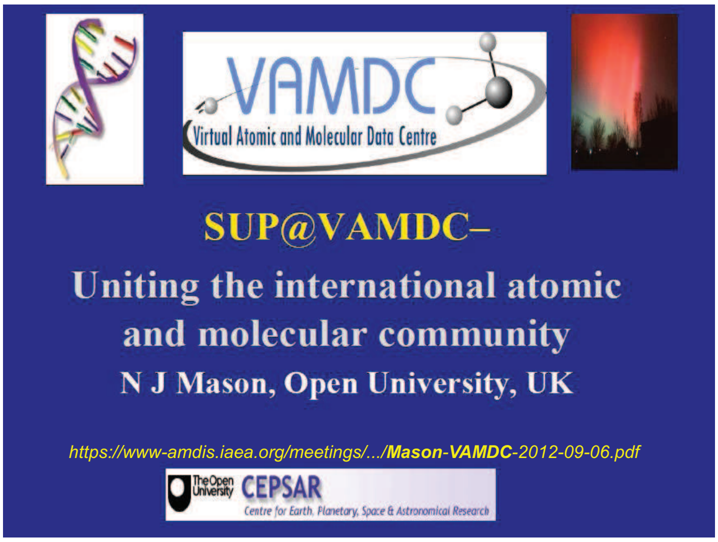

Forschungszentrum Jülich
in der Helmholtz-Gemeinschaft

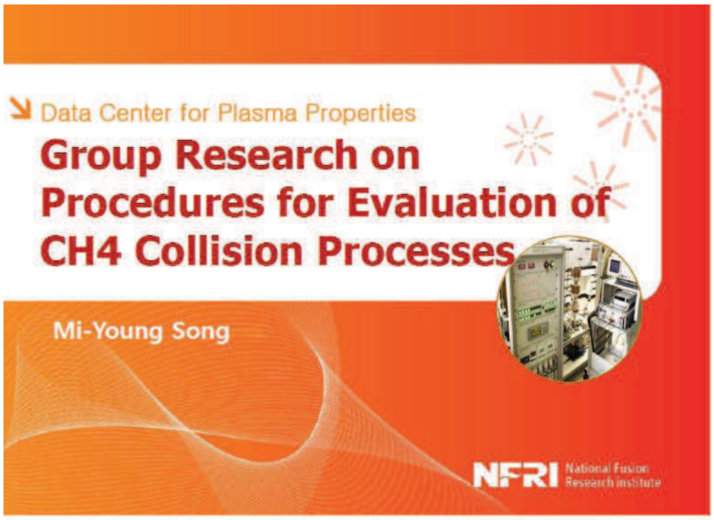
Institut für Plasmaphysik
EURATOM Association, Trilateral Euregio Cluster

Collision Processes in Low-Temperature Hydrogen Plasmas

Jül-4105
Dezember 2003
ISSN 0944-2952

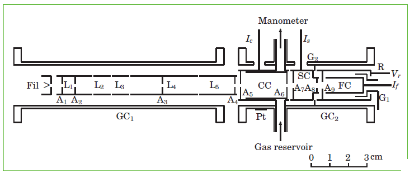
Ratko K. Janev, Detlev Reiter, Ulrich Samm



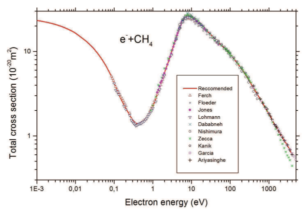


Experimental methods: total

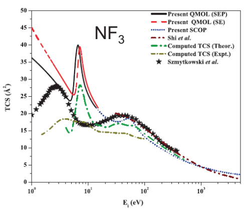
attenuation method $I = I_0 \exp(-\sigma n L)$; precision <5%



H. Nishimura et al., J.Phys. Soc. Japan **72** (2003) 1080

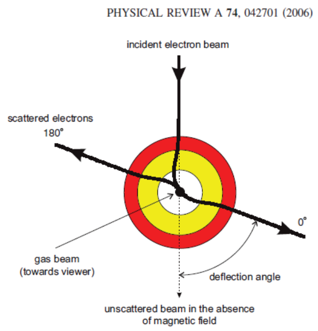


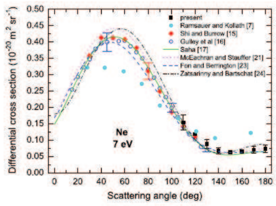
M.-Y. Song et al., to be published

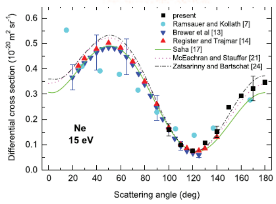


B. Goswami et al. PRA **88** (2013) 032707

Experimental methods: elastic

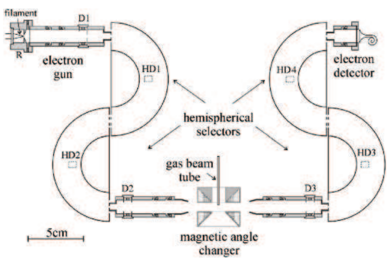




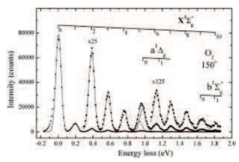


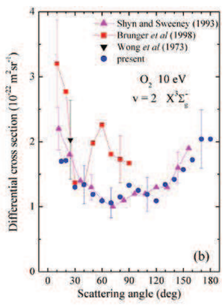
I. Linert, B. Mielewska, G. King, and M. Zubek, PRA (2006)

Experimental methods: excitation (electronic, vibrational)



