Consiglio Nazionale
delle Ricerche

Ab-initio
electron-molecule state-resolved dynamics for non-equilibrium plasmas modelling

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25th Data Center Network meeting, IAEA, Vienna, Austria – 1 October 2019

Plan of the presentation:

1. Theory: electron-molecule scattering

2. *ab-initio* state-resolved cross sections:
   A. **Nitrogen and Oxygen:** Atmospheric (re-)entry and hypersonic
   B. **Carbon dioxide:** Plasma-based CO_2 conversion
   C. **BeH^+, H_2^+, OH, ArH^+:** I.T.E.R and controlled fusion; Astrochemistry

3. Conclusions and perspectives

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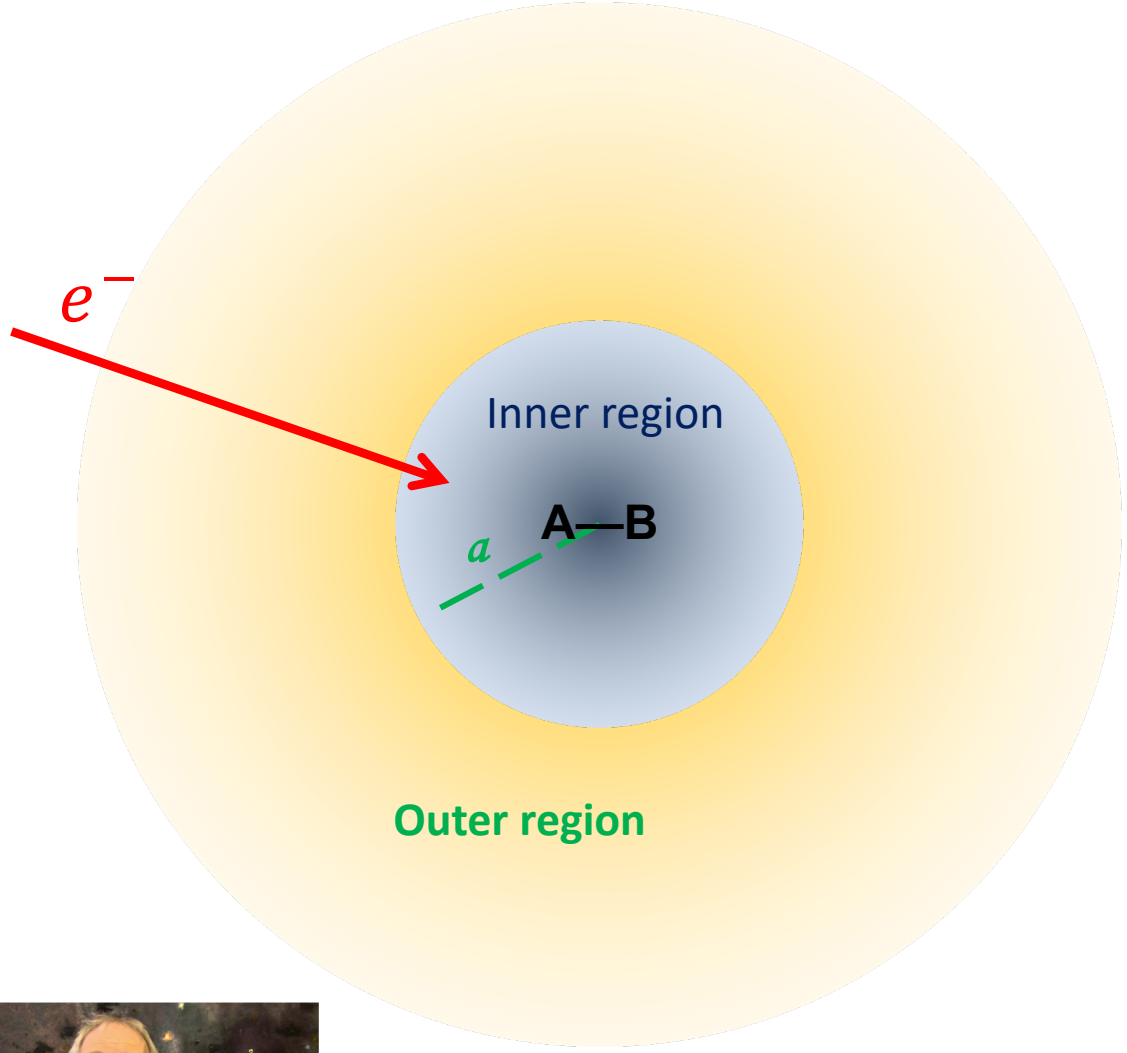
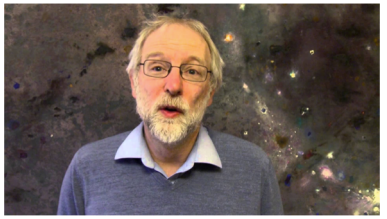
3. Conclusions and perspectives

The R-matrix method





J. Tennyson, Phys. Rep., **491**, 29 (2010)

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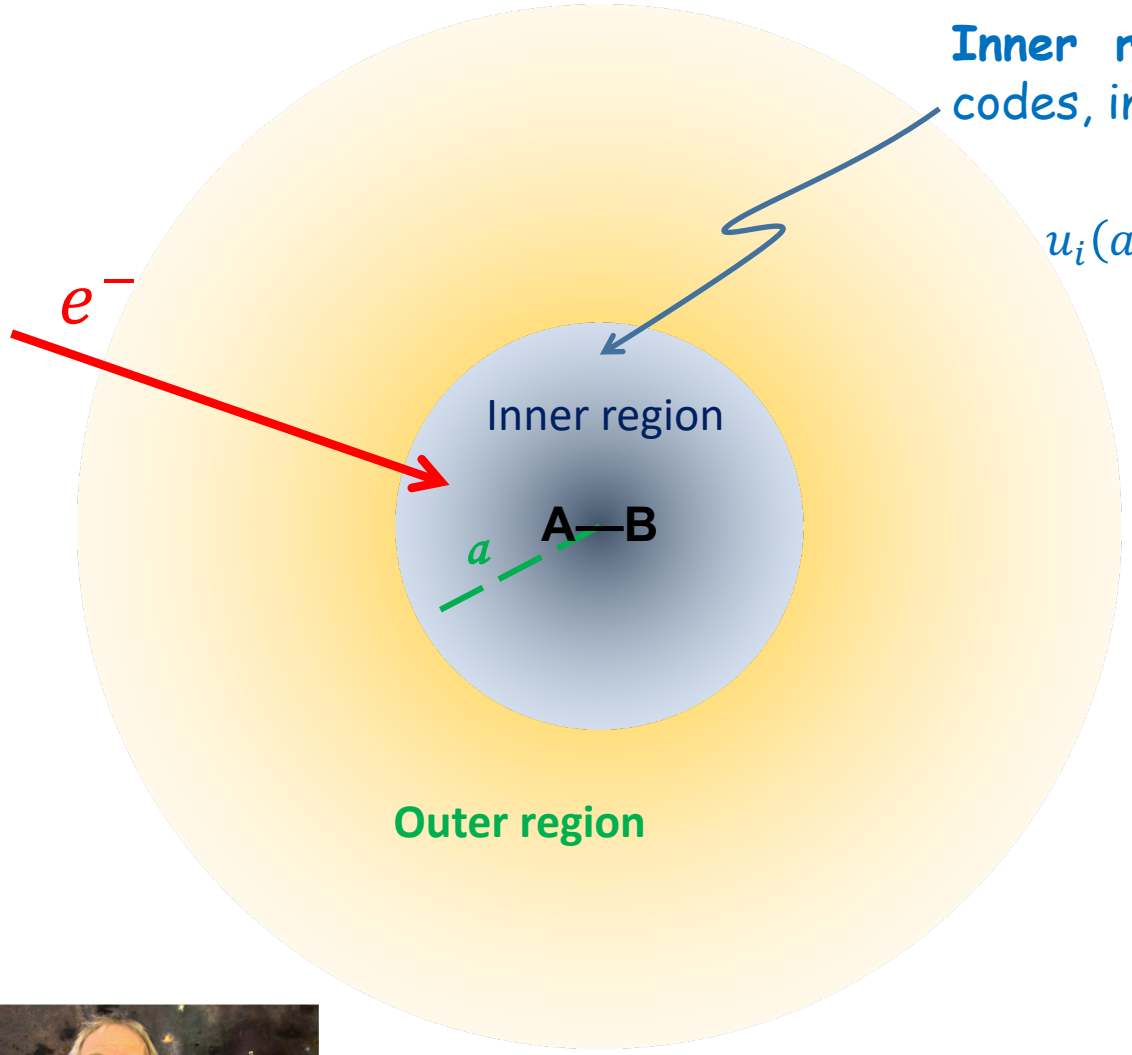
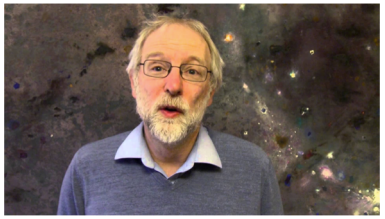


Inner region: N+1 electrons; *ab-initio* quantum chemistry codes, including exchange correlations; continuum orbitals

$$u_i(a) = \sum_j R_{ij}(a,E)\left[r\,u_j{}' - b\,u_j\right]_{r=a}$$

$$R_l(a,E) = \frac{1}{2}\sum_\lambda \frac{w_{\lambda l}(a)^2}{E_\lambda - E}$$



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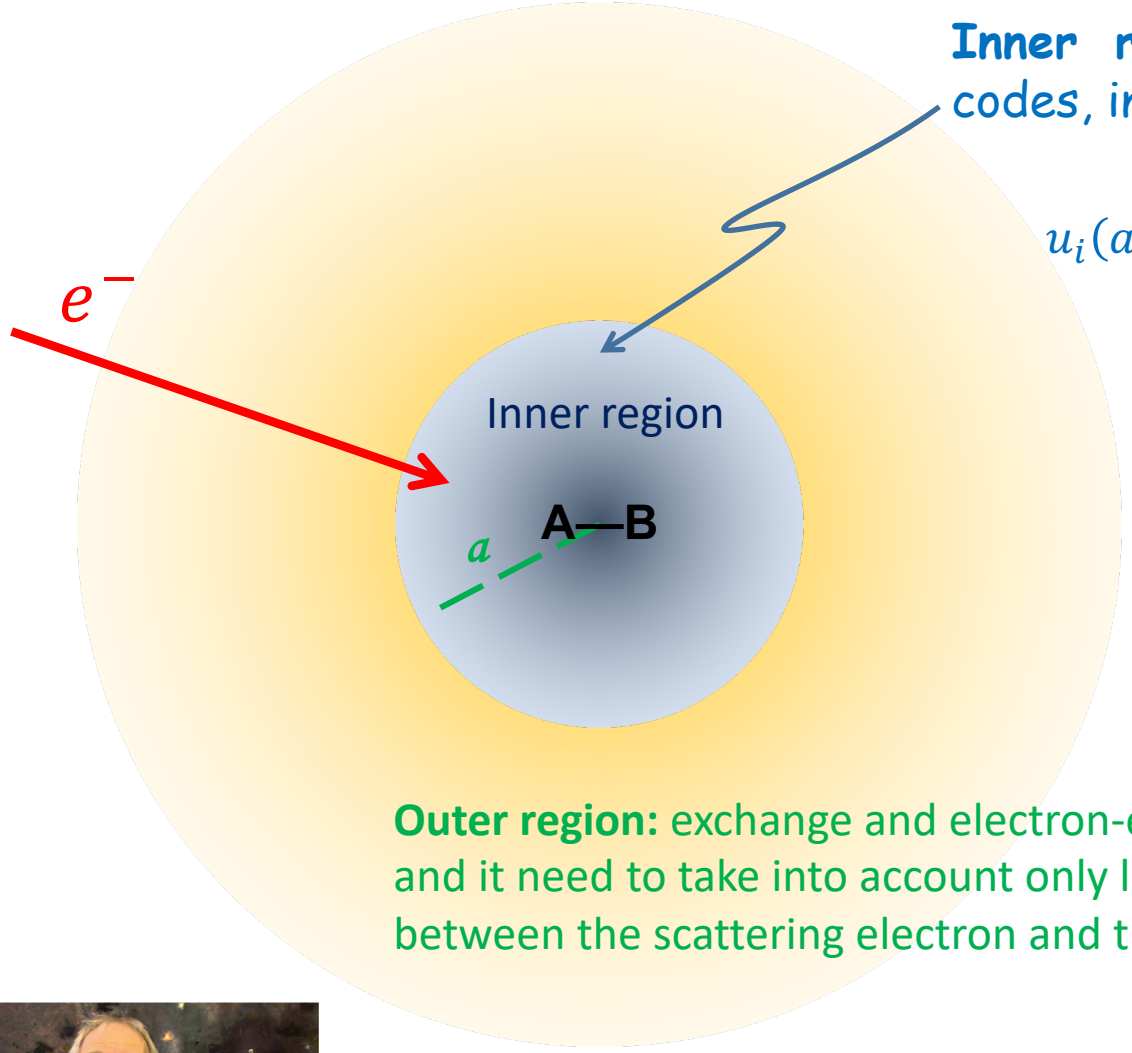

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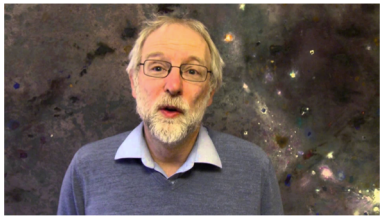
Outer region: exchange and electron-electron correlations are neglected and it need to take into account only long–range multi–polar interactions between the scattering electron and the target

$$u_l(r) \sim \frac{1}{\sqrt{k}}\left(\sin\varphi_l + \cos\varphi_l\, K_l\right)$$



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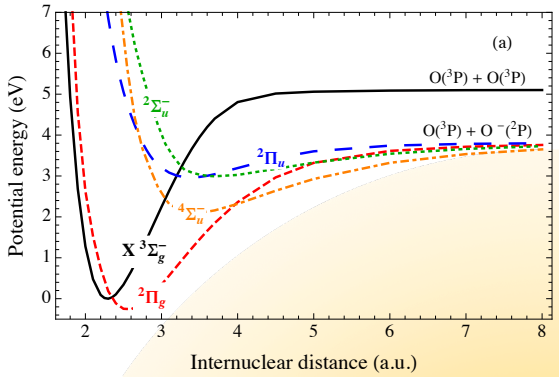

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Boundary: Target wavefunction has zero amplitude

$$K_l = e^{-2i\varphi_l}\,\frac{1 - R_l(L^* - b)}{1 - R_l(L - b)}\,,$$

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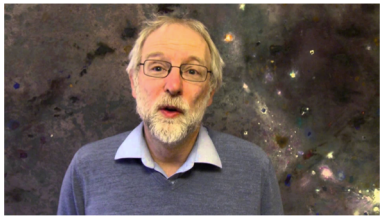


J. Tennyson, Phys. Rep., **491**, 29 (2010)

Basic formulas for electron-molecule scattering

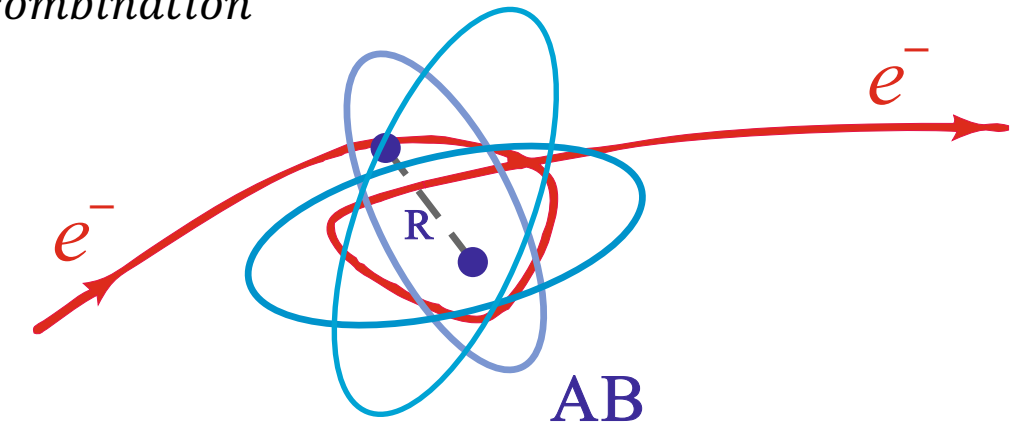
Processes occurring for resonant electron-molecule scattering:

$$e^- + AB(v) \rightarrow AB^- \rightarrow AB\,(w) + e^- \qquad Vibrational\ Excitation$$

$$\rightarrow A^- + B \qquad Dissociative\ Attachment$$

$$\rightarrow A\ + B + e^- \qquad Dissociative\ Excitation$$

$$e^- + AB^+(v) \rightarrow AB^* \rightarrow A\ + B \qquad Dissociative\ Recombination$$



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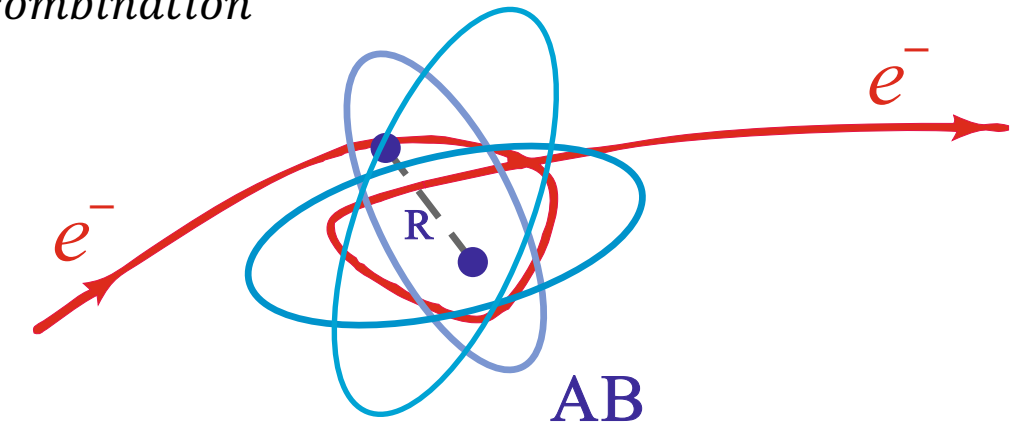


$$\left(T_N + V^- - \frac{i}{2}\Gamma - E\right)\xi(R) = -V^*_{dk}(\epsilon, R)\,\chi_i(R)\,,$$

