



*Vibrational excitation and dissociation
of deuterium molecule by electron impact*

Vincenzo Laporta
Istituto per la Scienza e Tecnologia dei Plasmi, CNR, Bari (Italy)

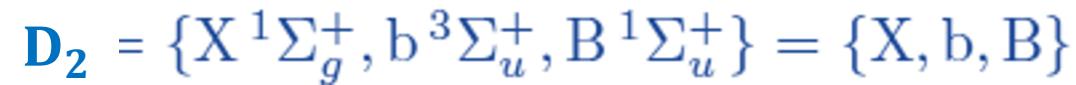
vincenzo.laporta@istp.cnr.it

The results of this presentation are in collaboration with:

R. Agnello, I. Furno (Swiss Plasma Center, Lausanne, Switzerland)
G. Fubiani (LAPLACE, Universite de Toulouse, France)
C. Hill (IAEA, Vienna, Austria)
D. Reiter (Heinrich-Heine-University, Dusseldorf, Germany)
F. Taccogna (ISTP, Bari, Italy)

Principal collaborators:

Ioan Schneider (Université du Havre, France)
Jonathan Tennyson (UCL, London, UK)
Marco Panesi (University of Illinois at Urbana-Champaign, US)
Kalyan Chakrabarti (Scottish Church College, Kolkata, India)



Local Complex Potential Model

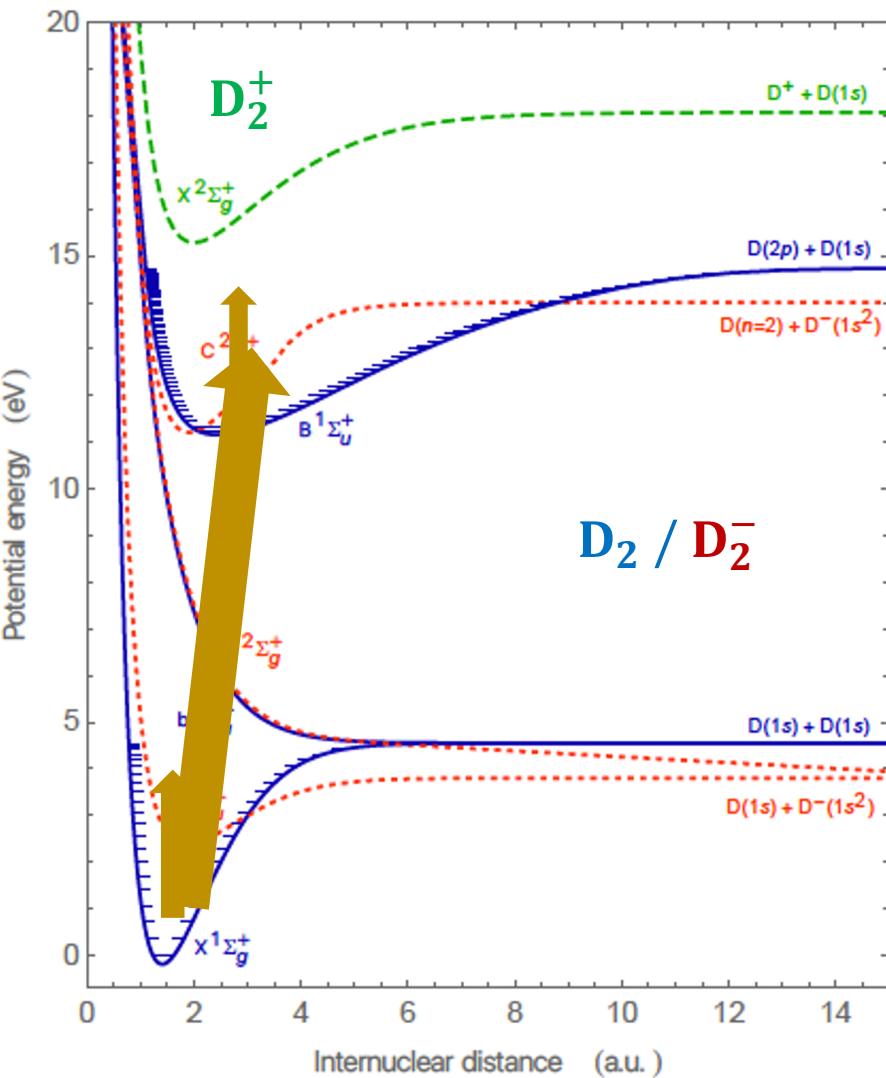
First time (in my knowledge) of using this approach to calculate vibrationally-electronically-excited collisions

Electron-D₂⁺ results will be presented by Ioan Schneider

$$\mathbf{D}_2^+ = \{\text{X}^1\Sigma_g^+, \text{b}^3\Sigma_u^+, \text{B}^1\Sigma_u^+\} = \{\text{X}, \text{b}, \text{B}\}$$

$$\mathbf{D}_2^- = \{\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+\} = \{\text{X}^-, \text{B}^-, \text{C}^-\}$$

Label	Reaction
<i>Vibrational excitation</i>	
VE1	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{X}^1\Sigma_g^+; v')$
VE2	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; v')$
VE3	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; v')$
<i>Dissociative electron attachment</i>	
DA1	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+) \rightarrow \text{D}(1s) + \text{D}^-(1s^2)$
DA2	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow \text{D}(n=2) + \text{D}^-(1s^2)$
DA3	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow \text{D}(n=2) + \text{D}^-(1s^2)$
<i>Dissociative excitation</i>	
DE1	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{X}^1\Sigma_g^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$
DE2	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{b}^3\Sigma_u^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$
DE3	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(2p) + \text{D}(1s)$
DE4	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(2p) + \text{D}(1s)$
DE5	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{b}^3\Sigma_u^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$
DE6	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{X}^1\Sigma_g^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$



$$\mathbf{D}_2^+ = \{\text{X}^1\Sigma_g^+, \text{b}^3\Sigma_u^+, \text{B}^1\Sigma_u^+\} = \{\text{X}, \text{b}, \text{B}\}$$

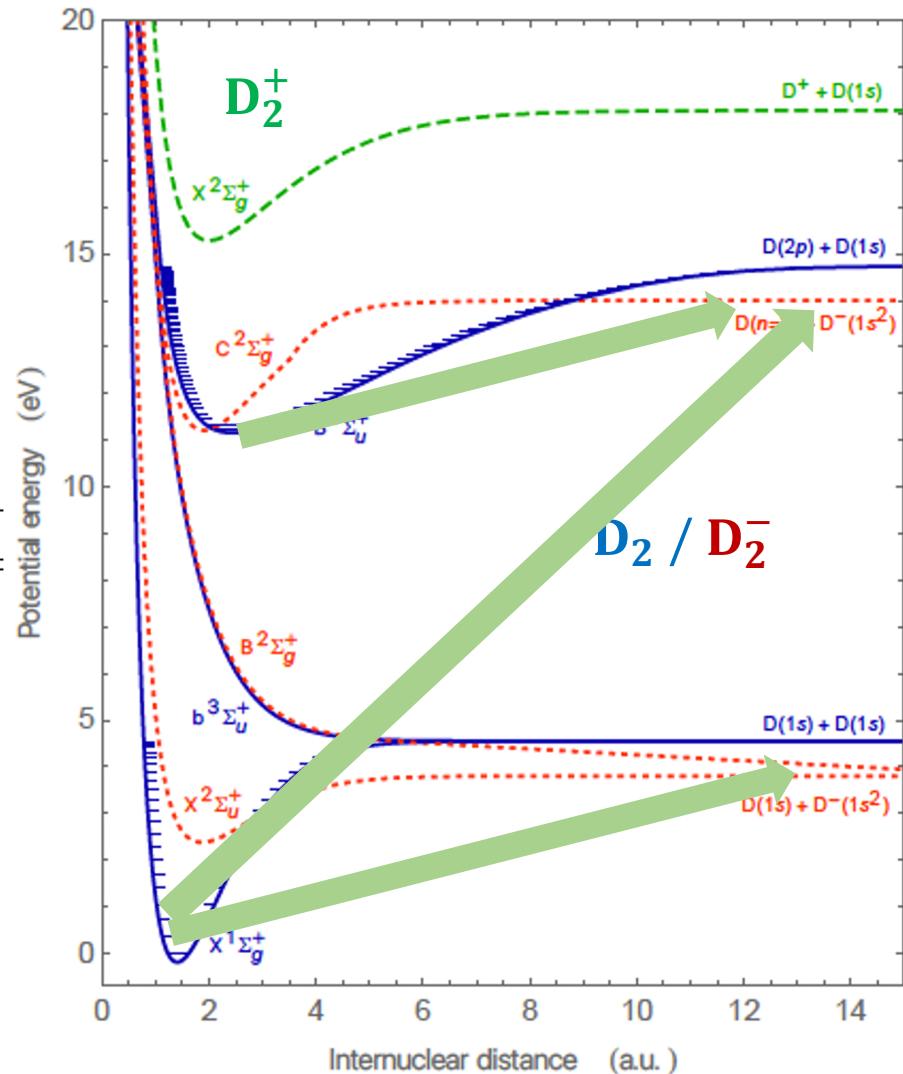
$$\mathbf{D}_2^- = \{\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+\} = \{\text{X}^-, \text{B}^-, \text{C}^-\}$$

Label	Reaction
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	<i>Vibrational excitation</i>
VE1	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{X}^1\Sigma_g^+; v')$
VE2	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; v')$
VE3	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; v')$

	<i>Dissociative electron attachment</i>
DA1	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+) \rightarrow \text{D}(1s) + \text{D}^-(1s^2)$
DA2	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow \text{D}(n=2) + \text{D}^-(1s^2)$
DA3	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow \text{D}(n=2) + \text{D}^-(1s^2)$