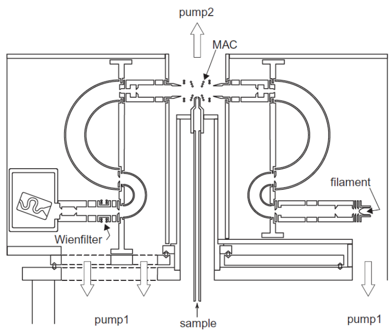
$e^- + O_2\ (v=0) - e^- + O_2\ (v=0, 1, 2, \text{etc.})$

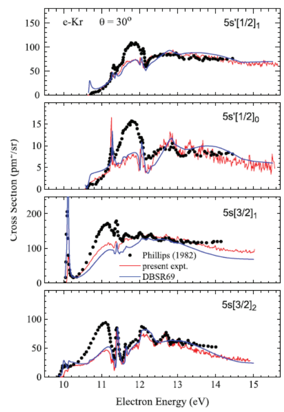




Experiments by:
I. Linert, M. Zubek (Gdansk) J. Phys. B **39** (2006)
M. Khakoo et al. (Fullerton California)
M. Allan (Freiburg University)

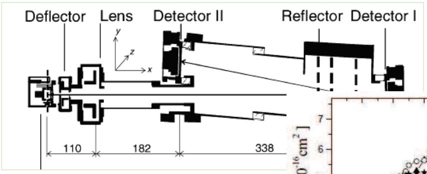
Experimental methods: electronic, vibrational, DA

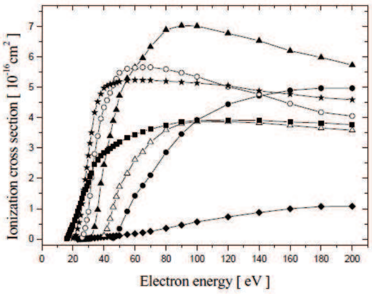




M. Allan, O. Zatsarinny. K. Bartschat, PRA (2011) **Kr: experiment and Dirac R-matrix**

Experimental methods: ionization (1)





$WF_6 \rightarrow$

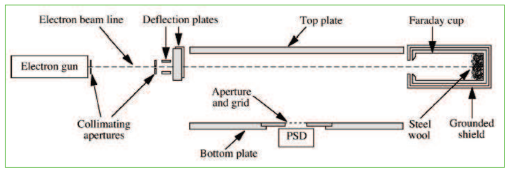
$WF_5^+ > WF_2^{+} >$

$WF_3^+ \approx WF_4^+$

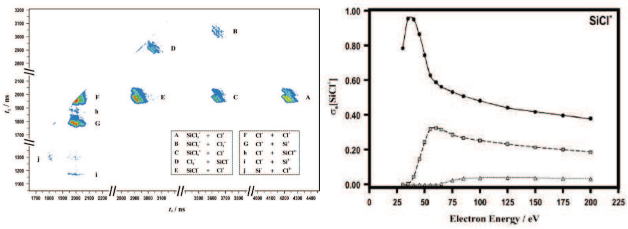
Accuracy: ±15%

R. Basner, M. Schmidt, K. Becker, Int. J. Mass Spectr. 233 (2004) 25

Experimental methods: ionization (2)



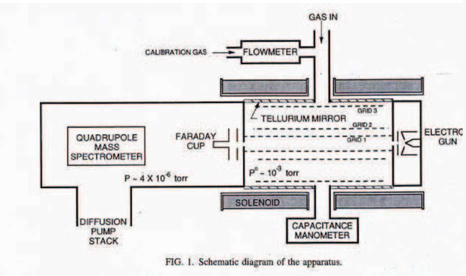
$SiCl^+$ from single, double, triple ionization of $SiCl_4$

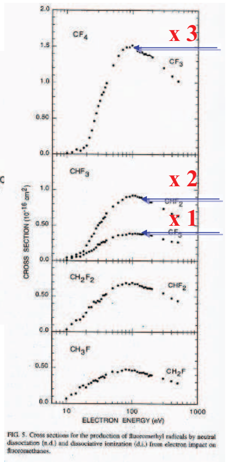


B. G. Lindsay et al., JCP **129** (2004), S J King nad S D Price, JCP**134** (2011) 074311

Dissociation into neutrals (CF_4, CH_3F…)

volatile organotellurides



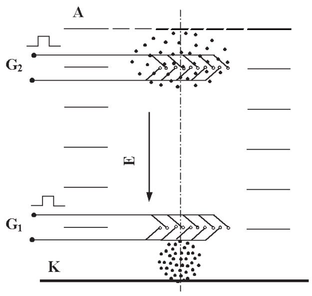


Additivity rule:
cross section = sum of paths

Motlagh and Moore, JCP**109** (1988) 432

Diffusion coefficients → electronic distribution function n_e ($\boldsymbol{r}$, $\boldsymbol{v}$, t)