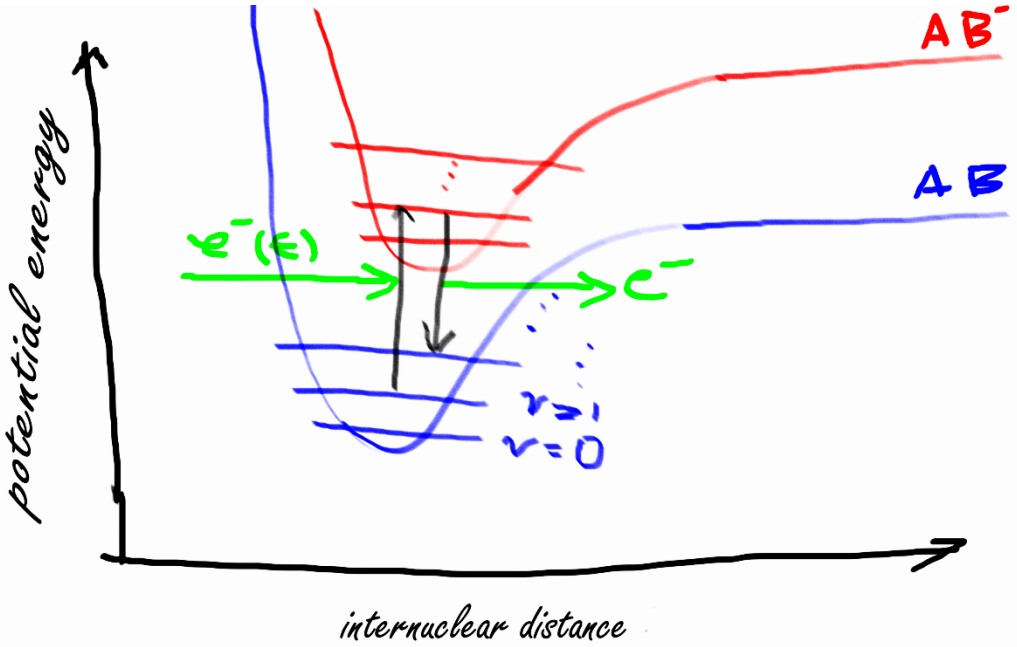
Neutral molecule

Resonant

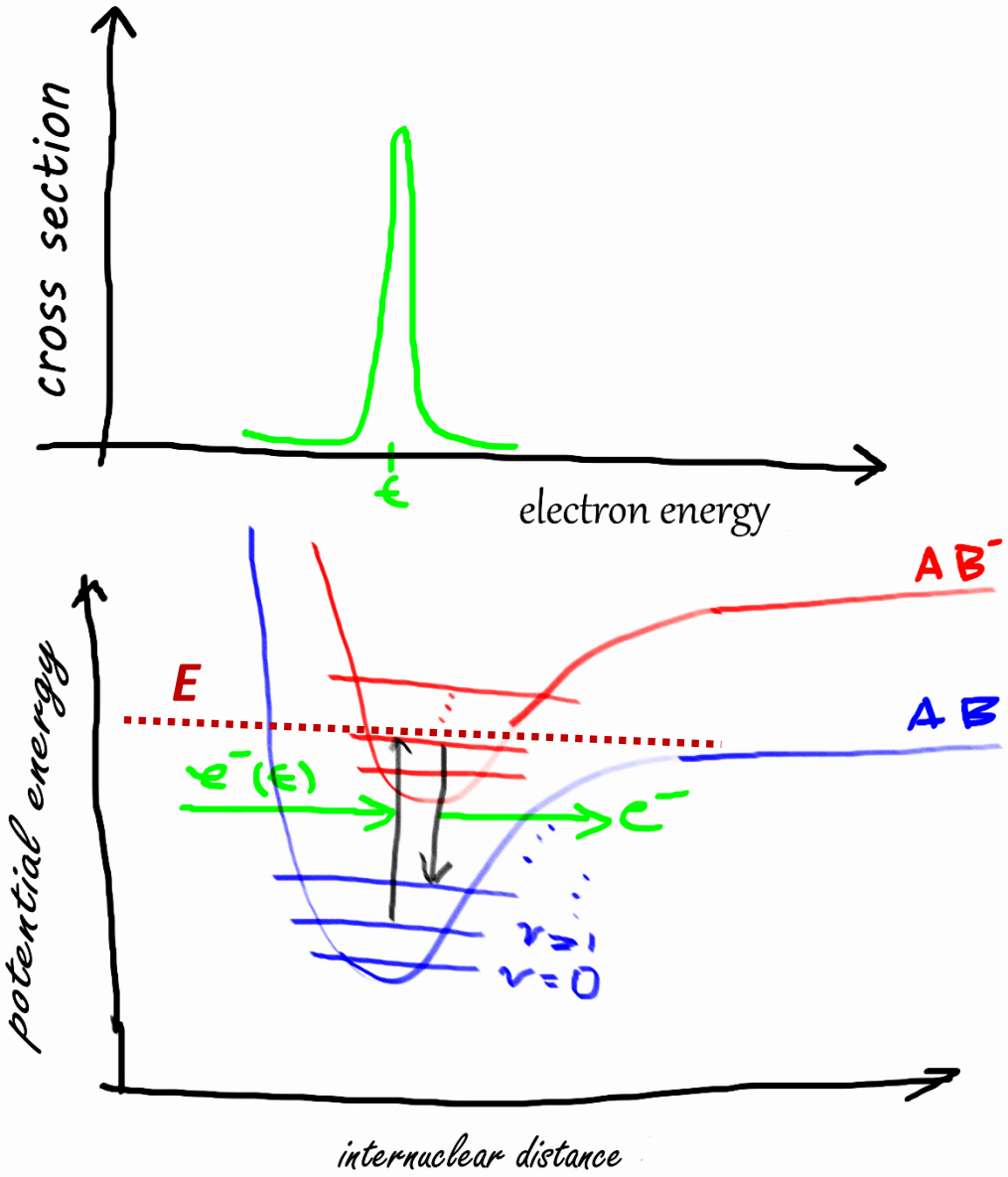
Vibrational-excitation

cross section

$$e + AB(v) \rightarrow AB^{-} \rightarrow AB(v') + e$$



J. N. Bardsley and F. Mandl, Reports on Progress in Physics, **31**, 471 (1968)



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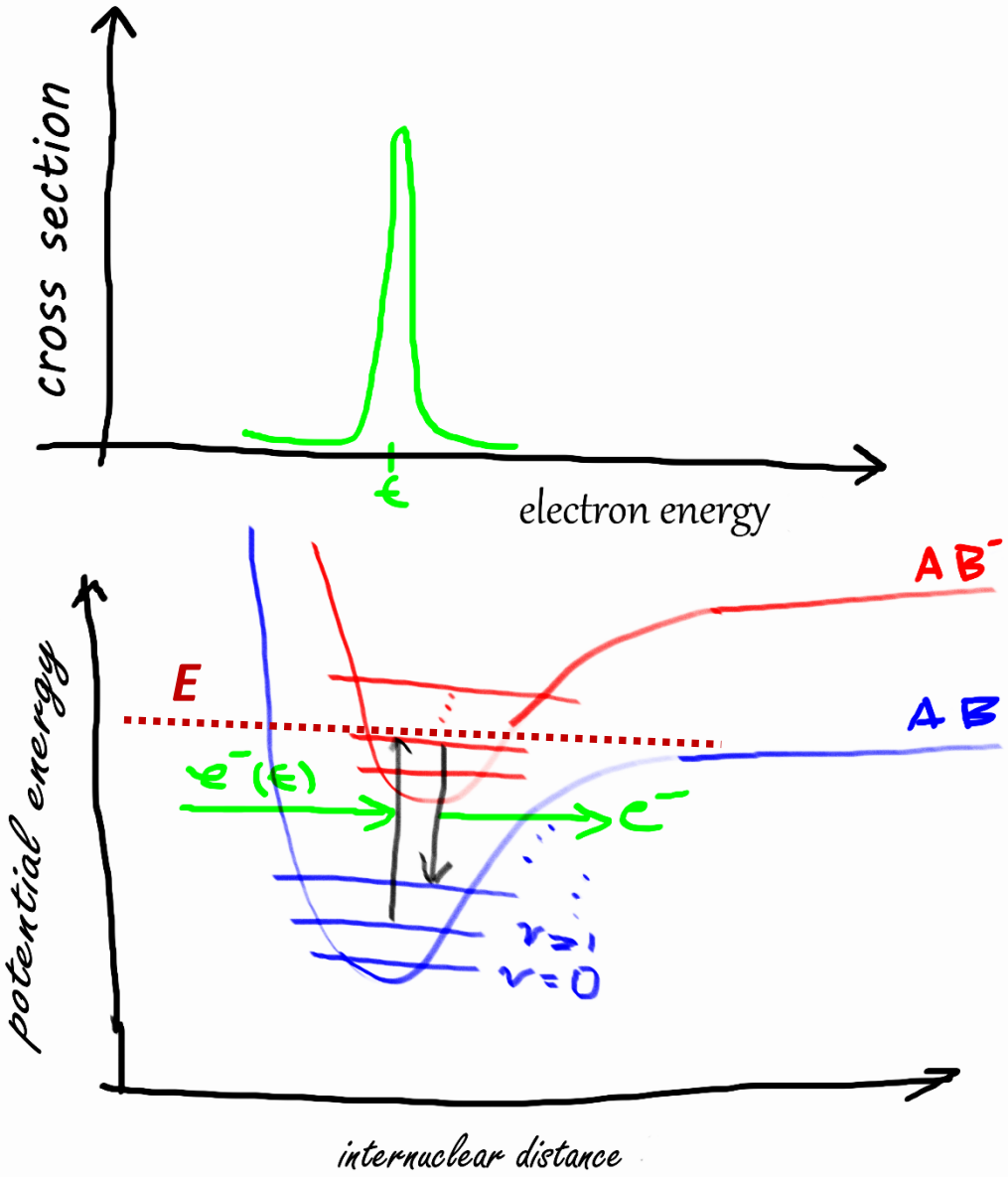

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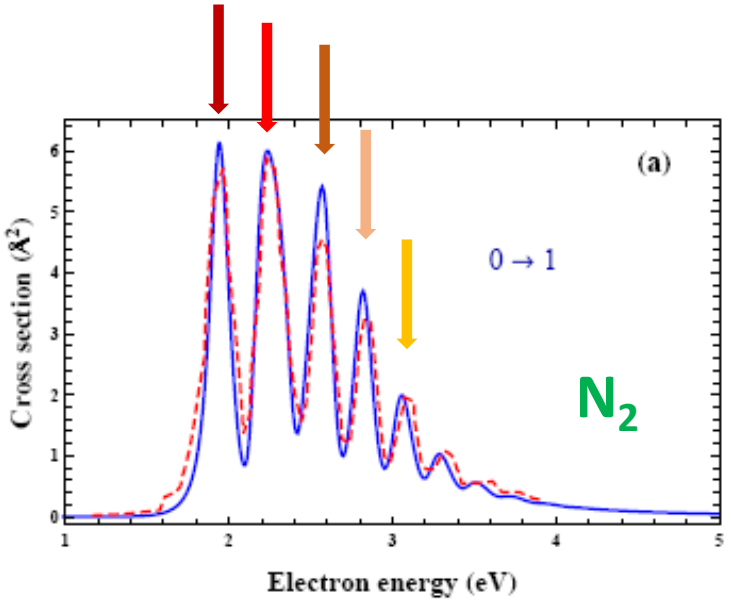

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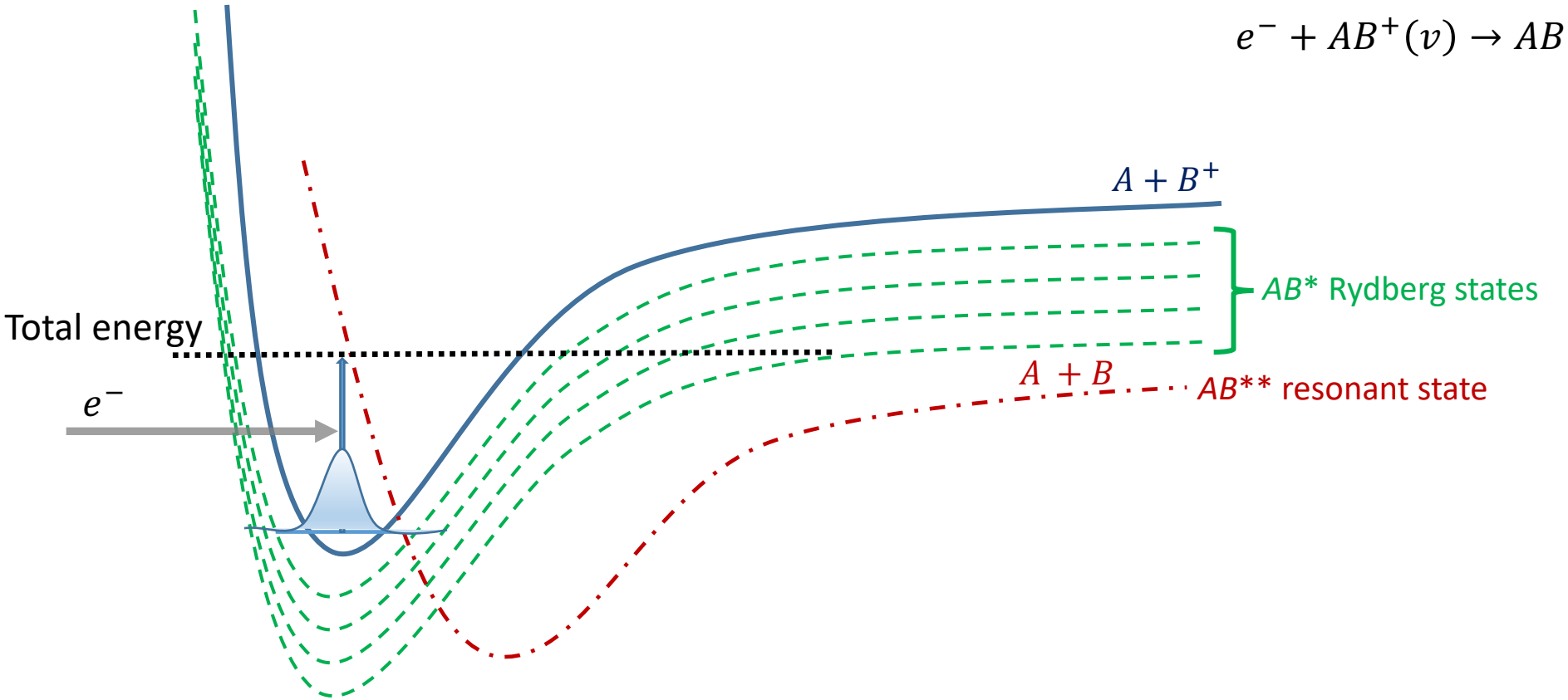
Dissociative recombination

$$e^- + AB^+(v) \rightarrow AB^*, AB^{**} \rightarrow A + B$$



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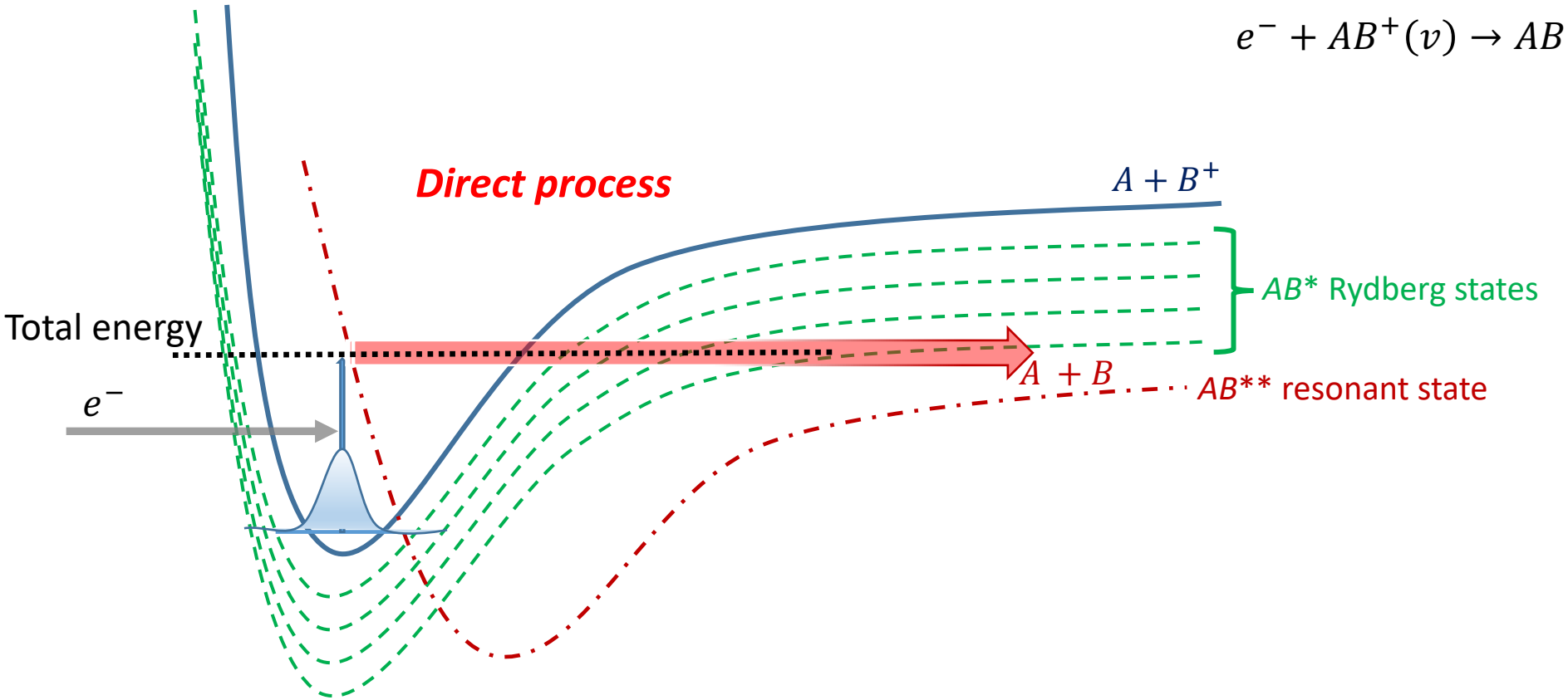

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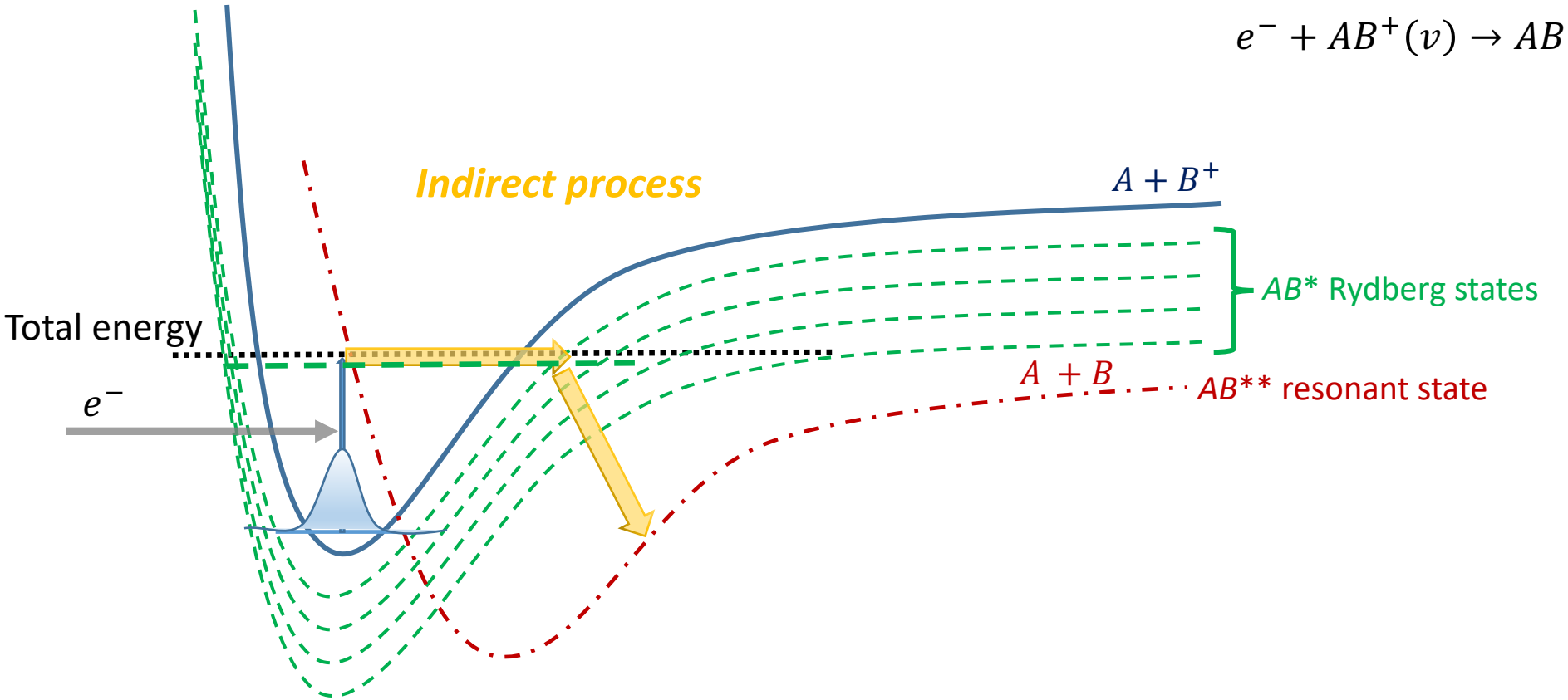

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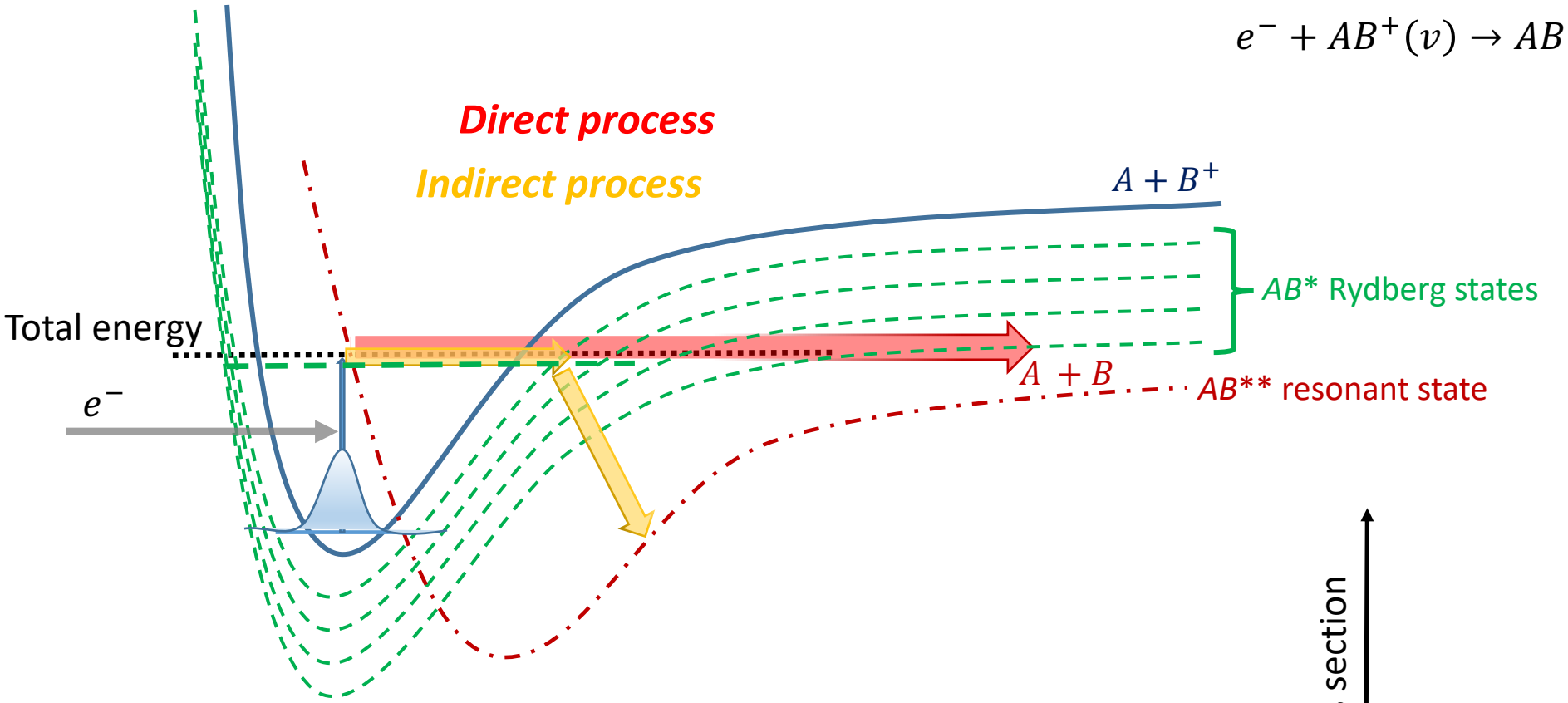
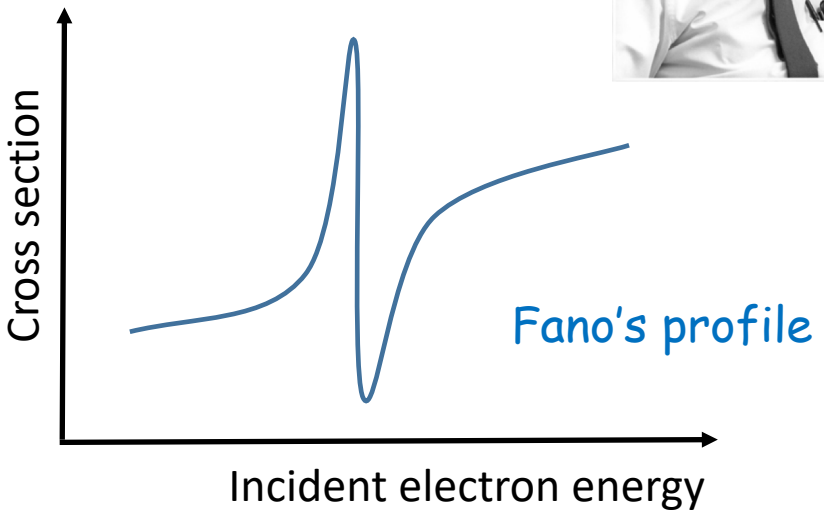


Multichannel Quantum Defect Theory



A Giusti, Journal of Physics B: Atomic and Molecular Physics, **13**, 3867 (1980)

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3. Conclusions and perspectives

electron-N_2 resonant scattering

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The resonance at 2.3 eV in electron-N_2 scattering is described in term of the resonant state $\mathbf{N_2^-(X\,^2\Pi_g)}$

The quantum chemistry codes MOLPRO and UK-R-Matrix have been used to calculate potential energy curves, resonance width and scattering

cc-pvQZ basis set **MR-CI model**

N_2 target: $(1\sigma_g, 1\sigma_u)^4(2\sigma_g, 2\sigma_u, 1\pi_u, 3\sigma_g, 1\pi_g, 3\sigma_u)^{10}$

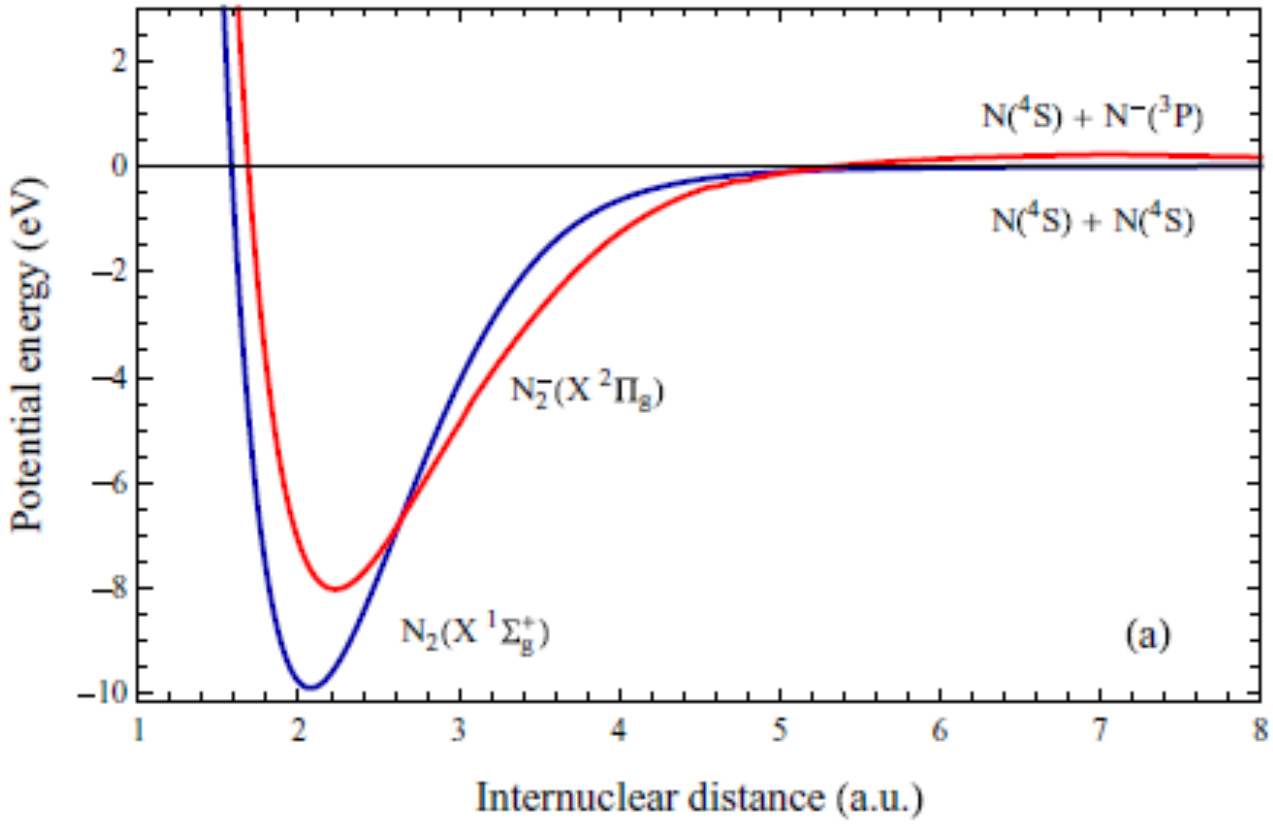
e+N_2 scattering: $(1\sigma_g, 1\sigma_u)^4(2\sigma_g, 2\sigma_u, 1\pi_u, 3\sigma_g, 1\pi_g, 3\sigma_u)^{11}$