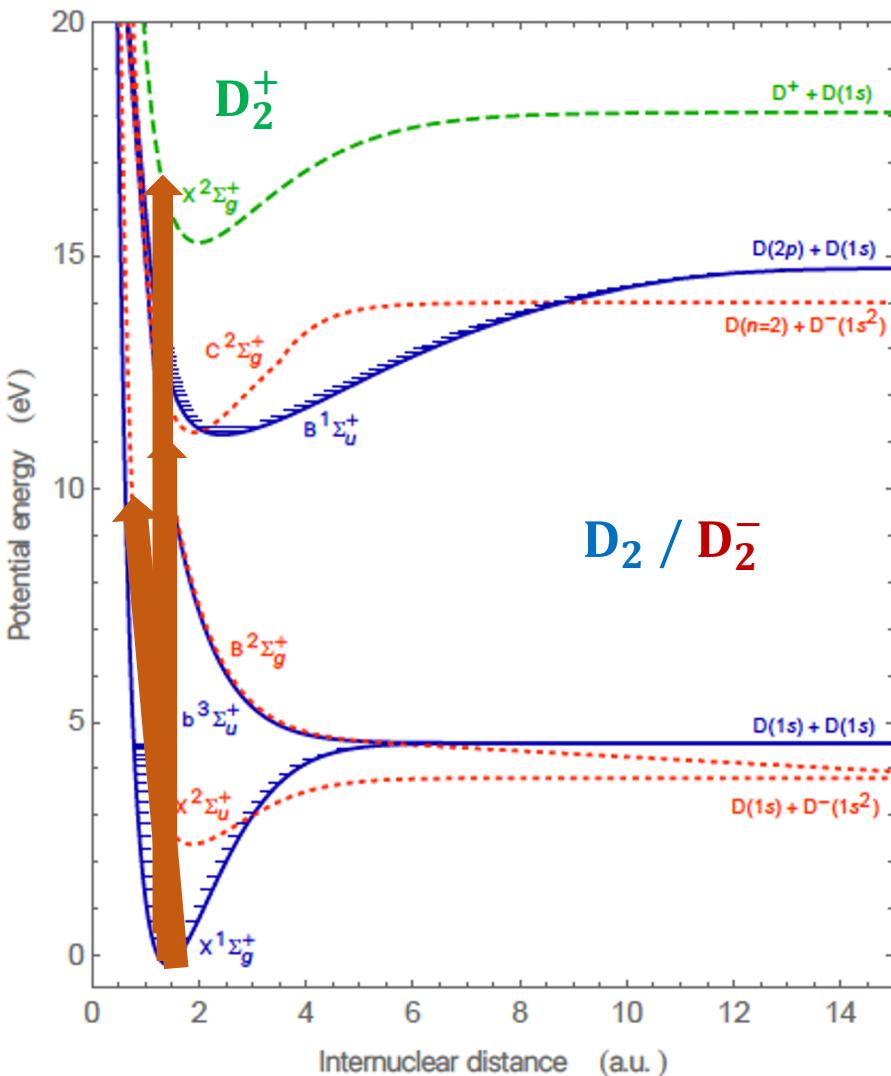
	<i>Dissociative excitation</i>
DE1	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{X}^1\Sigma_g^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$
DE2	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{b}^3\Sigma_u^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$
DE3	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(2p) + \text{D}(1s)$
DE4	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(2p) + \text{D}(1s)$
DE5	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{b}^3\Sigma_u^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$
DE6	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{X}^1\Sigma_g^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$



$$\mathbf{D}_2^+ = \{\text{X}^1\Sigma_g^+, \text{b}^3\Sigma_u^+, \text{B}^1\Sigma_u^+\} = \{\text{X}, \text{b}, \text{B}\}$$

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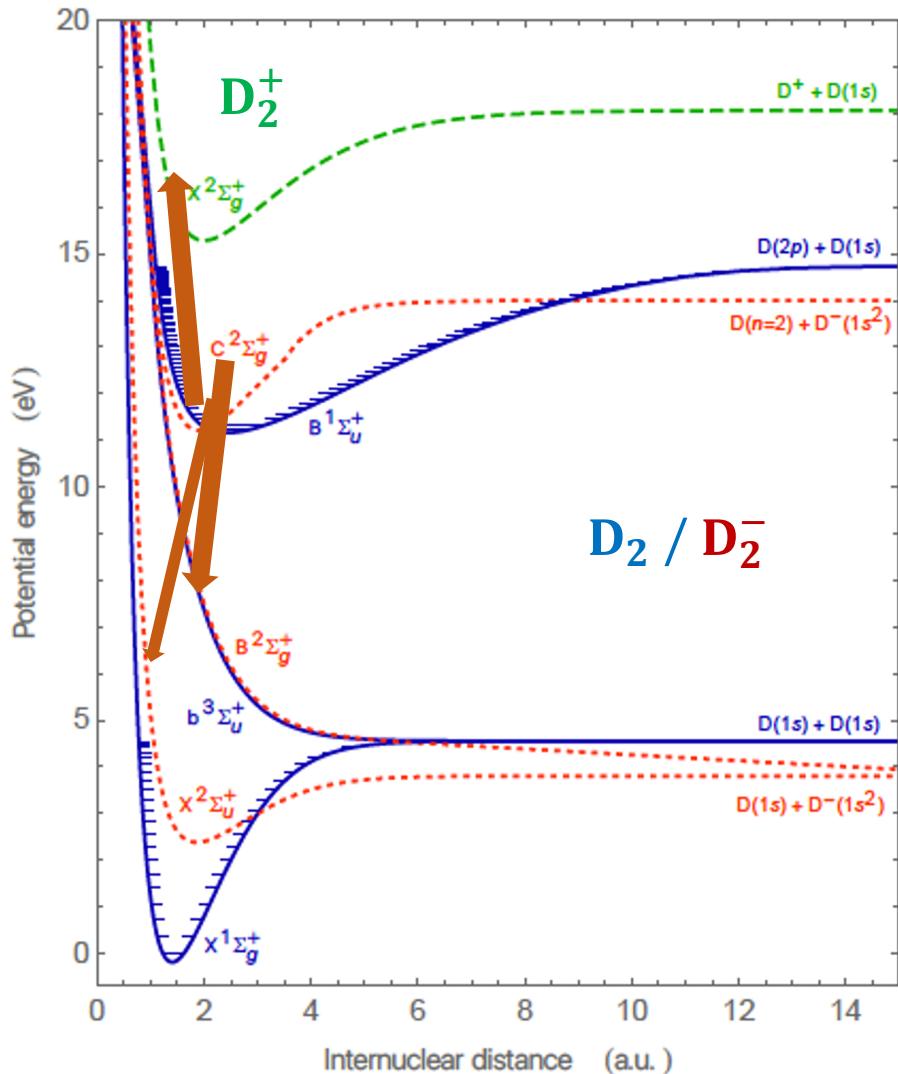
Label	Reaction
<i>Vibrational excitation</i>	
VE1	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{X}^1\Sigma_g^+; v')$
VE2	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; v')$
VE3	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; v')$
<i>Dissociative electron attachment</i>	
DA1	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+) \rightarrow \text{D}(1s) + \text{D}^-(1s^2)$
DA2	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow \text{D}(n=2) + \text{D}^-(1s^2)$
DA3	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow \text{D}(n=2) + \text{D}^-(1s^2)$
<i>Dissociative excitation</i>	
DE1	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{X}^1\Sigma_g^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$
DE2	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{b}^3\Sigma_u^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$
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DE4	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(2p) + \text{D}(1s)$
DE5	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{b}^3\Sigma_u^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$
DE6	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{X}^1\Sigma_g^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$



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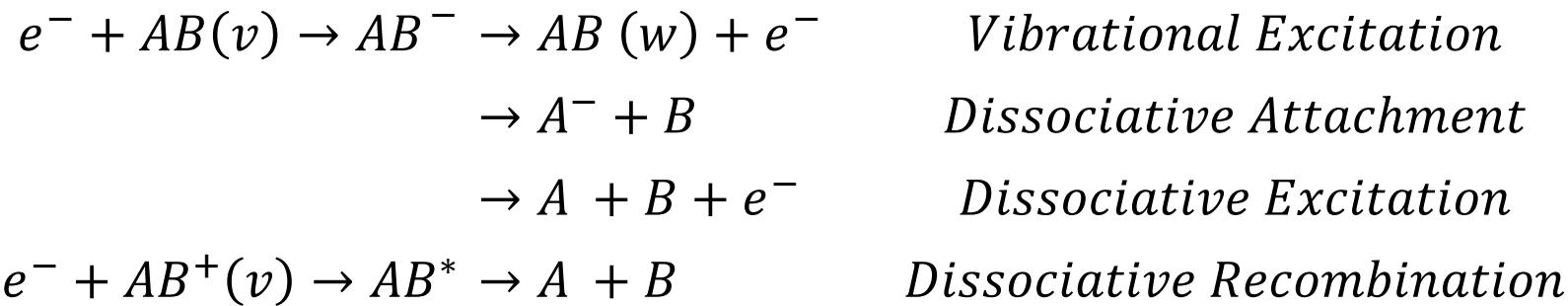
$$\mathbf{D}_2^- = \{\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+\} = \{\text{X}^-, \text{B}^-, \text{C}^-\}$$

Label	Reaction
<i>Vibrational excitation</i>	
VE1	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{X}^1\Sigma_g^+; v')$
VE2	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; v')$
VE3	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; v')$
<i>Dissociative electron attachment</i>	
DA1	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+) \rightarrow \text{D}(1s) + \text{D}^-(1s^2)$
DA2	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow \text{D}(n=2) + \text{D}^-(1s^2)$
DA3	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow \text{D}(n=2) + \text{D}^-(1s^2)$
<i>Dissociative excitation</i>	
DE1	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{X}^2\Sigma_u^+, \text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{X}^1\Sigma_g^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$
DE2	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{B}^2\Sigma_g^+, \text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{b}^3\Sigma_u^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$
DE3	$e(\epsilon) + \text{D}_2(\text{X}^1\Sigma_g^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(2p) + \text{D}(1s)$
DE4	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{B}^1\Sigma_u^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(2p) + \text{D}(1s)$
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DE6	$e(\epsilon) + \text{D}_2(\text{B}^1\Sigma_u^+; v) \rightarrow \text{D}_2^-(\text{C}^2\Sigma_g^+) \rightarrow e(\epsilon') + \text{D}_2(\text{X}^1\Sigma_g^+; \epsilon_c) \rightarrow e(\epsilon') + \text{D}(1s) + \text{D}(1s)$

