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Electron-molecule collisions in fusion plasmas: a long-standing collaboration with Professor Ratko Janev

R. Celiberto

30th Summer School and International Symposium on the Physics of Ionized Gases
24-28 August, 2020, Sabac (Serbia)

Jülich - 2012

Belgrade - 2016

Electron-molecule collisions

Electron-molecule collisions

- Non-equilibrium low temperature plasma modeling
  - Non-Boltzmann population
  - non-Maxwellian electron energy distribution function

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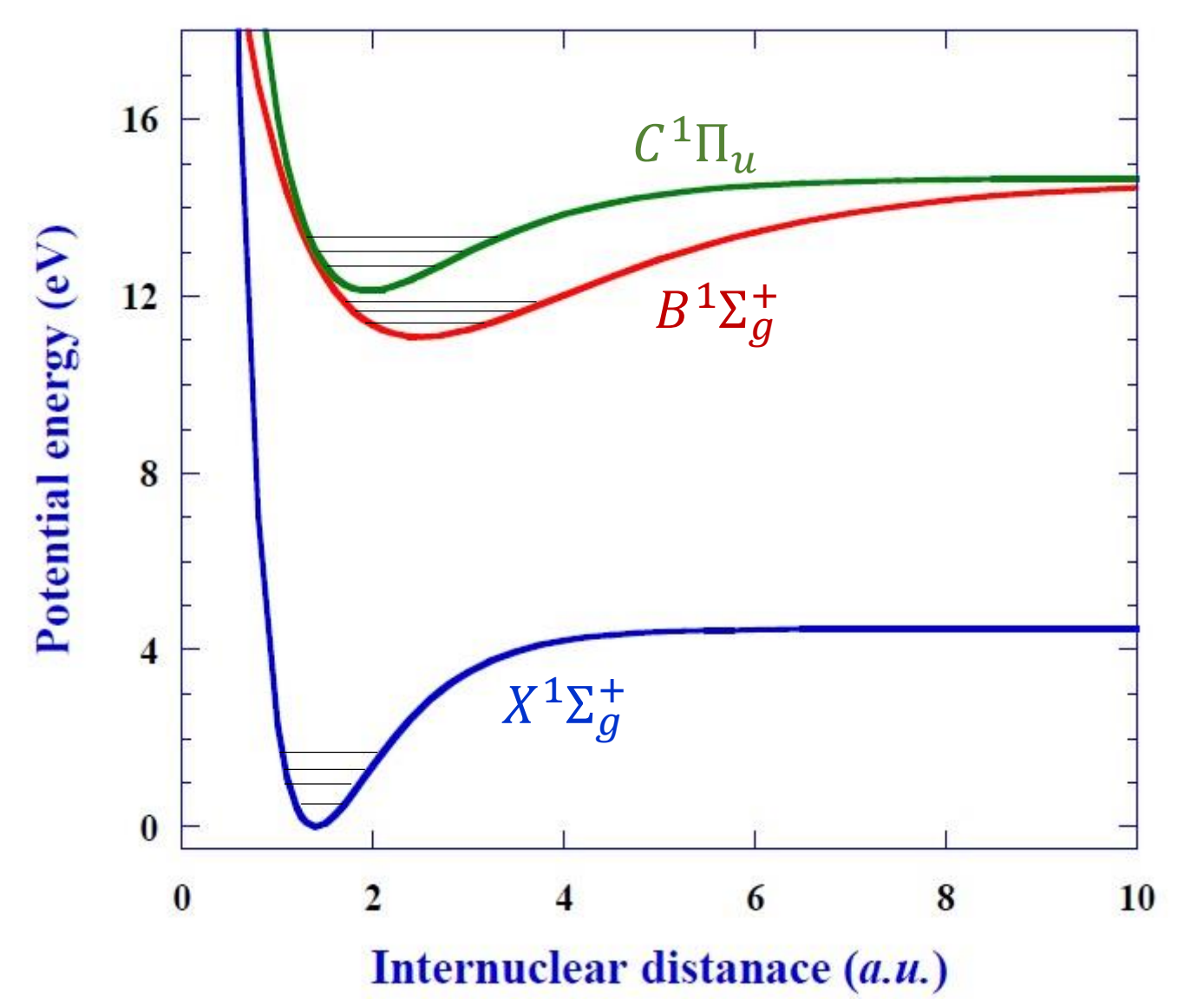
Electron-molecule collisions

- Non-equilibrium low temperature plasma modeling
  - Non-Boltzmann population
  - non-Maxwellian electron energy distribution function
- State-to-state vibrational kinetics
- Large sets of cross section data

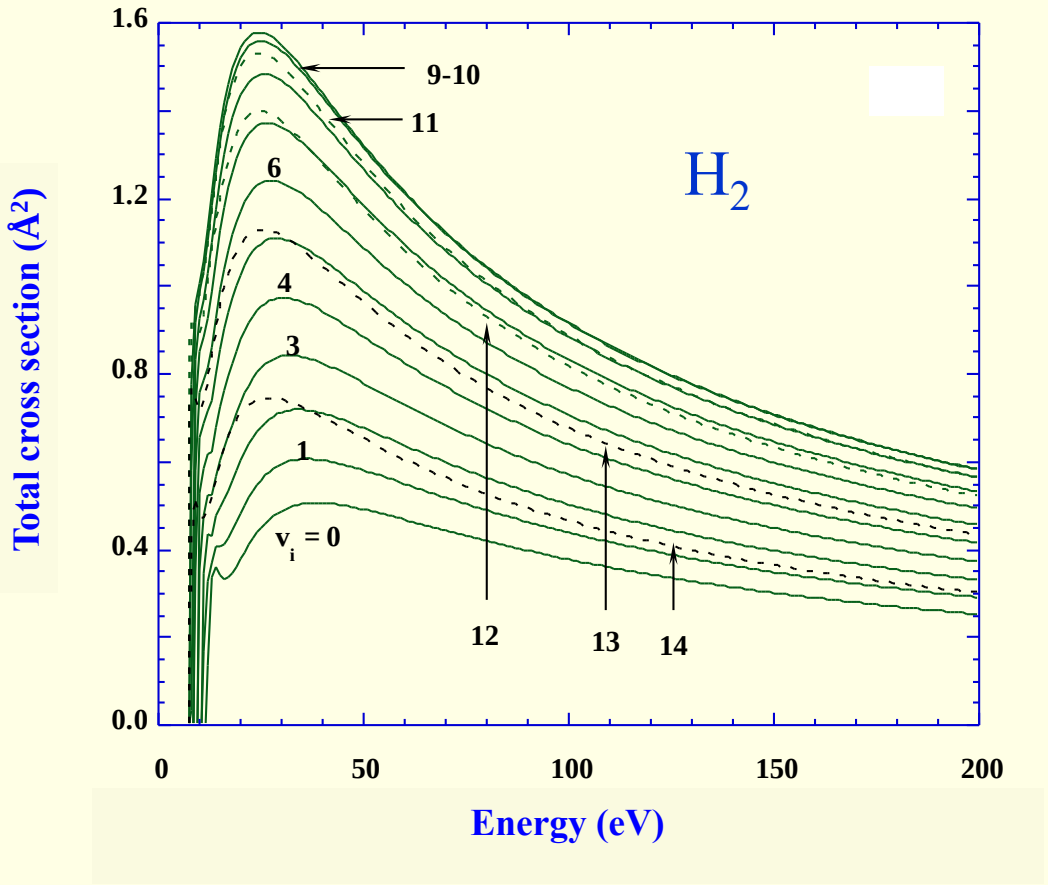
Electron-molecule collisions

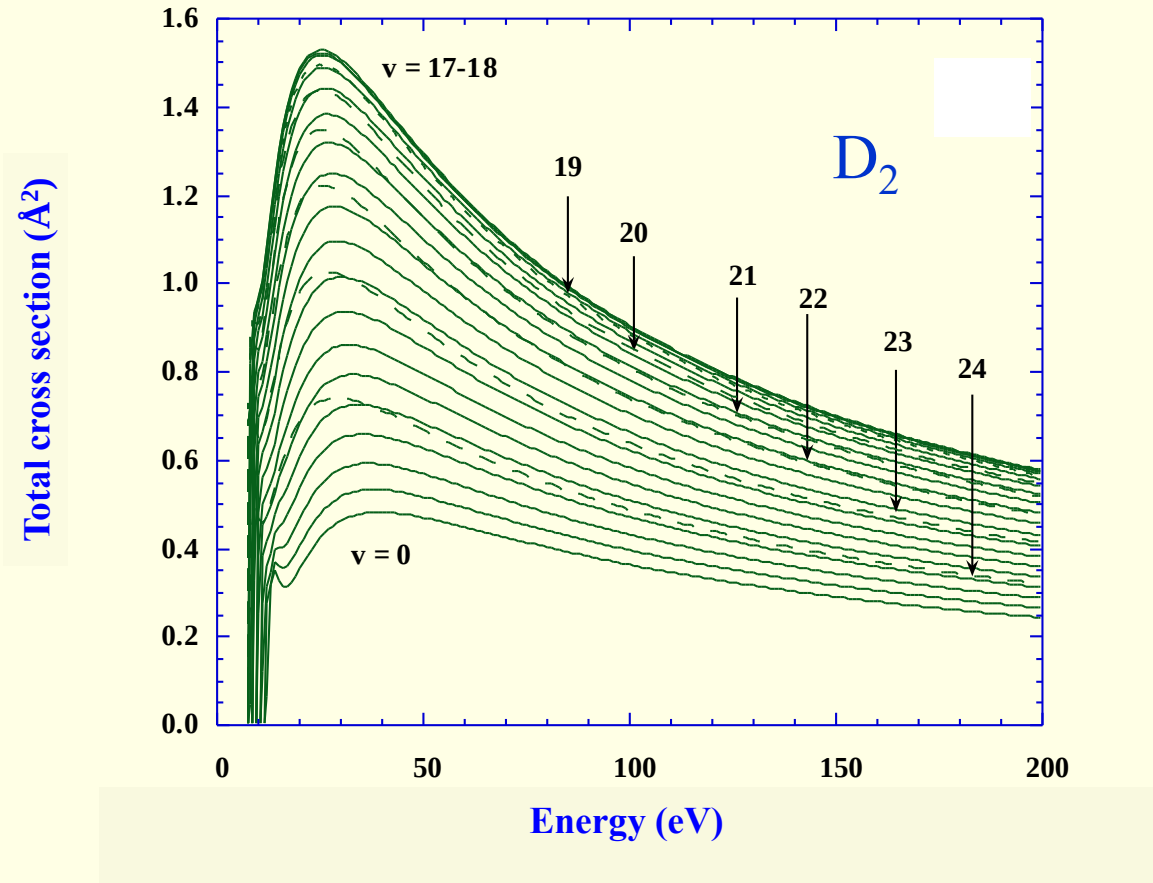
- Non-resonant processes
- Resonant processes

$$H_2(X; v_i) + e \rightarrow H_2(B\,^1\Sigma_g^+, C\,^1\Pi_u) + e$$



$$H_2/D_2(X^1\Sigma_g^+; v = 0 - 14) + e \rightarrow H_2/D_2(B^1\Sigma_g^+) + e$$





International Atomic Energy Agency

INDC(NDS)-333
Distr.:

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

ANALYTICAL REPRESENTATION OF ELECTRON IMPACT EXCITATION CROSS SECTIONS OF VIBRATIONALLY EXCITED H_2 AND D_2 MOLECULES

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International Atomic Energy Agency, Vienna, Austria