$(1\sigma_g, 1\sigma_u)^4(2\sigma_g, 2\sigma_u, 1\pi_u, 3\sigma_g, 1\pi_g, 3\sigma_u)^{10}(2\pi_u, 4\sigma_g, 5\sigma_g, 2\pi_g, 1\delta_g, 4\sigma_u)^1$

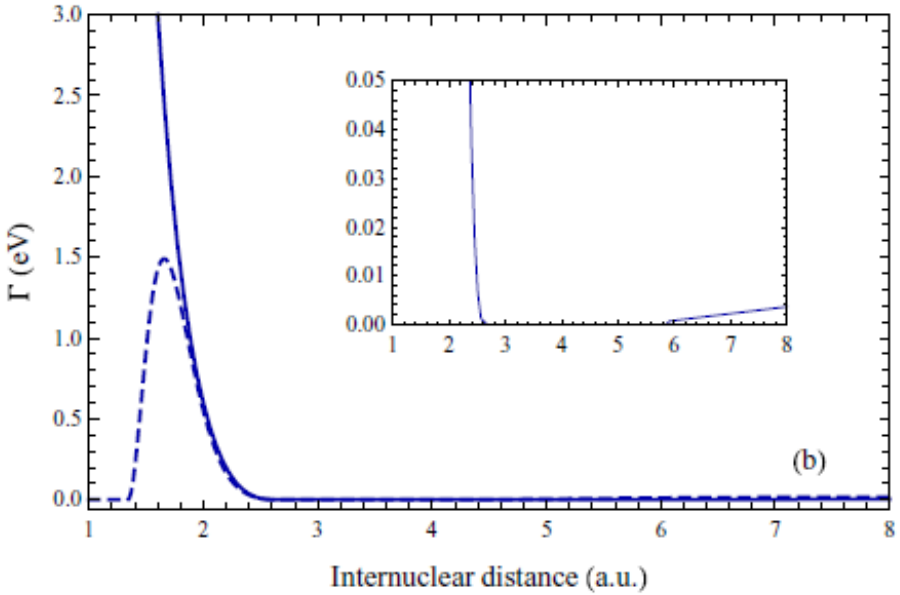
V. Laporta *et al.*, Plasma Sources Sci. Technol. **23**, 065002 (2014)
V. Laporta *et al.*, Plasma Sources Sci. Technol. **21**, 055018 (2012)

N_2

Potential energy curves



Coupling N_2^-/N_2



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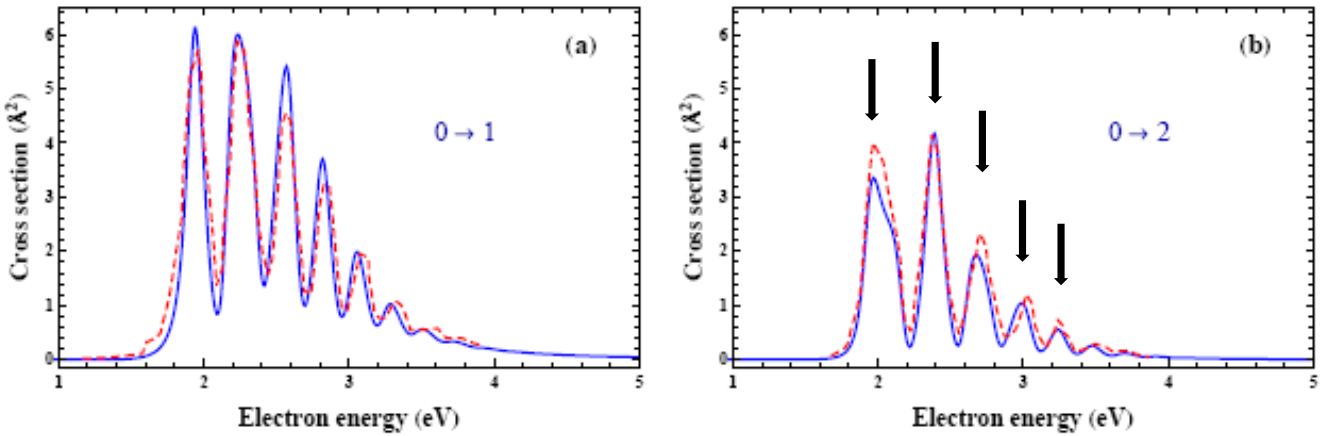
Comparison with experiments

Vibrational-excitation process:



$$e^- + \mathrm{N_2}\left(\mathrm{X}\,^1\Sigma_g^+;\, v, J\right) \longrightarrow \mathrm{N_2^-}\left(\mathrm{X}\,^2\Pi_g\right) \longrightarrow e^- + \mathrm{N_2}\left(\mathrm{X}\,^1\Sigma_g^+;\, v', J\right)$$

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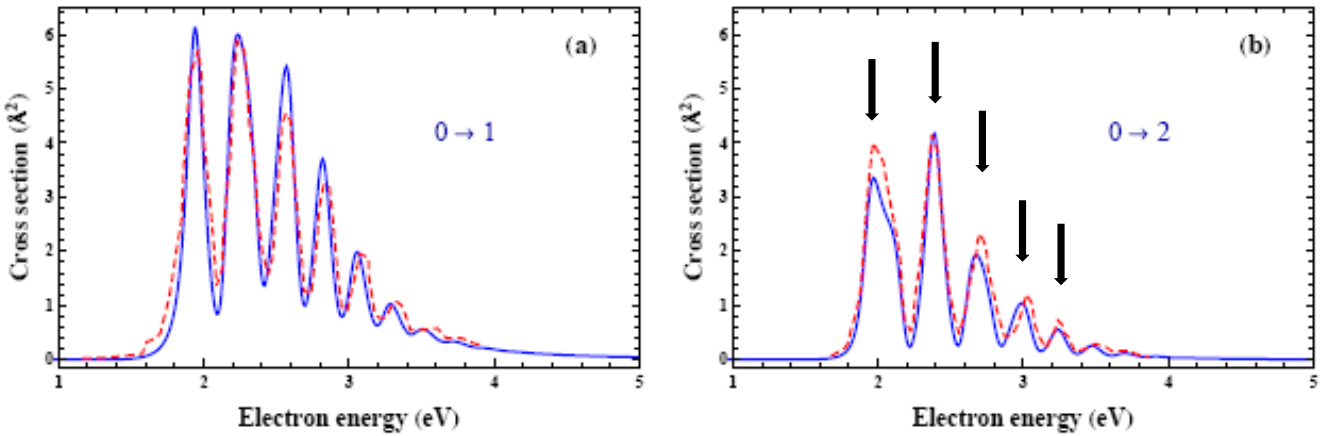

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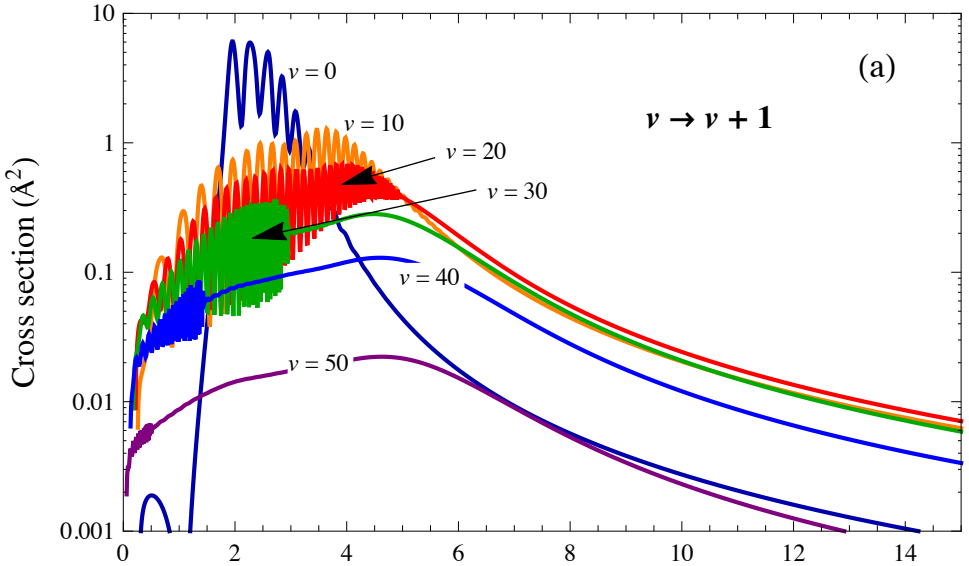

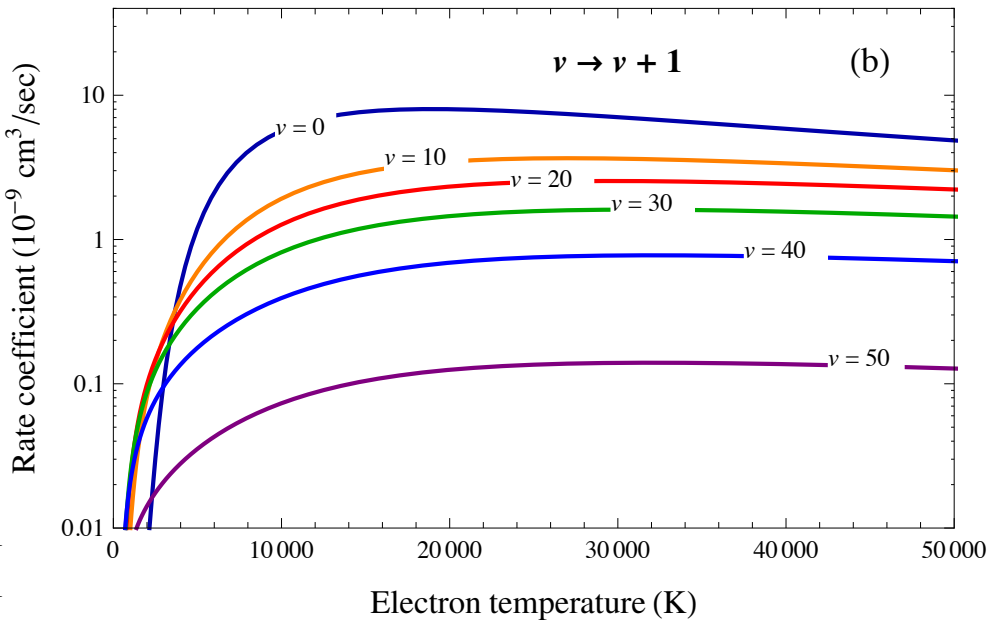

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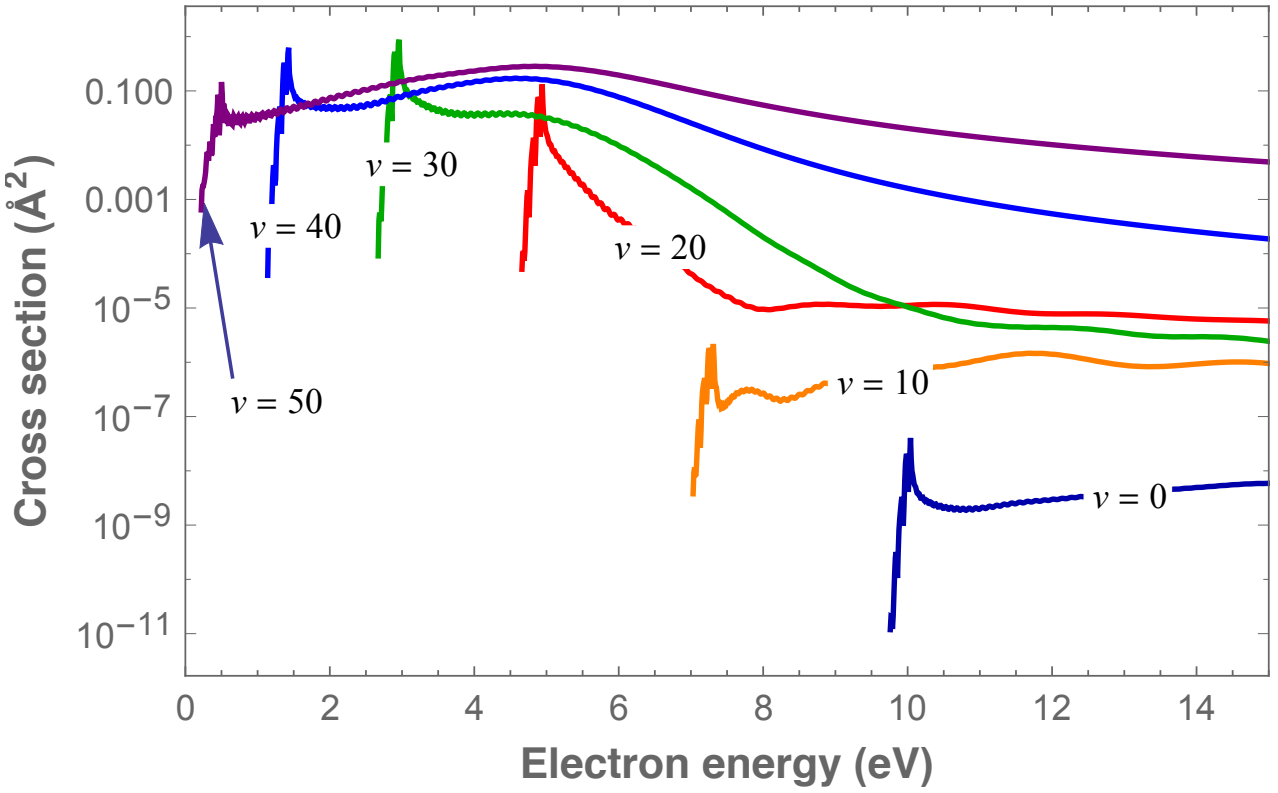
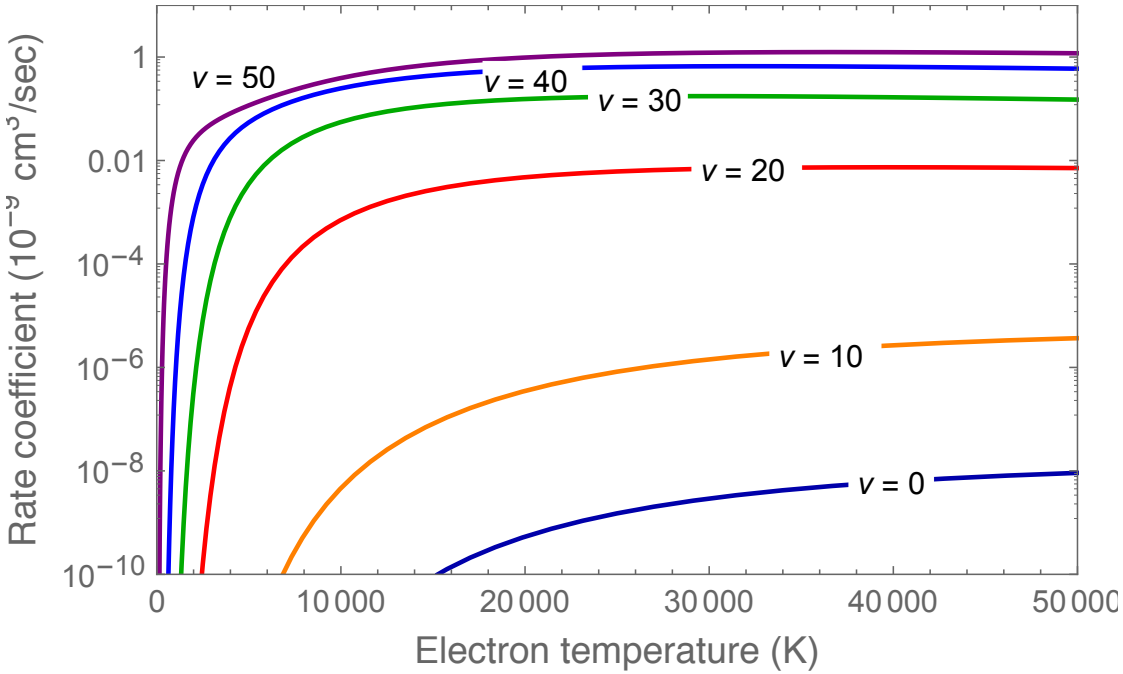
Electron-impact dissociation:

$$e^- + \mathrm{N}_2\left(\mathrm{X}\,^1\Sigma_g^+;\, v, J\right) \longrightarrow \mathrm{N}_2^-\left(\mathrm{X}\,^2\Pi_g\right) \longrightarrow e^- + 2\,\mathrm{N}(^4\mathrm{S})$$





electron-O_2(X, v) resonant scattering

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In order to describe the low-energy electron-$O_2(X\ ^3\Sigma_g^-)$ resonant scattering it needs to include in the calculations four resonant states, $^2\Pi_g$, $^2\Pi_u$, $^4\Sigma_u^-$, $^2\Sigma_u^-$ of O_2^-

Potential energy curves and resonance widths were obtained by MOLPRO and R-matrix within **aug-cc-pvQZ** basis-set and **MR-CI** model

Orbital configurations for **O_2 target**: $(2a_g, 1b_{1u})^6$ $(3a_g, 2b_{3u}, 2b_{2u}, 3b_{1u}, 1b_{2g}, 1b_{3g})^{10}$

3 core orbitals frozen electrons — 9 valence orbitals

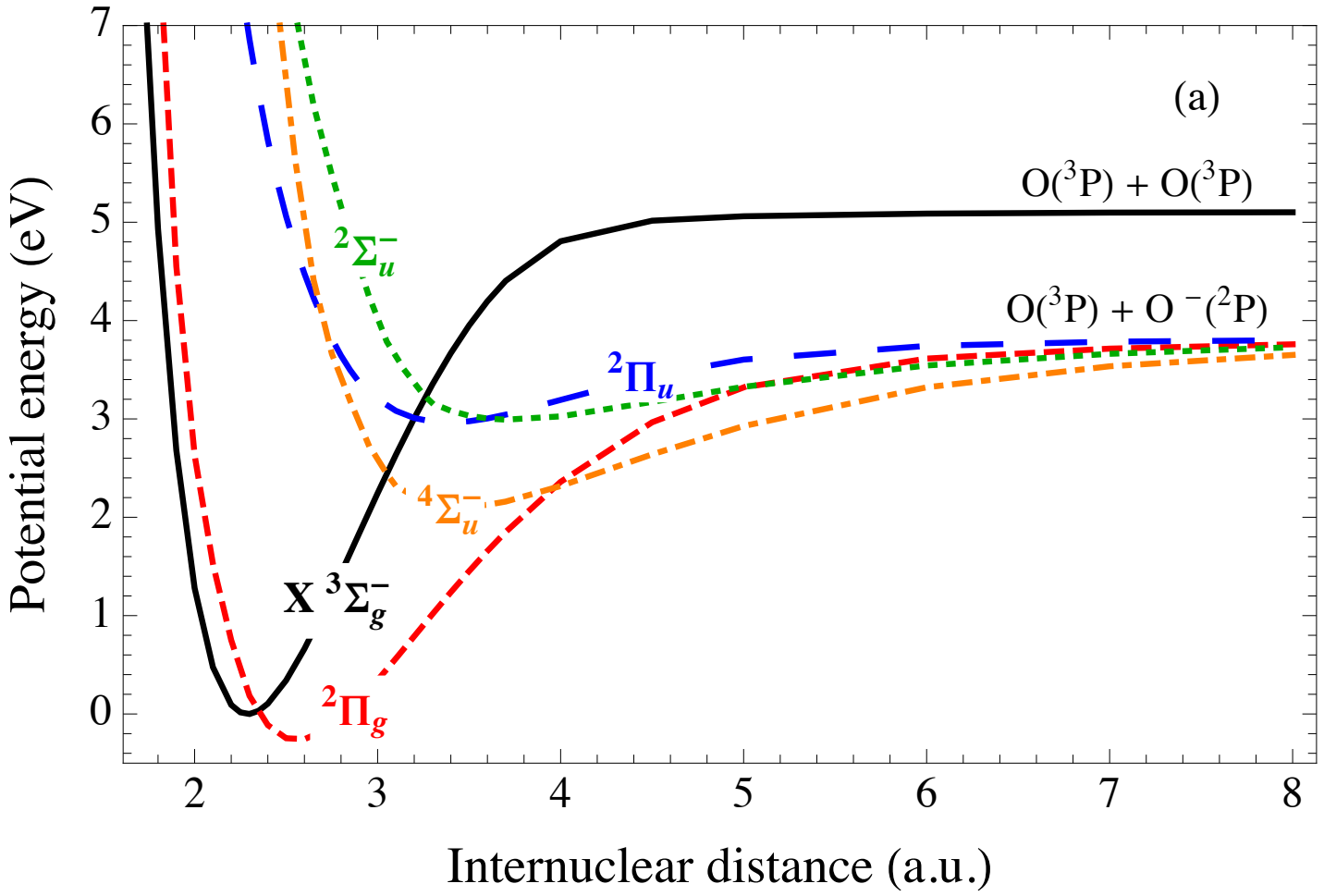
Two orbital configurations for **e + O_2 scattering**:

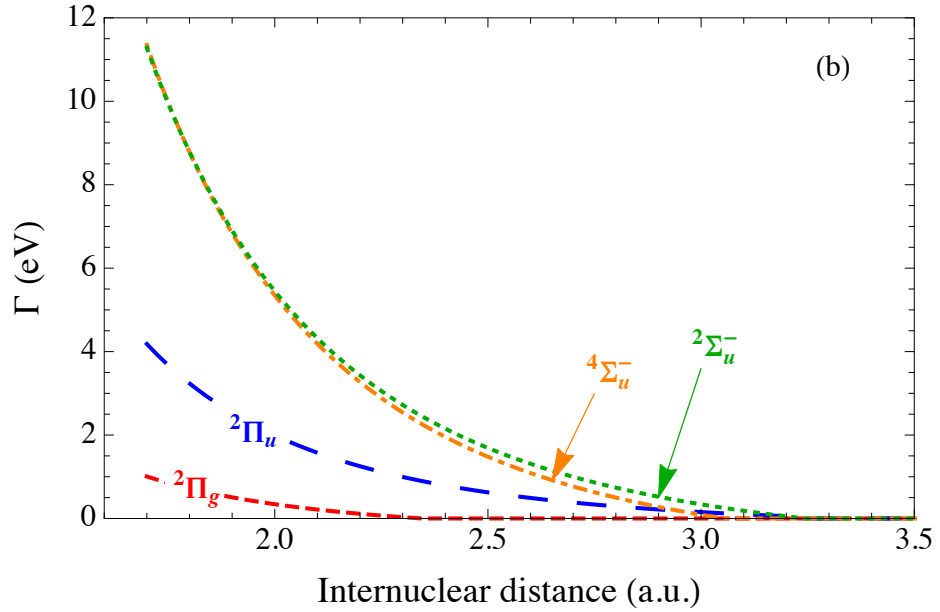
$(2a_g, 1b_{1u})^6$ $(5a_g, 2b_{3u}, 2b_{2u}, 4b_{1u}, 2b_{2g}, 2b_{3g})^{11}$

and

$(2a_g, 1b_{1u})^6$ $(5a_g, 2b_{3u}, 2b_{2u}, 4b_{1u}, 2b_{2g}, 2b_{3g})^{10}$ $(6a_g, 3b_{3u}, 3b_{2u}, 1b_{1g}, 5b_{1u}, 3b_{2g}, 3b_{3g}, 1a_u)^1$

O_2





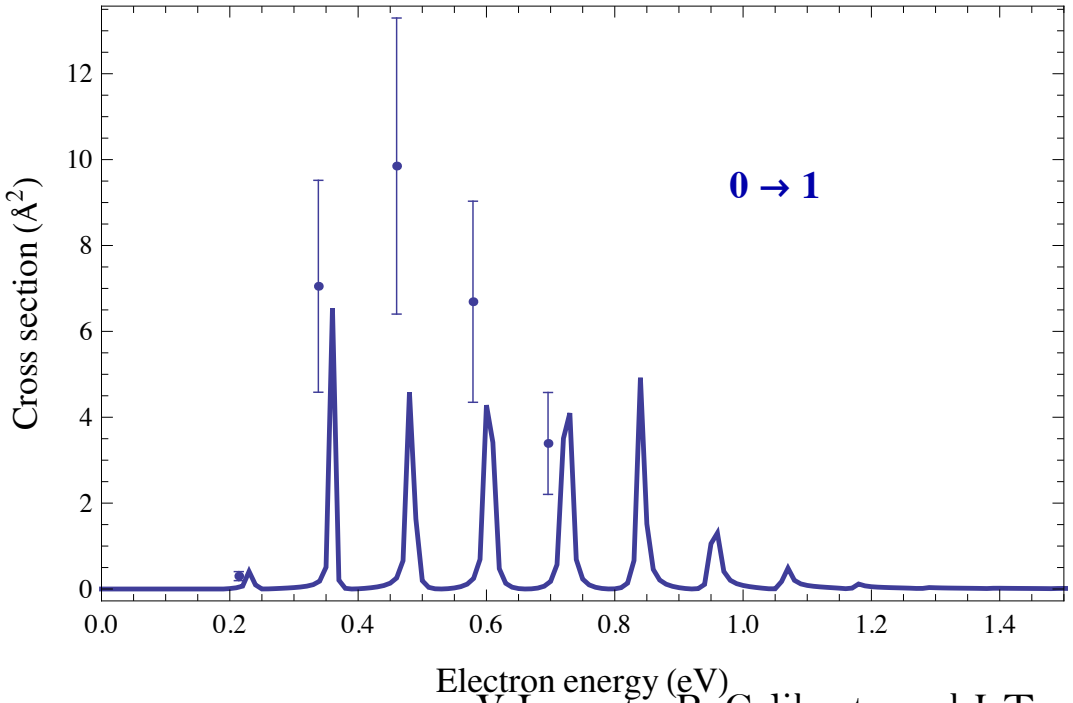
V. Laporta, R. Celiberto and J. Tennyson, *Phys. Rev.* ***A*****91**, 012701 (2015).