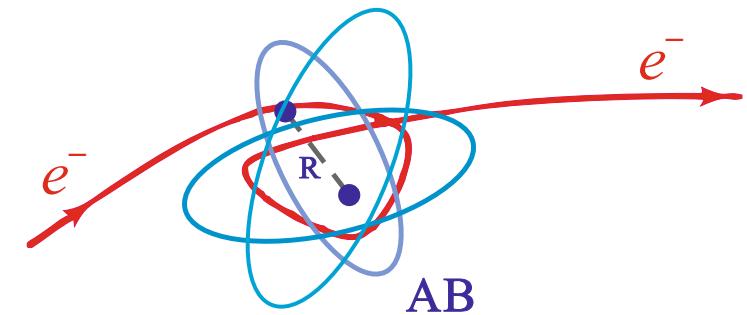


Local Complex Potential model for electron-molecule scattering

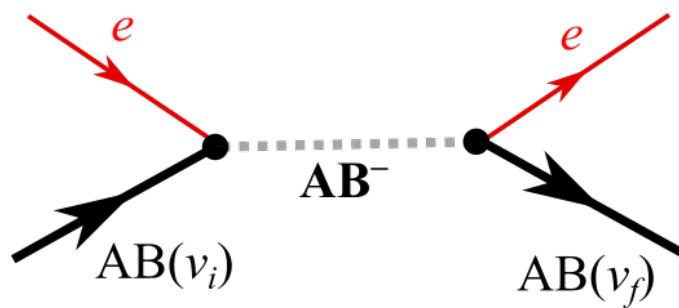
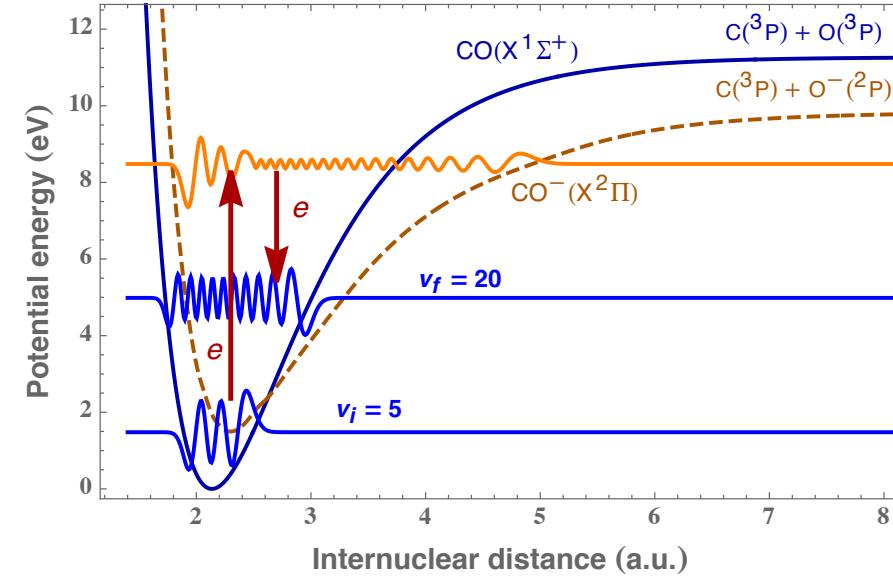
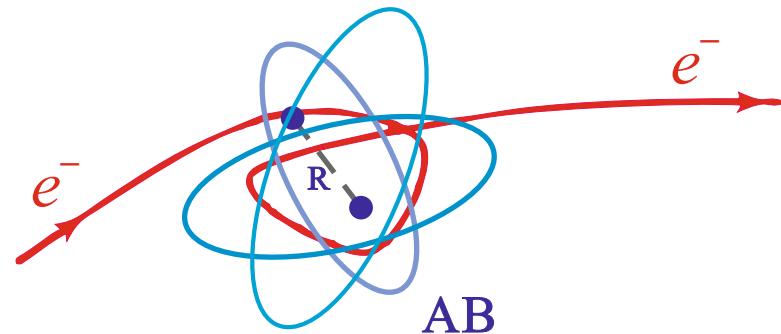
Processes occurring for resonant electron-molecule scattering:



MQDT approach for electron- D_2^+ will be presented by Ioan Schneider



Local Complex Potential model

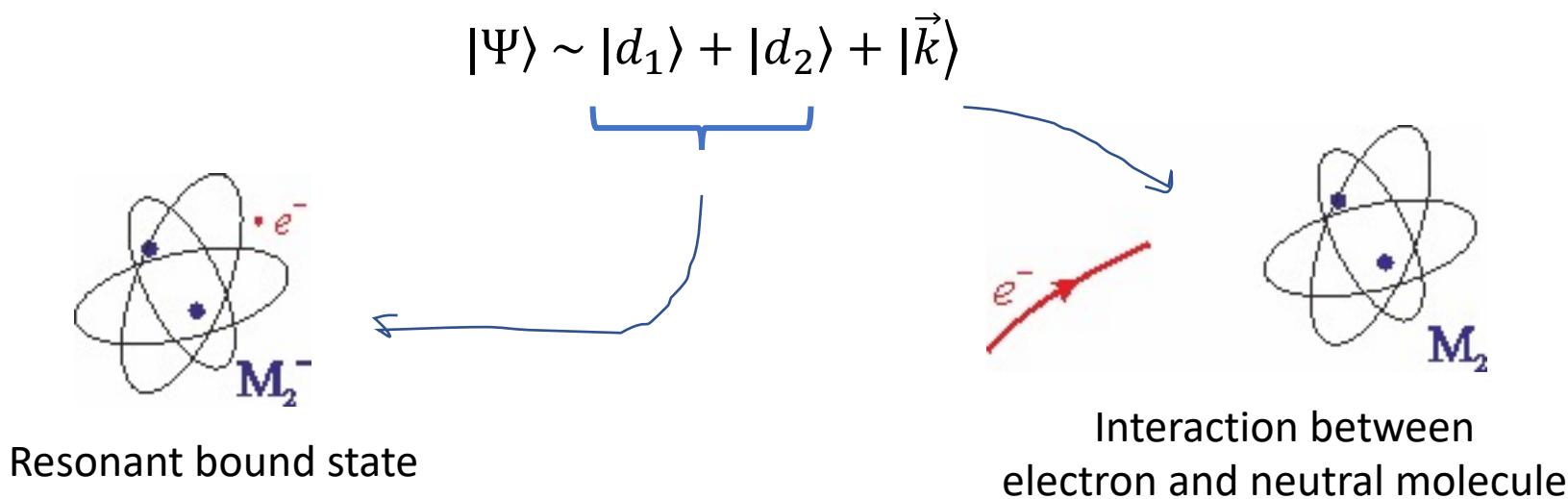


Some theoretical details

Let's consider electron-molecule scattering with the presence of two interacting resonances:



The process can be described by two discrete electronic states, $|d_1\rangle$ and $|d_2\rangle$, *embedded-in* and *interacting-with* a single electronic continuum $|\vec{k}\rangle$



The electron-molecule effective Hamiltonian

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{U} + \mathbf{V}$$

$$H_0 = |d_1\rangle(T_N + V_0 + \epsilon_1)\langle d_1| + |d_2\rangle(T_N + V_0 + \epsilon_2)\langle d_2| + \int d\vec{k} |\vec{k}\rangle(T_N + V_0 + \epsilon_{\vec{k}})\langle \vec{k}|$$

~~$$U = |d_1\rangle U_{12} \langle d_2| + \text{h.c.}$$~~

$$V = \int d\vec{k} |d_1\rangle V_{1k} \langle \vec{k}| + |d_2\rangle V_{2k} \langle \vec{k}| + \text{h.c.}$$

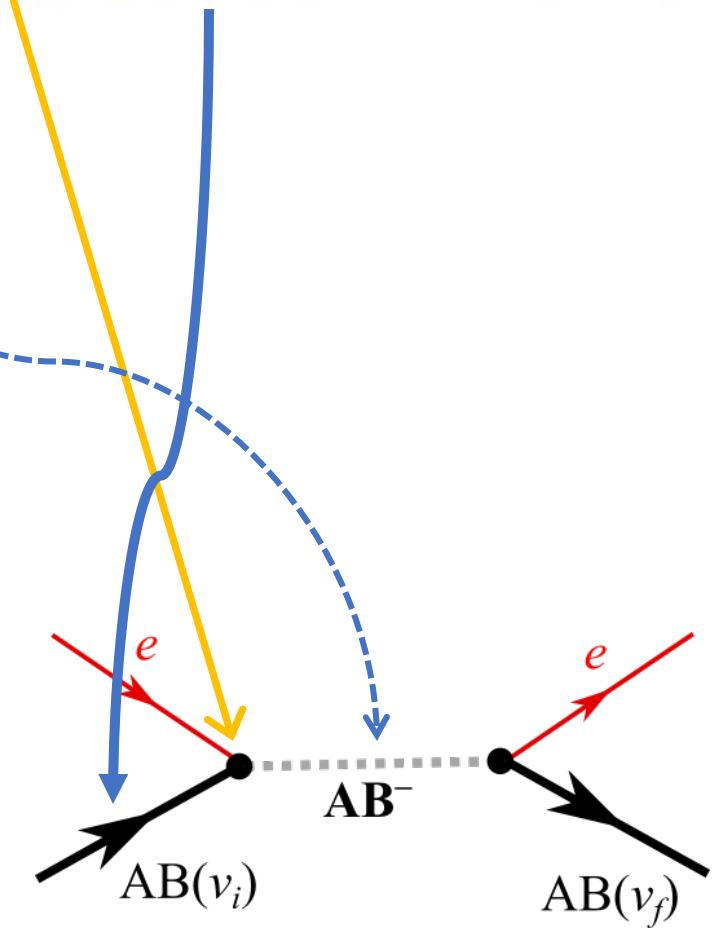
- V_0 is the neutral molecule potential
- $\epsilon_{1,2}$ are the resonance energies respect to V_0
- U describes the coupling between the discrete states
- V couples the discrete states with the continuum states

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dR^2} + V_r^-(R) - \frac{i}{2} \Gamma_r(R) - E \right] \xi_{s,v}^r(R) = -\mathcal{V}_r^s(R) \chi_v^s(R), \quad r \in \mathcal{R},$$

$$\mathcal{V}_r^{s2} = \frac{\hbar}{2\pi} \frac{\Gamma_r^s}{k}, \quad \Gamma_r = \sum_{s \in \mathcal{S}} \Gamma_r^s, \quad r \in \mathcal{R}.$$

$$\mathcal{S} = \{X\,{}^1\Sigma_g^+, b\,{}^3\Sigma_u^+, B\,{}^1\Sigma_u^+\} = \{X, b, B\}$$

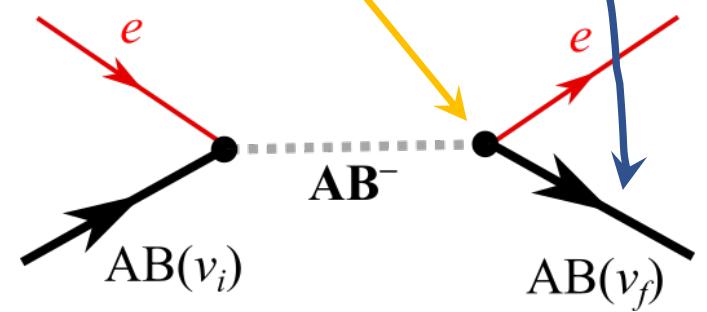
$$\mathcal{R} = \{X\,{}^2\Sigma_u^+, B\,{}^2\Sigma_g^+, C\,{}^2\Sigma_g^+\} = \{X^-, B^-, C^-\}$$