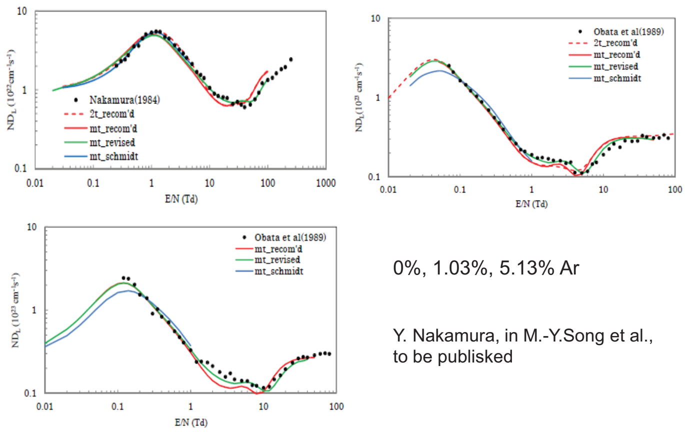
$$\frac{\partial}{\partial t}n_e(\mathbf{r},t) = -w\frac{\partial}{\partial z}n_e(\mathbf{r},t) + D_T\left[\frac{\partial^2}{\partial x^2}n_e(\mathbf{r},t) + \frac{\partial^2}{\partial y^2}n_e(\mathbf{r},t)\right] + D_L\frac{\partial^2}{\partial z^2}n_e(\mathbf{r},t)$$



$$w = -\left(\frac{2}{m}\right)^{1/2}\frac{eF}{3N}\int_0^\infty \frac{E}{\sigma_m(E)}\frac{df_0(E)}{dE}dE$$

$$D_T = \left(\frac{2}{m}\right)^{1/2}\frac{1}{3N}\int_0^\infty \frac{E}{\sigma_m(E)}f_0(E)dE$$

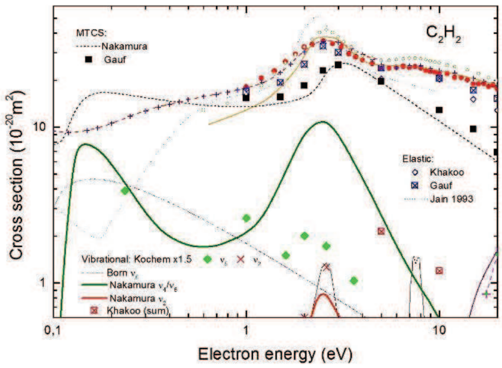
Methane: swarm in mixtures



0%, 1.03%, 5.13% Ar

Y. Nakamura, in M.-Y.Song et al., to be published

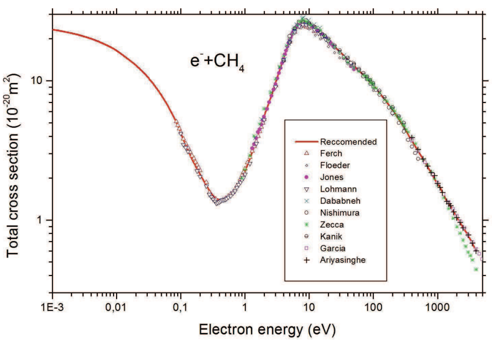
Acetylene: swarm ↔ beam: vibrational, MTCS



Swarm MTCS and vibrational (Nakamura, 2010)
seem to be better than beam measurement (Kochem, 1986)

Review case study: CH_4

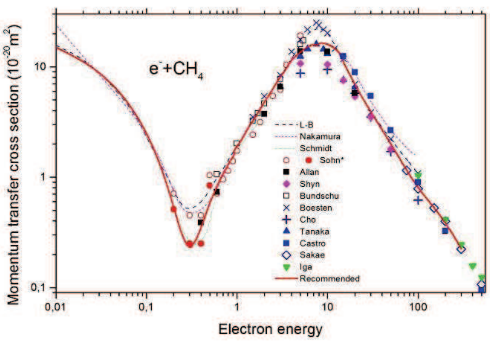
1. Total cross section: ±5%



M.-Y. Song, J. S. Yoon, H. Cho, Y. Itikawa, G. Karwasz, V. Kukooulin, Y. Nakamura, J. Tennyson, to be published

Review case study: CH_4

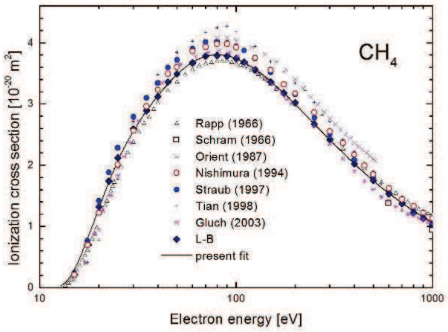
2. Momentum transfer (and elastic) cross sections: ±15%



M.-Y. Song, J. S. Yoon, H. Cho, Y. Itikawa, G. Karwasz, V. Kukooulin, Y. Nakamura, J. Tennyson, to be published

Review case study: CH_4

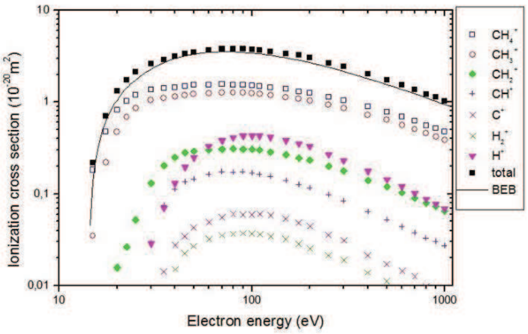
3. Ionization total: ±10%



M.-Y. Song, J. S. Yoon, H. Cho, Y. Itikawa, G. Karwasz, V. Kukooulin, Y. Nakamura, J. Tennyson, to be published

Review case study: CH_4

3a. Ionization partial: ±10%



M.-Y. Song, J. S. Yoon, H. Cho, Y. Itikawa, G. Karwasz, V. Kukooulin, Y. Nakamura, J. Tennyson, to be published