V. Laporta, R. Celiberto and J. Tennyson, *Plasma Sources Sci. Technol.* ***22***, *025001 (2013)*

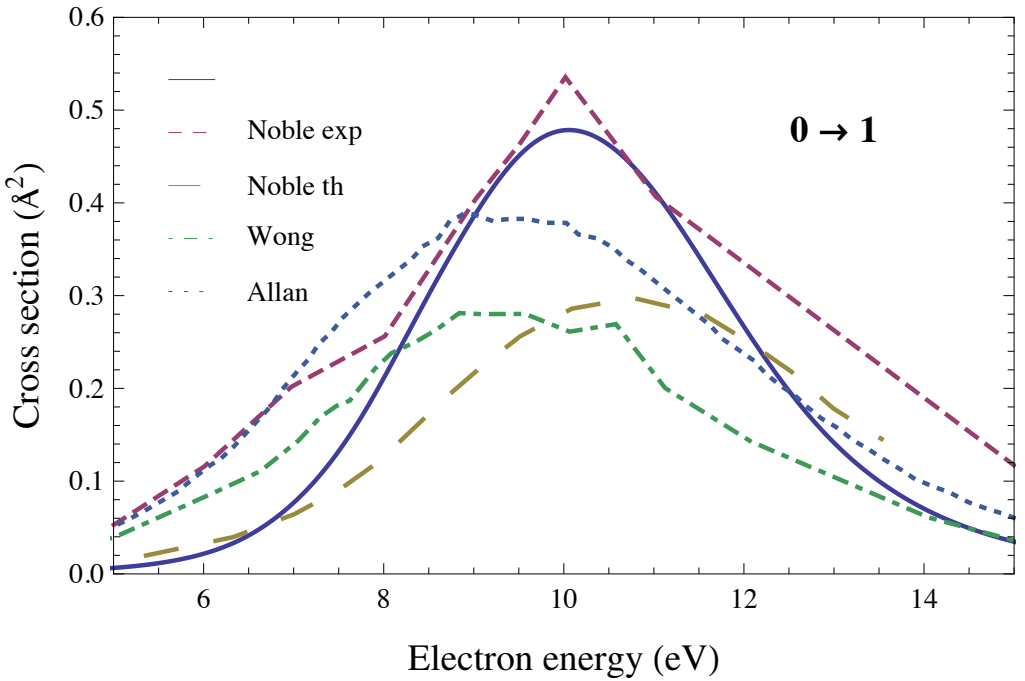
Vibrational-Excitation process:

$$e^- + O_2\left(X\,^3\Sigma_g^-;\ v\right) \longrightarrow O_2^-\left(^2\Pi_g, ^2\Pi_u, ^4\Sigma_u^-, ^2\Sigma_u^-\right) \longrightarrow e^- + O_2\left(X\,^3\Sigma_g^-;\ v'\right)$$

Low energy dominated by $^2\Pi_g$ symmetry
comparison with Allan's results



Resonance at 10 eV dominated by $^4\Sigma_u^-$ symmetry



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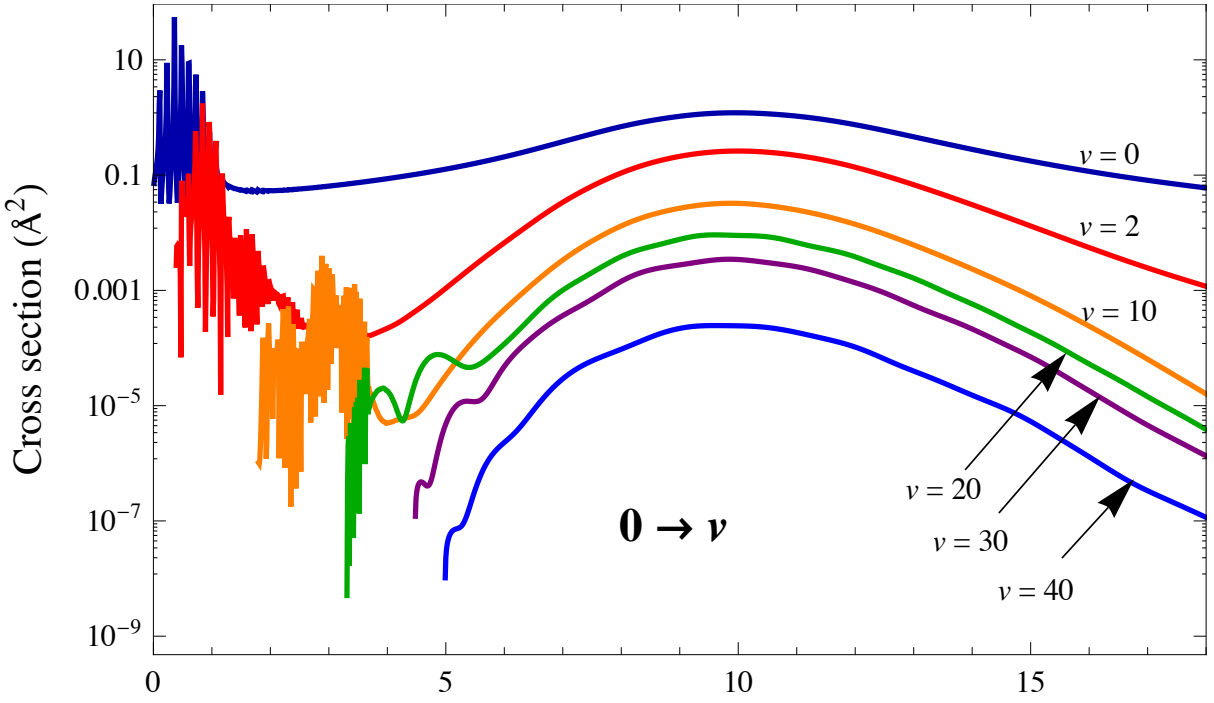
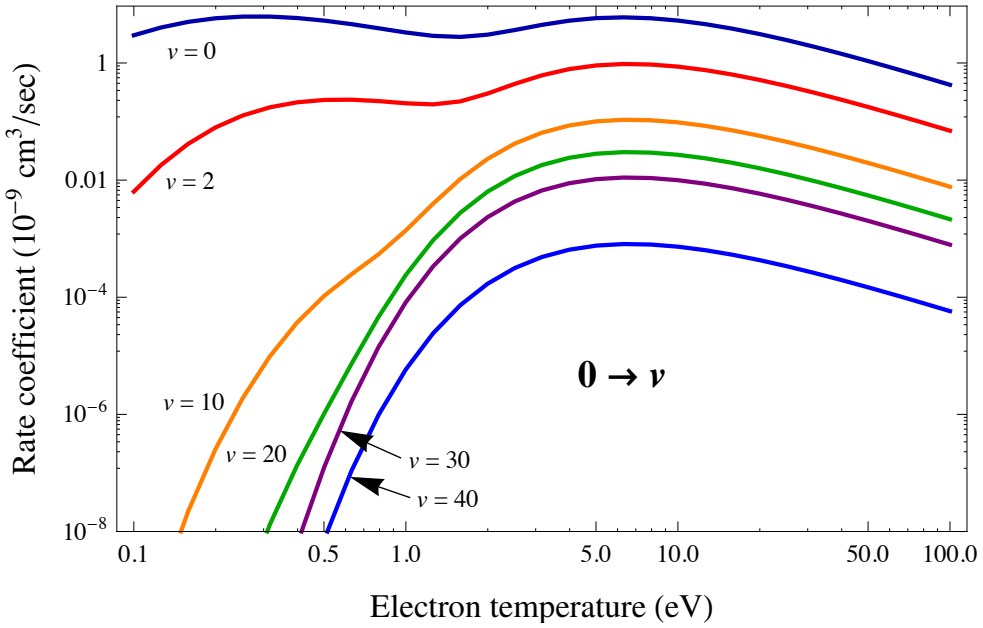
Full set of *Vibrational Excitation* cross sections for *j* = 1…



…and the corresponding rate coefficients



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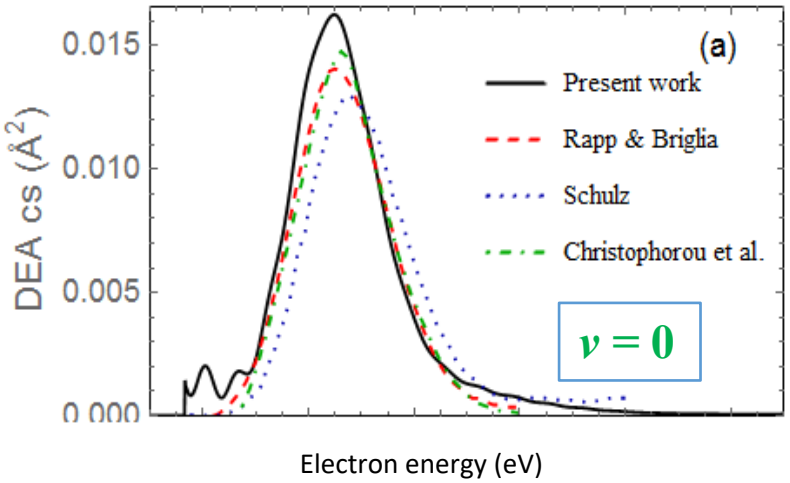
Dissociative-Electron-Attachment

$$e^- + O_2\left(X\,^3\Sigma_g^-;\, v\right) \longrightarrow O_2^-\left(^2\Pi_g, ^2\Pi_u, ^4\Sigma_u^-, ^2\Sigma_u^-\right) \longrightarrow O(^3P) + O^-(^2P)$$



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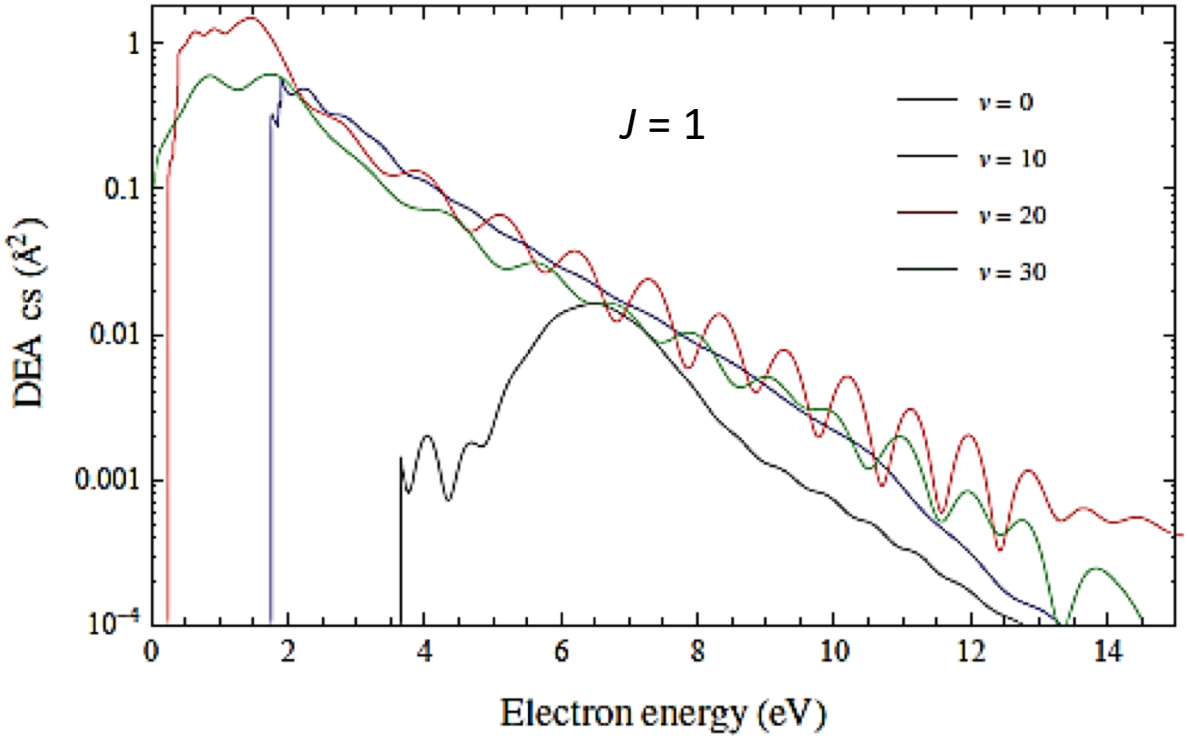
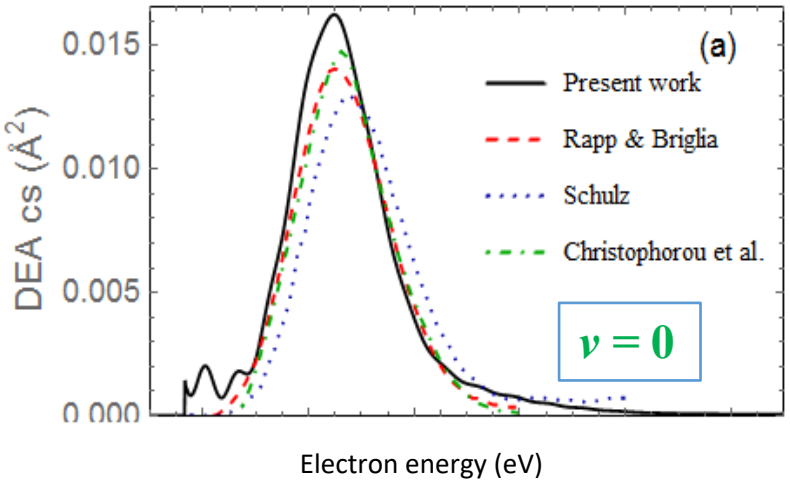
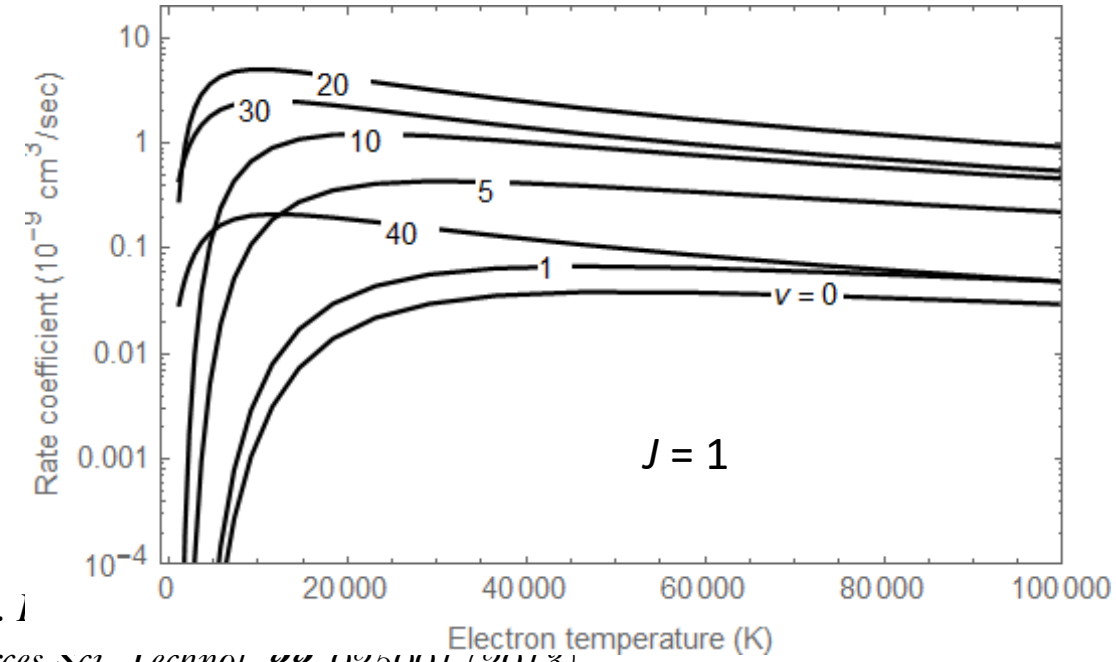
Dissociative-Electron-Attachment

$$e^- + O_2(X\,^3\Sigma_g^-;\, v) \longrightarrow O_2^-(^2\Pi_g, ^2\Pi_u, ^4\Sigma_u^-, ^2\Sigma_u^-) \longrightarrow O(^3P) + O^-(^2P)$$





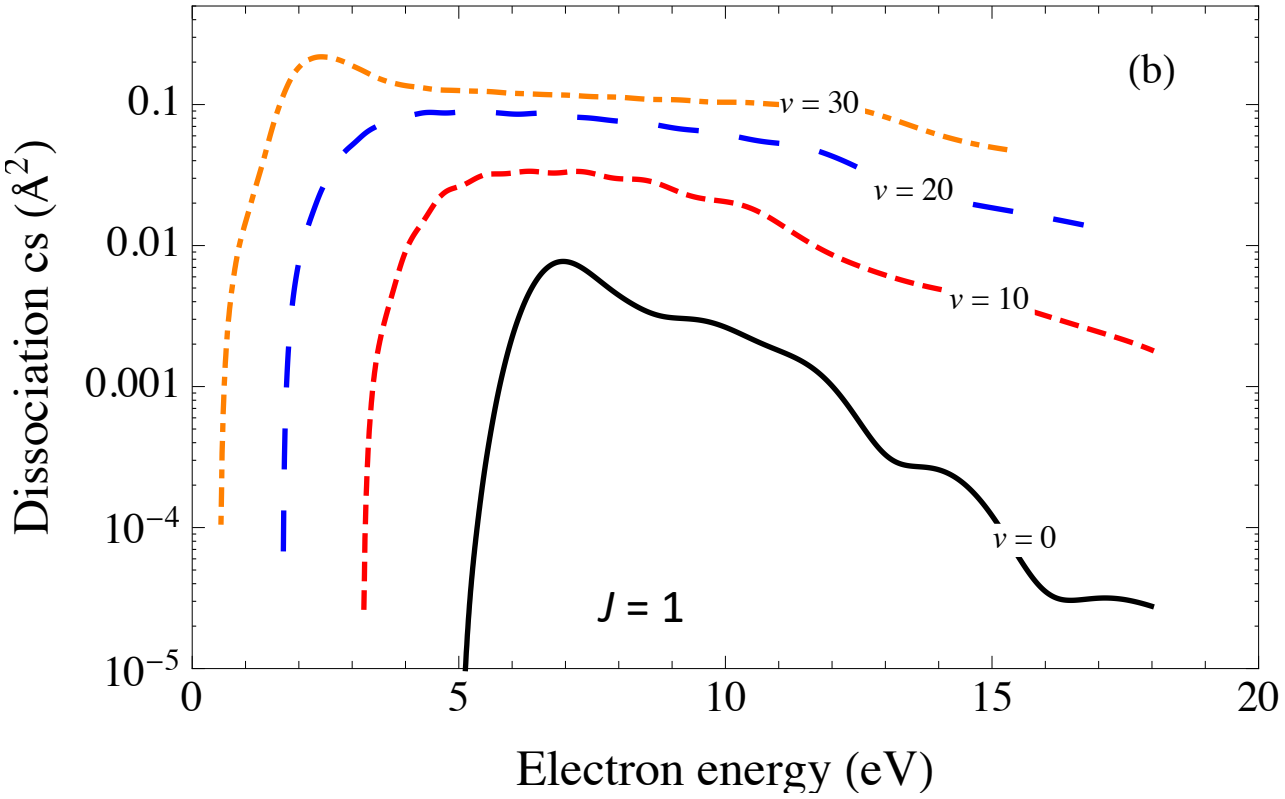


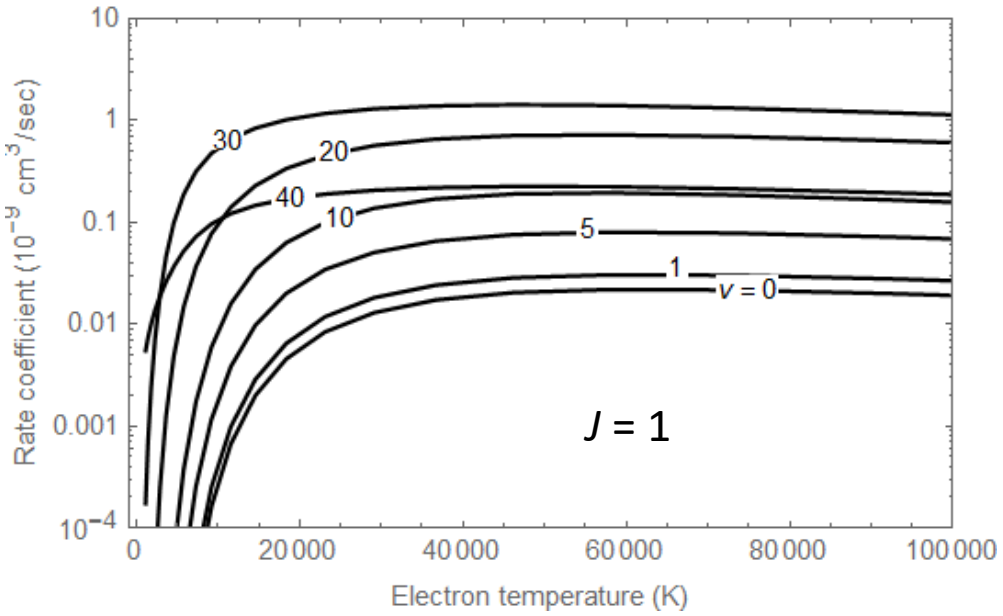
V. Laporta, R. Celiberto and J. Tennyson, *Phys. R*

V. Laporta, R. Celiberto and J. Tennyson, *Plasma Sources Sci. Technol.* **22**, 025001 (2013)

Electron-impact dissociative excitation:

$$e^- + O_2\left(X^3\Sigma_g^-;\ v\right) \longrightarrow O_2^-\left(^2\Pi_g, ^2\Pi_u, ^4\Sigma_u^-, ^2\Sigma_u^-\right) \longrightarrow e^- + 2\,O(^3P)$$





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

V. Laporta, R. Celiberto and J. Tennyson, *Plasma Sources Sci. Technol.* ***22***, *025001 (2013)*

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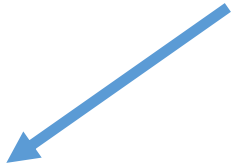
1. Theory: electron-molecule scattering