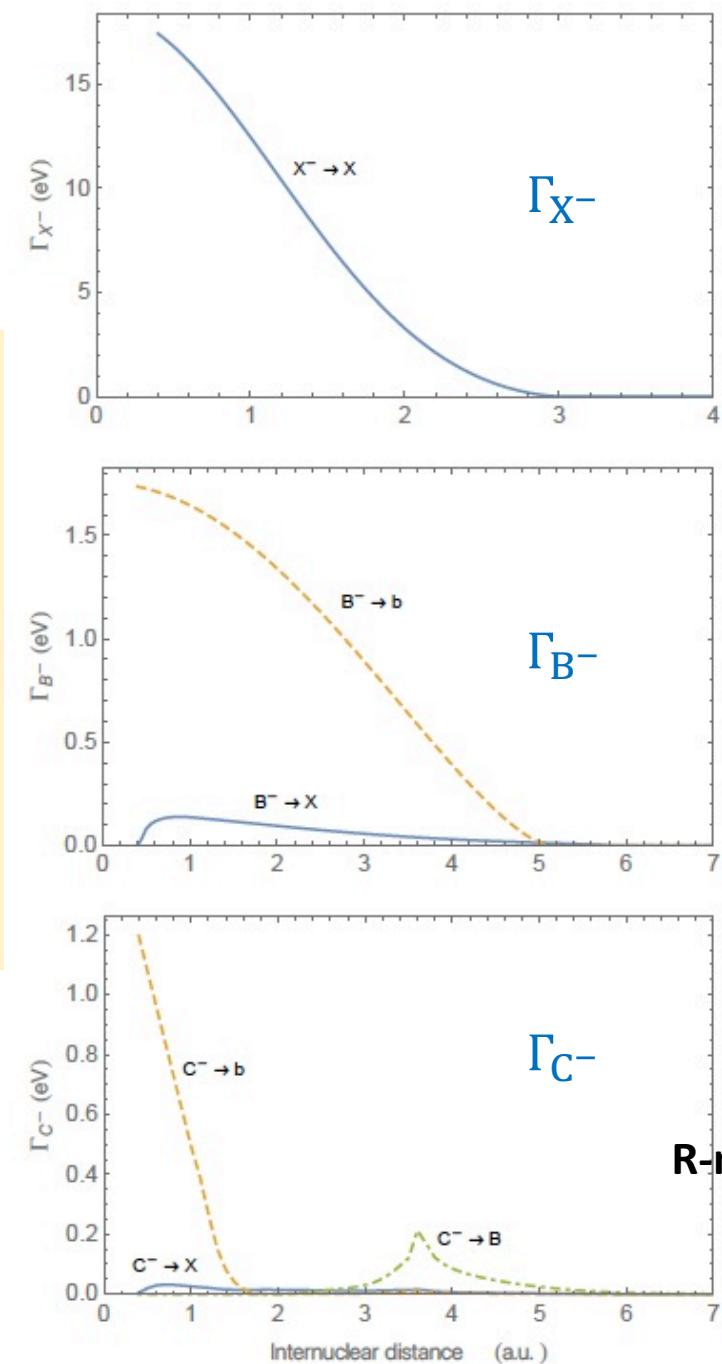
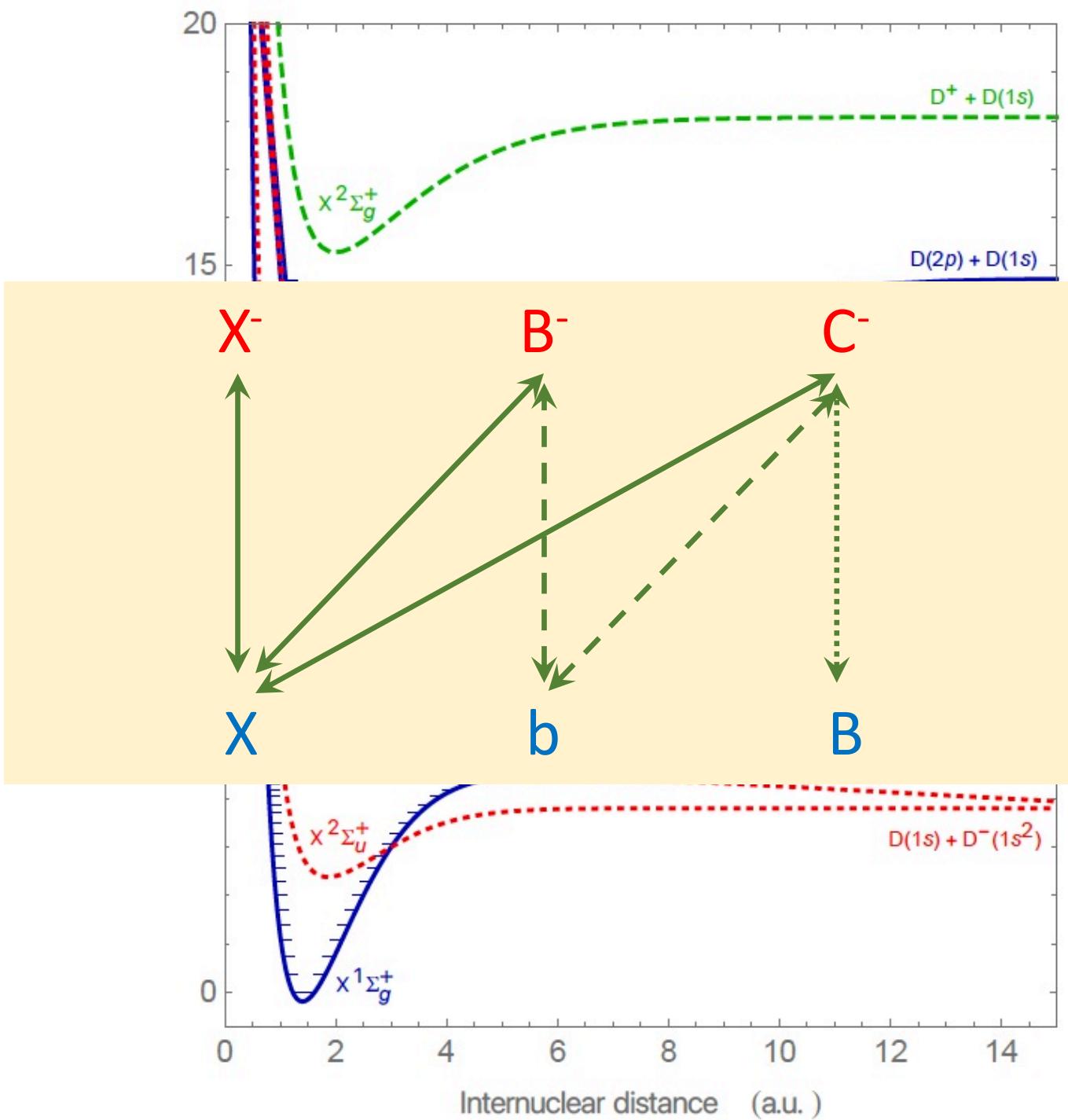


$$\begin{aligned}
\sigma_{s,v \rightarrow s',v'}^{\text{VE}}(\epsilon) &= \sum_{r \in \mathcal{R}} \frac{2S_r + 1}{(2S_s + 1)} \frac{g_r}{2} \frac{64\pi^5 m^2}{\hbar^4} \frac{k'}{k} \left| \langle \chi_{v'}^{s'} | \mathcal{V}_r^{s'} | \xi_{s,v}^r \rangle \right|^2, \quad s, s' \in \mathcal{S}, \\
\sigma_{s,v}^{\text{DA}}(\epsilon) &= \sum_{r \in \mathcal{R}} \frac{2S_r + 1}{(2S_s + 1)} \frac{g_r}{2} 2\pi^2 \frac{K}{\mu} \frac{m}{k} \lim_{R \rightarrow \infty} |\xi_{s,v}^r(R)|^2, \quad s \in \mathcal{S}, \\
\sigma_{s,v}^{\text{DE}}(\epsilon) &= \sum_{r \in \mathcal{R}} \frac{2S_r + 1}{(2S_s + 1)} \frac{g_r}{2} \frac{64\pi^5 m^2}{\hbar^4} \int_{\epsilon^{th}}^{\epsilon^{max}} d\epsilon_c \frac{k'}{k} \left| \langle \chi_c^{s'} | \mathcal{V}_r^{s'} | \xi_{s,v}^r \rangle \right|^2, \quad s, s' \in \mathcal{S},
\end{aligned}$$

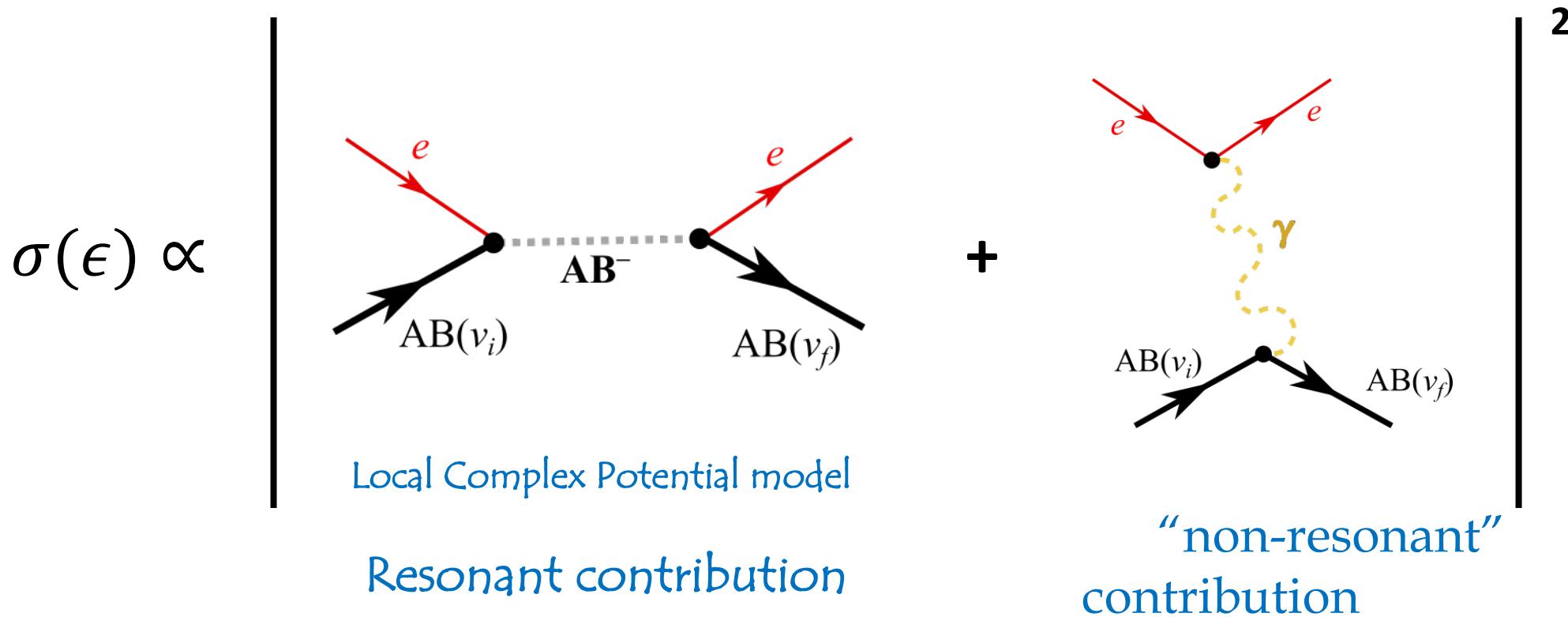
$$\mathcal{S} = \{\text{X } ^1\Sigma_g^+, \text{b } ^3\Sigma_u^+, \text{B } ^1\Sigma_u^+\} = \{\text{X, b, B}\}$$

$$\mathcal{R} = \{\text{X } ^2\Sigma_u^+, \text{B } ^2\Sigma_g^+, \text{C } ^2\Sigma_g^+\} = \{\text{X}^-, \text{B}^-, \text{C}^-\}$$