Review case study: CH_4

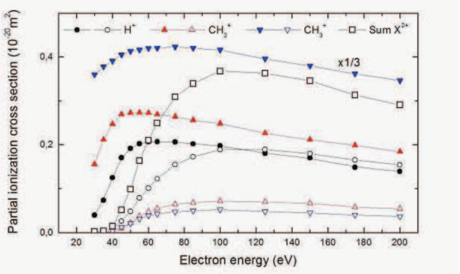
3a. **Ionization partial**: channel resolved

e.g. $e + CH_4 \rightarrow CH_3^+ + H^+ + 2e$

or $e + CH_4 \rightarrow (CH_4^+)^* + e \rightarrow CH_3^+ + H^+ + 2e$

or $e + CH_4 \rightarrow CH_3 + H^+ + e$

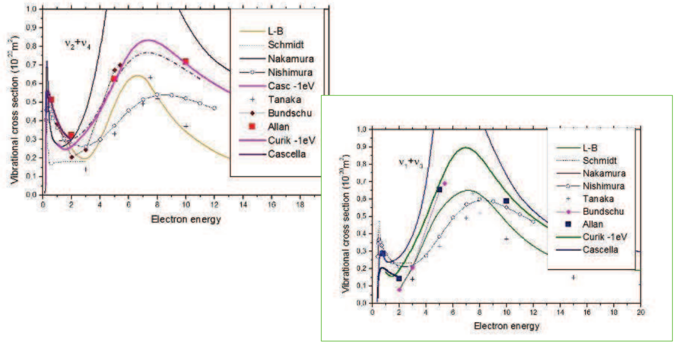
Experimental data (coincidence measurements): Ward et al.. 2011



to be **done...**

Review case study: CH_4

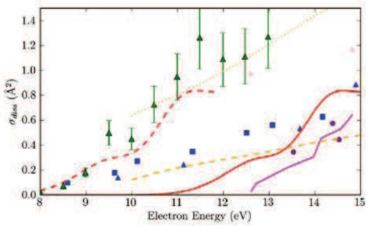
4. Vibrational: disagreement between swarm, beam, theory



M.-Y. Song, J. S. Yoon, H. Cho, Y. Itikawa, G. Karwasz, V. Kukooulin, Y. Nakamura, J. Tennyson, to be published

Review case study: CH_4

5. Electronic excitation: reasonable agreement between dissociation into-neutrals experiment and R-Matrix calculation

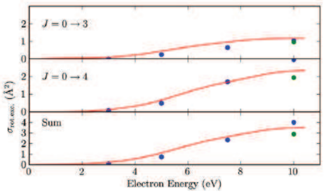


W. J. Brigg, J. Tennyson, M. Plummer
J. Phys. B **47** (2014) 185203
R-Matrix

Figure 13. Electron impact dissociation cross section. Theory: red solid line: present work; red dashed line: present work, shifted to lower energy by 3.2 eV; purple solid line: Hayashi (1991); orange dashed line: CH_2 of Ziółlkowski *et al* (2012); orange dotted line: CH_3 of Ziółlkowski *et al* (2012). Experiment: blue squares: CH_2 of Nakano *et al* (1991); blue triangles: CH_3 of Nakano *et al* (1991); green triangles: CH_3 of Makochekanwa *et al* (2006); pink triangles: CH_3 of Motlagh and Moore (1998); purple circles: Winters (1975).

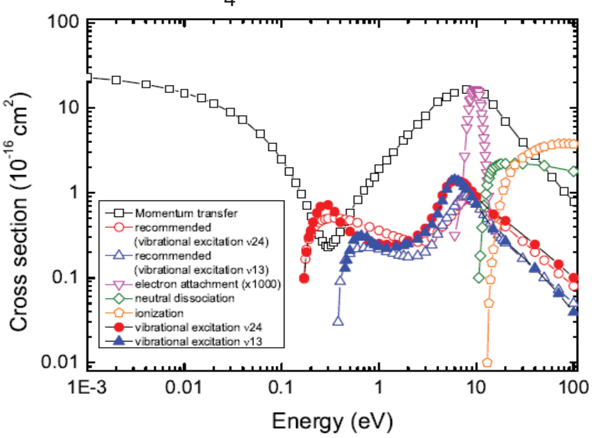
Review case study: CH_4

6. Rotational excitation: experiment (Kochem et al.. 1985) really difficult; cross sections from R-matrix calculations adopted



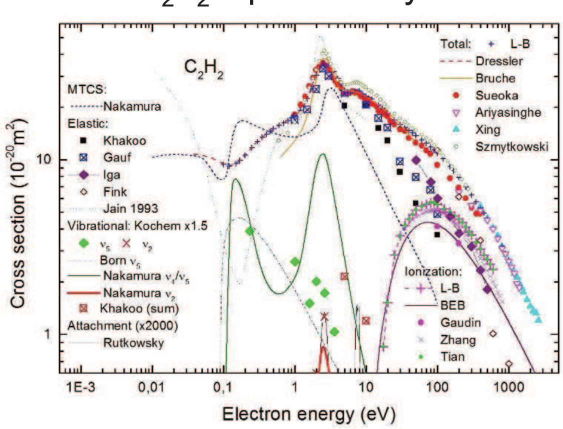
W. J. Brigg, J. Tennyson, M. Plummer, J. Phys. B **47** (2014) 185203
R-Matrix

CH_4 - overview



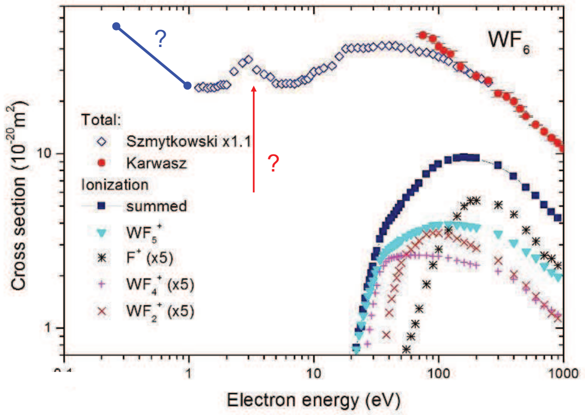
M.-Y. Song, J. S. Yoon, H. Cho, Y. Itikawa, G. Karwasz, V. Kukooulin, Y. Nakamura, J. Tennyson, to be published