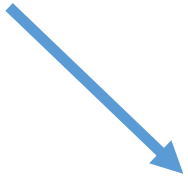
2. *ab-initio* state-resolved cross sections:
   A. **Nitrogen and Oxygen:** Atmospheric (re-)entry and hypersonic
   B. Carbon dioxide: Plasma-based CO_2 conversion
   C. **BeH^+, H_2^+, OH, ArH^+:** I.T.E.R and controlled fusion; Astrochemistry

3. Conclusions and perspectives

CO_2 Plasma based conversion

Recently, worldwide attention has been focused on





increasing emissions of greenhouse gases

CO_2

decreasing reserves of traditional energy sources

CH_4

CO_2 Plasma based conversion

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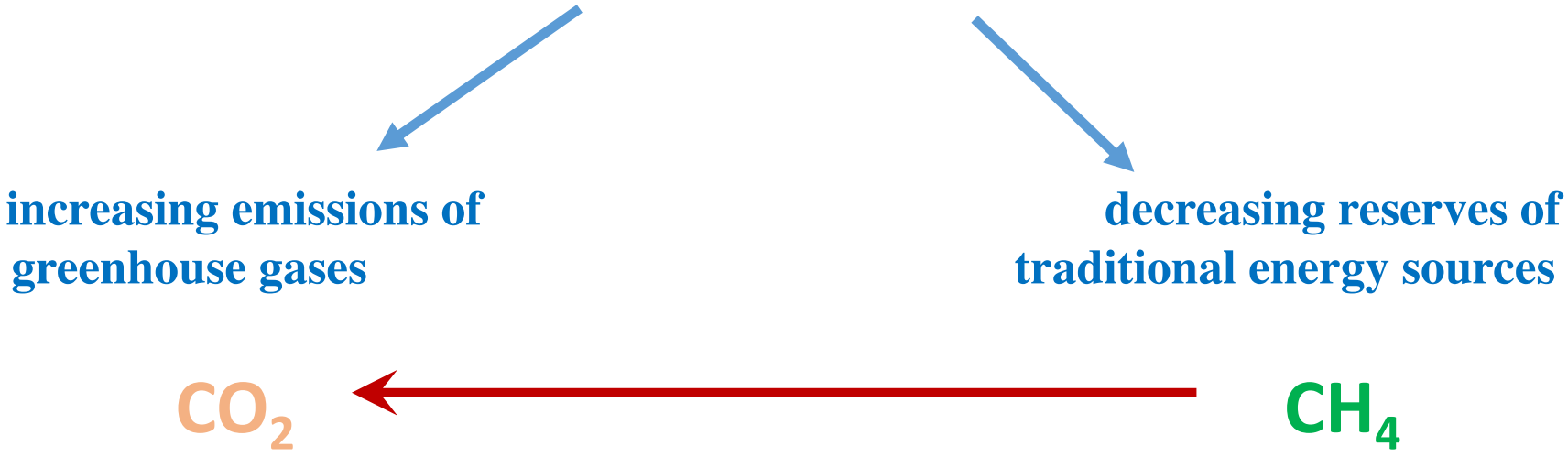

CO_2 Plasma based conversion

Recently, worldwide attention has been focused on

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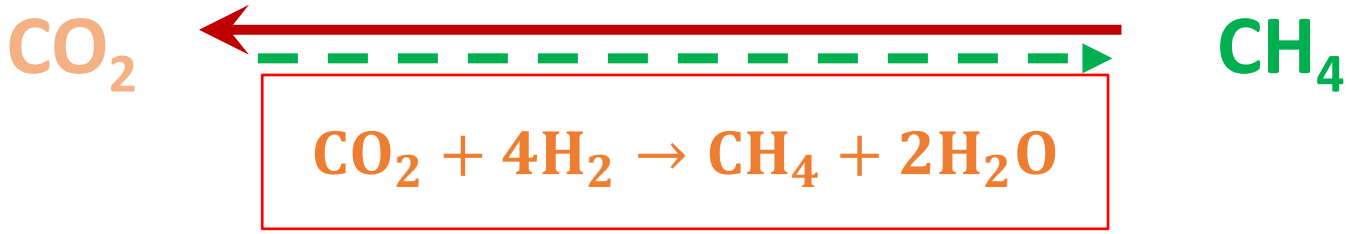


Highly endothermic carbon dioxide dissociation is one of the key processes affecting the overall reaction efficiency

A promising approach for this conversion involves the non-equilibrium chemistry in the plasma phase by electric discharges

Electron-CO_2 cross sections

Vibrational-excitation

$$e + \mathbf{CO_2}(\mathbf{X}\ ^1\boldsymbol{\Sigma}_\mathbf{g}^+, v) \rightarrow \mathbf{CO_2^-}(^2\boldsymbol{\Pi}_\mathbf{u}) \rightarrow e + \mathbf{CO_2}(\mathbf{X}\ ^1\boldsymbol{\Sigma}_\mathbf{g}^+, v')$$

CO_2 SYMMETRIC MODE

MOLPRO (MRCI model, aug-cc-pVQZ basis set, D_{2h}):

3 CORE ORBITALS: $(2A_g + 0B_{3u} + 0B_{2u} + 0B_{1g} + 1B_{1u} + 0B_{2g} + 0B_{3g} + 0A_u)^6$

12 VALENCE ORBITALS: $(3A_g + 2B_{3u} + 2B_{2u} + 0B_{1g} + 3B_{1u} + 1B_{2g} + 1B_{3g} + 0A_u)^{16}$

CO_2 BENDING/ANTISYMMETRIC MODE

MOLPRO (MRCI model, aug-cc-pVQZ basis set, C_{2v}):

3 CORE ORBITALS: $(2A_1 + 0B_1 + 1B_2 + 0A_2)^6$

12 VALENCE ORBITALS: $(5A_1 + 2B_1 + 4B_2 + 1A_2)^{16}$

Plasma Sources Sci. Technol. **25** (2016) 06LT02 (5pp) doi:10.1088/0963-

Letter

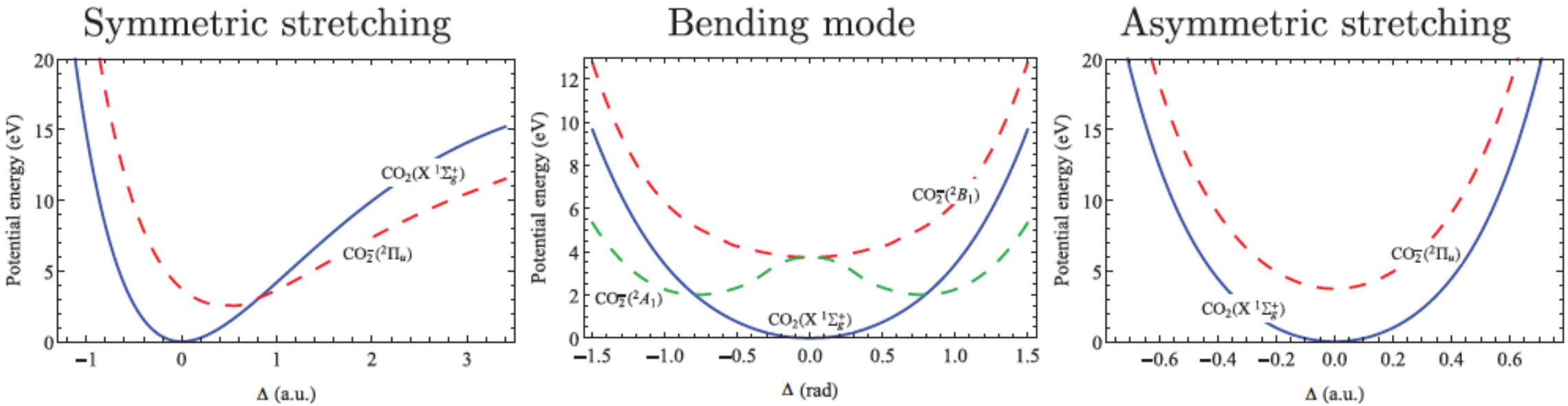
Calculated low-energy electron-impact vibrational excitation cross sections for CO_2 molecule

V Laporta[1,2], J Tennyson[2] and R Celiberto[1,3]

Vibrational-excitation

$$e + CO_2(X\ ^1\Sigma_g^+, v) \rightarrow CO_2^-(^2\Pi_u) \rightarrow e + CO_2(X\ ^1\Sigma_g^+, v')$$

R-Matrix potential energy curves



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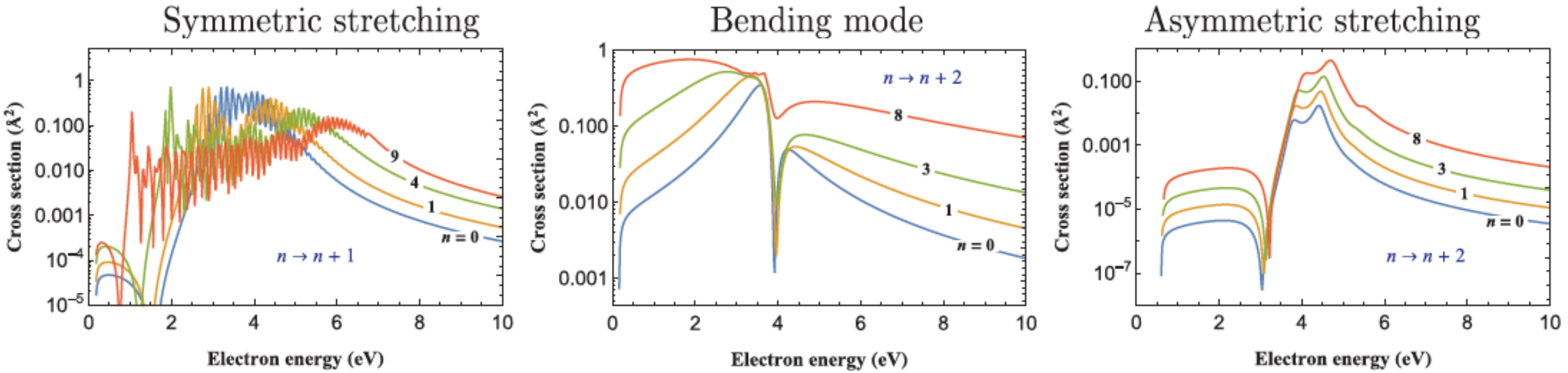


Dissociative-attachment for CO_2

$$e + \mathrm{CO_2(X)} \rightarrow \mathrm{CO(X)} + \mathrm{O^-(^2P)}$$

Dissociative-excitation for CO_2

$$e + \mathrm{CO_2(X)} \rightarrow \mathrm{CO(X)} + \mathrm{O(^3P)} + e$$

CO_2/CO_2^-

MOLPRO (MRCI model, aug-cc-pVQZ basis set, C_{2v}):

5 CORE ORBITALS: $(5A_1 + 0B_1 + 0B_2 + 0A_2)^{10}$

10 VALENCE ORBITALS: $(4A_1 + 3B_1 + 3B_2 + 0A_2)^{16}$

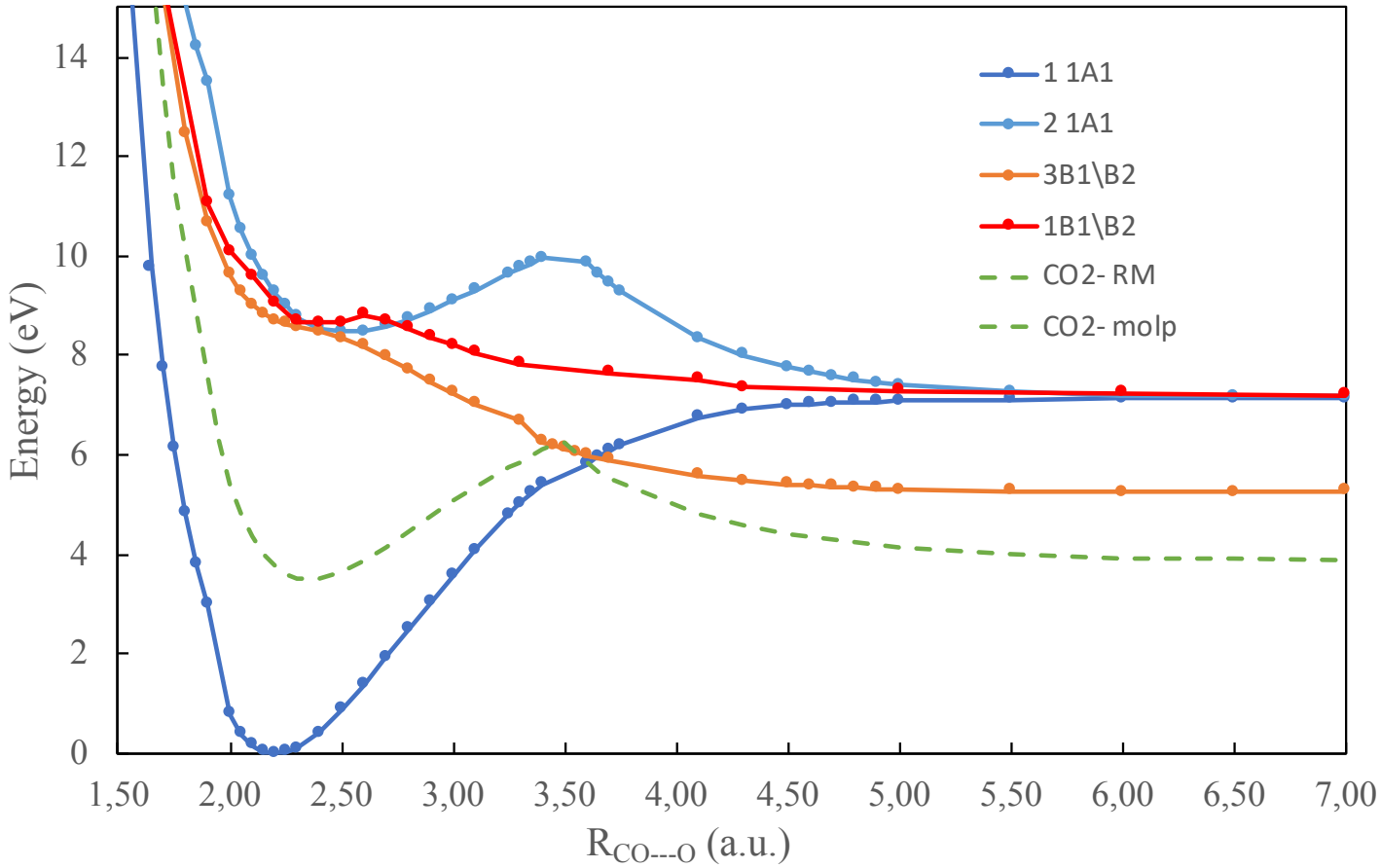
In preparation…

Dissociative-attachment for CO_2

$$e + CO_2(X) \rightarrow CO(X) + O^-(^2P)$$

Dissociative-excitation for CO_2

$$e + CO_2(X) \rightarrow CO(X) + O(^3P) + e$$



Abdillah Abdoulanziz

In preparation…

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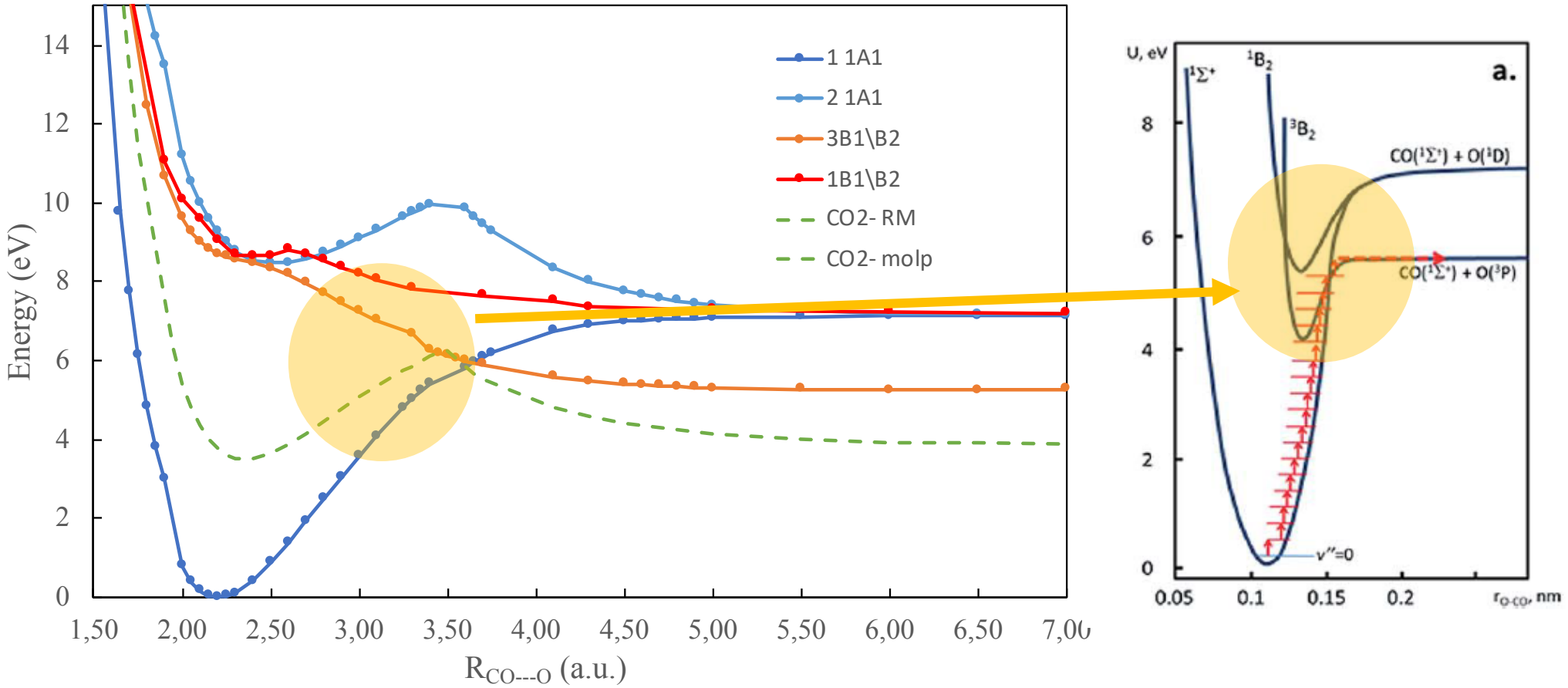

Abdillah Abdoulanziz

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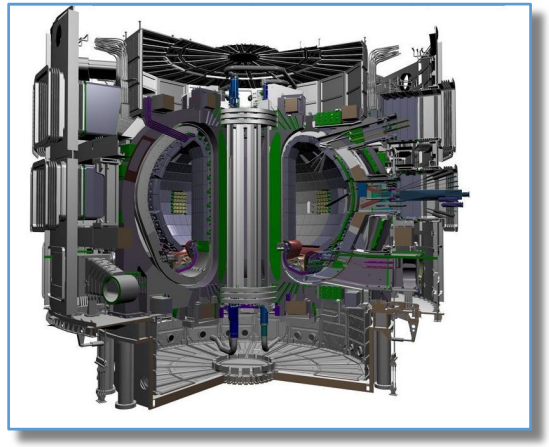
electron-BeH^+ and -BeD^+ scattering

$$e + \mathrm{BeH}^+\left(\mathrm{X}\,^1\Sigma^+; v, j\right) \rightarrow \mathrm{BeH}^+\left(\mathrm{X}\,^1\Sigma^+; v', j'\right) + e \qquad \text{(VE)}$$

$$\rightarrow \mathrm{Be}^*(n = 1 \ldots 12) + \mathrm{H}(^2S) \qquad \text{(DR)}$$

$$\rightarrow \mathrm{Be}^+(^2S) + \mathrm{H}(^2S) + e \qquad \text{(DE)}$$



I.T.E.R.

*V. Laporta, K. Chakrabarti, et al., Plasma Phys. Control. Fusion **59**, 045008 (2017)*
*S. Niyonzima, V. Laporta, et al., Plasma Sources Sci. Technol. **27**, 025015 (2018)*

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$$e + \mathrm{BeH}^+\left(\mathrm{X}\,^1\Sigma^+; v, j\right) \rightarrow \mathrm{BeH}^+\left(\mathrm{X}\,^1\Sigma^+; v', j'\right) + e \qquad \text{(VE)}$$

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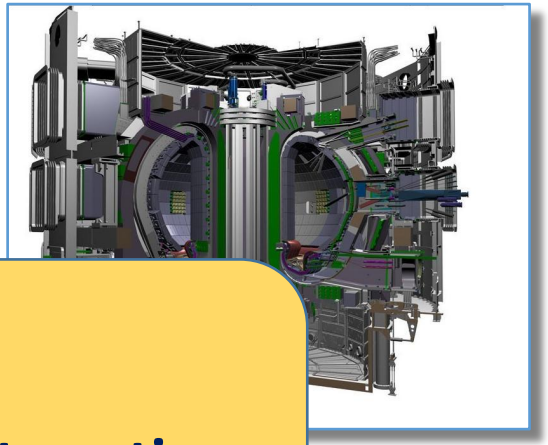


plasmas Be-wall interaction

.E.R.