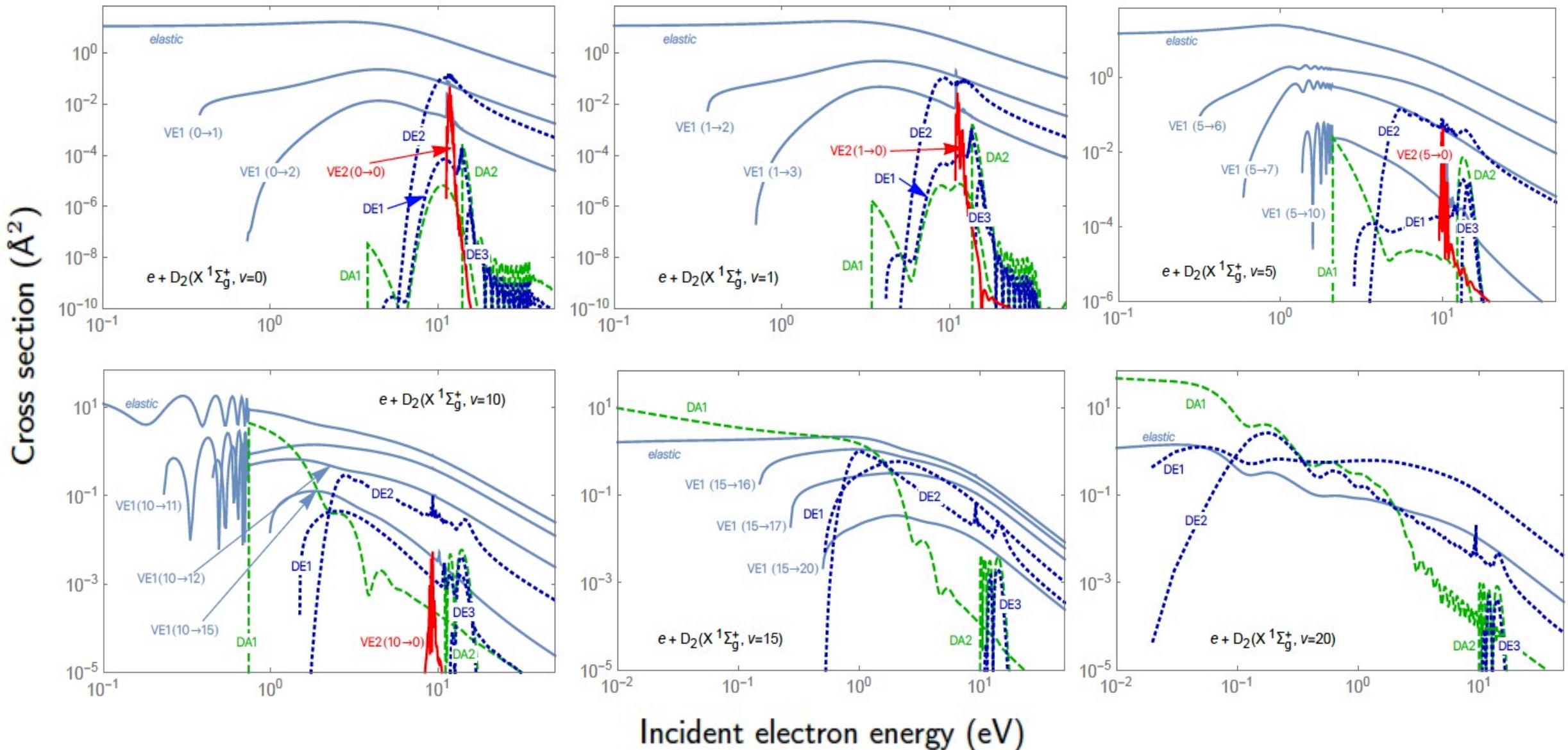


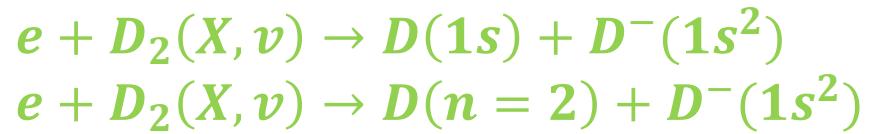


Beyond LCP model...



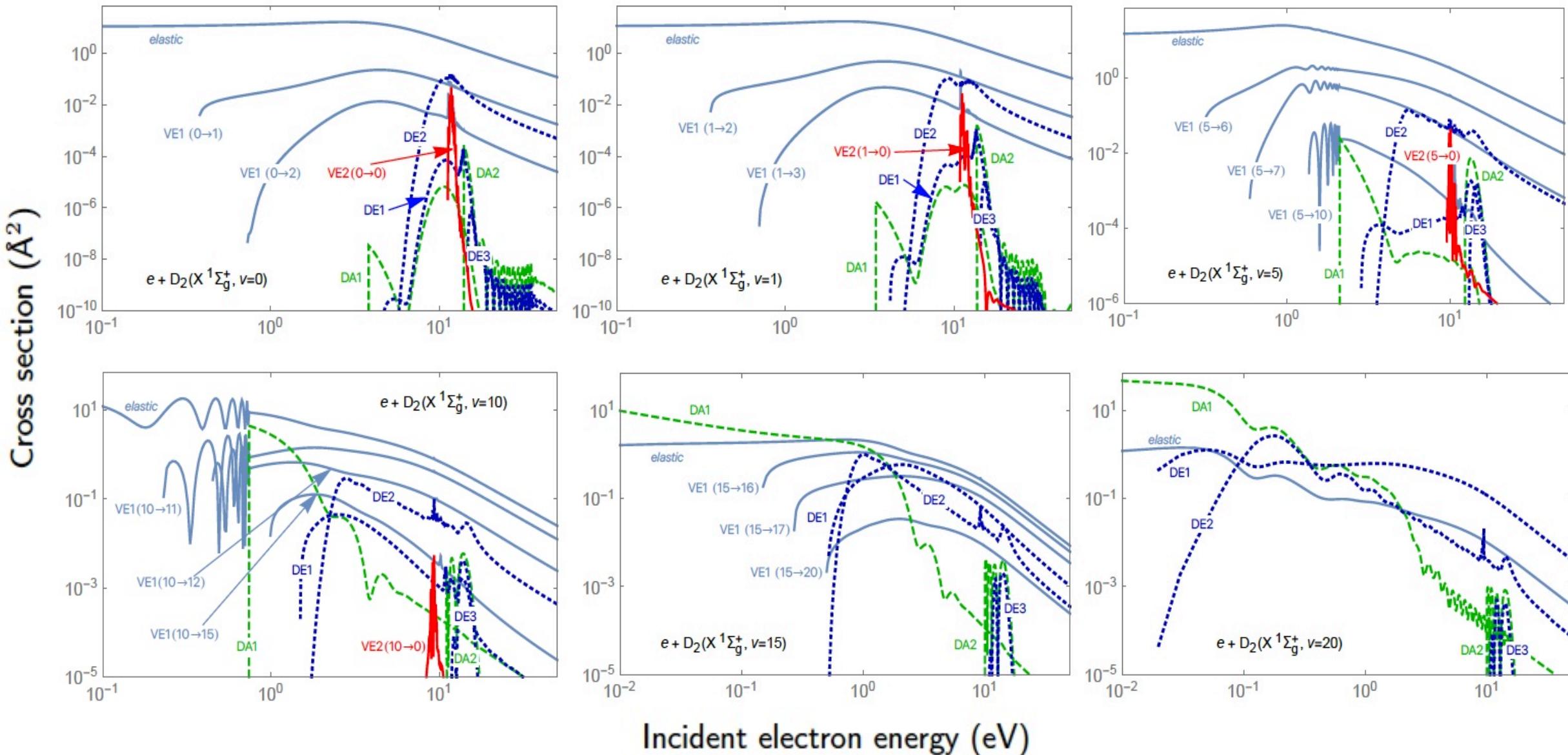
$e + D_2(X, v) \rightarrow e + D_2(X, w)$ elastic, VE1

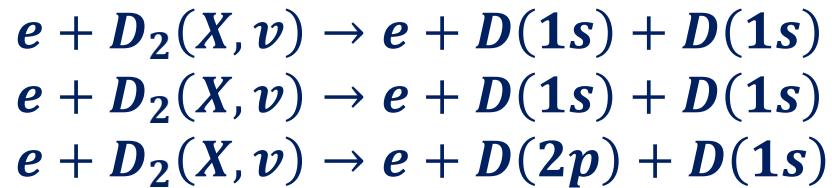




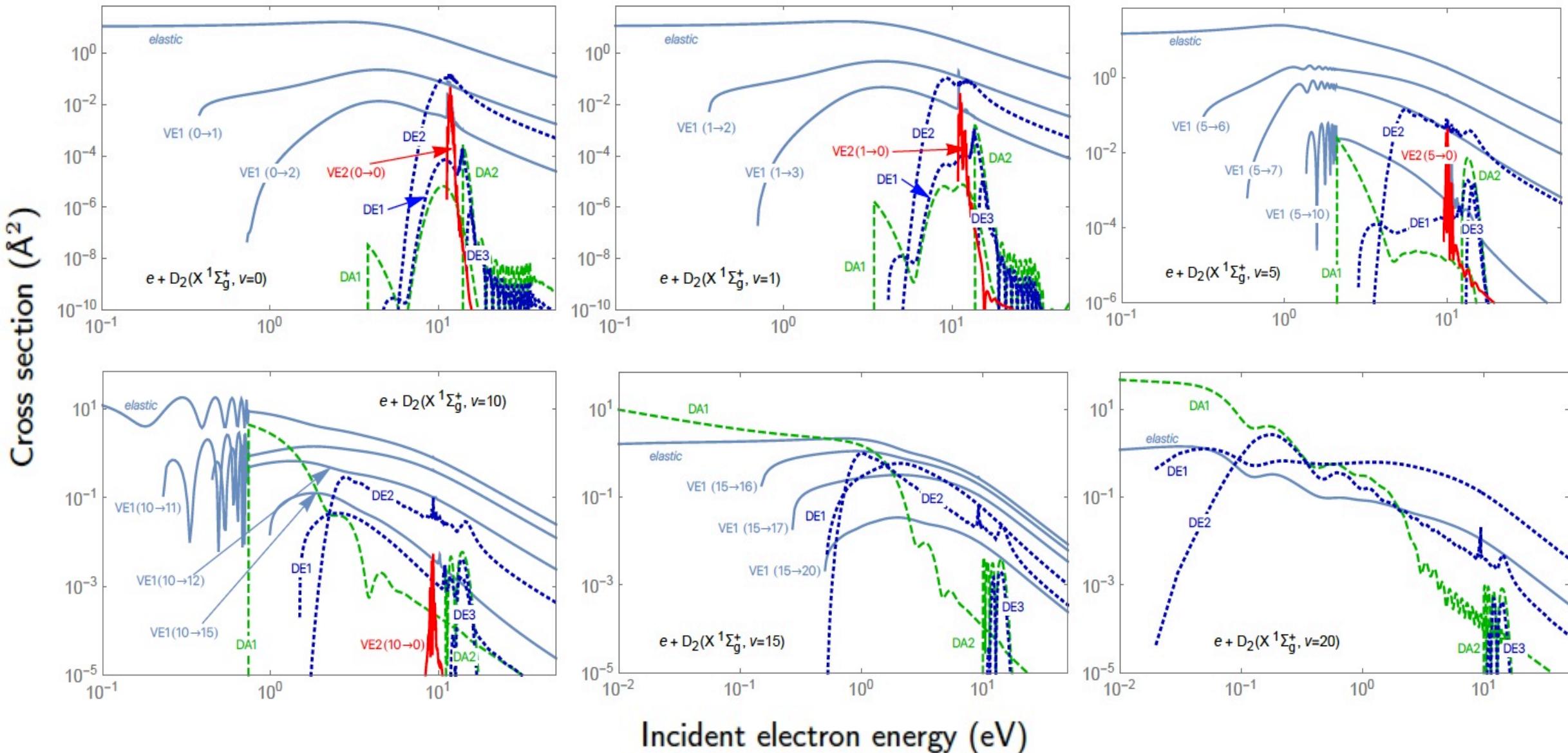
DA1

DA2



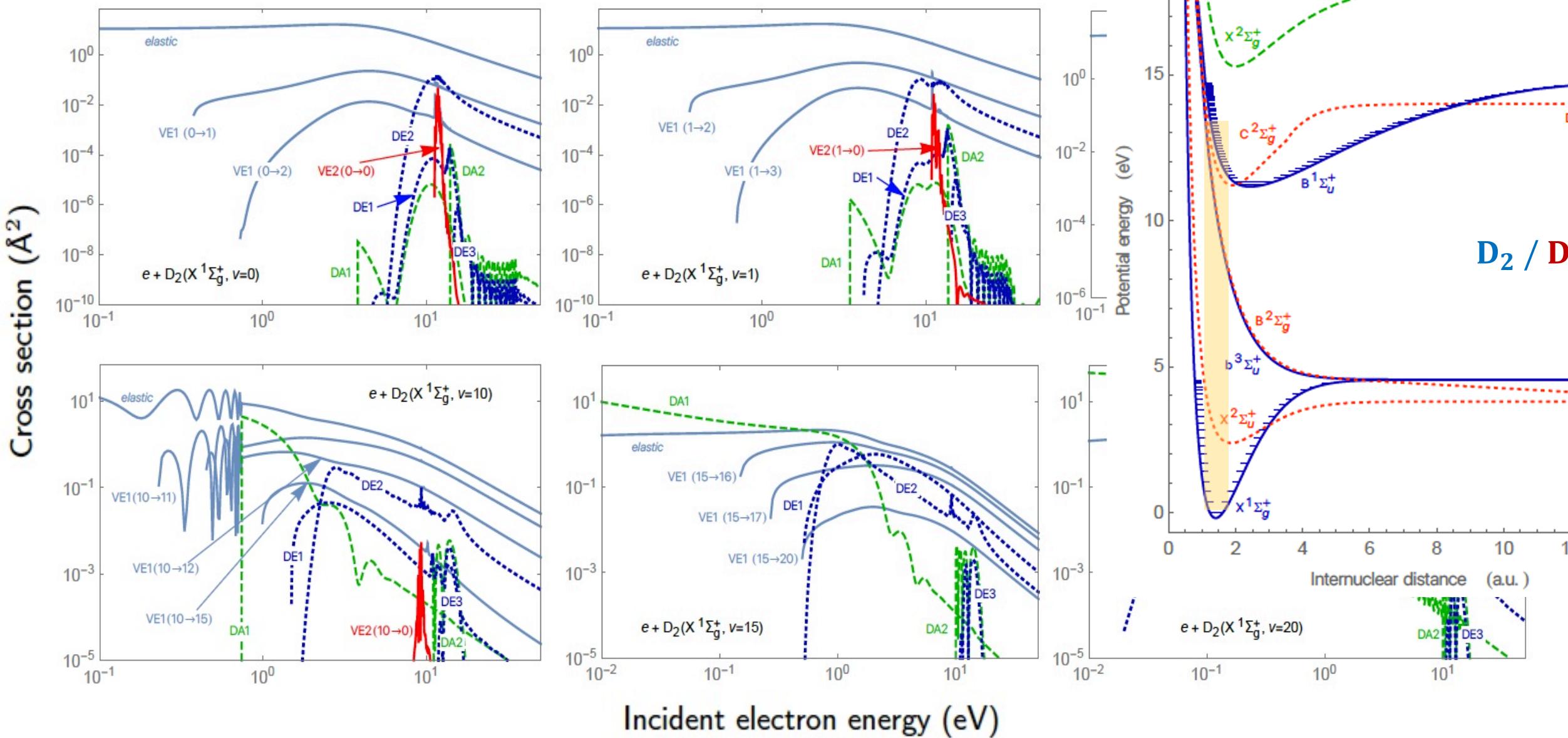


DE1
DE2
DE3

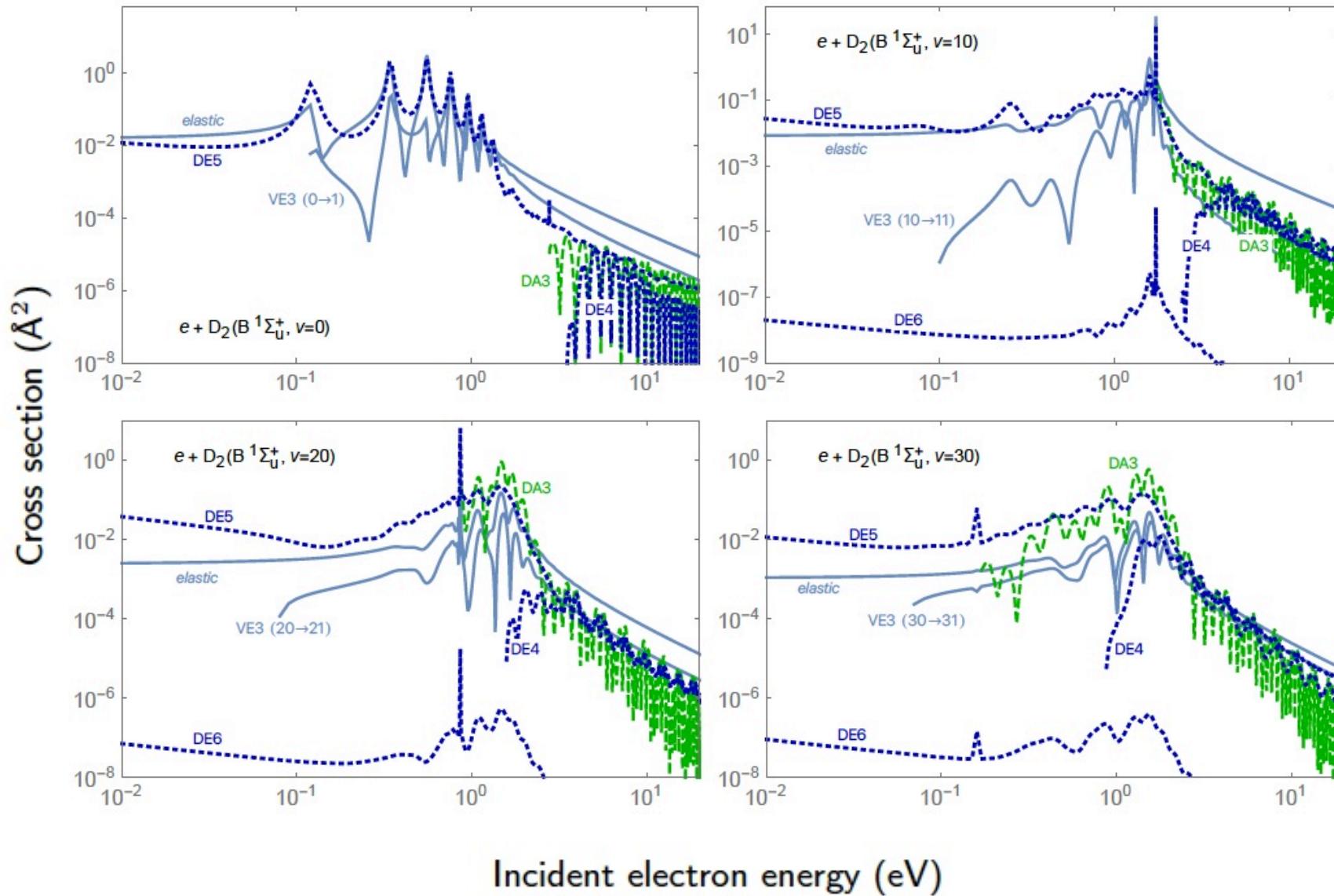