C_2H_2 - preliminary



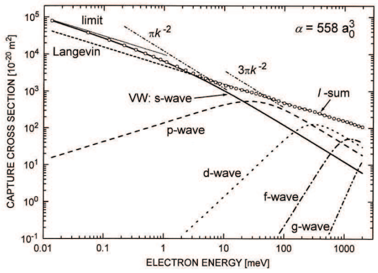
M.-Y. Song, J. S. Yoon, H. Cho, Y. Itikawa, G. Karwasz, V. Kukooulin, Y. Nakamura, J. Tennyson, work in progress

WF$_6$ - few data



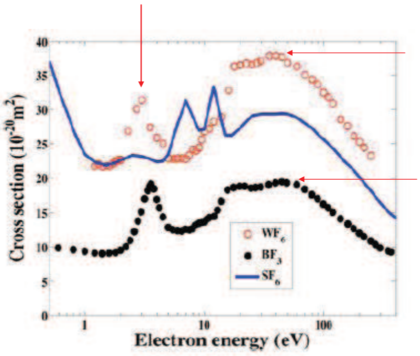
GK, work in progress

Semi-empirical methods - zero-energy cross section: Langevin, Voigth-Wannier



Allan et al., Advances At. Mol. Phys. (2004)

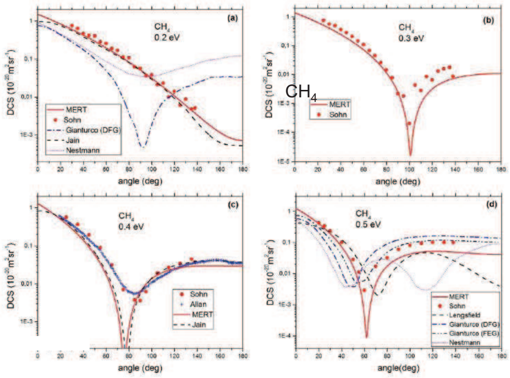
Searching analogies (2): „resonances" in total cross sections



G. Karwasz, K. Fedus, FS&T (2013), experimental data: Szmytkowski and collaborators

Semi-empirical methods: elastic (MERT)

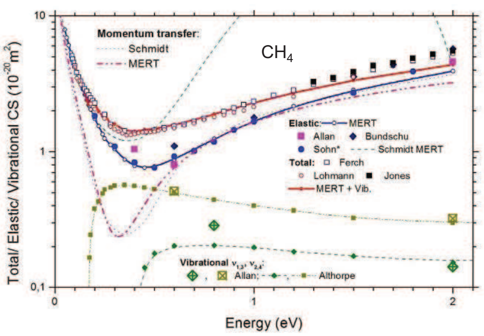
Link between elastic, total, MTCS: in some simple cases, and low energies



K. Fedus, G. Karwasz, Eur. J. Phys. D (2014)

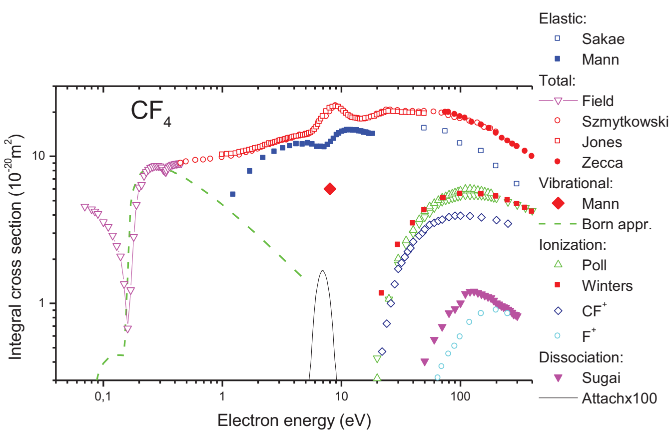
Semi-empirical methods: elastic (MERT)

Link between elastic, total, MTCS: in some simple cases, and low energies



K. Fedus, G. Karwasz, Eur. J. Phys. D (2014)

Semi-empirical methods: vibrational (Born)



G.P.Karwasz, A.Zecca, R.S.Brusa, La Rivista del Nuovo Cimento 24 No.4 (2001) 1-101

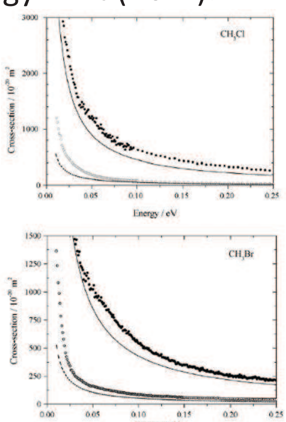
Rotational, very low energy limit (Born):

Polar molecules:

$$\sigma(J,K;J',K') = \xi(2J+1)\begin{pmatrix} J & J' & 1 \\ K & -K' & 0 \end{pmatrix}^2$$

$$\times \ln\left|\frac{k^2+k'^2-2kk'\cos\theta_2}{k^2+k'^2-2kk'\cos\theta_1}\right|^{1/2}$$