V. Laporta, K. Chakrabarti, et al., Plasma Phys. Control. Fusi

S. Niyonzima, V. Laporta, et al., Plasma Sources Sci. Technol.

UK-R-Matrix

Potential energy curves and couplings

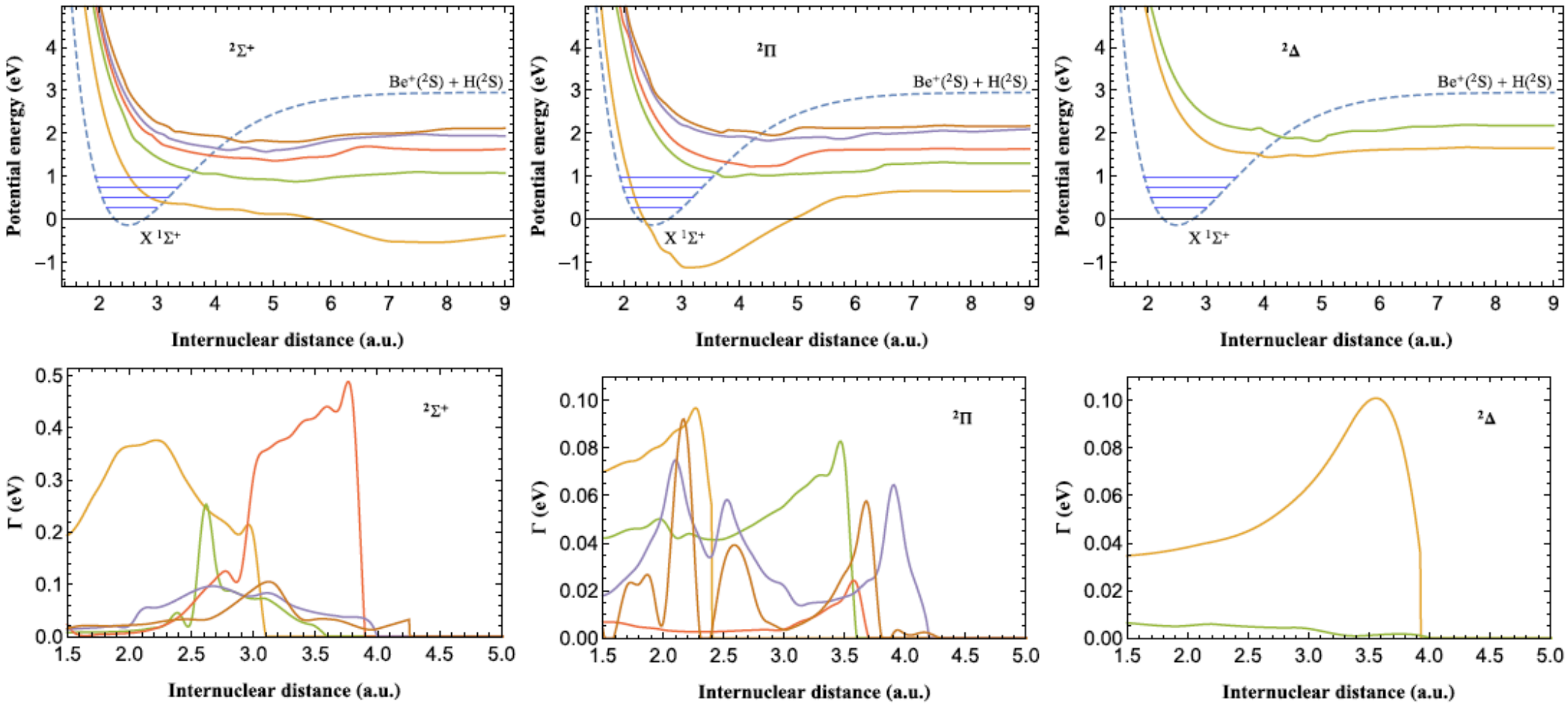
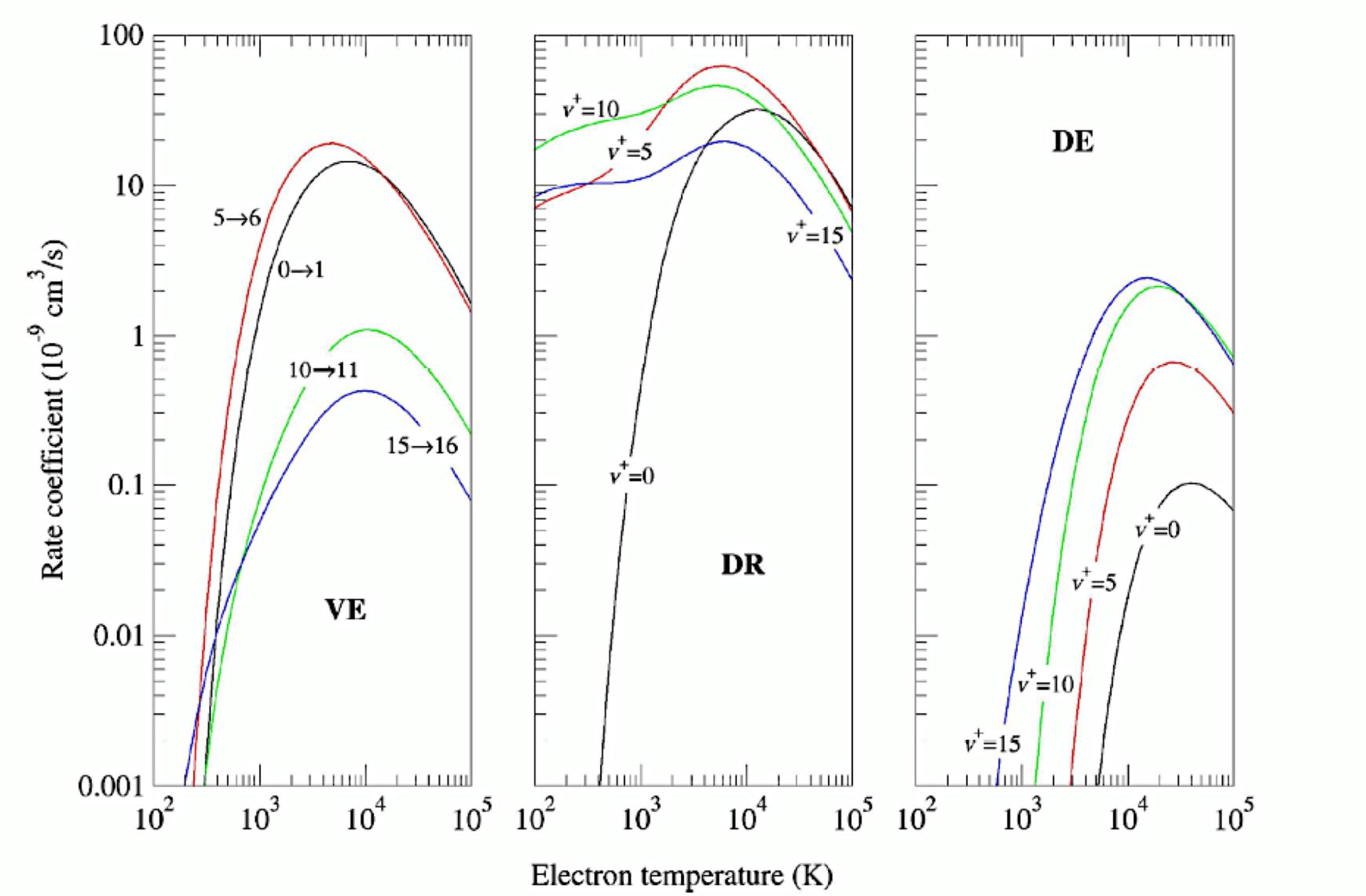
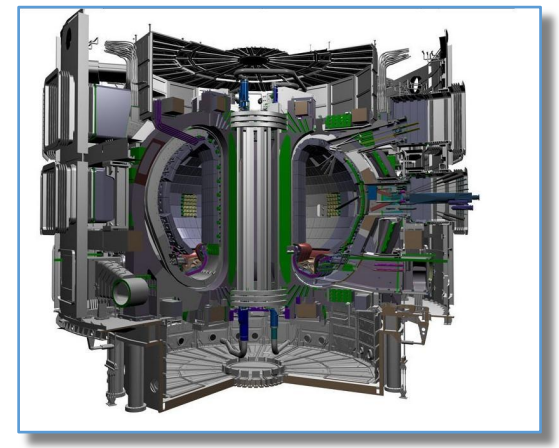


Figure 1. Potential energy curves (top line) and widths (bottom line) for BeH** resonant states in $^2\Sigma^+$, $^2\Pi$ and $^2\Delta$ scattering channels for $j^+ = 0$. Dashed line refers to potential energy curve for BeH^+ ground electronic state where the first vibrational levels are marked.

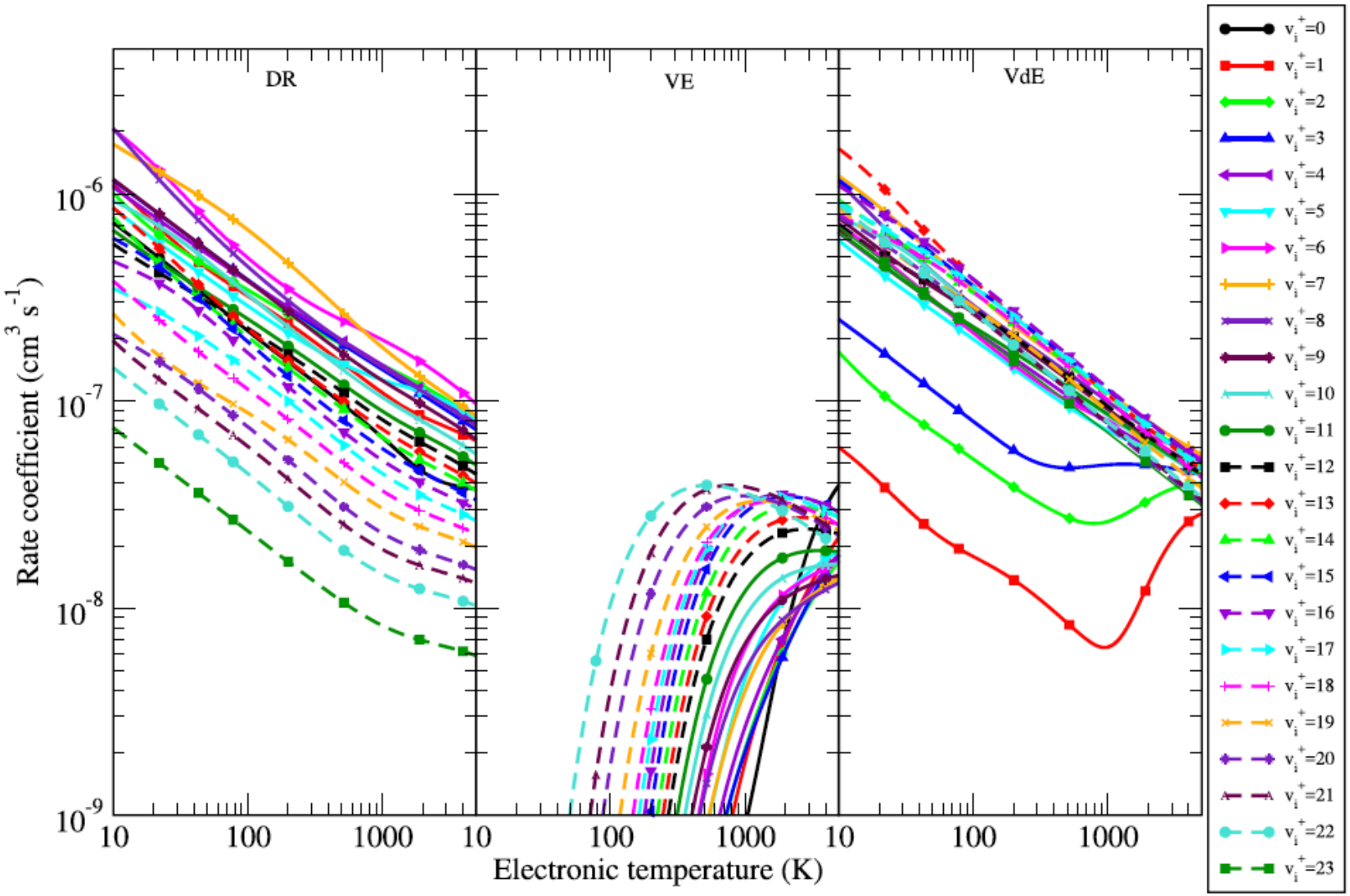
$e + \mathrm{BeH}^+$

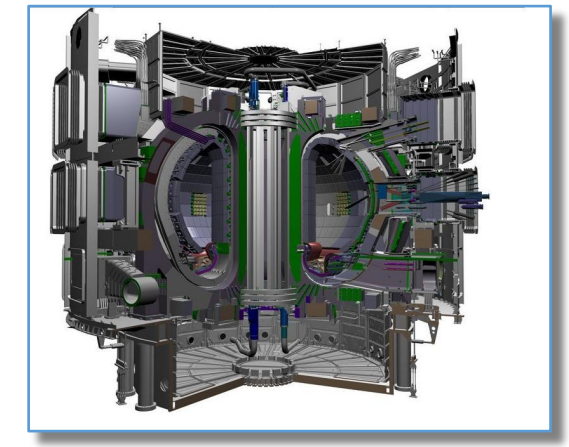




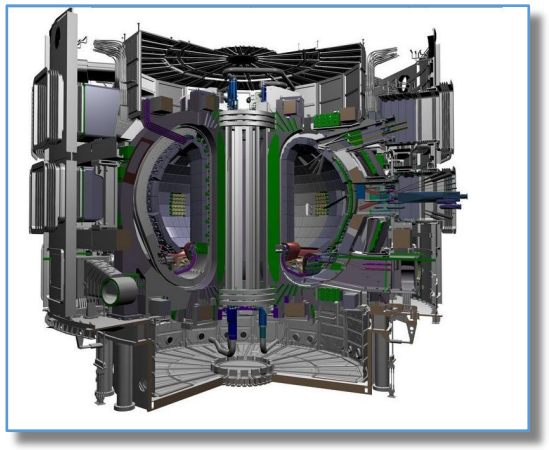
I.T.E.R.

$e + \mathrm{BeD}^+$





I.T.E.R.



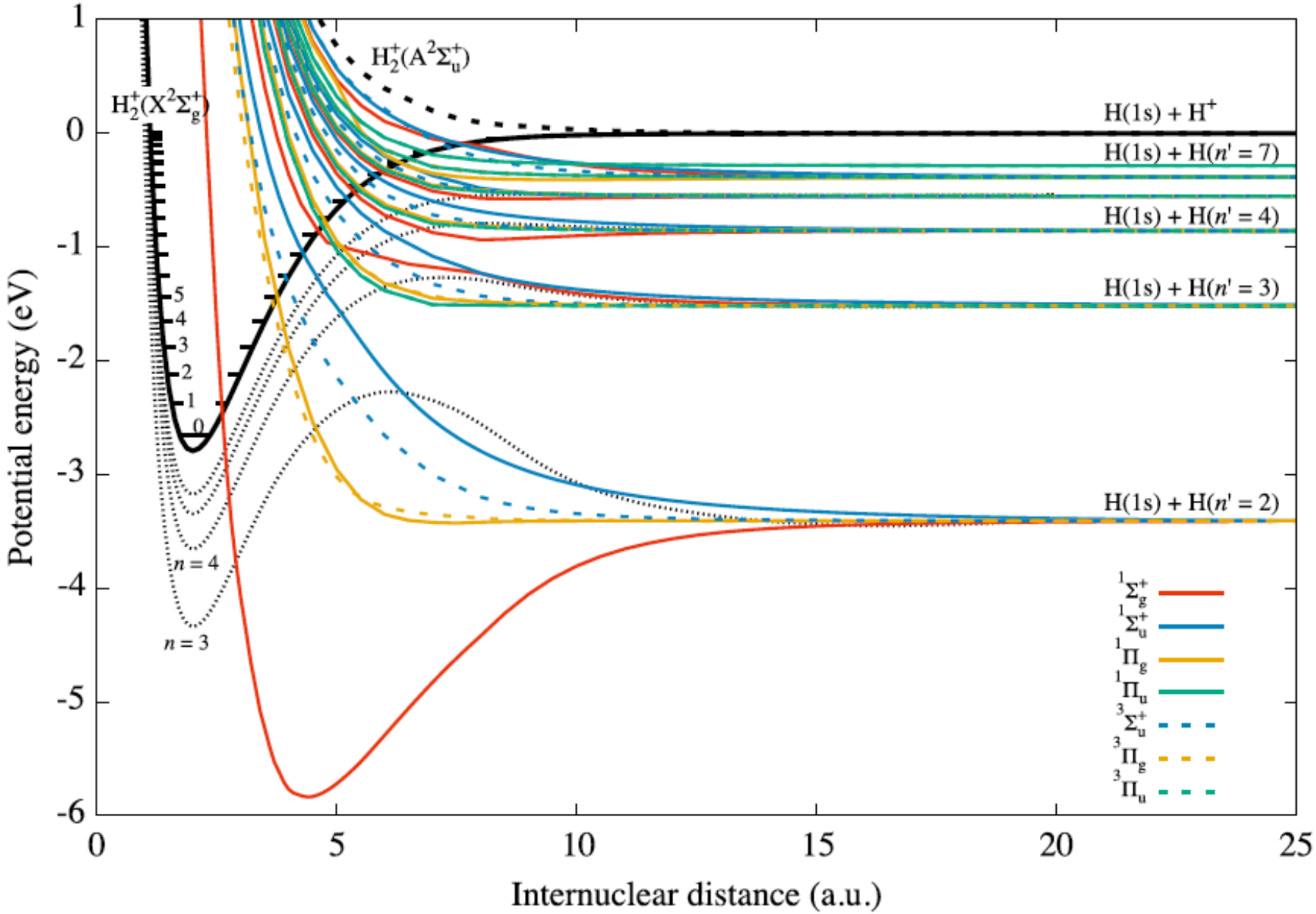
electron-H_2^+

$$H_2^+(N_i^+, v_i^+) + e^-(\varepsilon) \longrightarrow H + H\,,$$ Dissociative Recombination

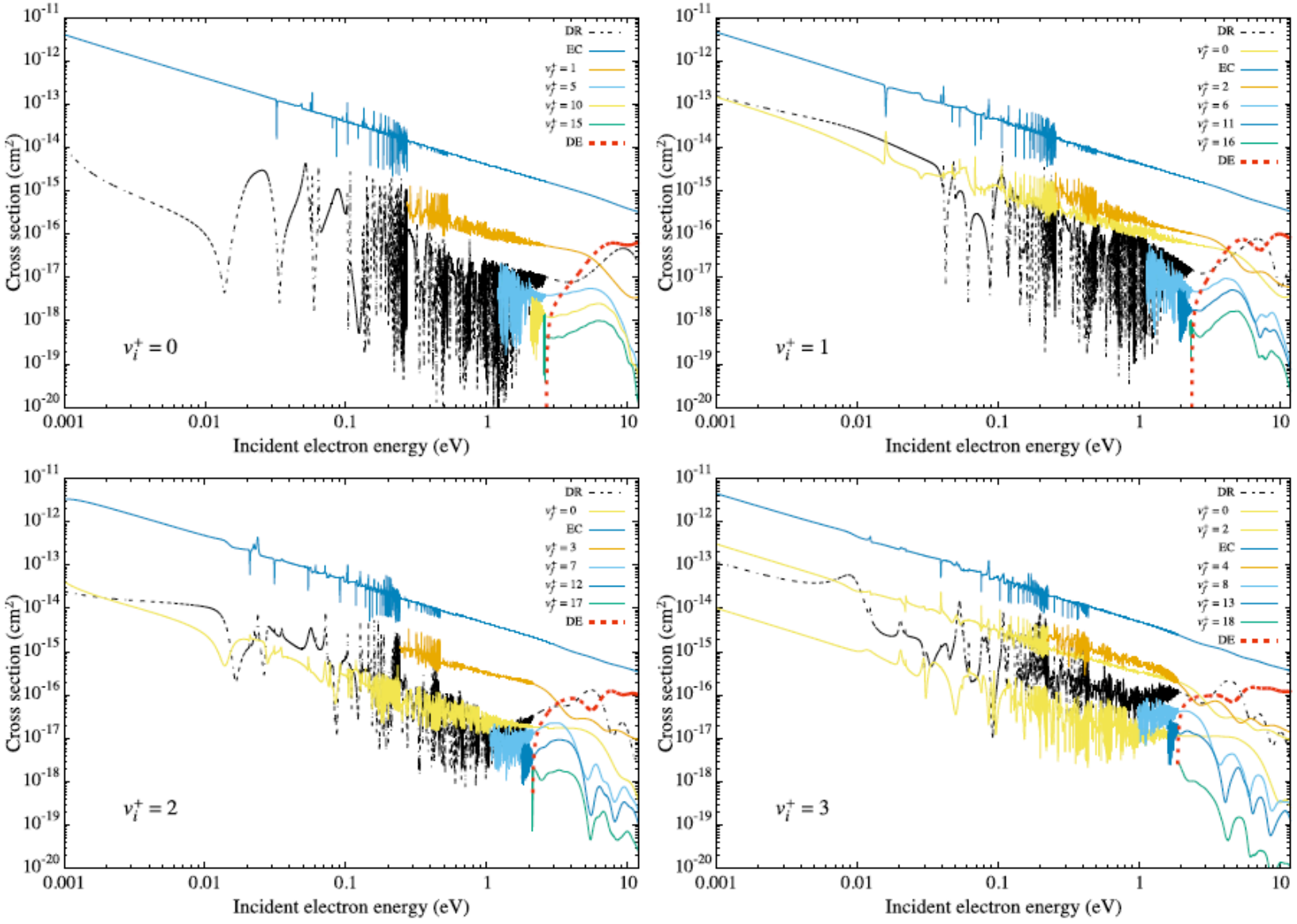
$$H_2^+(N_i^+, v_i^+) + e^-(\varepsilon) \longrightarrow H_2^+(N_f^+, v_f^+) + e^-(\varepsilon_f)\,,$$ Vibrational Excitation

$$H_2^+(N_i^+, v_i^+) + e^-(\varepsilon) \longrightarrow H + H^+ + e^-(\varepsilon_f)\,.$$ Dissociative Excitation

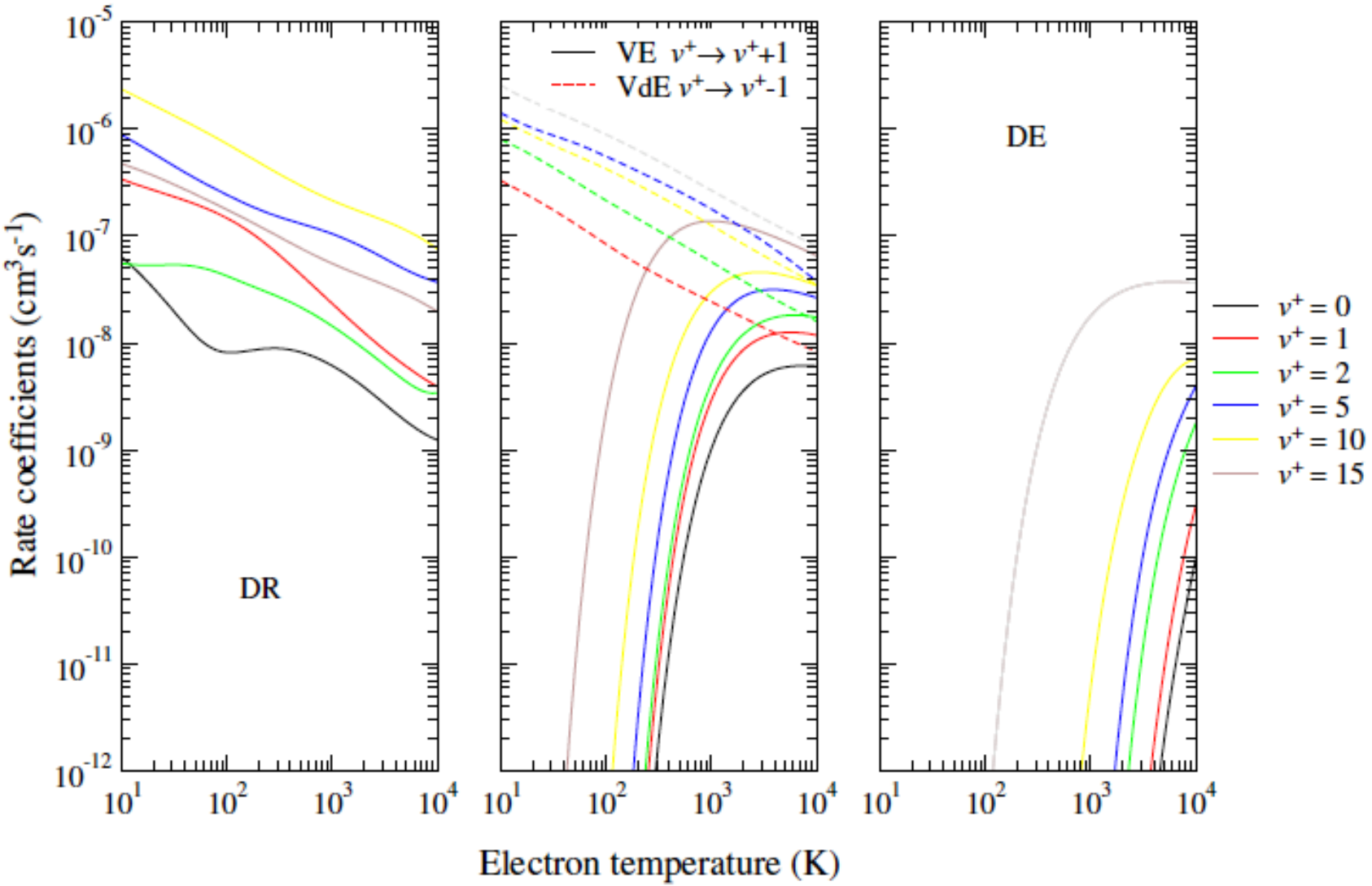
V. Laporta et al. *In preparation…*


Potential energy (eV)
Internuclear distance (a.u.)
1
0
-1
-2
-3
-4
-5
-6
0
5
10
15
20
25
$H_2^+(A^2\Sigma_u^+)$
$H_2^+(X^2\Sigma_g^+)$
H(1s) + H^+
H(1s) + H(n' = 7)
H(1s) + H(n' = 4)
H(1s) + H(n' = 3)
H(1s) + H(n' = 2)
5
4
3
2
1
0
n = 4
n = 3
$^1\Sigma_g^+$
$^1\Sigma_u^+$
$^1\Pi_g$
$^1\Pi_u$
$^3\Sigma_u^+$
$^3\Pi_g$
$^3\Pi_u$

electron-H_2^+


Cross section (cm²)
Incident electron energy (eV)
$v_i^+ = 0$
DR
EC
$v_f^+ = 1$
$v_f^+ = 5$
$v_f^+ = 10$
$v_f^+ = 15$
DE
$v_i^+ = 1$
$v_f^+ = 0$
$v_f^+ = 2$
$v_f^+ = 6$
$v_f^+ = 11$
$v_f^+ = 16$
$v_i^+ = 2$
$v_f^+ = 3$
$v_f^+ = 7$
$v_f^+ = 12$
$v_f^+ = 17$
$v_i^+ = 3$
$v_f^+ = 4$
$v_f^+ = 8$
$v_f^+ = 13$
$v_f^+ = 18$

electron-H_2^+


Rate coefficients (cm^{3}s^{-1})
Electron temperature (K)
DR
VE $v^+ \rightarrow v^+$+1
VdE $v^+ \rightarrow v^+$-1
DE
v^+ = 0
v^+ = 1
v^+ = 2
v^+ = 5
v^+ = 10
v^+ = 15