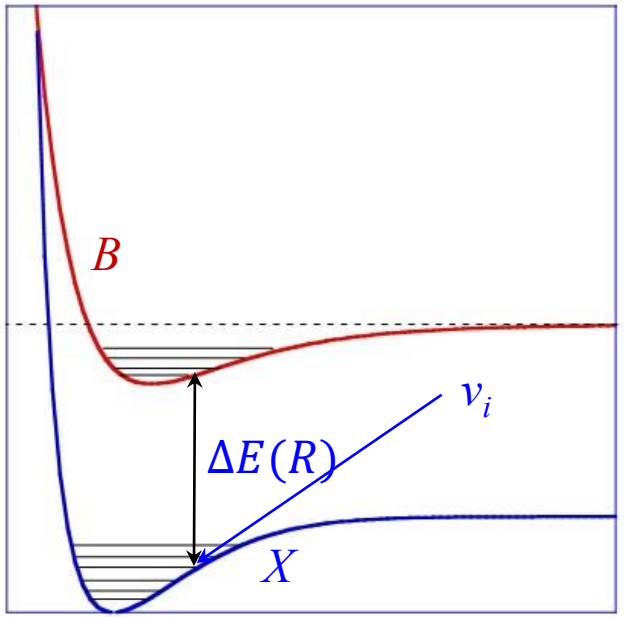
February 1995

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

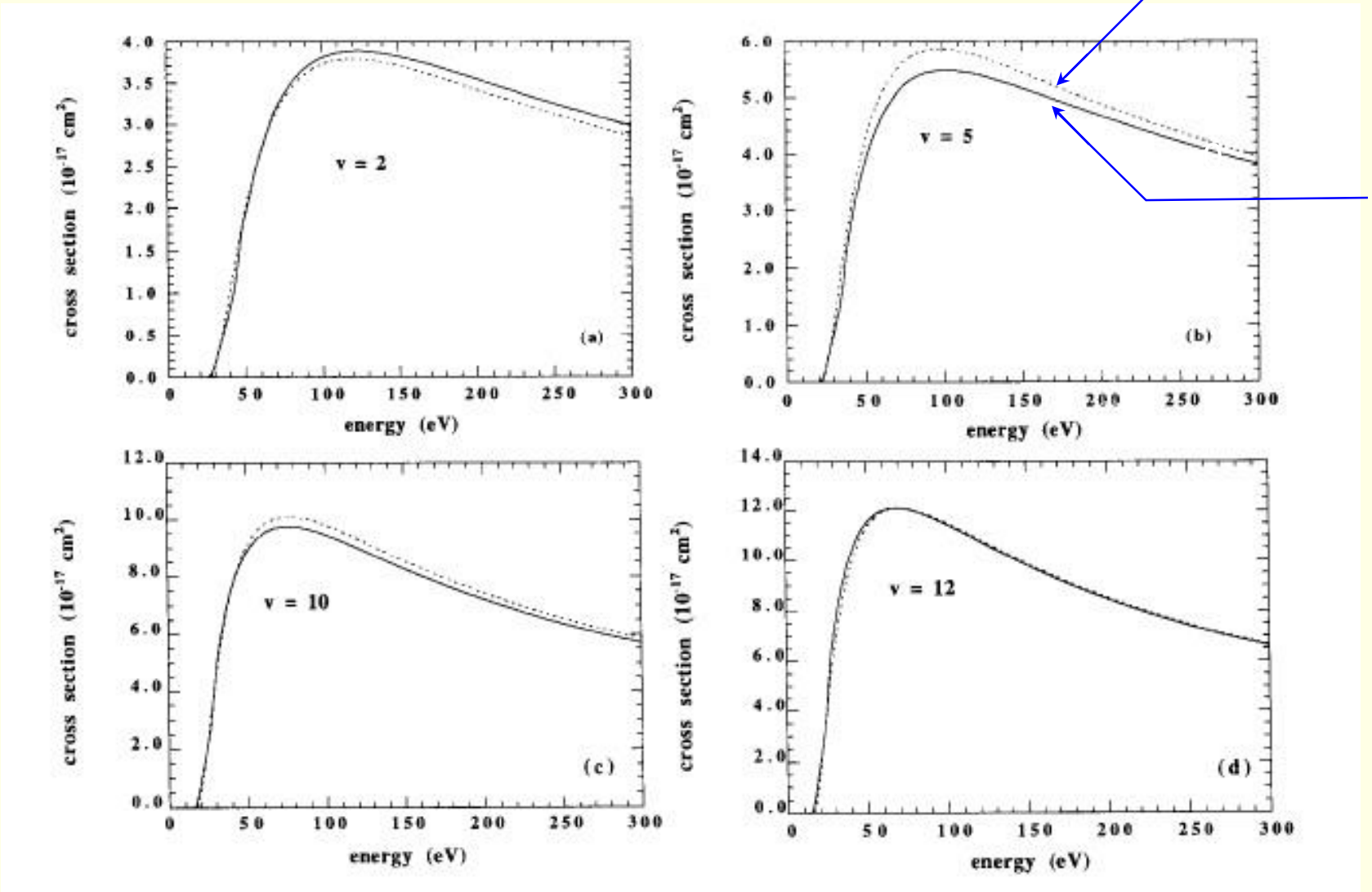
$$\sigma_{v_i}^{X\to B}(x) \approx \tilde{\sigma}(x)\frac{1}{\left|\Delta E_{X,B}(R_{v_i})\right|^3}$$

$$x = E / \Delta E_{X,B}(R_{v_i})$$

$$\tilde{\sigma}(x) = \frac{20013}{x}\left(\frac{x}{x-1}\right)^{2.6323}\left(1+0.57363\ln x\right)$$



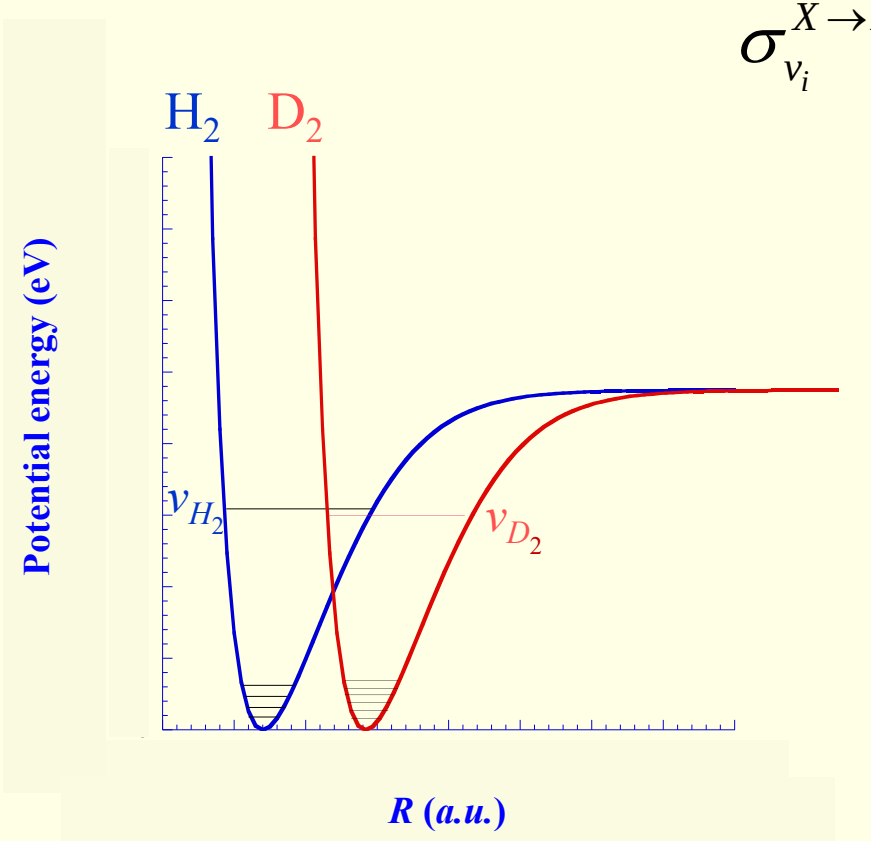
$$H_2(X) + e \rightarrow H_2(B) + e$$



Analytic expression

calculated

$$\sigma_{v_i}^{X\to B}(x) \approx \tilde{\sigma}(x)\frac{1}{\left|\Delta E_{X\to B}(R_{v_i})\right|^{\gamma}}$$



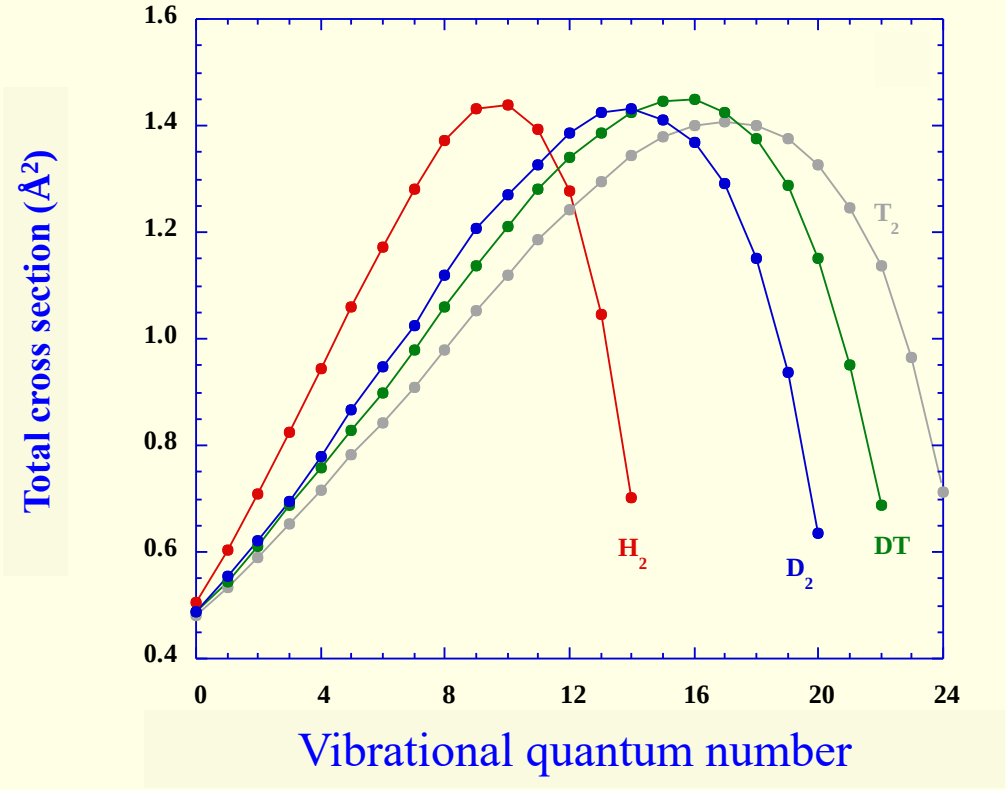
$$E_{v_{H_2}} \approx E_{v_{D_2}} \qquad \hbar\omega_{H_2} v_{H_2} \approx \hbar\omega_{D_2} v_{D_2}$$

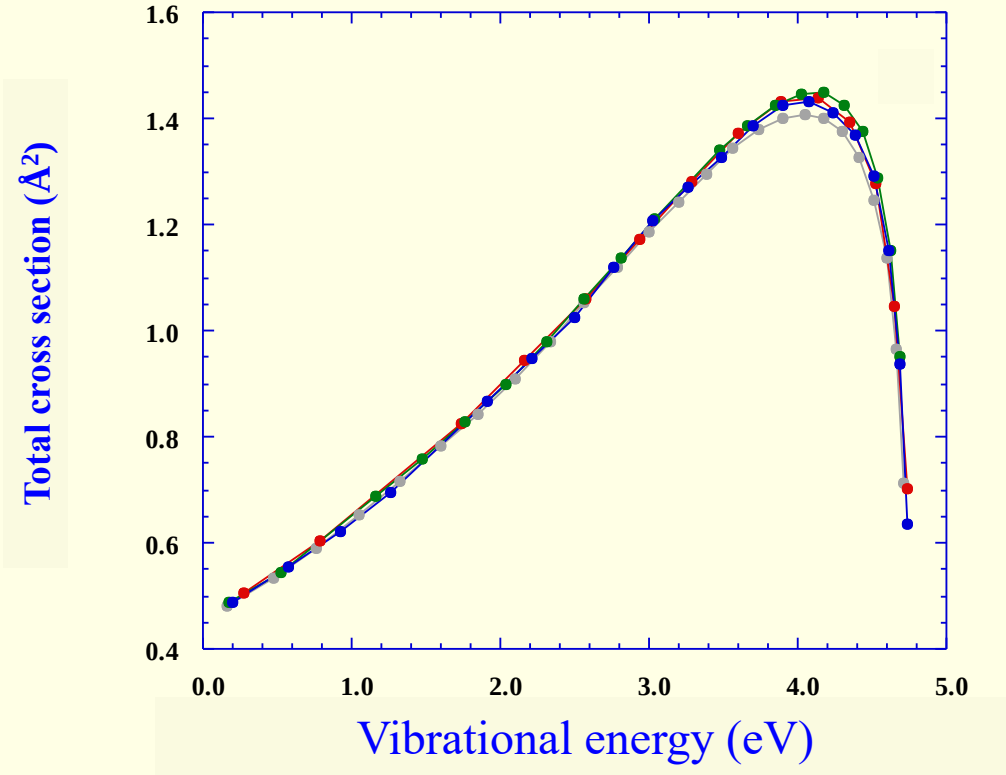
$$v_{H_2} \approx v_{D_2}\frac{\omega_{D_2}}{\omega_{H_2}} \qquad v_{H_2} \approx v_{D_2}\sqrt{\frac{m_{H_2}}{m_{D_2}}}$$

$$v_{H_2} \approx v_{D_2}\sqrt{\frac{1}{2}}$$

$$X \rightarrow B$$

$$E = 40 \text{ eV}$$





R. Celiberto, A. Laricchiuta, R. K. Janev
Physica Scripta (2001)

Atomic Data and Nuclear Data Tables 77, 161–213 (2001)
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CROSS SECTION DATA FOR ELECTRON-IMPACT INELASTIC PROCESSES OF VIBRATIONALLY EXCITED MOLECULES OF HYDROGEN AND ITS ISOTOPES

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An extensive cross section database for the electron-impact inelastic processes of vibrationally excited molecules of hydrogen and its isotopes is presented. The following inelastic processes are covered: electronic excitation (dissociative and nondissociative), direct ionization (dissociative and nondissociative), excitation-radiative decay vibrational excitation and dissociation, and dissociative electron attachment. The data have been compiled partly from the literature and partly generated theoretically for the present report. The data are presented in graphical form. The data are also presented by sufficiently accurate analytic fit functions. Mass-scaling relations are provided for cross section evaluation of those isotope molecules for which calculated data are not available. © 2001 Academic Press

Vibro-electronic transitions

Dissociation

$$H_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow H_2(B\,^1\Sigma_u^+) + e \rightarrow 2H + e$$
$$D_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow D_2(B\,^1\Sigma_u^+) + e \rightarrow 2D + e$$
$$T_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow T_2(B\,^1\Sigma_u^+) + e \rightarrow 2T + e$$
$$DT(X\,^1\Sigma_g^+, v_i) + e \rightarrow DT(B\,^1\Sigma_u^+) + e \rightarrow D + T + e$$

$$H_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow H_2(C\,^1\Pi_u) + e \rightarrow 2H + e$$
$$D_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow D_2(C\,^1\Pi_u) + e \rightarrow 2D + e$$
$$T_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow T_2(C\,^1\Pi_u) + e \rightarrow 2T + e$$
$$DT(X\,^1\Sigma_g^+, v_i) + e \rightarrow DT(C\,^1\Pi_u) + e \rightarrow D + T + e$$

$$H_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow H_2(B'\,^1\Sigma_u^+) + e \rightarrow 2H + e$$
$$D_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow D_2(B'\,^1\Sigma_u^+) + e \rightarrow 2D + e$$

$$H_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow H_2(D\,^1\Pi_u) + e \rightarrow 2H + e$$
$$D_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow D_2(D\,^1\Pi_u) + e \rightarrow 2D + e$$

$$H_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow H_2(B''\,^1\Sigma_u^+) + e \rightarrow 2H + e$$
$$D_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow D_2(B''\,^1\Sigma_u^+) + e \rightarrow 2D + e$$

$$H_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow H_2(D'\,^1\Pi_u) + e \rightarrow 2H + e$$
$$D_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow D_2(D'\,^1\Pi_u) + e \rightarrow 2D + e$$

$$H_2(B\,^1\Sigma_u^+, v_i) + e \rightarrow H_2(I\,^1\Pi_g) + e \rightarrow 2H + e$$

$$H_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow H_2(b\,^3\Sigma_u^+) + e \rightarrow 2H + e$$
$$D_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow D_2(b\,^3\Sigma_u^+) + e \rightarrow 2D + e$$

Total excitation

$$H_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow H_2(B\,^1\Sigma_u^+) + e$$
$$D_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow D_2(B\,^1\Sigma_u^+) + e$$
$$T_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow T_2(B\,^1\Sigma_u^+) + e$$
$$DT(X\,^1\Sigma_g^+, v_i) + e \rightarrow DT(B\,^1\Sigma_u^+) + e$$

$$H_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow H_2(C\,^1\Pi_u) + e$$
$$D_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow D_2(C\,^1\Pi_u) + e$$
$$T_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow T_2(C\,^1\Pi_u) + e$$
$$DT(X\,^1\Sigma_g^+, v_i) + e \rightarrow DT(C\,^1\Pi_u) + e$$

$$H_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow H_2(B'\,^1\Sigma_u^+) + e$$
$$D_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow D_2(B'\,^1\Sigma_u^+) + e$$

$$H_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow H_2(D\,^1\Pi_u) + e$$
$$D_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow D_2(D\,^1\Pi_u) + e$$

$$H_2(X\,^1\Sigma_g^+, v_i) + e \rightarrow H_2(B''\,^1\Sigma_u^+) + e$$
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$$H_2(B\,^1\Sigma_u^+, v_i) + e \rightarrow H_2(I\,^1\Pi_g) + e$$

Ionization

Dissociative

$$H_2(X\,{}^1\Sigma_g^+, v_i) + e \rightarrow H_2^+(X\,{}^2\Sigma_g^+) + 2e \rightarrow H + H^+ + 2e$$

$$D_2(X\,{}^1\Sigma_g^+, v_i) + e \rightarrow D_2^+(X\,{}^2\Sigma_g^+) + 2e \rightarrow D + D^+ + 2e$$

$$H_2(X\,{}^1\Sigma_g^+, v_i) + e \rightarrow H_2^+({}^2\Sigma_u^+) + 2e \rightarrow H + H^+ + 2e$$

$$D_2(X\,{}^1\Sigma_g^+, v_i) + e \rightarrow D_2^+({}^2\Sigma_u^+) + 2e \rightarrow D + D^+ + 2e$$

Non-dissociative

$$D_2(X\,{}^1\Sigma_g^+, v_i) + e \rightarrow D_2^+(X\,{}^2\Sigma_g^+) + 2e$$

Radiative decay

($M_2 \equiv H_2, D_2$)

Vibrational excitation

$$M_2(X\ ^1\Sigma_g^+, v_i) + e \rightarrow M_2(B\ ^1\Sigma_u^+, C\ ^1\Pi_u) + e \rightarrow M_2(X\ ^1\Sigma_g^+, v_f) + e + h\nu$$

Dissociation

$$M_2(X\ ^1\Sigma_g^+, v_i) + e \rightarrow M_2(B^1\Sigma_u^+, C\ ^1\Pi_u) + e \rightarrow M_2\,(X\ ^1\Sigma_g^+, \text{continuum}) + e + h\nu$$

$$\downarrow$$

$$M(1s) + M(1s)$$

Resonant processes

($M_2 \equiv H_2, D_2, T_2, HD, HT, DT$)

Dissociative electron attachment (DEA)

$$M_2(X\ ^1\Sigma_g^+, v_i) + e \rightarrow M_2^-(\text{resonant state}) \rightarrow M + M^-$$

Resonant vibrational excitation (RVE)

$$M_2(X\ ^1\Sigma_g^+, v_i) + e \rightarrow M_2^-(\text{resonant state}) \rightarrow M_2(X\ ^1\Sigma_g^+, v_f)$$

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$$CH + e^- \rightarrow CH^* + e^-$$

(R. Celiberto, R.K. Janev and D. Reiter, 2009)

$$BeH^+ + e^- \rightarrow BeH^{+*} + e^-$$

(R. Celiberto, R.K. Janev and D. Reiter, 2012)

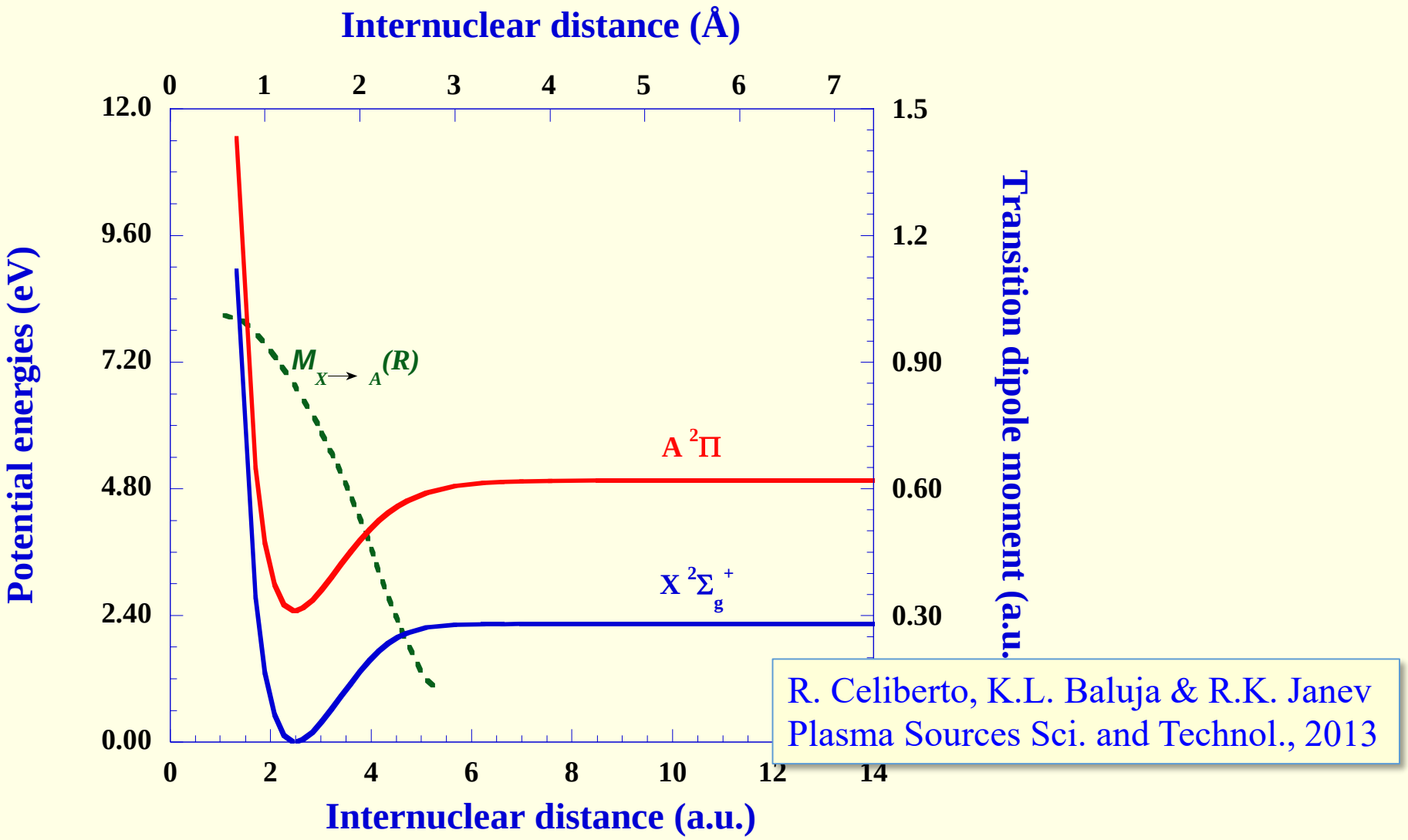
$$BeH + e^- \rightarrow BeH^* + e^-$$

(R. Celiberto, K.L. Baluja and R.K. Janev, 2013)

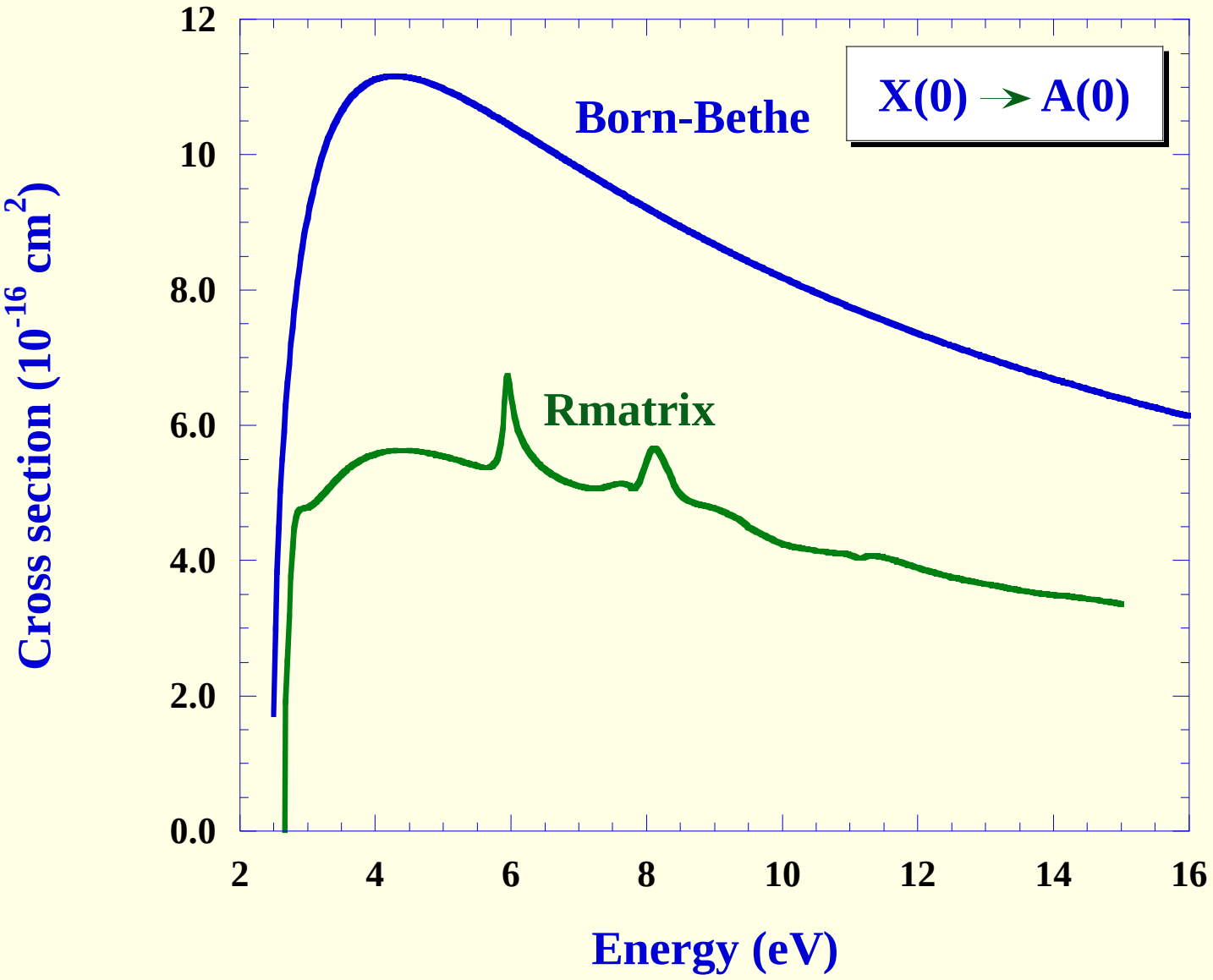
$$He_2^+ + e^- \rightarrow He_2^{+*} + e^-$$

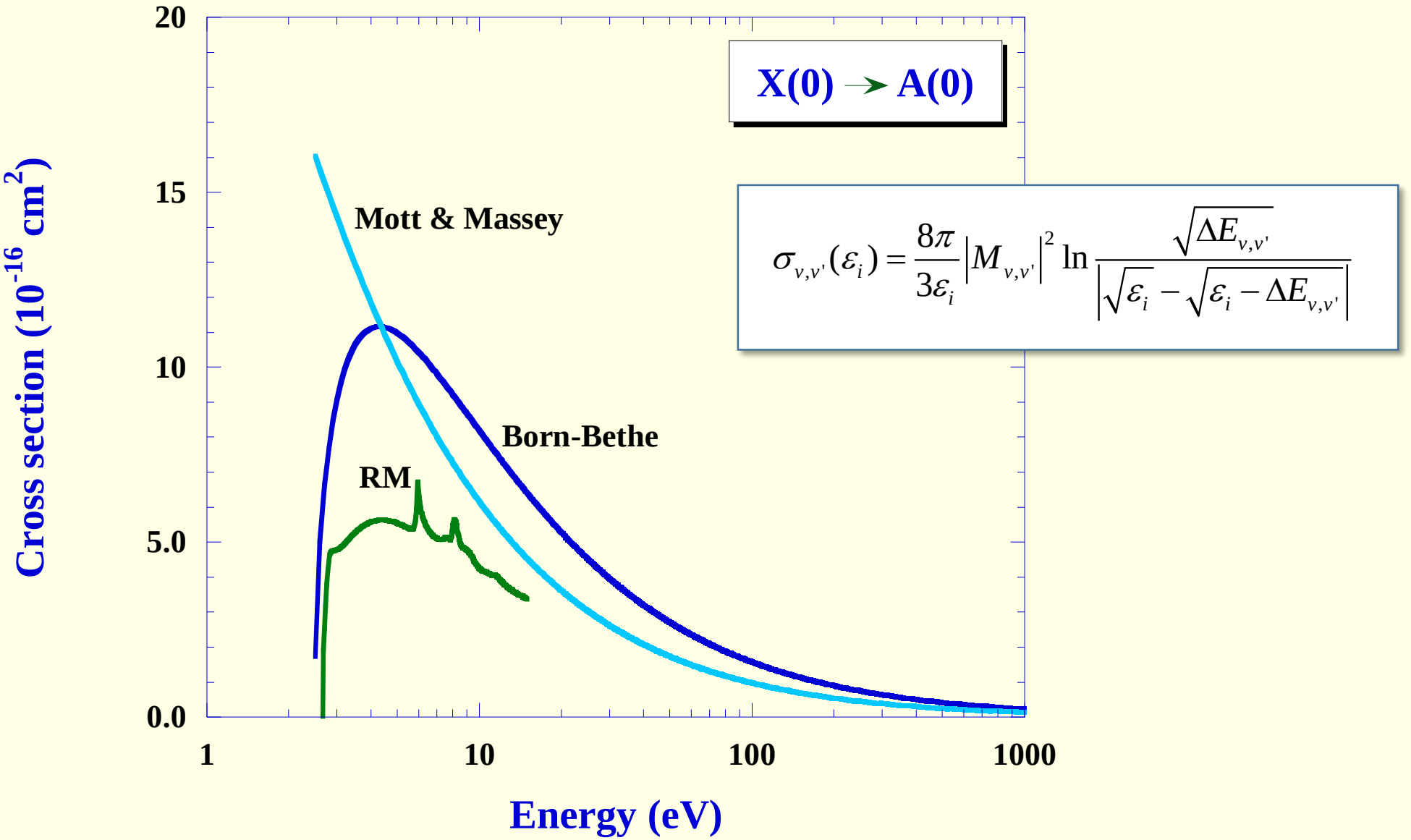
(R Celiberto, K L Baluja, R K Janev and V Laporta, 2015)

$$\mathrm{BeH}(X\,^2\Sigma^+, v_i) + e \rightarrow \mathrm{BeH}(A\,^2\Sigma^+, v_f) + e$$

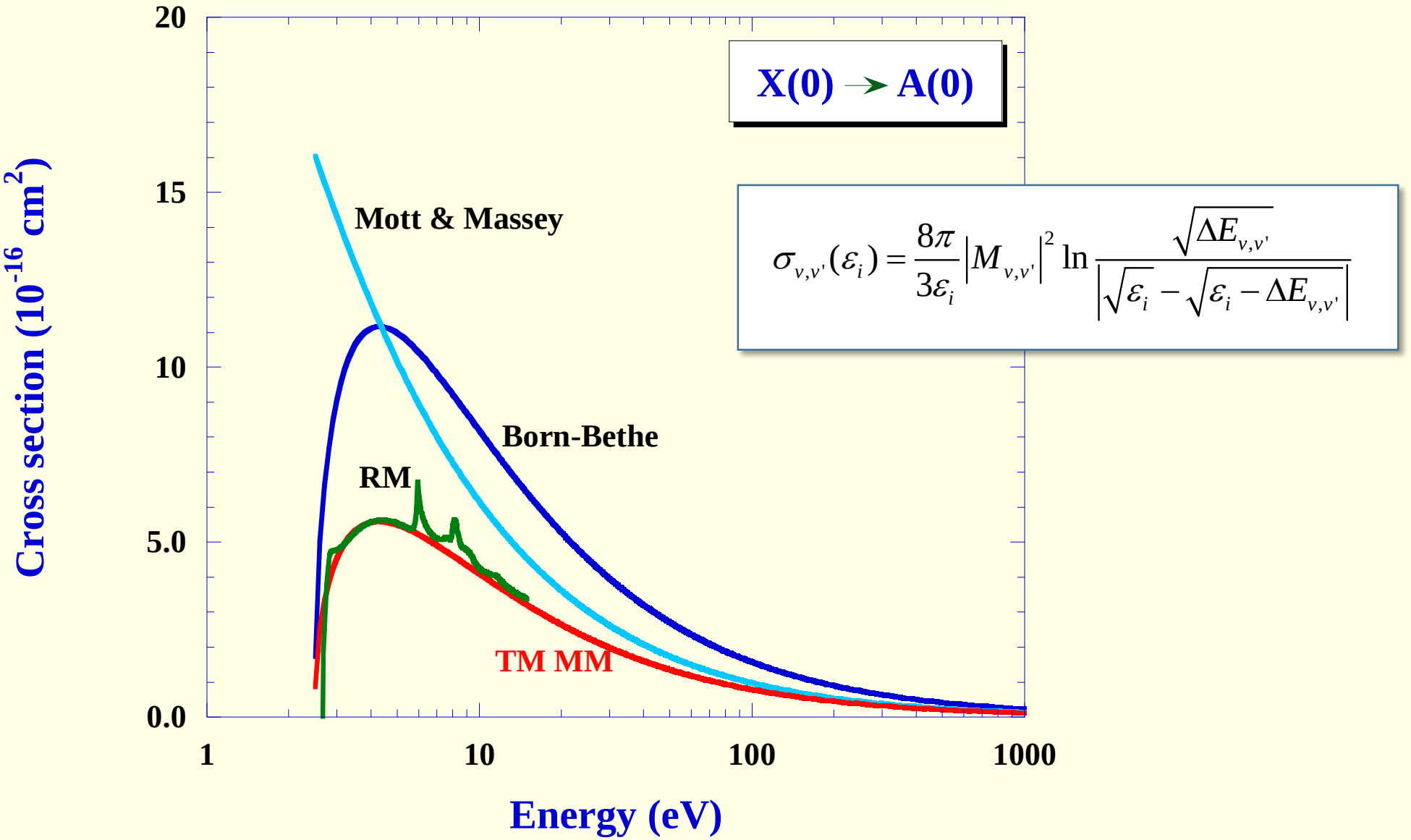


R. Celiberto, K.L. Baluja & R.K. Janev
Plasma Sources Sci. and Technol., 2013

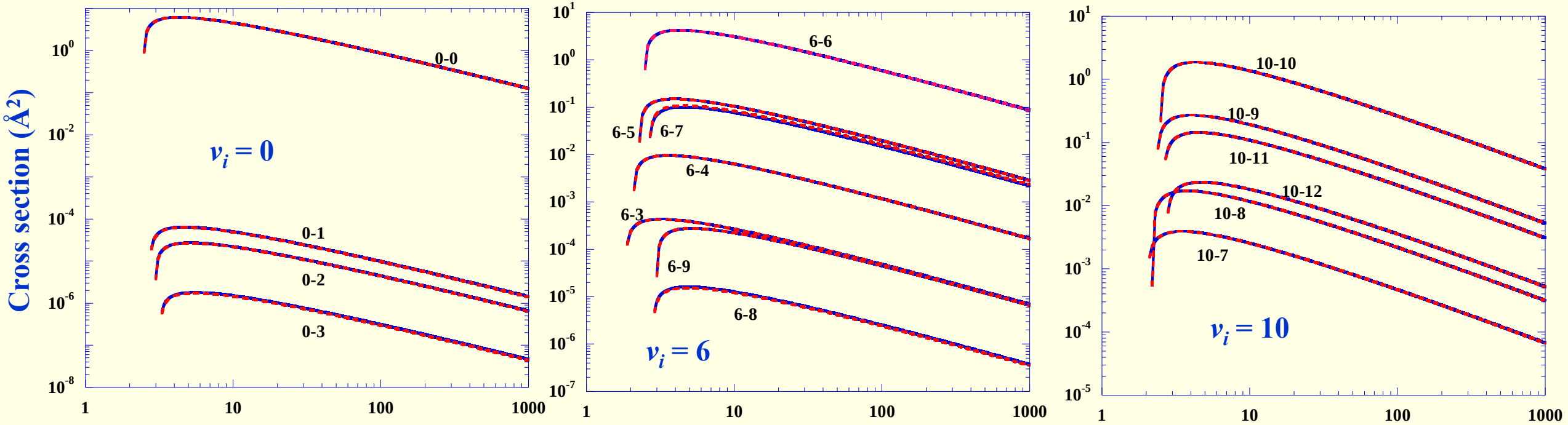

X(0) → A(0)
Born-Bethe
Rmatrix
Cross section (10^{-16} cm^2)
Energy (eV)
0.0
2.0
4.0
6.0
8.0
10
12
2
4
6
8
10
12
14
16



$$\sigma_{v,v'}(\varepsilon_i) = \frac{8\pi}{3\varepsilon_i}\left|M_{v,v'}\right|^2 \ln \frac{\sqrt{\Delta E_{v,v'}}}{\left|\sqrt{\varepsilon_i} - \sqrt{\varepsilon_i - \Delta E_{v,v'}}\right|}$$


X(0) → A(0)
Mott & Massey
Born-Bethe
RM
TM MM
Cross section (10^{-16} cm^2)
Energy (eV)
20
15
10
5.0
0.0
1
10
100
1000
$\sigma_{v,v'}(\varepsilon_i) = \frac{8\pi}{3\varepsilon_i}\left|M_{v,v'}\right|^2 \ln \frac{\sqrt{\Delta E_{v,v'}}}{\left|\sqrt{\varepsilon_i} - \sqrt{\varepsilon_i - \Delta E_{v,v'}}\right|}$

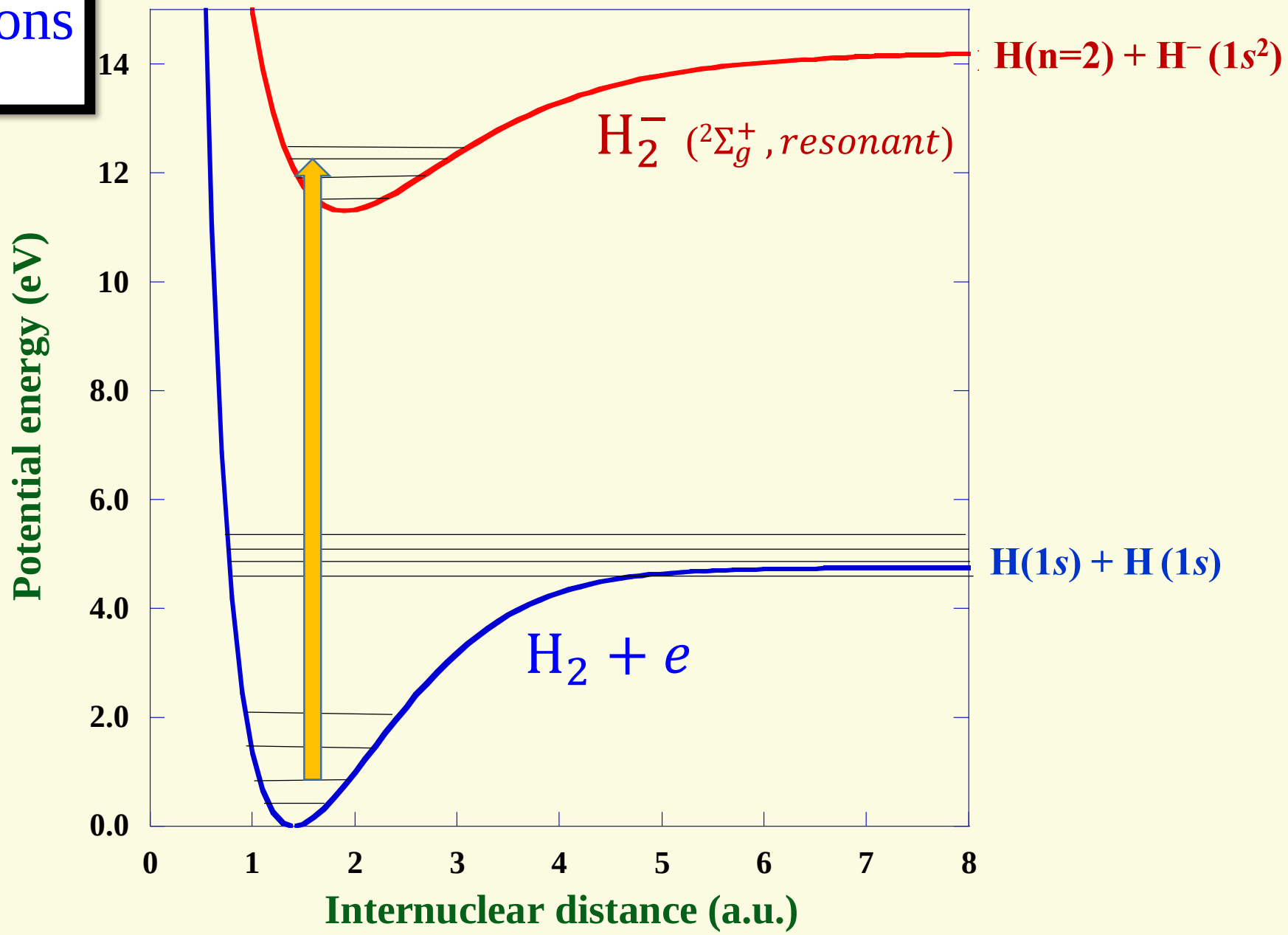
$$\mathrm{BeH}(X\,^2\Sigma^+, v_i) + e \rightarrow \mathrm{BeH}(A\,^2\Sigma^+, v_f) + e$$



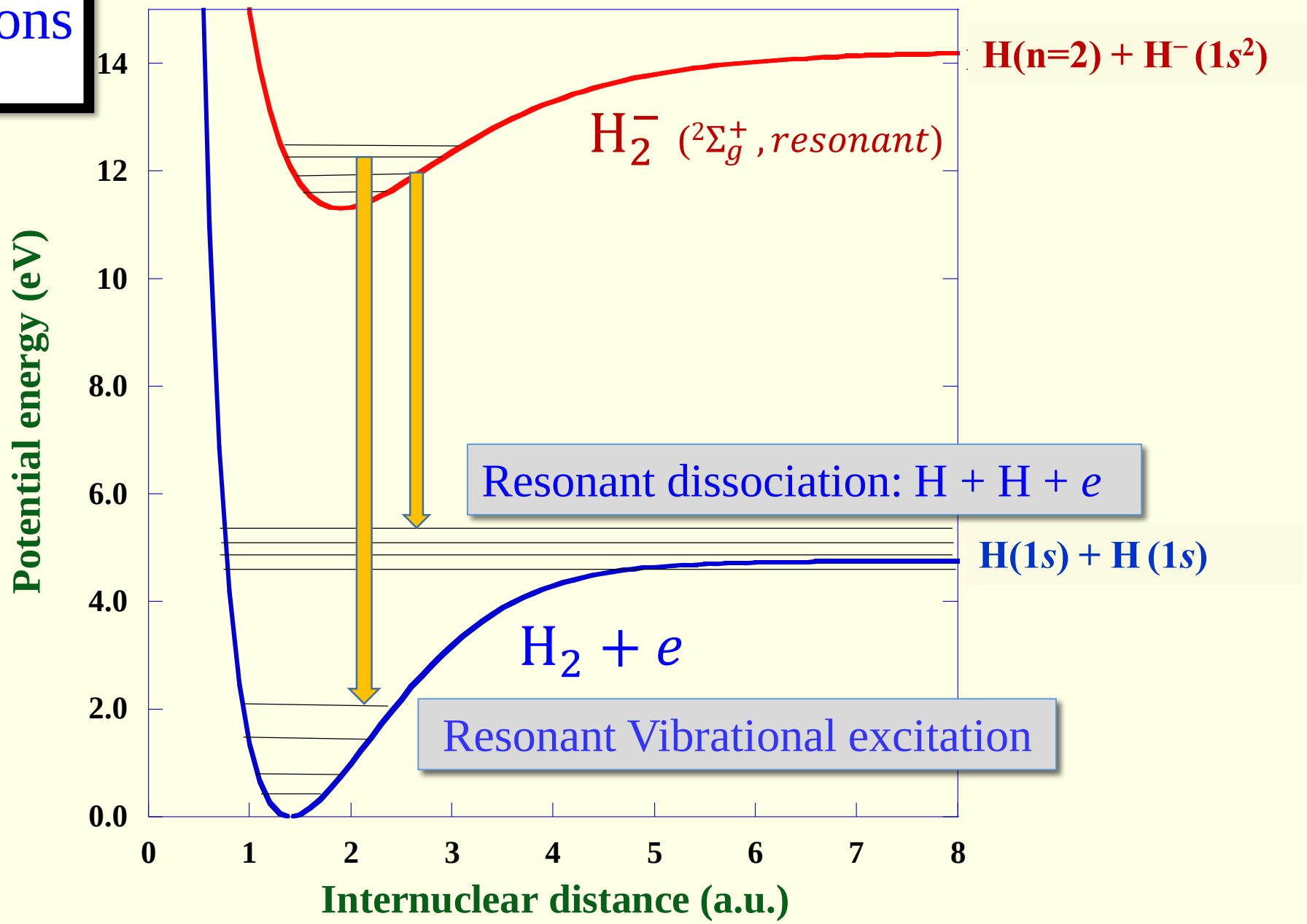
$$\sigma_{v,v'}(x) = \sigma_{0,0}(x)\frac{M^2_{v,v'}}{\Delta E_{v,v'}}$$

Resonant collisions

Resonant collisions

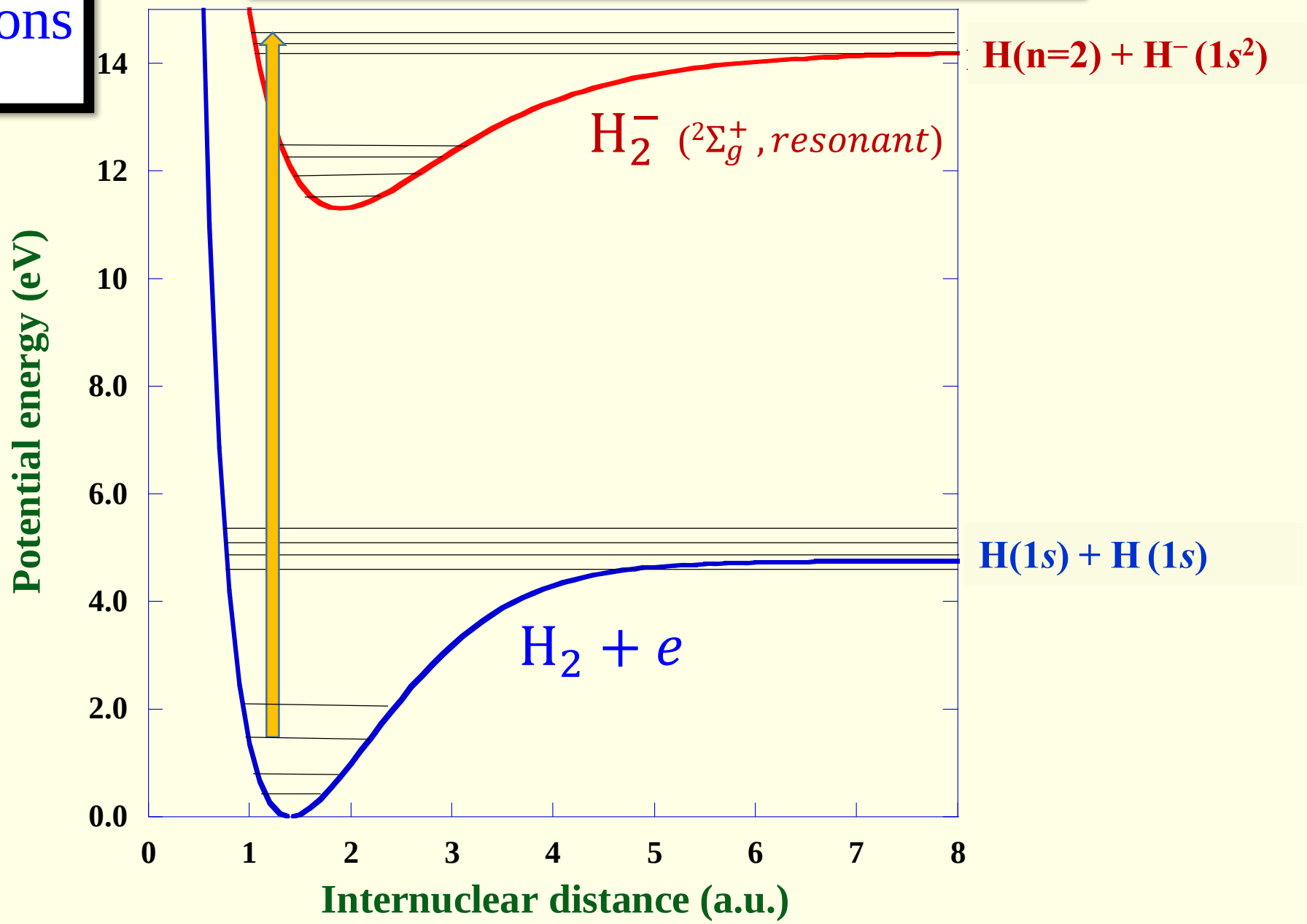


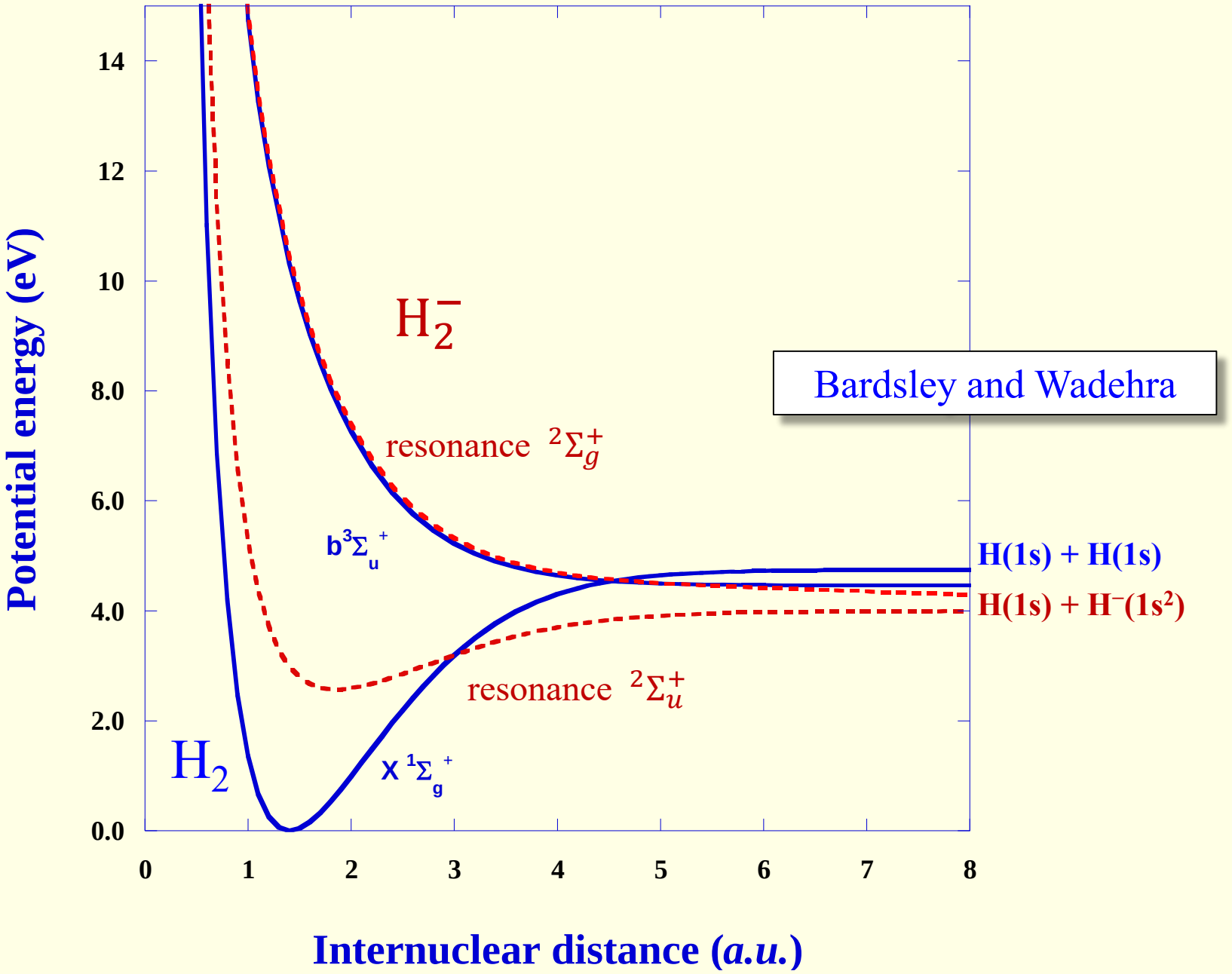
Resonant collisions

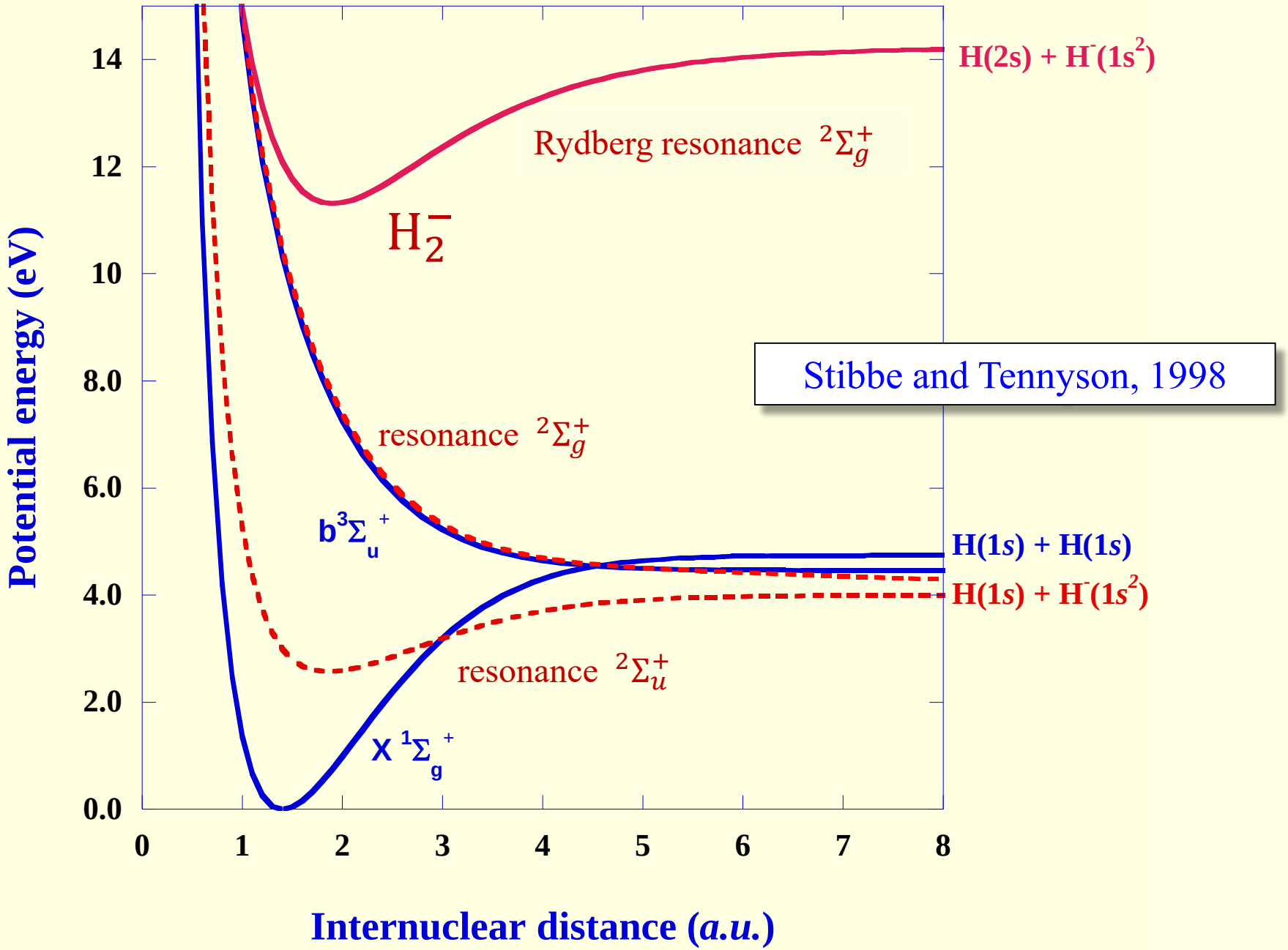


Resonant collisions

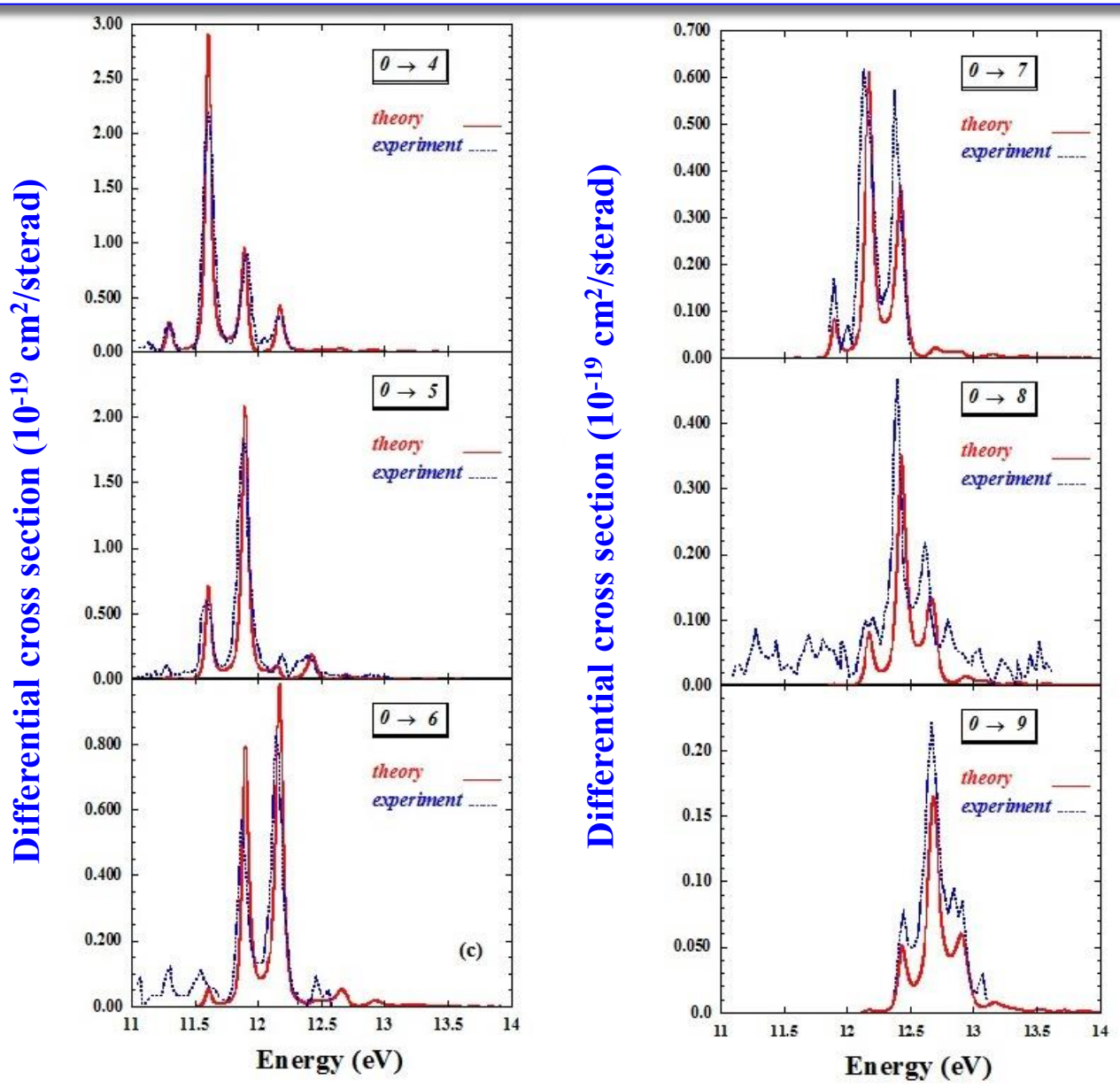
Dissociative electron attachment: H + H⁻




Potential energy (eV)
14
12
10
8.0
6.0
4.0
2.0
0.0
0
1
2
3
4
5
6
7
8
Internuclear distance (a.u.)
H_2^-
resonance $^2\Sigma_g^+$
$b^3\Sigma_u^+$
resonance $^2\Sigma_u^+$
H_2
$X\,^1\Sigma_g^+$
Bardsley and Wadehra
H(1s) + H(1s)
H(1s) + H⁻(1s²)


Potential energy (eV)
14
12
10
8.0
6.0
4.0
2.0
0.0
0
1
2
3
4
5
6
7
8
Internuclear distance (a.u.)
H(2s) + H⁻(1s²)
Rydberg resonance ²Σg+
H2−
resonance ²Σg+
b³Σu+
H(1s) + H(1s)
H(1s) + H⁻(1s²)
resonance ²Σu+
X ¹Σg+
Stibbe and Tennyson, 1998

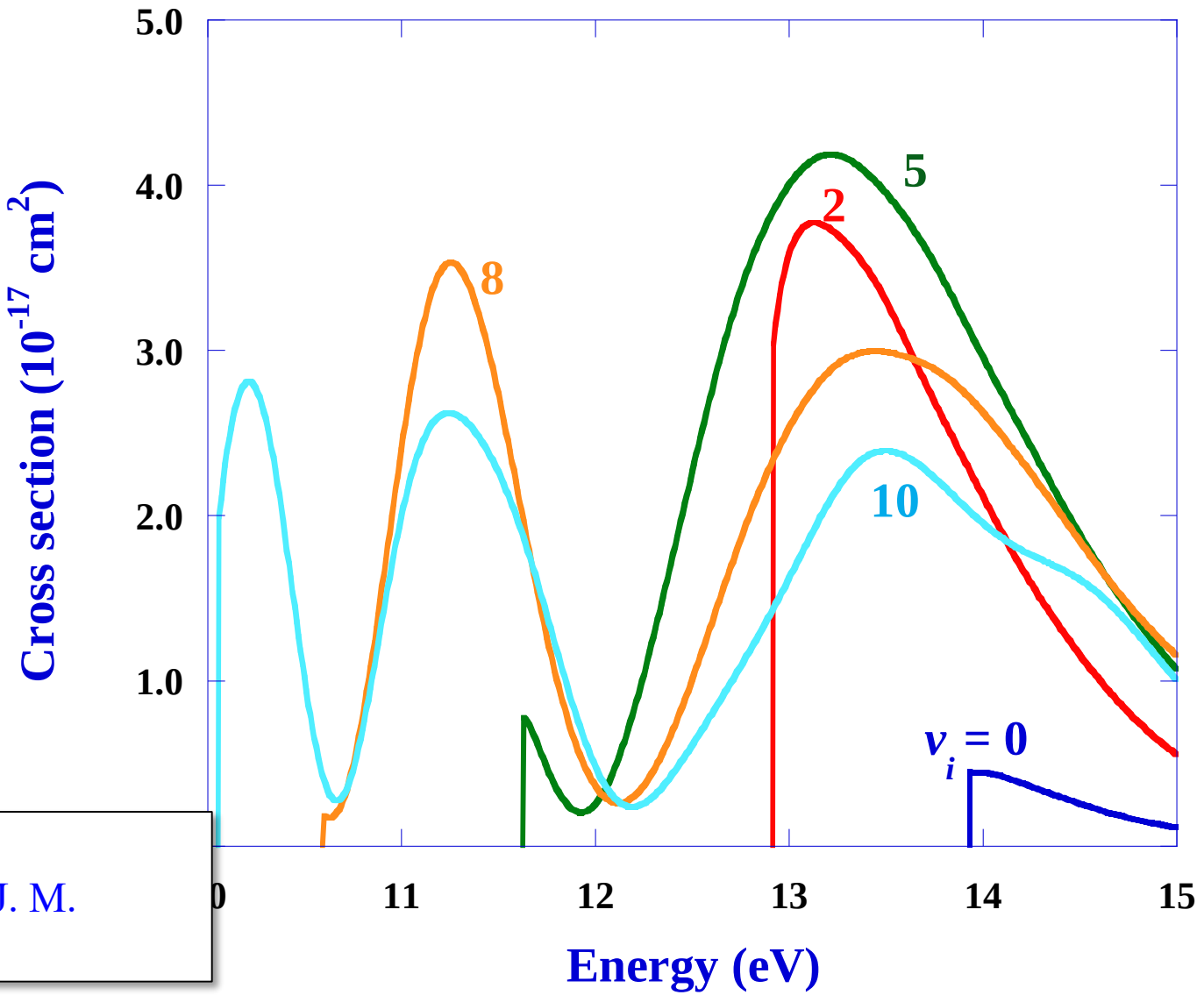
$$H_2(v_i = 0) + e \rightarrow H_2^-(^2\Sigma_g^+, \text{Rydberg}) \rightarrow H_2(v_f) + e$$



Experiment from
Comer & Read (1971)

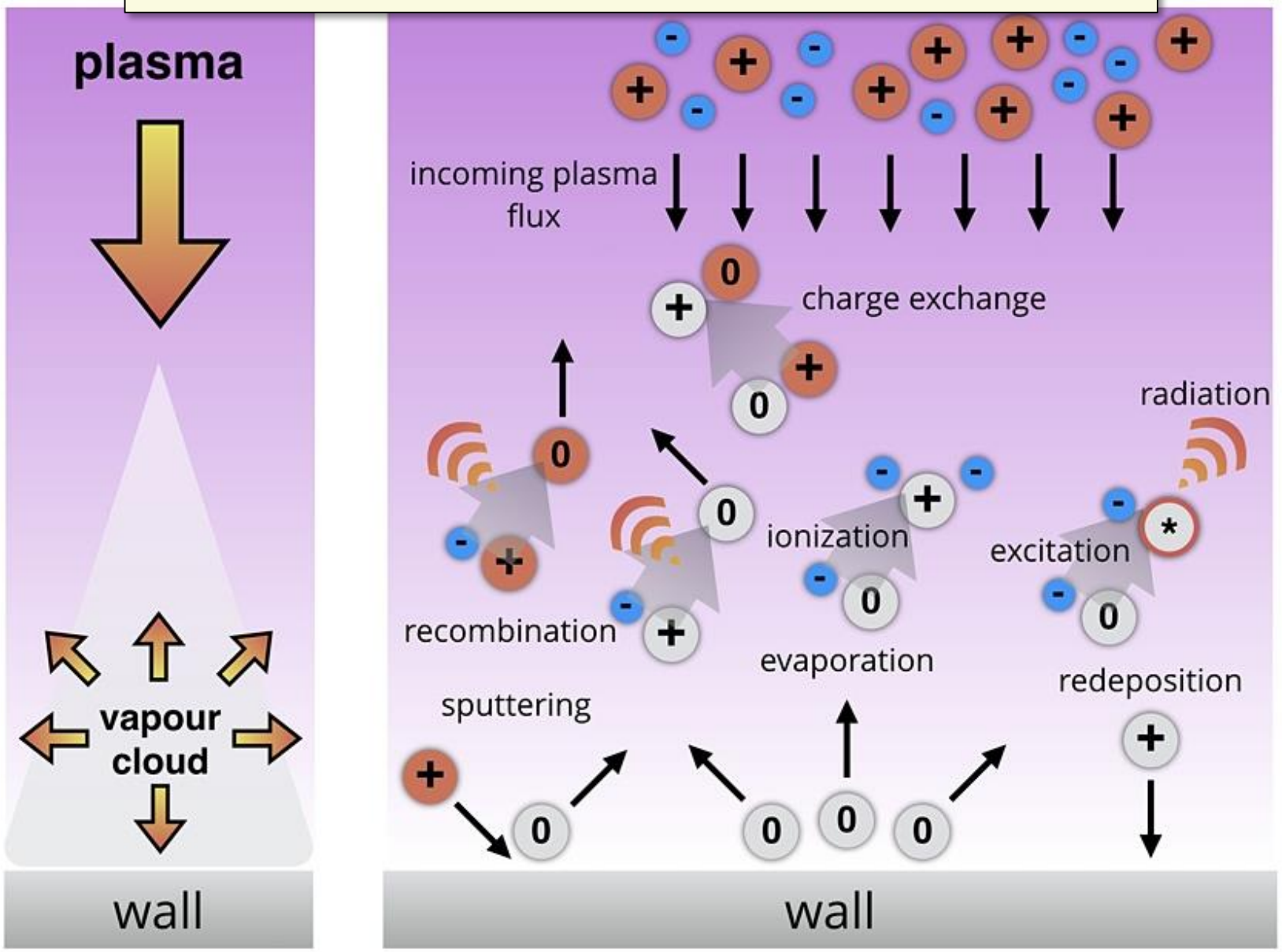
R. Celiberto, R. K. Janev, J. M. Wadehra, and A. Laricchiuta
Phys. Rev. (2008)

$H_2(v_i) + e \rightarrow (H_2^-, \text{Rydberg}) \rightarrow H(n = 2) + H^-$

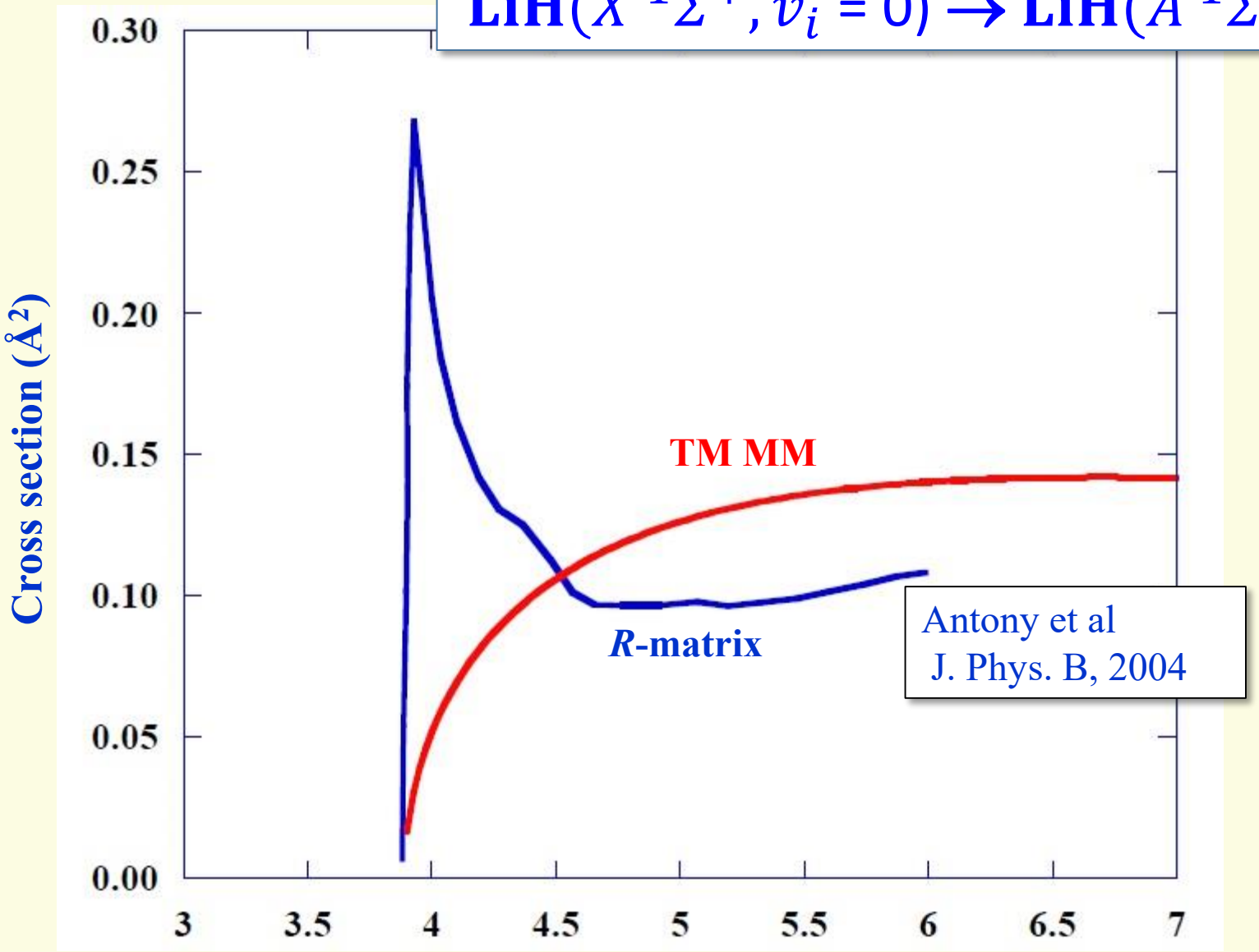


Chem Phys, 2013
R. Celiberto, R. K. Janev, J. M. Wadehra, J. Tennyson

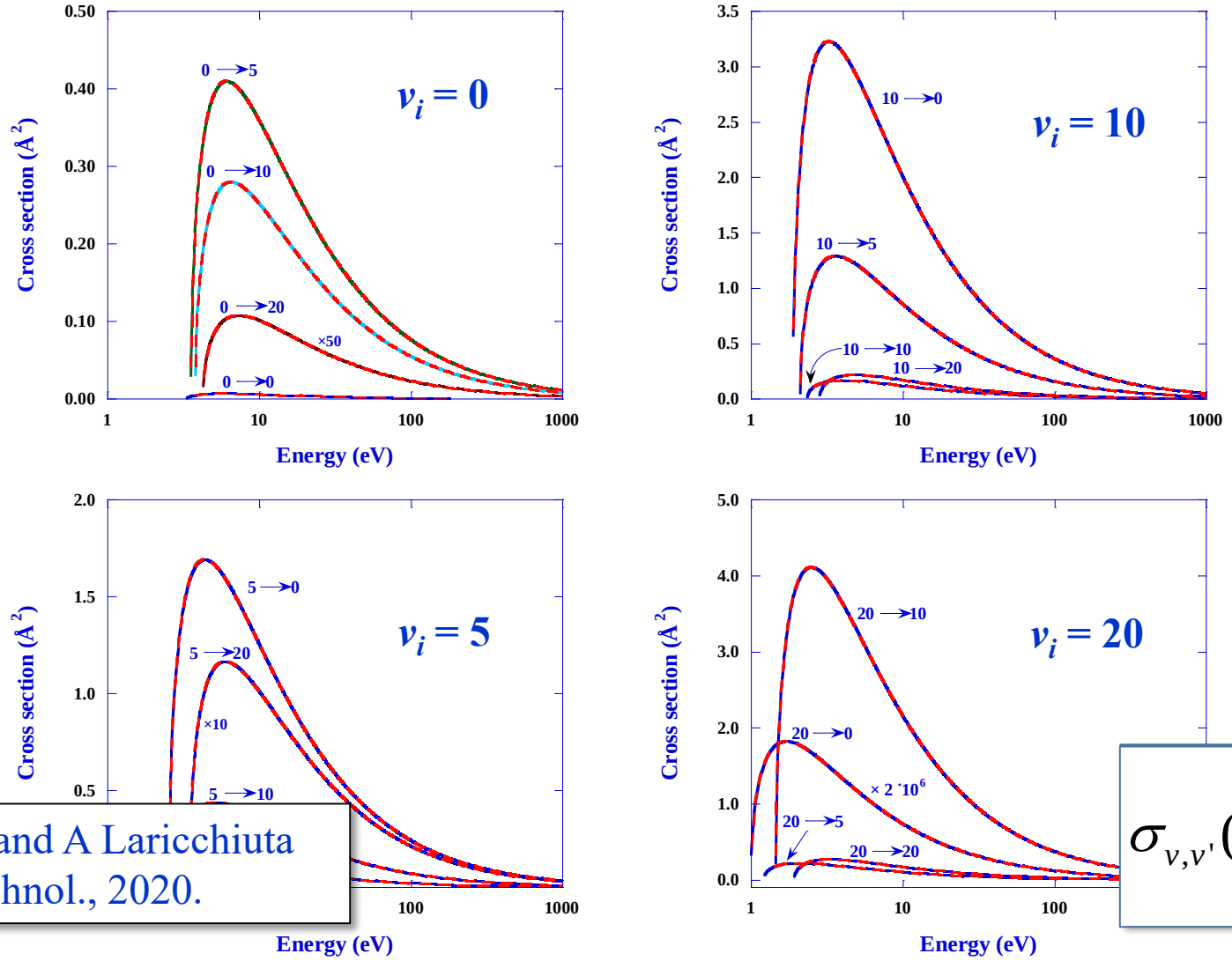
Vapour shielding project



$\mathbf{LiH}(X\,^1\Sigma^+, v_i = 0) \rightarrow \mathbf{LiH}(A\,^1\Sigma^+, v_i = 12)$



$\mathbf{LiH}(X\,^1\Sigma^+, v_i) \rightarrow \mathbf{LiH}(A\,^1\Sigma^+, v_f)$



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Plasma Sources Sci. Technol., 2020.

$$\sigma_{v,v'}(x) = \sigma_{0,0}(x)\frac{M^2_{v,v'}}{\Delta E_{v,v'}}$$

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