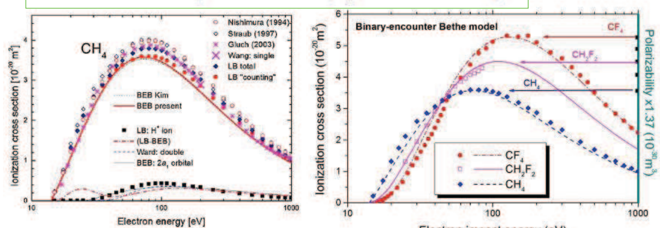
$$\xi=(4\pi/3k^2)(\mu^2/[ea_0]^2).$$



N C Jones et al. Intr. J. Mass Spectr. 277 (2008) 91

Ionization: semiempirical formulae

$$\sigma[\mathrm{cm}^2] = \frac{10^{-13}}{IE}\left\{A_1 \ln(E/I) + \sum_{i=2}^{N} A_i \left(1-\frac{I}{E}\right)^{i-1}\right\},$$



$$\sigma = \sum_n 4\pi a_0^2 \xi_n \left(\frac{R}{I_n}\right)^2 \frac{1}{t+u_n+1}\left\{1-\frac{1}{t}+\frac{\ln t}{2}\left(1-\frac{1}{t^2}\right)-\frac{\ln t}{t+1}\right\}$$

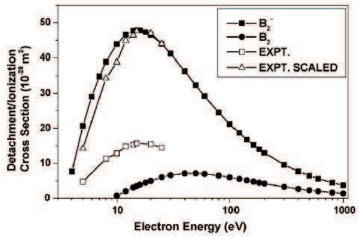
Normalized energies: $t = E/I_n$; $u_n = E_{kin}/I_n$ Only two values needed from QCh

Y.-K. Kim and M. E. Rudd, Phys. Rev. A 50 (1994) 3954
G. Karwasz, P. Mozejko, M.-Y. Song, Int. J. Mass Spectrometry (2014)

Electron detachment(D-M): B_2^{-}, BO^-, O_2^-, CN^-)

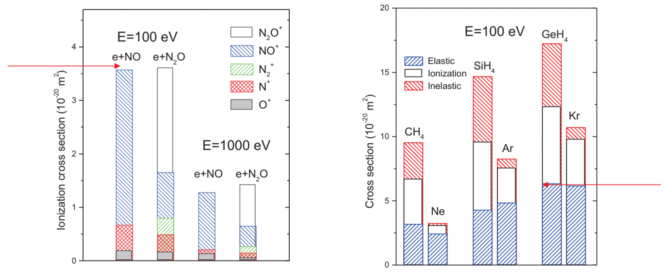
Deutsche-Mark formalism

$$\sigma(u) = \sum_{n,l} g_{nl} \pi r_{nl}^2 \xi_{nl} b_{nl}^{(q)}(u) \left[\frac{\ln(c_{nl}u)}{u}\right] \qquad b_{nl}^{(q)} = \frac{A_1 - A_2}{1 + (u/A_3)^p} + A_2$$



H. Deutsch et al. Int. J. Mass Spectr. **277** (2008) 151

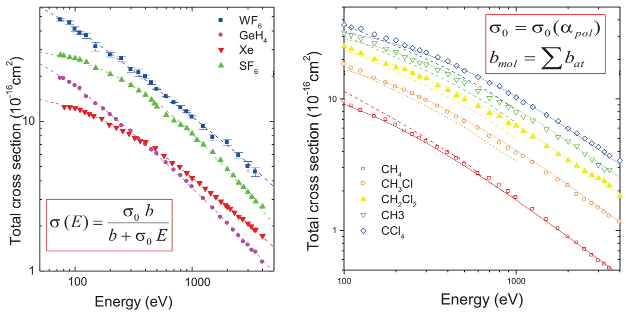
Searching analogies (1): partitioning into elastic & ionization



G. P. Karwasz, J.Phys. B 28 (1995) 1301-9
A. Zecca, G. P. Karwasz, R. S. Brusa and T. Wróblewski, Int. J.Mass Spectr. 223-224 (2003) 205

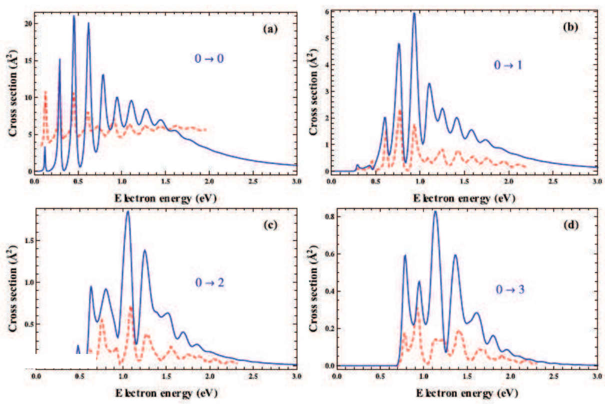
High energies: in search for additivity rule

CH_4, CF_4, SiH_4, ... WF_6 → CH_2F_2, SiF_4 ...
→ H, C, Si, ... W



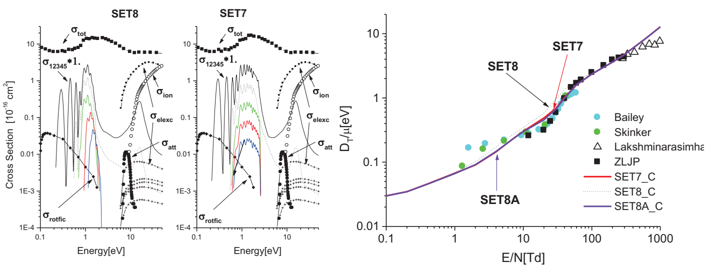
G. Karwasz et al., Phys. Rev. A **59** (1999) 1341

Theoretical progress: resonances in NO (R-matrix)



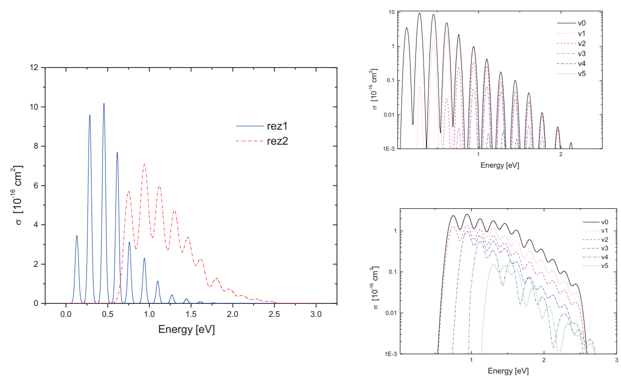
Laporta, ... J Tennyson, Plasma Sources Sci. Technol. 21 (2012) 055018

Swarm analysis: resonances in NO



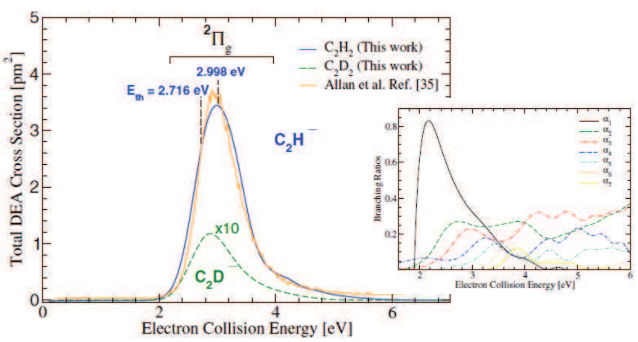
M. Josic, J. Mechlińska-Drewko, Z. Petrovic, G. Karwasz, Chem. Phys. Lett. (2003)

Overlapping resonances: NO (swarm analysis)



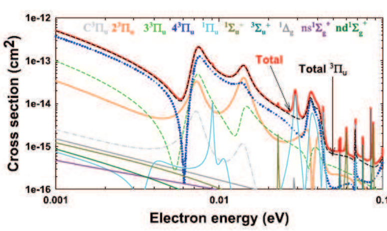
M. Josic, J. Mechlińska-Drewko, Z. Petrovic, G. Karwasz, Chem. Phys. Lett. (2003)

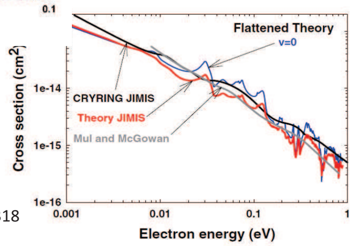
Theoretical progress - Kohn variational: dissociative attachment (C_2H_2)



S. T. Chorou and A. E. Orel, Phys. Rev. A. **77** (2009) 042079

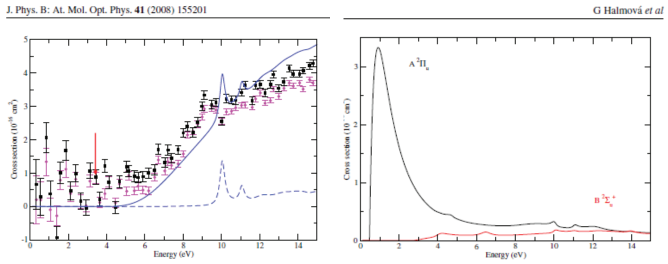
Theoretical progress: dissociative recombination ($N_2^+ + e^- \rightarrow N^* + N^*$)





S. L. Guberman, J. Chem. Phys. 139 (2013) 124318
also Tennyson and collaborators, PRA (2014)

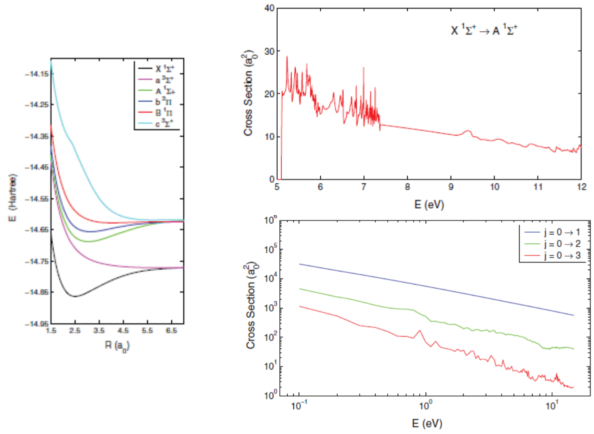
C_2^- – electron detachment, electronic excitation



solid line – with Born correction
broken – without Born correction

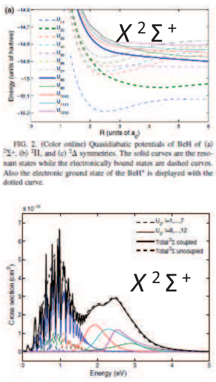
Halnova, Gorkenfield, J Tennyson, JPB 41 (2008)
UK Molecular R-matrix code: electronic, rotational

BeH^+ – electronic and rotational excitation



K Chakrabarti and J Tennyson, Eur. Phys. J. D 66 (2012) 31
UK Molecular R-matrix code: electronic, rotational

BeH^+ dissociative recombination



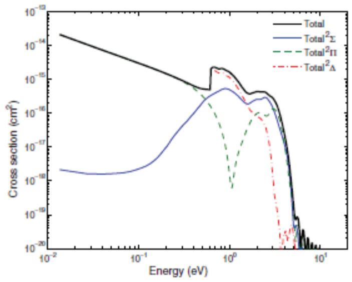


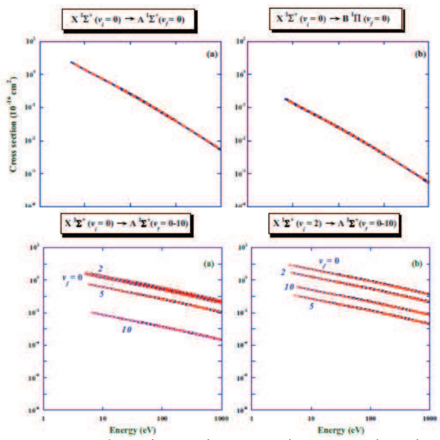
TABLE I. Parameters for the fitted form of the dissociative recombination cross sections at low collision energies.

Ion	Vibrational level	σ_0 (10^{-16}cm^2 eV^b)	b
BeH^+	$v=0$	3.10	0.99
BeH^+	$v=1$	6.90	0.93
BeD^+	$v=0$	3.32	1.02
BeD^+	$v=1$	4.72	1.05

σ/E^b

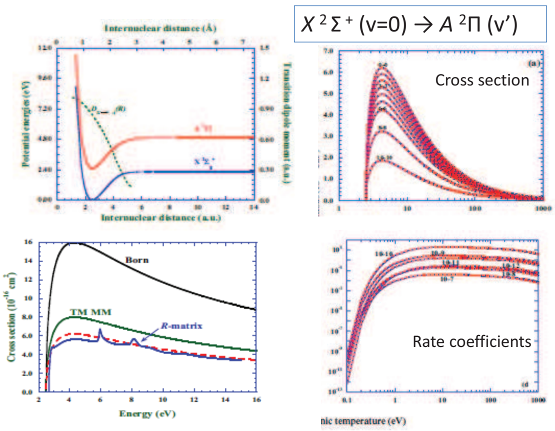
Roos,..Orel, PRA 80 (2009) 012501
Variational Kohn method

BeH^+ – electronic and vibrational excitation



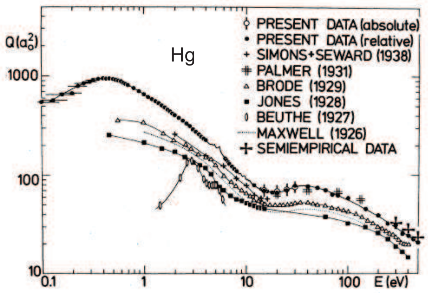
R Celiberto, R K Janev, D Reiter, Plasma Phys. Control. Fusion **54** (2012) 035012
Coulomb-Born approximation: cross sections, excitation rates T=0.1-10,000 eV)

BeH: electronic and vibrational excitation



R Celiberto, K L Baluja and R K Janev, Plasma Sources Sci. Technol. **22** (2013) 015008
Mott-Massey Schr. eq.

Metals: Hg, Au, Ru



K. Jost and B. Ohnemus,
Phys. Rev. A **19** (1979) 641

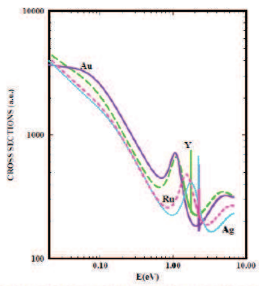
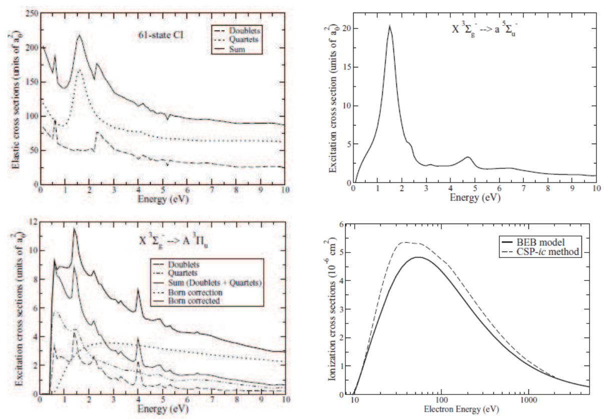


Figure 1 Electron elastic TCSs for Au, Y, Ru and Ag in the region of negative ion formation

A. Z. Msezane, Z. Felfli, D Sokolovski
J. Phys.: Conf Series, **388** (2012) 042002
Thomas-Fermi potential

Metal molecules (B_2): electronic excitation



J. S. Rajvanshi & K. L. Baluja, Phys. Rev. A 86 (2012) 032794: R-Matrix

Conclusions – state of art

1. Total cross sections (for "easy" molecules) OK
2. Elastic (and therefore total also): theory OK
3. Vibrational: theory on a promising way
4. Ionization: abundant data and models
5. Dissociative attachment (and dissociative neutralization) – theory proves OK, work needed
6. Electronic excitation (and dissociation) – remains the most challenging

Conclusions (2) - perspectives:

1. „Physical" cross sections still needed
2. „Chemical" cross sections even more
3. Reviews for new targets: Be, BeH_2, W ?
4. Simple theories and scalling laws useful
5. Advanced theories „at reach"
6. Lab experiments still needed
7. and ITER-like experiment even more

→ constructing cooperative networks

Acknowledgments:

International Atomic Energy Agency
Atomic Molecular Data Services
Provided by the Nuclear Data Section

플라즈마물성데이터센터
Data Center for Plasma Properties

Greetings from Toruń!