$e + ArH^+$ collisions

$$e(\varepsilon) + \mathrm{ArH}^+(\mathrm{X}\,^1\Sigma^+, v^+) \rightarrow \mathrm{Ar} + \mathrm{H}\ , \ (\mathrm{DR})$$

A. Abdoulanziz, F. Colboc, D.A. Little, Y. Moulane, J.Zs. Mezei, E. Roueff, J. Tennyson, I.F. Schneider and V. Laporta, MNRAS 479, 2415 (2018)

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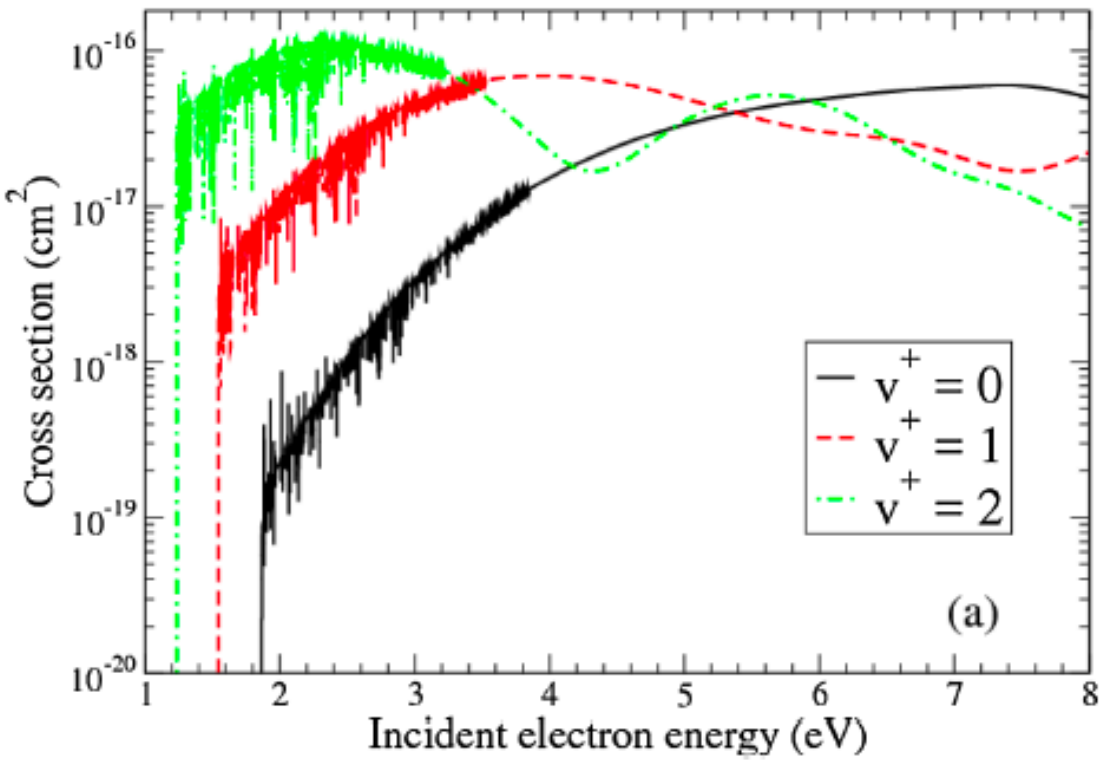

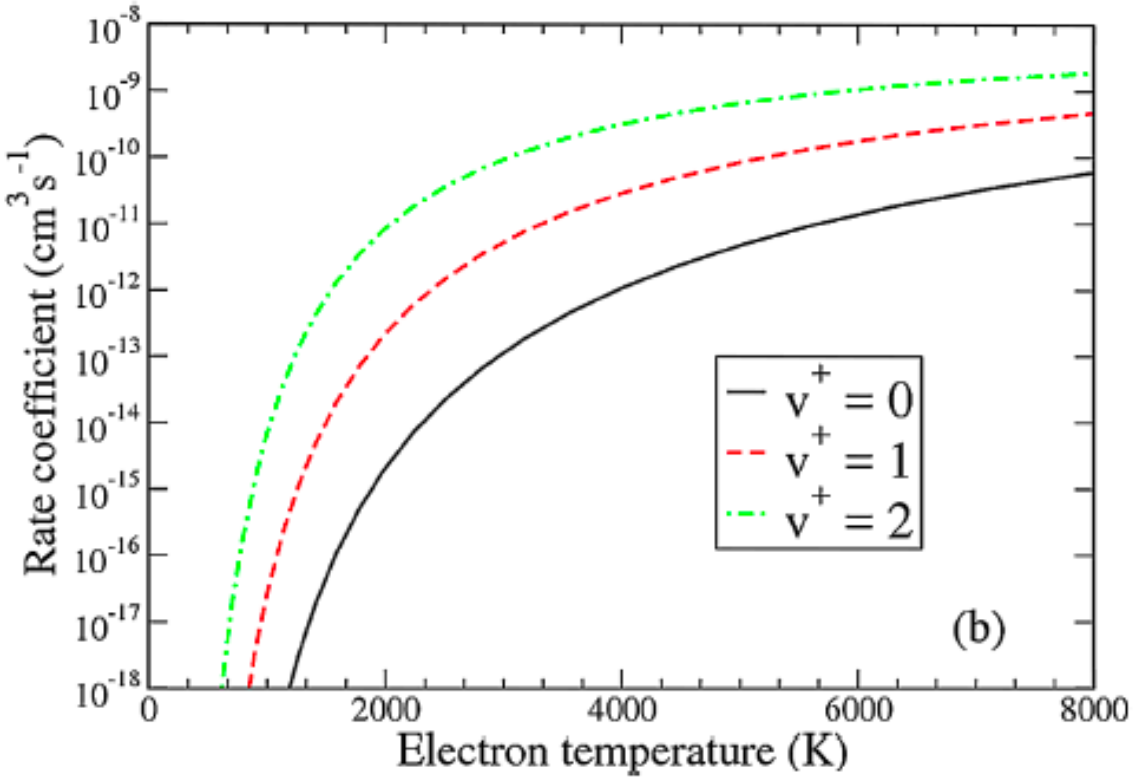

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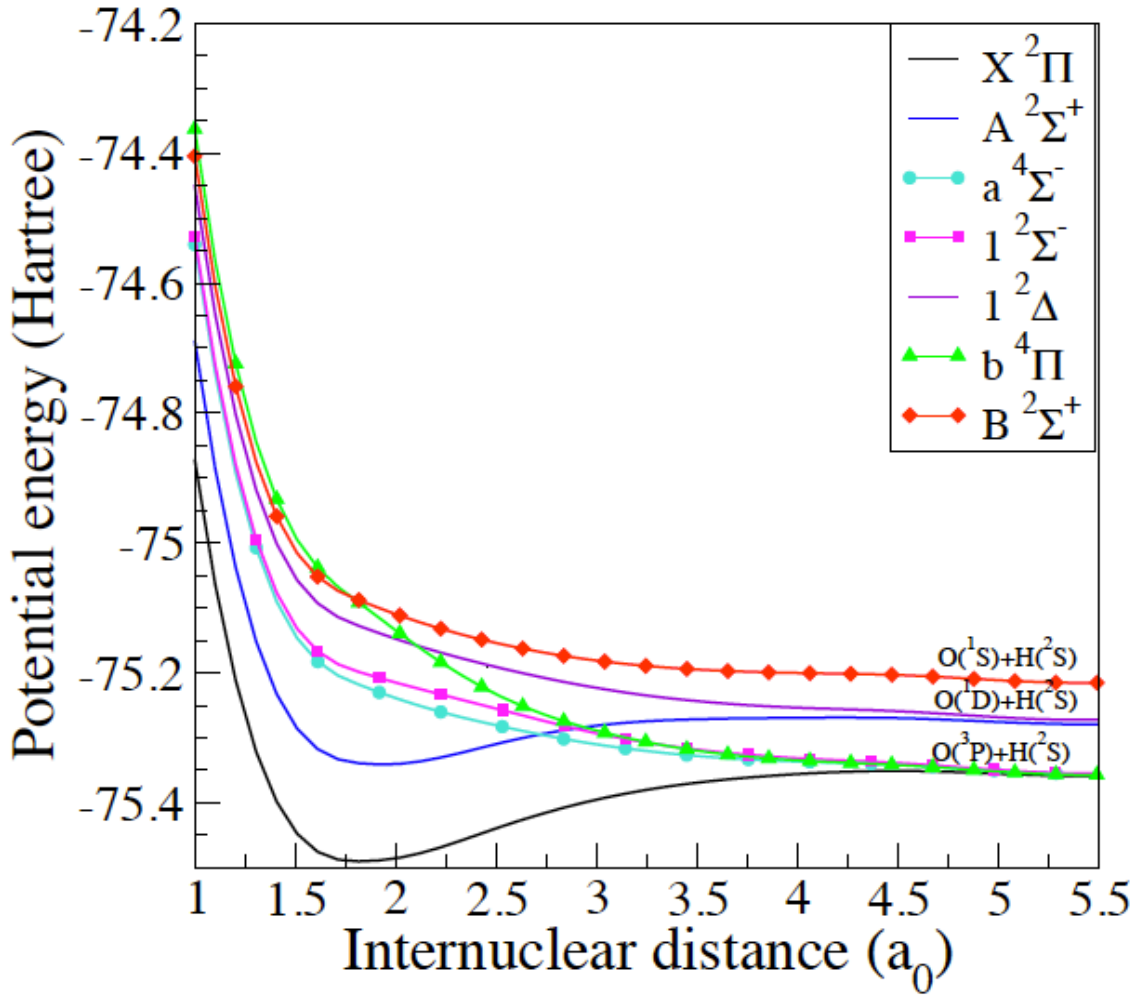
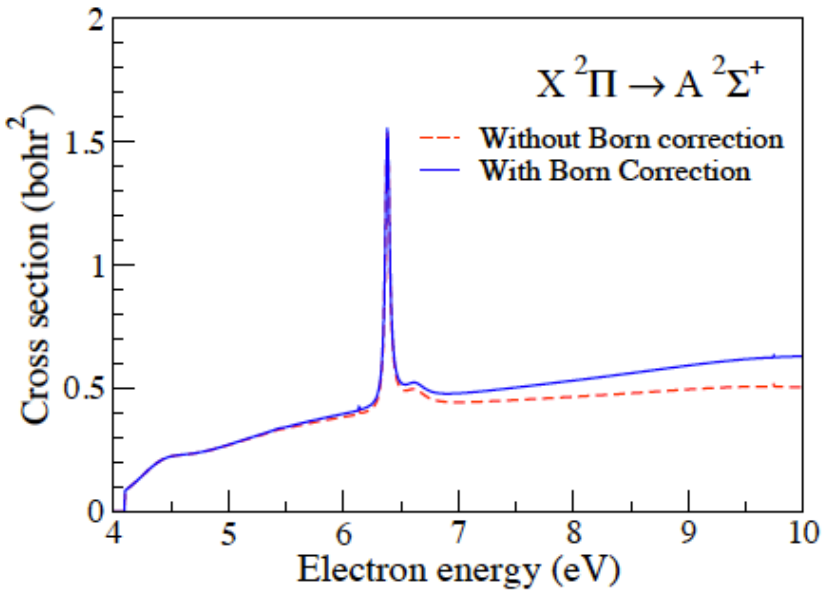
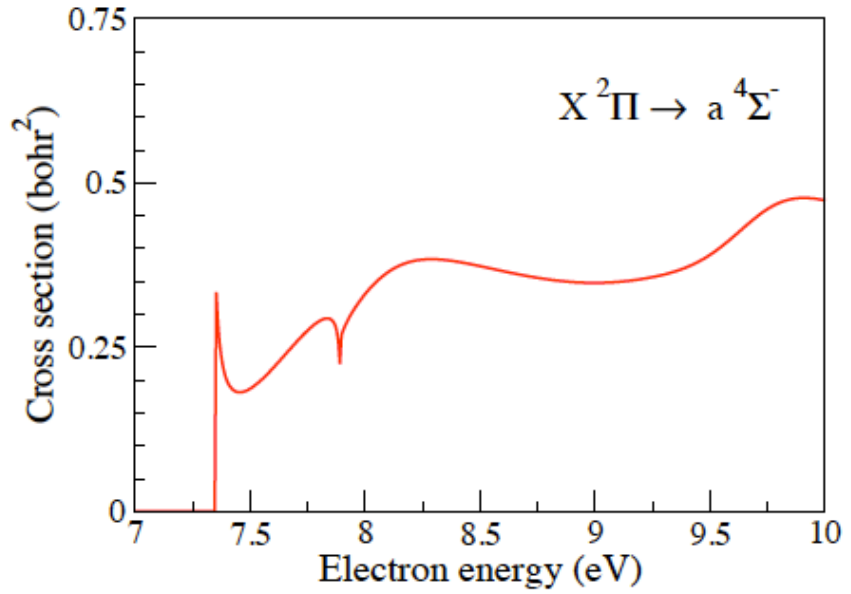
e + OH collisions

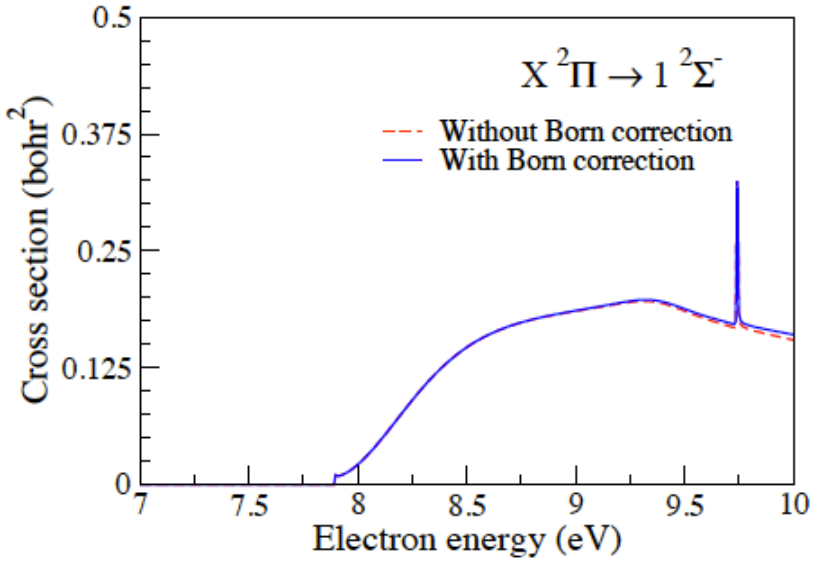
$$
\begin{aligned}
e + \mathrm{OH}(\mathrm{X}\,^2\Pi) &\rightarrow e + \mathrm{OH}(\mathrm{A}\,^2\Pi, \mathrm{a}\,^4\Sigma^-, 1\,^2\Sigma^-)\,, && \text{(EE)}\\
&\rightarrow e + \mathrm{O}(^3\mathrm{P}) + \mathrm{H}(^2\mathrm{S})\,, && \text{(DE)}\\
&\rightarrow e + \mathrm{O}(^1\mathrm{D}) + \mathrm{H}(^2\mathrm{S})\,. && \text{(DE)}\\
&\rightarrow \mathrm{O}^-(^2\mathrm{P}) + \mathrm{H}(^2\mathrm{S}) && \text{(DA)}
\end{aligned}
$$

K. Chakrabarti, V. Laporta, and Jonathan Tennyson, *submitted*, 2019


-74.2
-74.4
-74.6
-74.8
-75
-75.2
-75.4
Potential energy (Hartree)
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Internuclear distance (a0)
X 2Π
A 2Σ+
a 4Σ-
1 2Σ-
1 2Δ
b 4Π
B 2Σ+
O(1S)+H(2S)
O(1D)+H(2S)
O(3P)+H(2S)

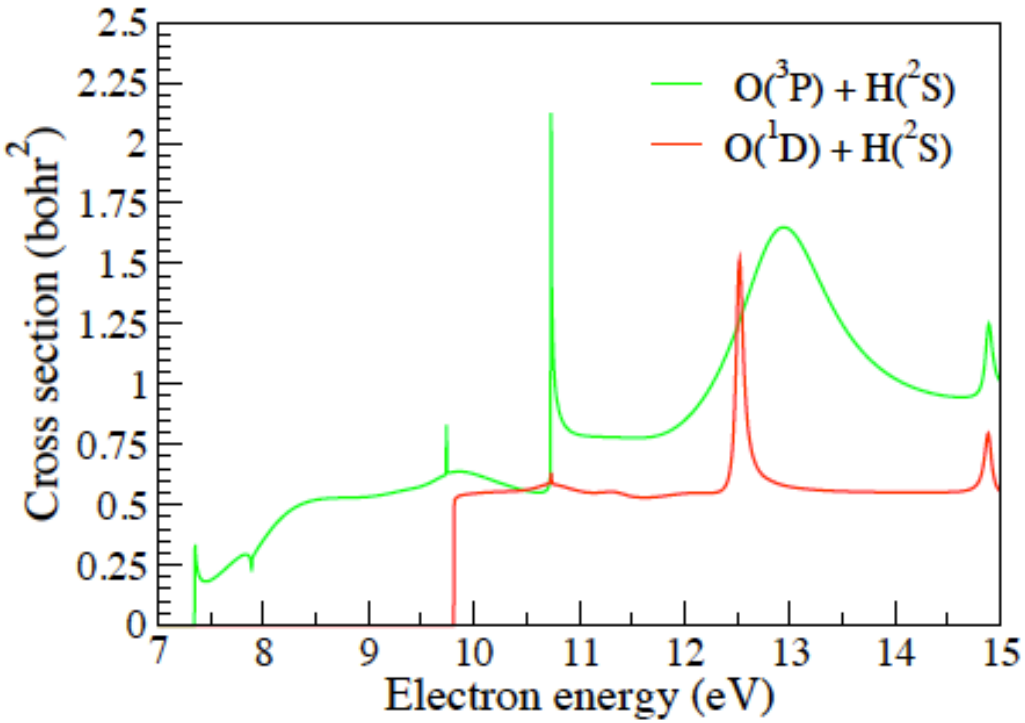

X $^2\Pi \rightarrow$ A $^2\Sigma^+$
Without Born correction
With Born Correction
Cross section (bohr^2)
Electron energy (eV)


X $^2\Pi \rightarrow$ a $^4\Sigma^-$
Cross section (bohr^2)
Electron energy (eV)

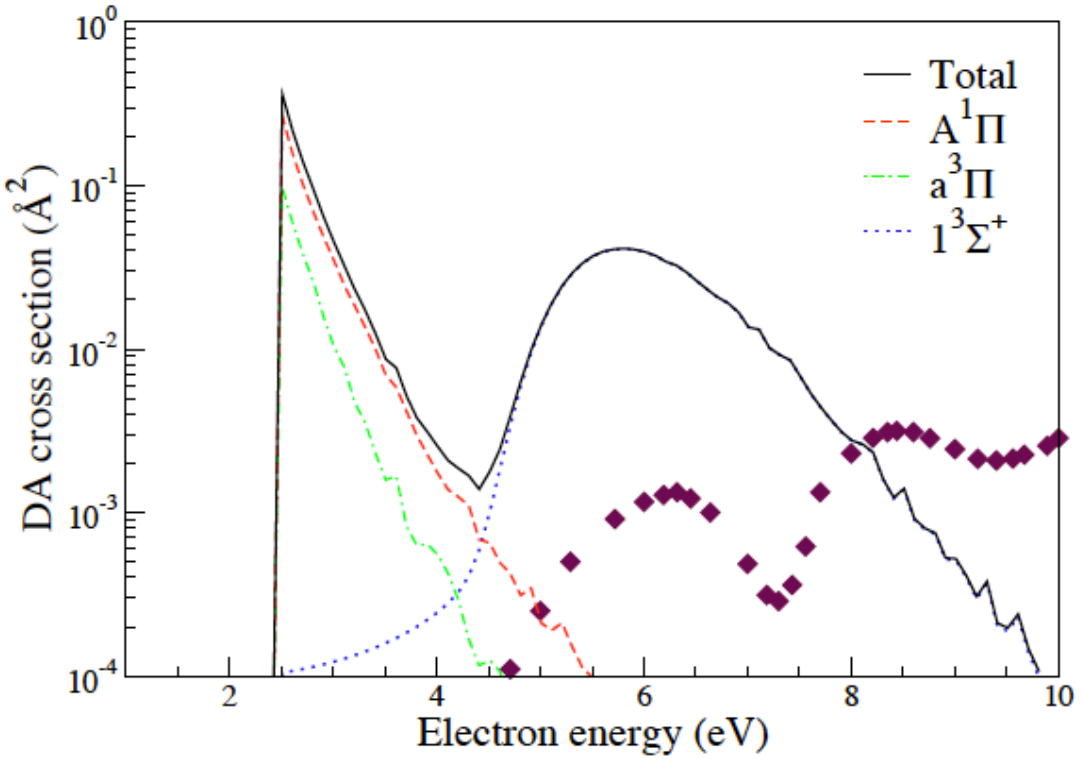

X $^2\Pi \rightarrow$ 1 $^2\Sigma^-$
Without Born correction
With Born correction
Cross section (bohr^2)
Electron energy (eV)

@ $R=R_{eq}$

Dissociation



Dissociative electron attachment



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   A. **Nitrogen and Oxygen:** Atmospheric (re-)entry and hypersonic
   B. **Carbon dioxide:** Plasma-based CO_2 conversion
   C. **BeH^+, H_2^+, OH, ArH^+:** I.T.E.R and controlled fusion; Astrochemistry

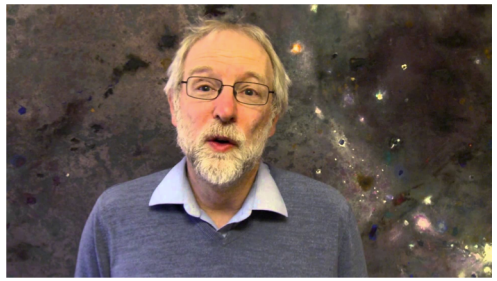
3. Conclusions and perspectives

Conclusions and perspectives

- *Ab-initio* molecular Quantum dynamics*;*
- State specific cross sections and rate coefficients for vibrational excitation, dissociative attachment, dissociative recombination and dissociative excitation processes;
- Non-equilibrium molecular plasmas modelling;
- Extensions to atom-molecule and molecule-molecule scattering in particular for the reaction:

$$Be^+ + H_2 \rightarrow BeH^+ + H$$
$$Be^+ + H_2 \rightarrow BeH + H^+$$

- Data base for e + H_2 and e + H_2^+ collisions.