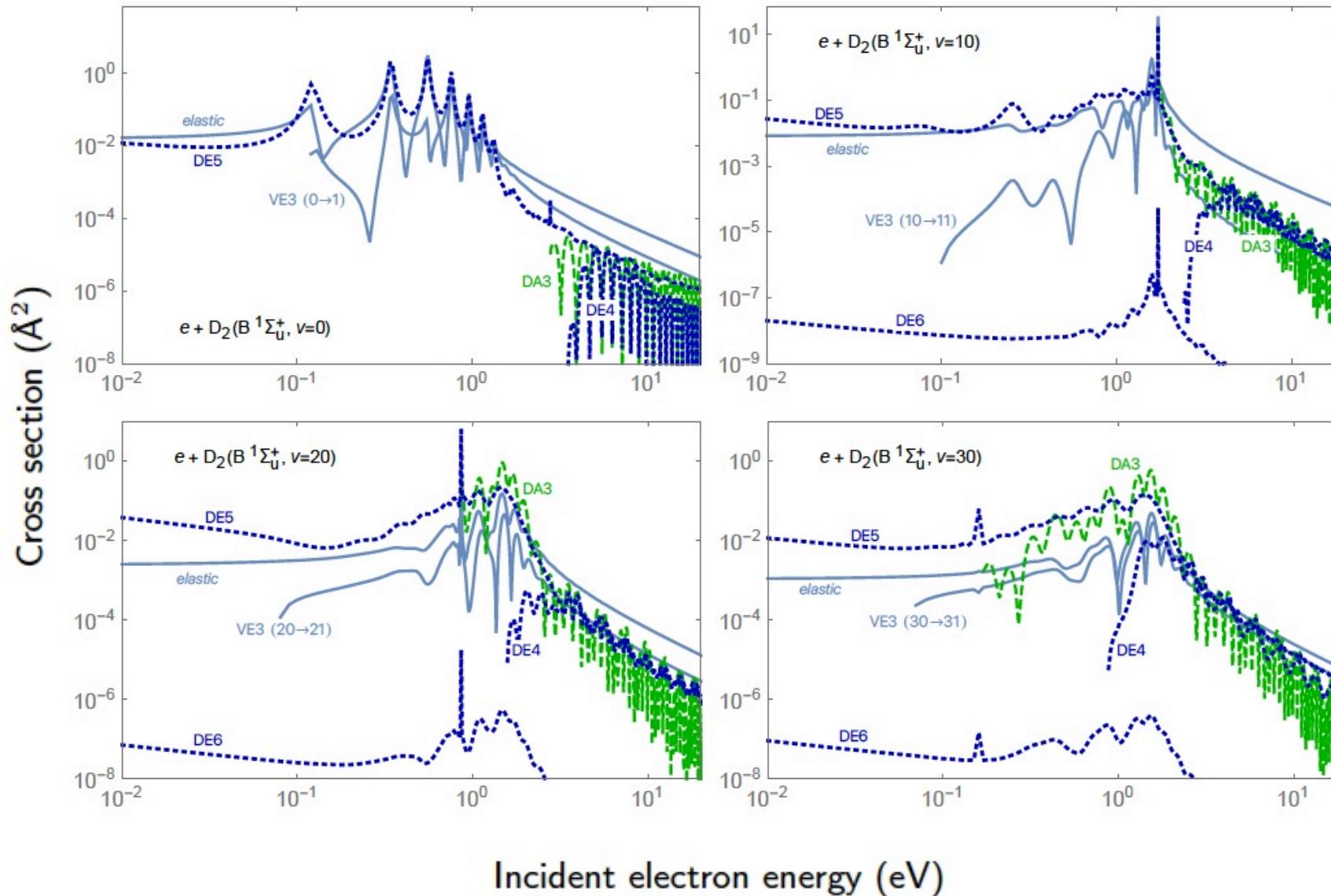


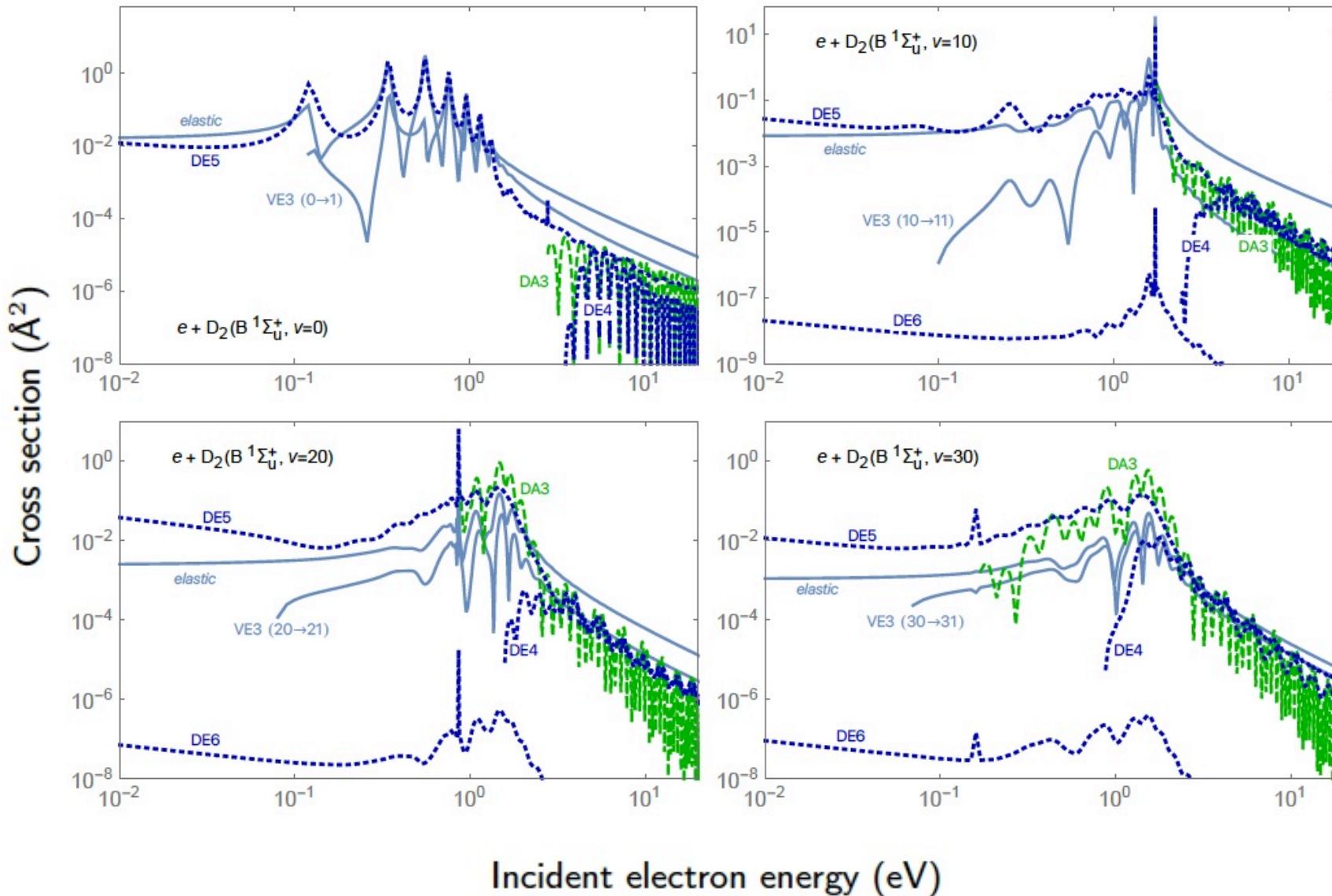
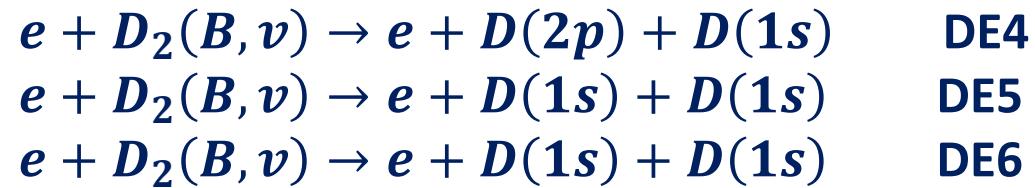
VE2



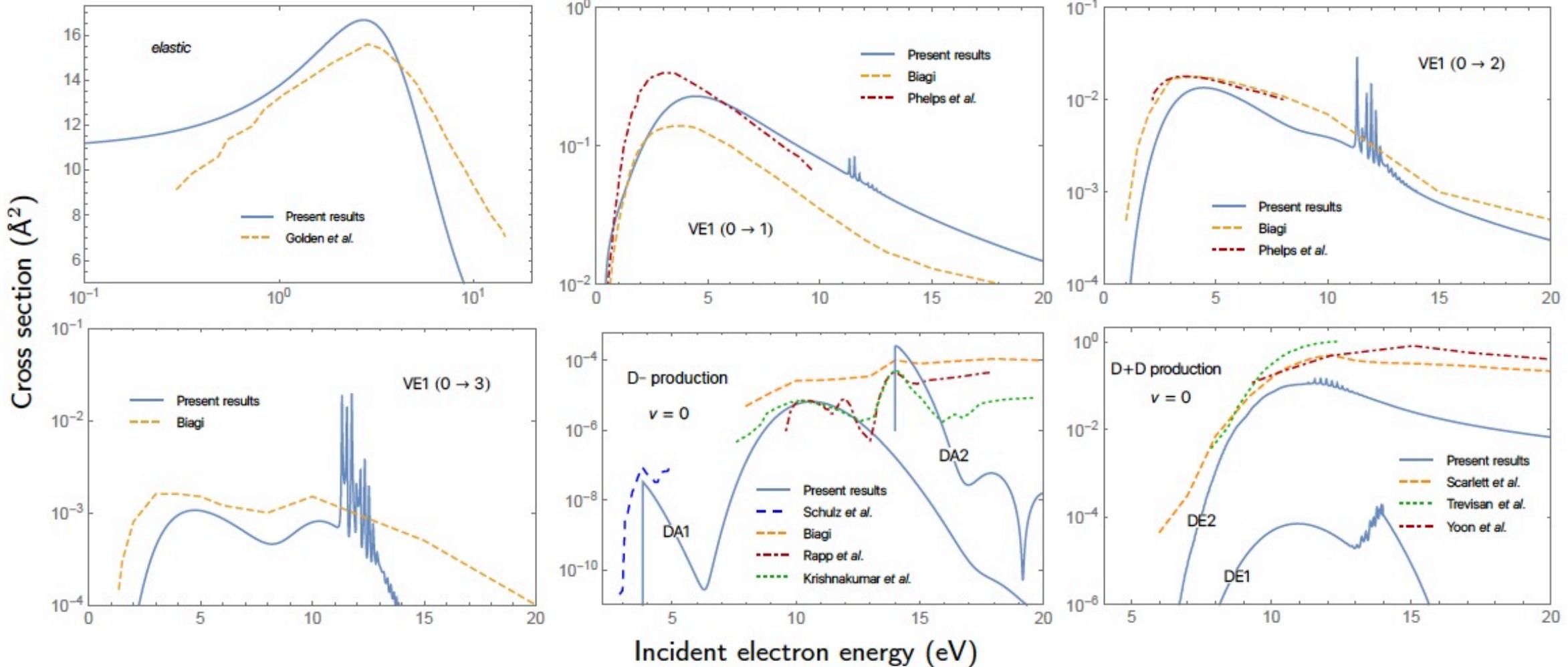
$e + D_2(B, v) \rightarrow e + D_2(B, w)$ elastic, VE3



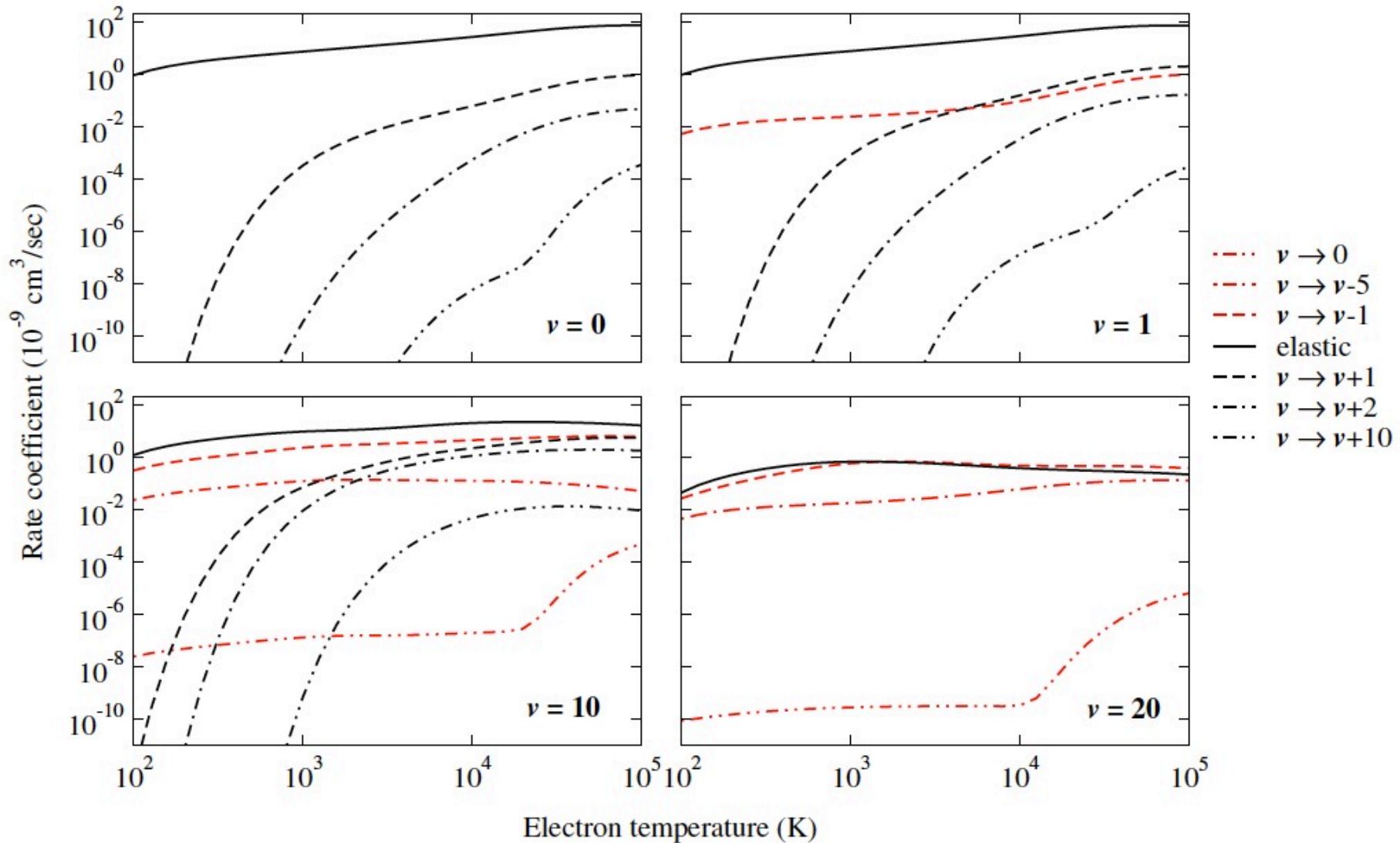




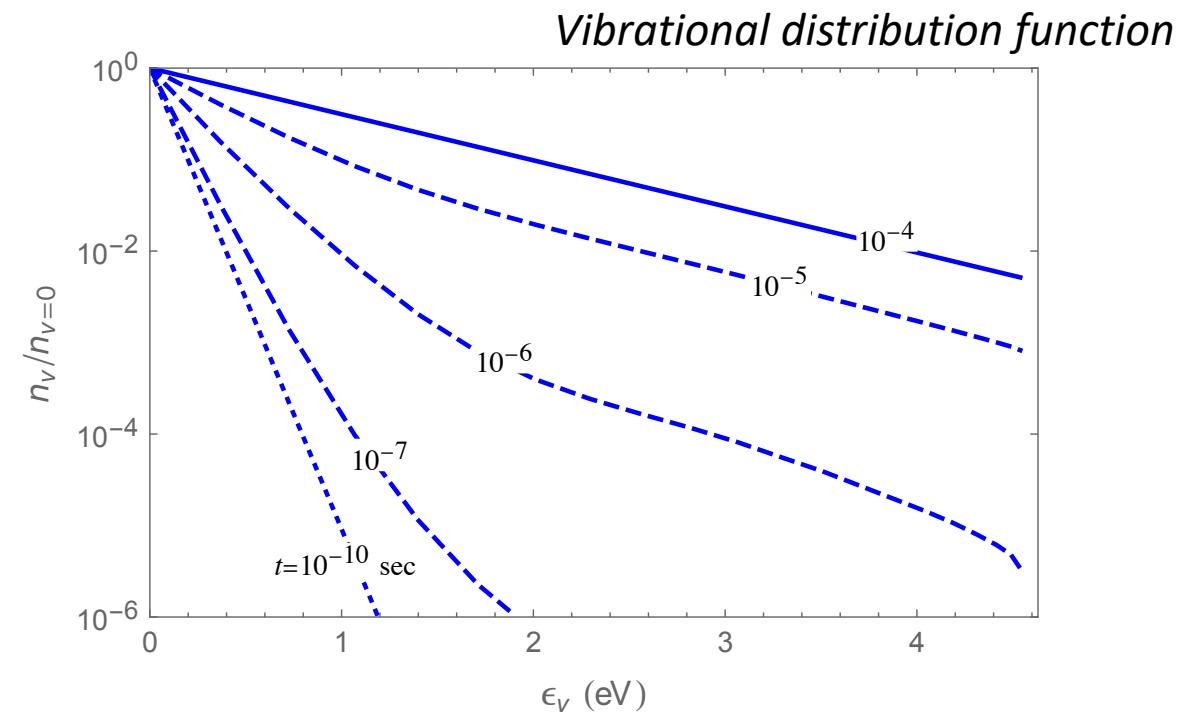
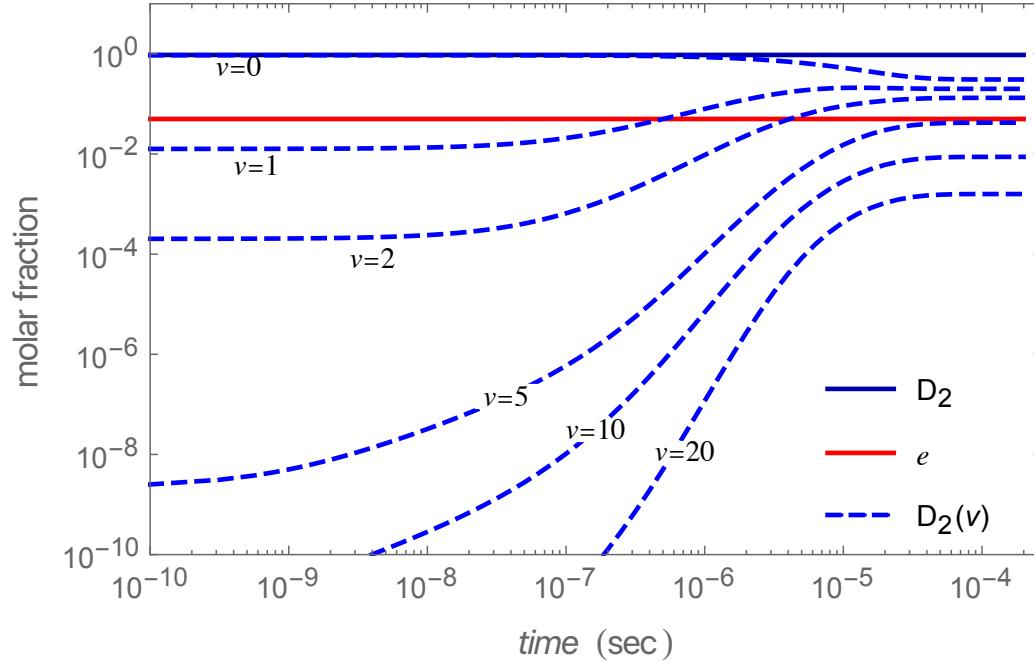
Comparison with data in literature



Vibrational relaxation of $D_2(X)$



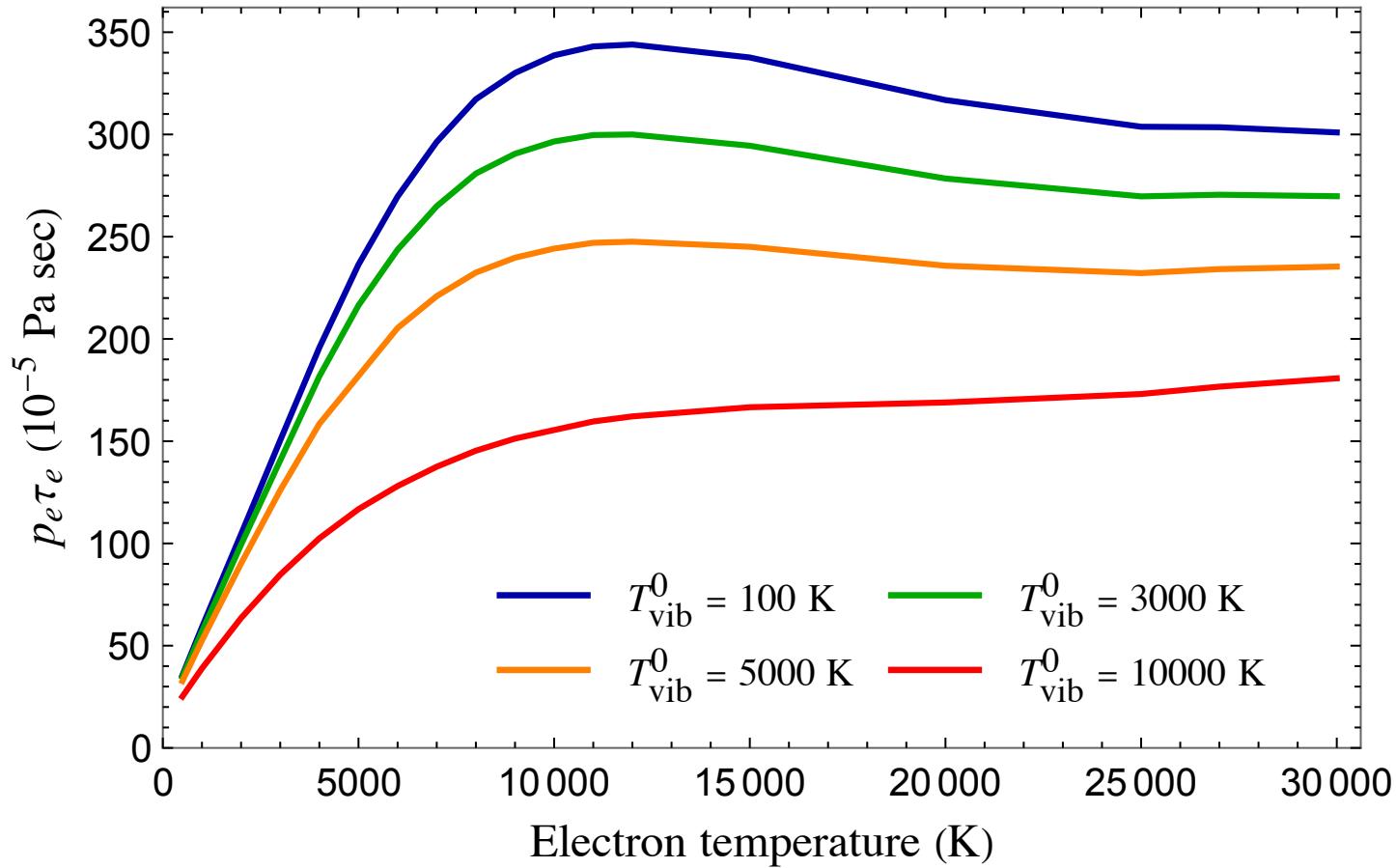
Vibrational relaxation of D₂(X)



$$\frac{dn_v}{dt} = n_e \sum_{w=0}^{20} [k_{w,v} n_w - k_{v,w} n_v], \quad v = 0, \dots, 20,$$

$n_{\text{tot}} = 10^{22} \text{ part/m}^3$
95% of D₂ 5% of e
 $T_{\text{gas}} = 10000 \text{ K}$
 $T^0_{\text{vib}} = 1000 \text{ K}$

Vibrational relaxation of D₂(X)



Conclusions

LCP (this presentation) and MQDT (loan Schneider's presentation) models are the only serious theoretical frameworks - **completely ab initio** - to describe state-resolved electron-molecule collisions which are able to take into account correctly **nuclear vibrations (and rotations)**.

I showed the LCP extension to calculate the vibrationally and electronically excited cross sections.

LCP and MQDT models are the only approaches able to calculate **Dissociative Attachment** and **Dissociative Recombination** processes.

Molecular input data come from ab initio quantum chemistry approaches, e.g. **R-Matrix**.

Outlook...

Inclusion of the other electronically excited states

H_2 cross sections and isotopic effects (work in progress...)

Including rotational motion

Inclusion of ‘non-resonant’ contributions

Extension of the LCP model for ionization cross sections

Thank you for your attention