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Thank you for your attention

Carte du monde "électron-molécule"

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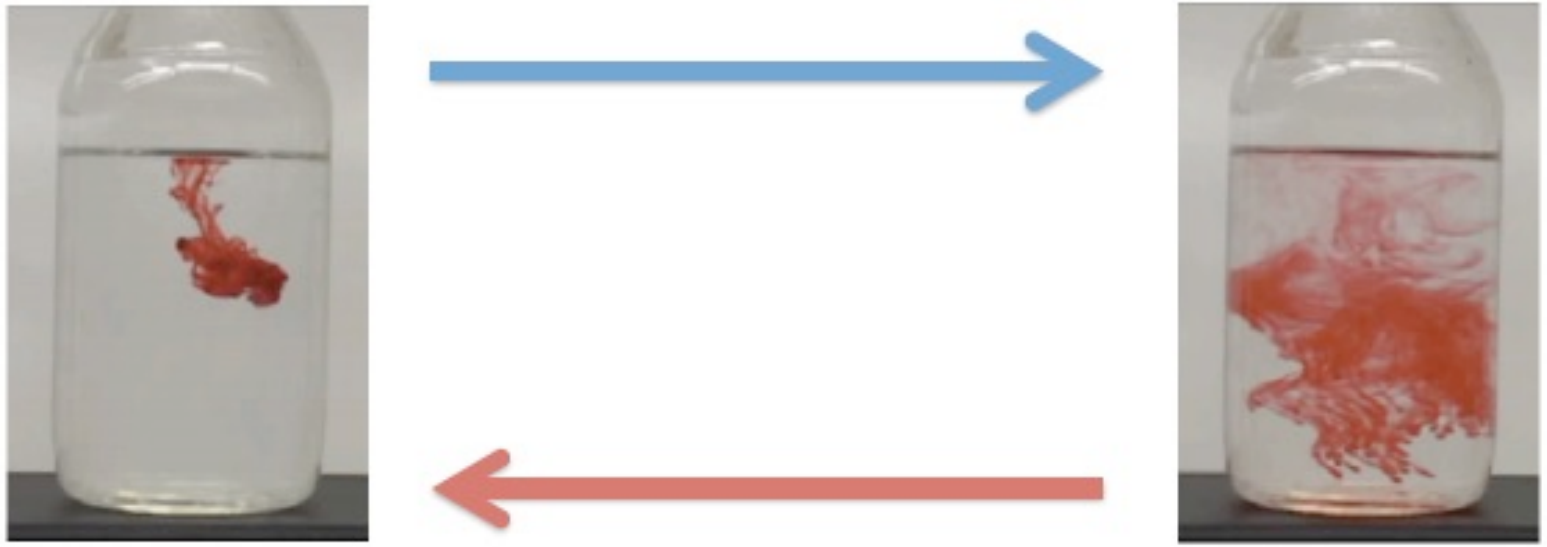
Non-equilibrium molecular plasmas modelling

- *Non-equilibrium thermodynamics* is an extension of equilibrium thermodynamics it attempts to describe the physical processes in their ***time-courses*** in continuous detail.

- A central role in non-equilibrium thermodynamics is played by ***transport equations*** which are the corresponding to equations of state in equilibrium thermodynamics.

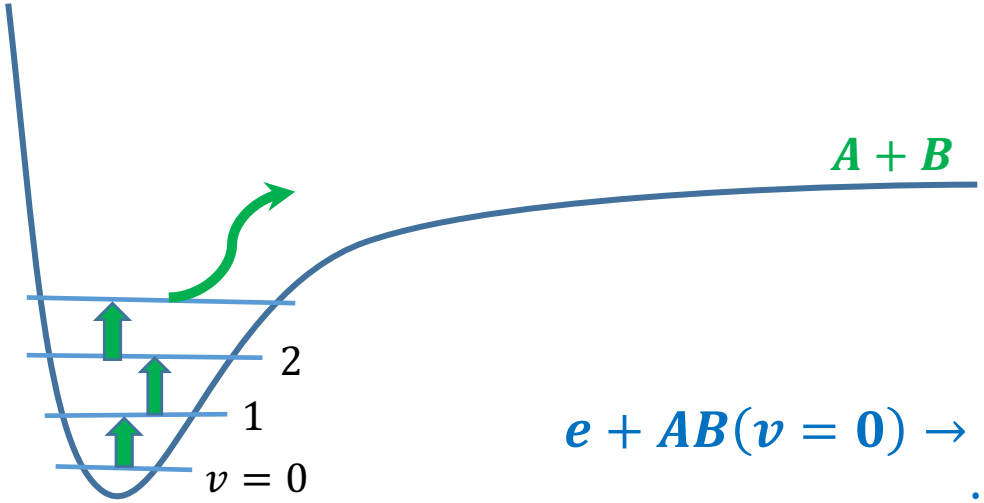
- Transport equations describe the amount of heat, mass, electrical charge… which are transferred per unit time between different systems and different regions of a system as a response to a non-homogeneity in temperature *T*, molar concentration *c*, electric potential φ_e…

$$\boldsymbol{q} = -\lambda \nabla T \quad \text{(Fourier's law)},$$
$$\boldsymbol{J} = -D \nabla c \quad \text{(Fick's law)},$$
$$\boldsymbol{I} = \sigma_{\mathrm{e}} \nabla \varphi_{\mathrm{e}} \quad \text{(Ohm's law)}.$$



Applications: non-equilibrium dissociation mechanism

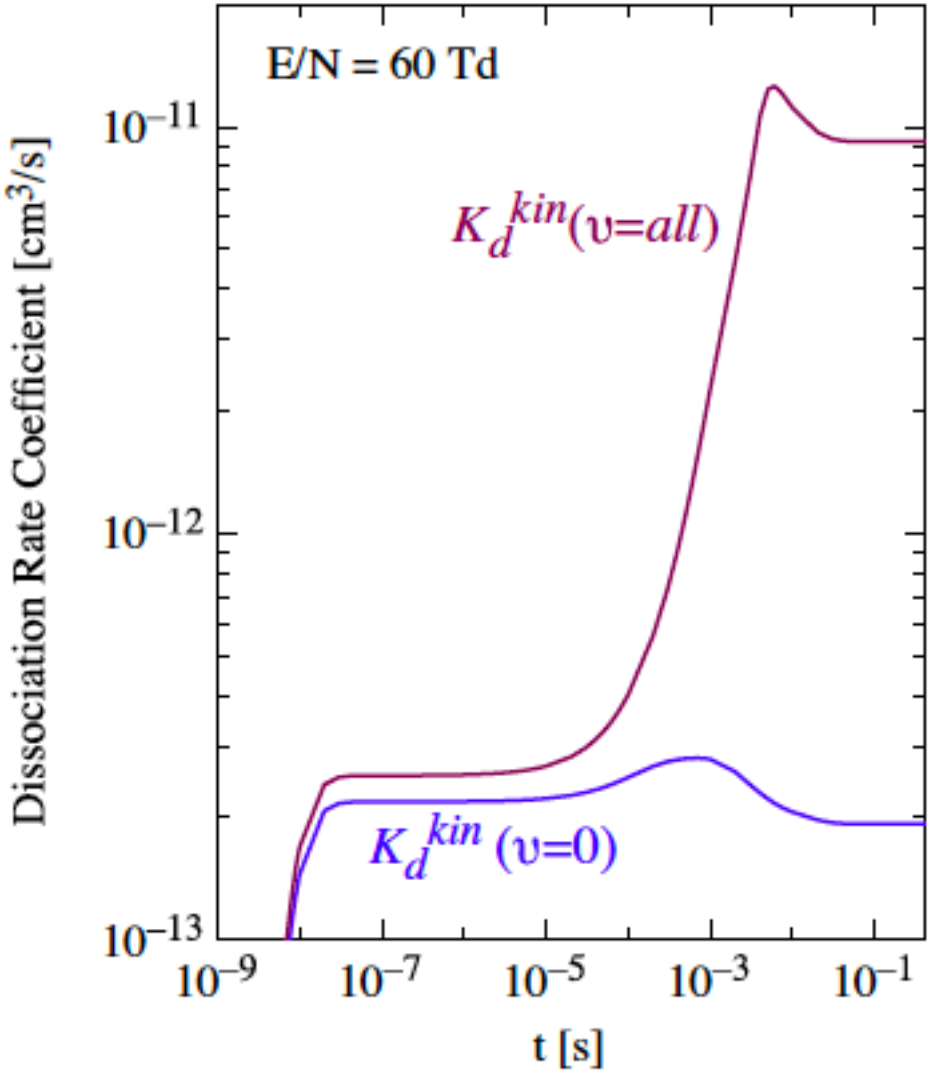
- Despite its apparent simplicity, the dissociation rate for a molecule is very difficult to be determined
- Polak shows that experimental dissociation rates cannot be reproduced by direct electron impact dissociation involving vibrational ground state of molecules.
- The “pure-vibrational-mechanism” is the theoretical framework to explain the dissociation rate

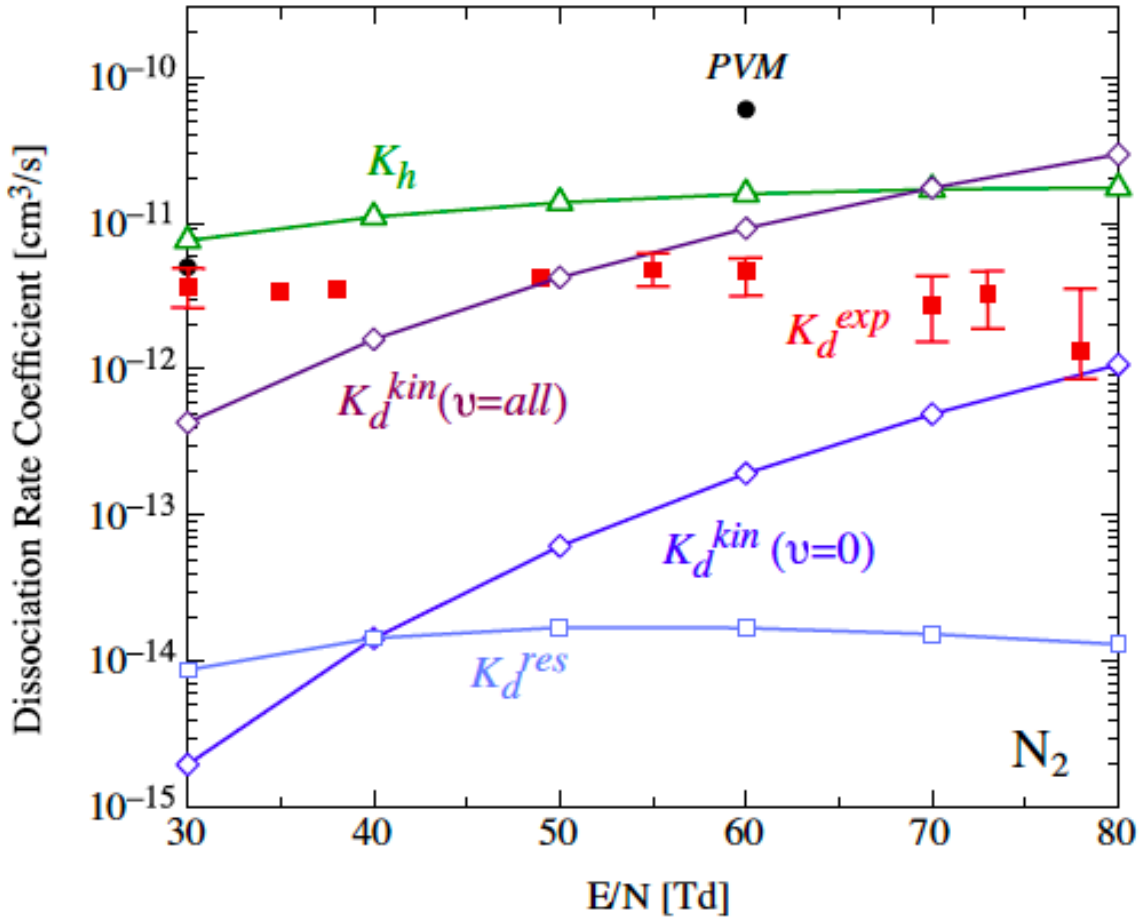


$$k_d^{kin} = \sum_{v=0}^{v_{max}} k_d^{kin}(v) \frac{N_v}{N_{tot}}$$

$$\boldsymbol{e + AB(v = 0)} \rightarrow e + AB(v = 1) \rightarrow \cdots$$
$$\cdots e + AB(v = n) \rightarrow \boldsymbol{A + B + e}$$

M. Capitelli, G. Colonna, V. Laporta et al., Chemical Physics 438, 31 (2014)





M. Capitelli, G. Colonna, V. Laporta et al., Chemical Physics 438, 31 (2014)

Titres universitaires :

2007 – Doctorat en physique, Université de Bari, Italie (séjours à Lyon et au CERN à Genève)
2010 – Qualification pour maitre de conférences - section 29 (France)
2017 – Qualification pour maitre de conférences - section 30 (France)
2017 – Habilitation scientifique national - section 02/B2 et 03/A2 (Italie)
2017 – Habilitation à Diriger les Recherches, Université du Havre, France
2018 – Qualification pour professeur - section 30 (France)

Parcours professionnel après la thèse :

2006 – 2007 Centre de Physique Théorique, CNRS-École Polytechnique, Palaiseau Cedex, France
2007 – 2009 Dipartimento interateneo di fisica, Università di Bari, Italia
2009 – 2010 Institut de Physique Nucléaire de Lyon, Université Claude Bernard Lyon-1, France **(A.T.E.R.)**
2010 – 2011 Istituto di Metodologie Inorganiche e dei Plasmi, Consiglio Nazionale delle Ricerche, Bari, Italie
2011 – 2013 Department of Physics and Astronomy, University College London, London (UK); Prof. J. Tennyson
2013 – 2015 Istituto di Nanotecnologia-CNR et DICATECh-Politecnico di Bari (Italie)
Juillet 2013 Ames Research Center, NASA, Moffett Field (CA), USA; Prof. R.L. Jaffe;
2015 – 2015 Ohio Aerospace Institute et Air Force Research Laboratory-WPAFB, Dayton (OH) - USA
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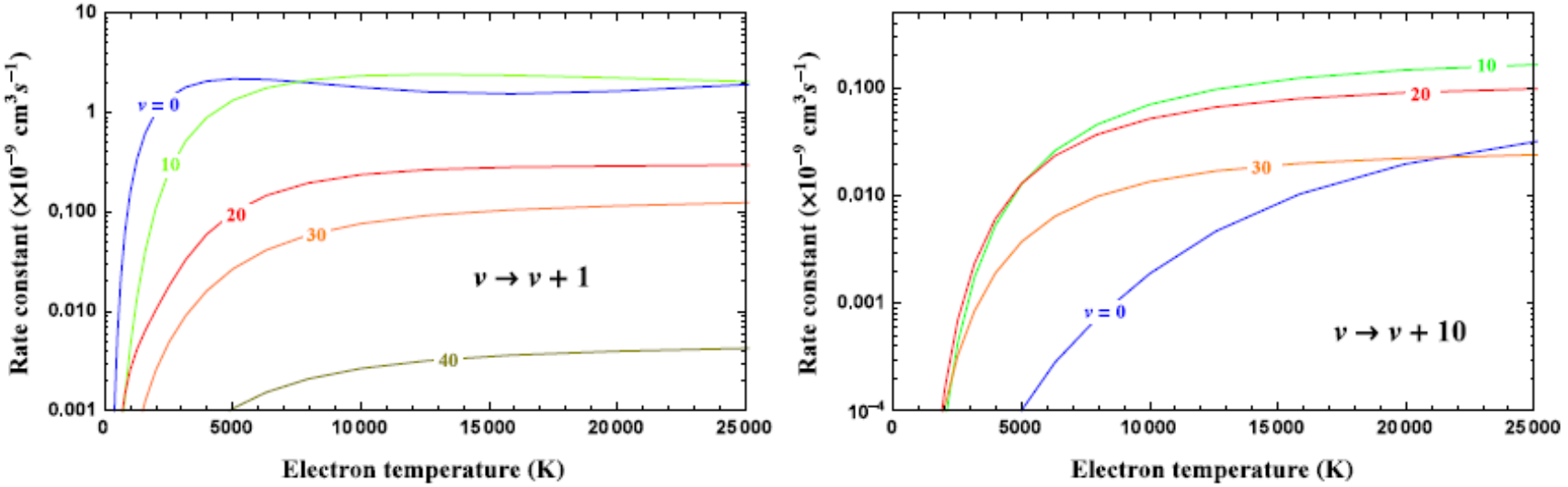
Application: Electron-vibration relaxation in oxygen plasmas

$$e + \mathrm{O}_2(\mathrm{X}^3\Sigma_g^-; v, j) \rightleftarrows e + \mathrm{O}_2(\mathrm{X}^3\Sigma_g^-; w, j), \quad \text{(VE)}$$

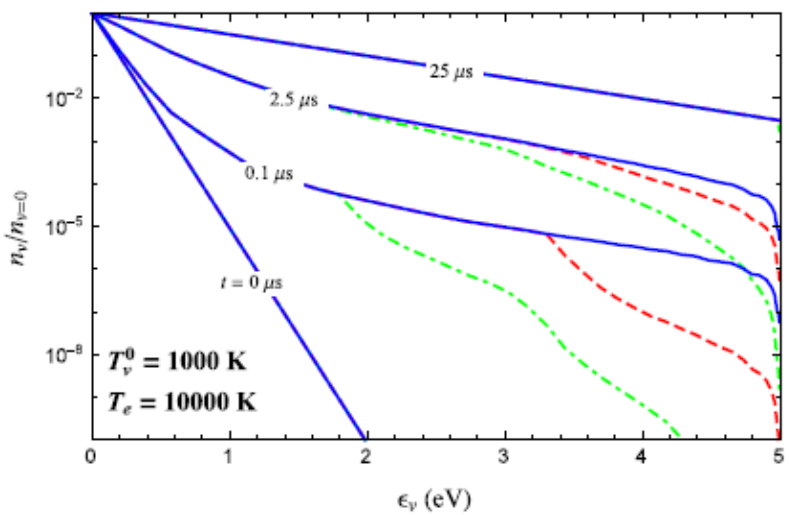
- State-to-State vibrational kinetics
- Vibrational relaxation time is comparable to chemical relaxation: **vibrational non-equilibrium**

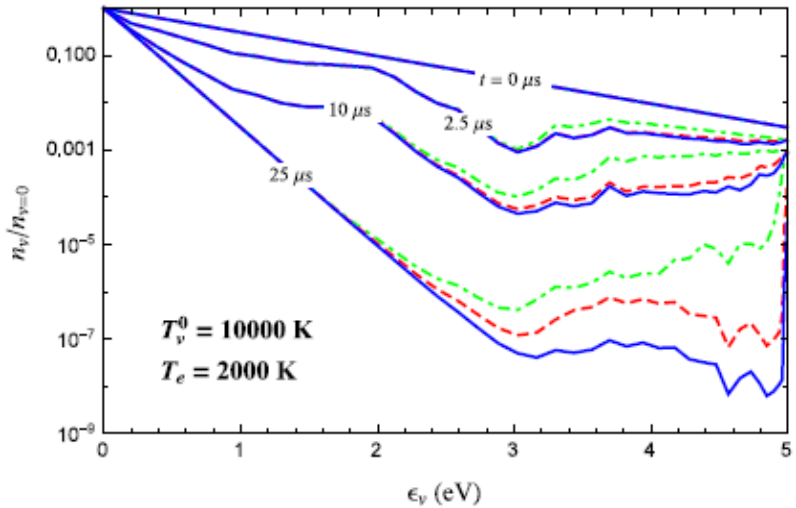
$$\frac{dn_v}{dt} = n_e \sum_{w \in \mathcal{V}} [k_{w,v}\, n_w - k_{v,w}\, n_v], \quad v \in \mathcal{V},$$



V. Laporta, K.L. Heritier and M. Panesi, Chemical Physics **472** (2016) 44–49

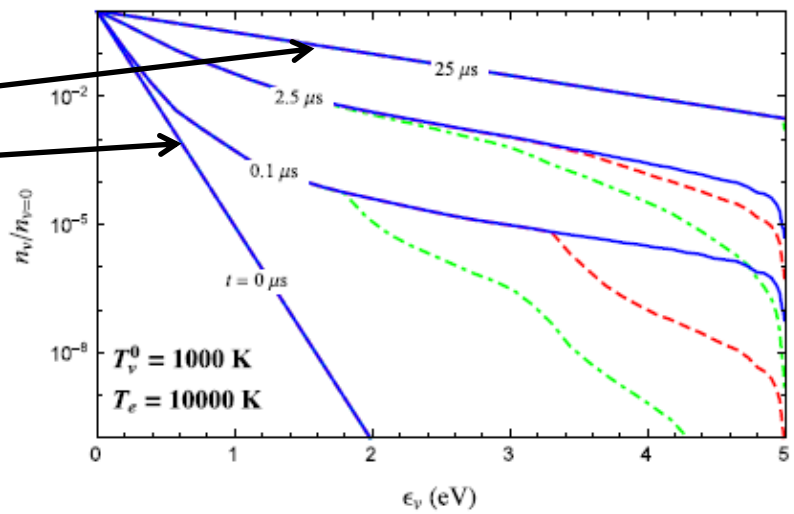
Time evolution of **non-equilibrium** vibrational distribution function:

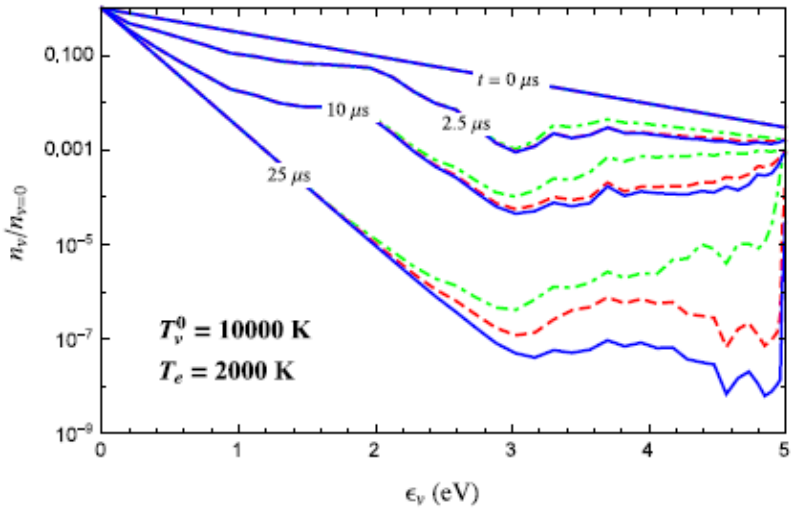




Time evolution of **non-equilibrium** vibrational distribution function:

Equilibrium distribution

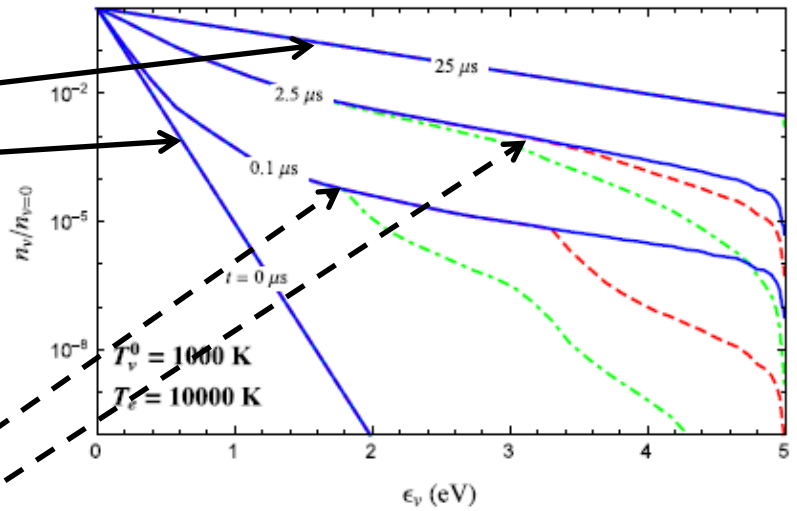


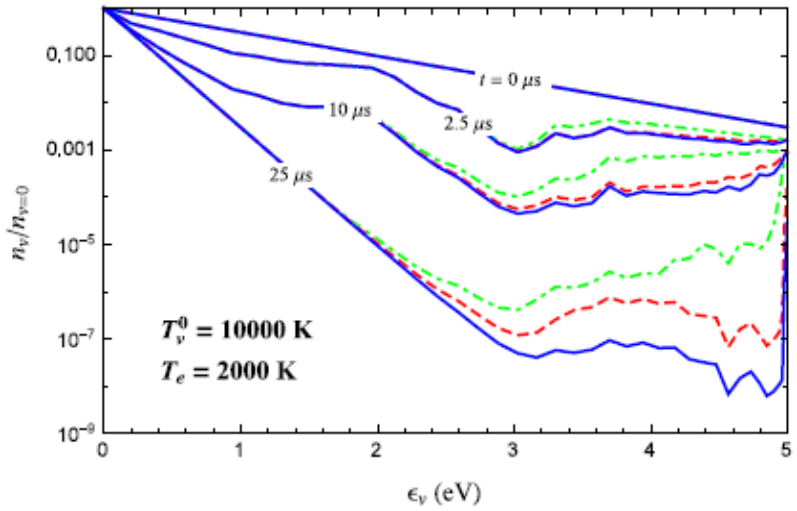


Time evolution of **non-equilibrium** vibrational distribution function:

Equilibrium distribution

Non-equilibrium distribution





Vibrational relaxation time: