Stockholms universitet

Theoretical studies of electron interactions with molecular ions and mutual neutralization

- HeH and BeH

Åsa Larson

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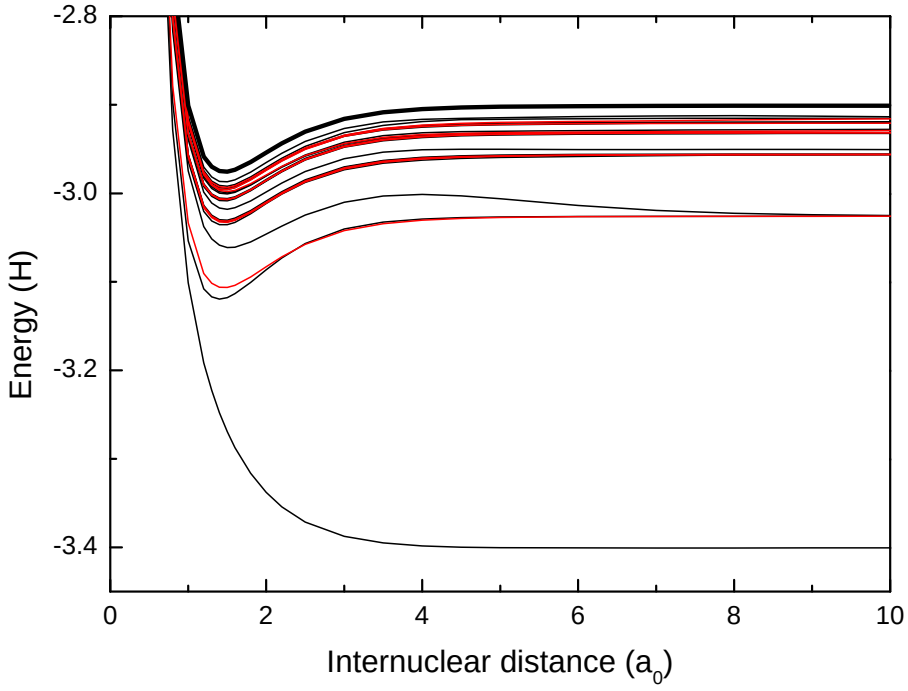
The HeH system

Low-energy DR $HeH^+ + e^- \rightarrow He + H$



Via non-adiabatic interactions
Rydberg states

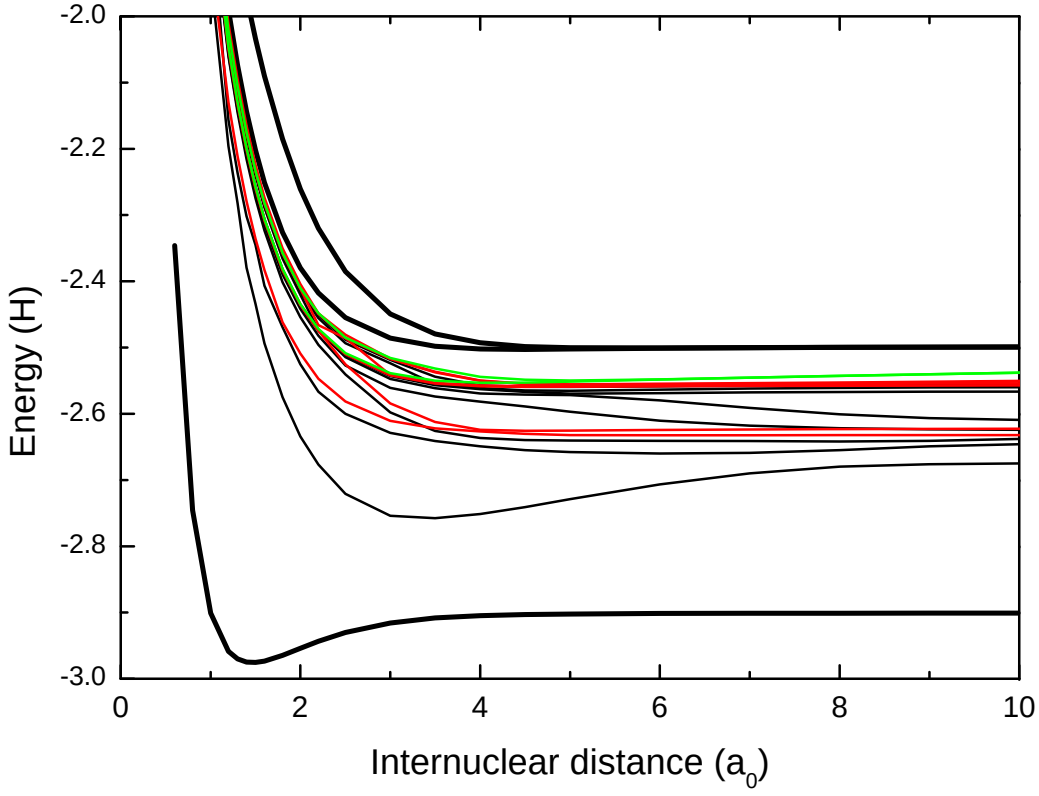
MQDT

Takagi et al, PRA 70 022709 (2004)

Haxton & Greene, PRA 79 022701 (2009).

The HeH system

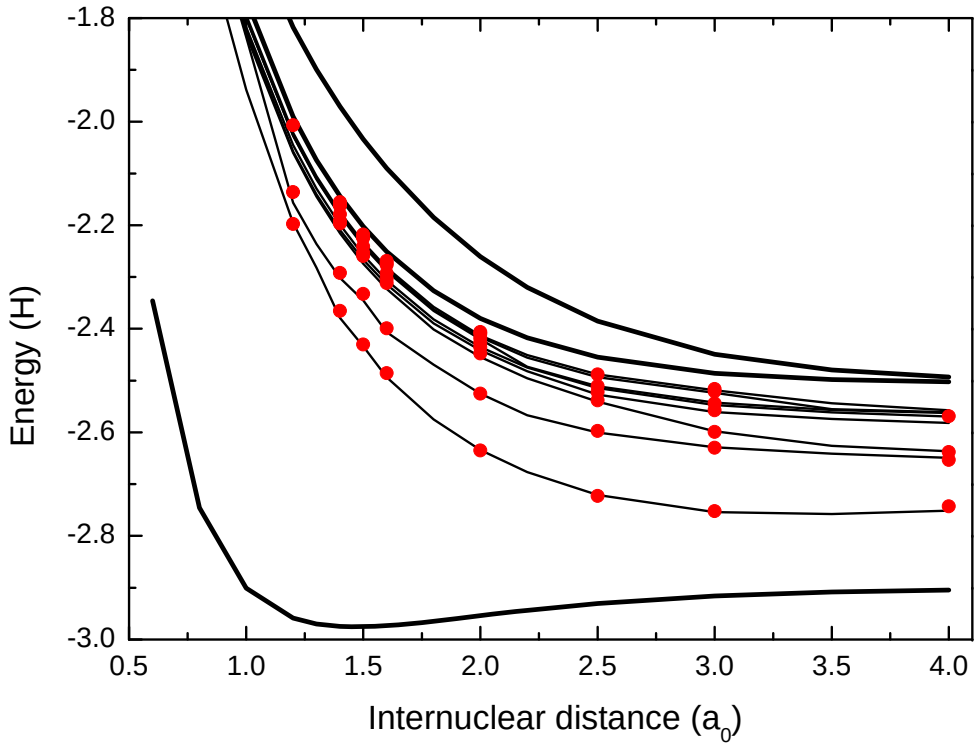
High-energy resonant states



- Calculation of potential curves (full CI, good basis, very highly excited states)

The HeH system

High-energy resonant states

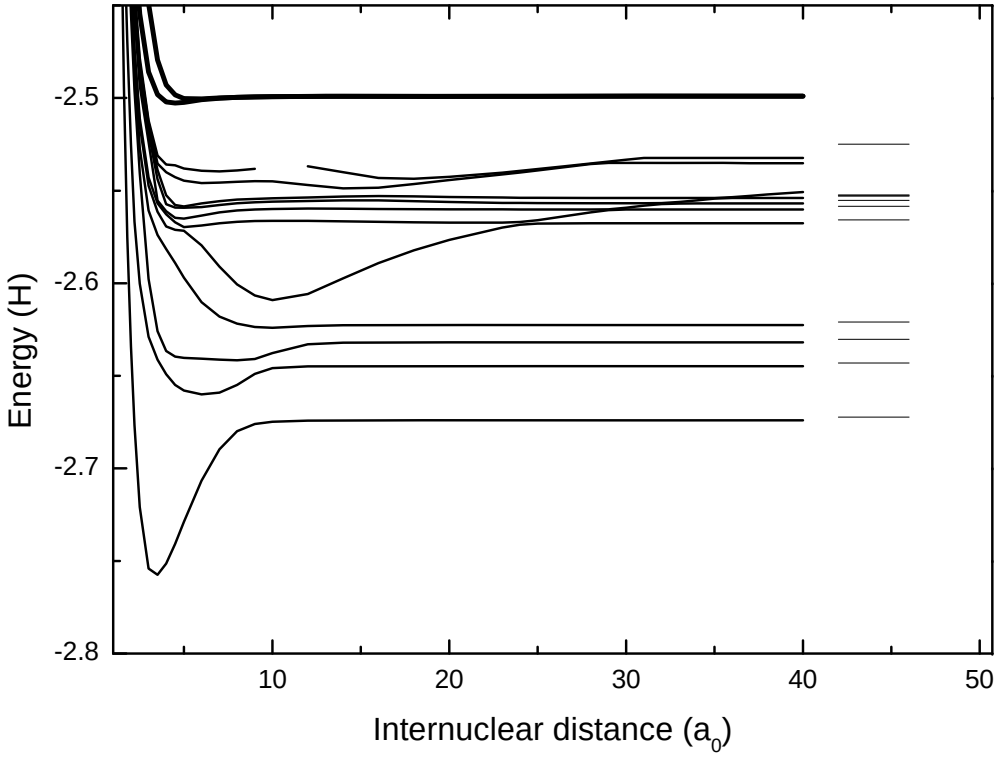


- Electron scattering calculations (Complex-Kohn variational method with a MRCI target wf)

⇒ Γ(R)

The HeH system

High-energy resonant states



- Non-adiabatic couplings (full-CI)

Sidis formula:

$$\left\langle \Phi_i \left| \frac{\partial}{\partial R} \right| \Phi_j \right\rangle = R^{-1} \left\{ \frac{1}{2} \left(E_i - E_j \right) \left\langle \Phi_i \left| \sum_k r_k^2 \right| \Phi_j \right\rangle + \left(E_i - E_j \right)^{-1} \left\langle \Phi_i \left| T \right| \Phi_j \right\rangle \right\}$$

V. Sidis, JCP 55, 5838 (1971)

The HeH system

Reactions to study

Resonant vibrational excitation:

(VE) $$HeH^+(v) + e^- \rightarrow HeH^* \rightarrow HeH^+(v') + e^-$$

Resonant dissociative excitation:

(DE) $$HeH^+(v) + e^- \rightarrow HeH^* \rightarrow He + H^+ + e^-$$

Studied here

The HeH system

Reactions to study

High-energy dissociative recombination:

(DR) $HeH^+(v) + e^- \rightarrow HeH^* \rightarrow He^* + H$

Ion-pair formation:

(RIP) $HeH^+(v) + e^- \rightarrow HeH^* \rightarrow He^+ + H^-$

previous study [1]

Mutual neutralization:

(MN) $He^+ + H^- \rightarrow HeH^* \rightarrow He^* + H$

[1] Å. Larson & A. E. Orel, PRA 59 3601 (1999).

The HeH system

VE & DE – Theoretical treatment

Driven Schrödinger eq. $\left(T + V_i - \frac{i}{2}\Gamma_i - E\right)\Psi_v^i = -\sqrt{\frac{\Gamma_i}{2\pi}}\chi_v$

⇨ Local approximation

⇨ No couplings between neutral states

T-matrix: $T_{vv'}^i(E) = \left\langle \chi_{v'} \middle| \sqrt{\frac{\Gamma_i}{2\pi}} \middle| \Psi_v^i \right\rangle$

⇨ Coherent sum for states of the same symmetry

$$T_{vv'} = \sum_i T_{vv'}^i$$

The HeH system

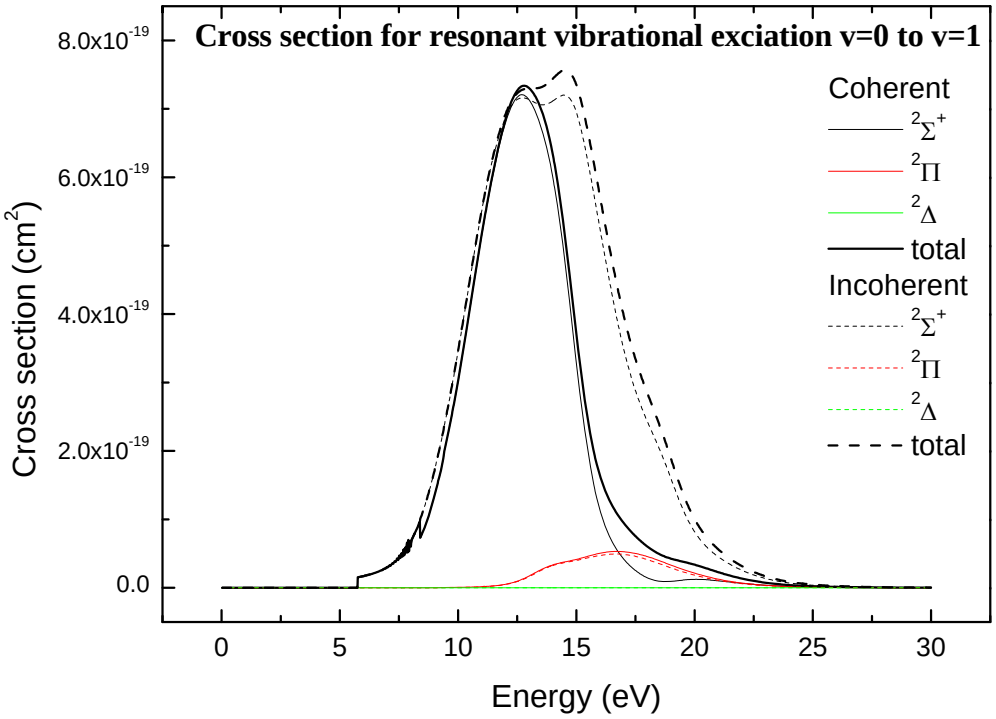
VE & DE – Theoretical treatment

VE cross section $$\sigma_{vv'} = \frac{2\pi^3}{E} g \left| T_{vv'} \right|^2$$

DE cross section $$\sigma_{v} = \frac{2\pi^3}{E} g \int \left| T_{v\varepsilon} \right|^2 d\varepsilon$$

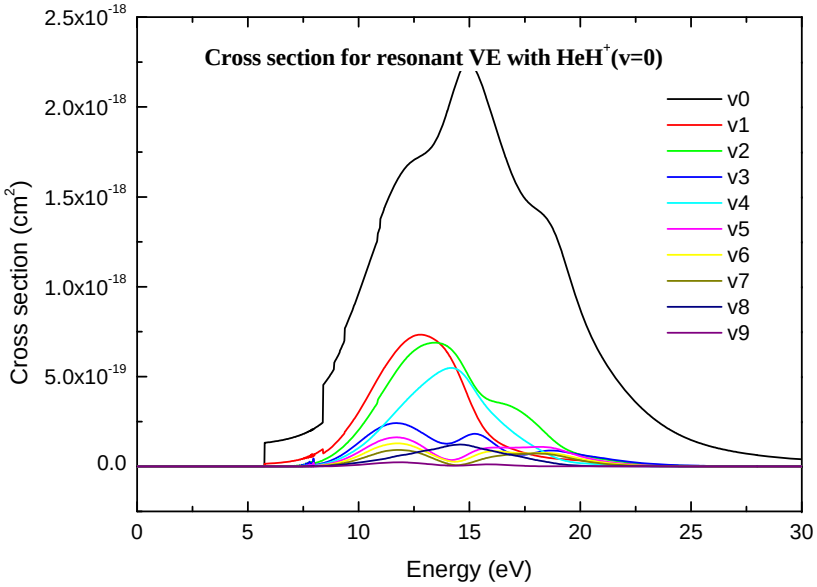
The HeH system

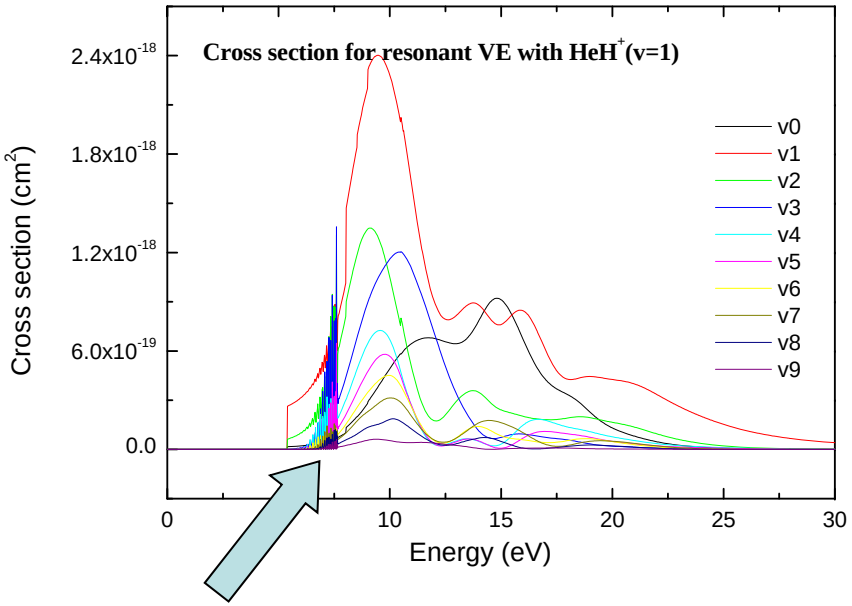
VE v = 0 → v = 1 Coherent/Incoherent



The HeH system

VE cross sections

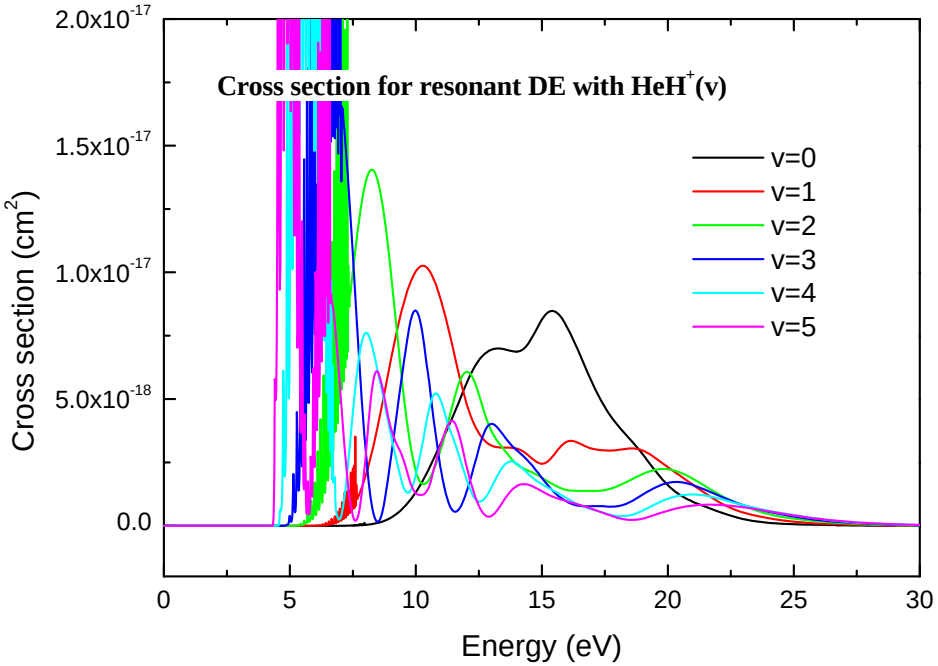




Structures due to capture into quasibound vibrational states in $^2\Sigma^+$ resonant states

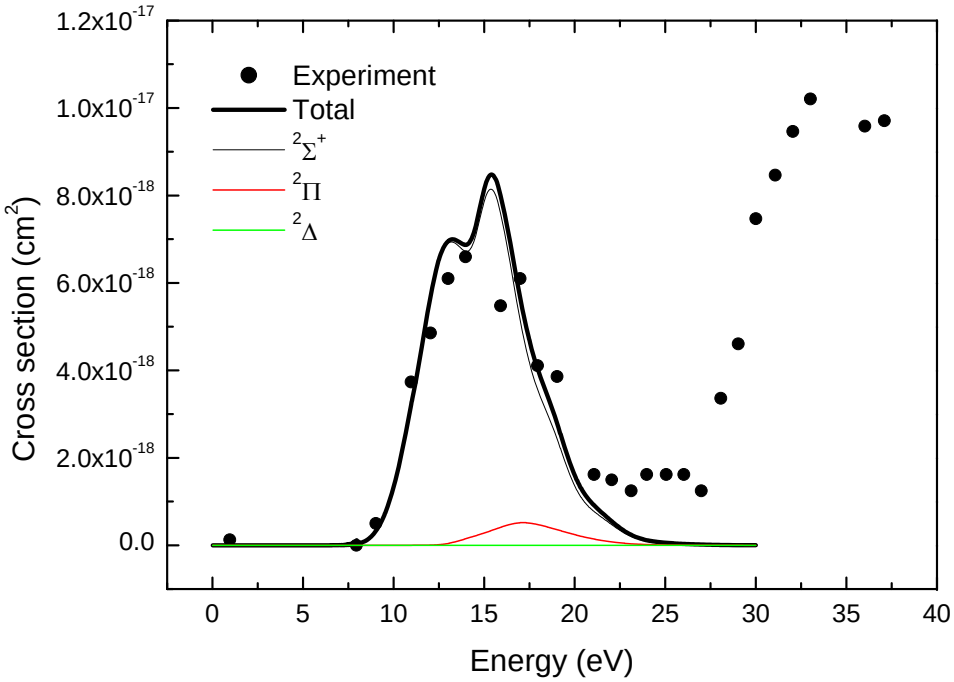
The HeH system

DE cross section



The HeH system

DE cross section



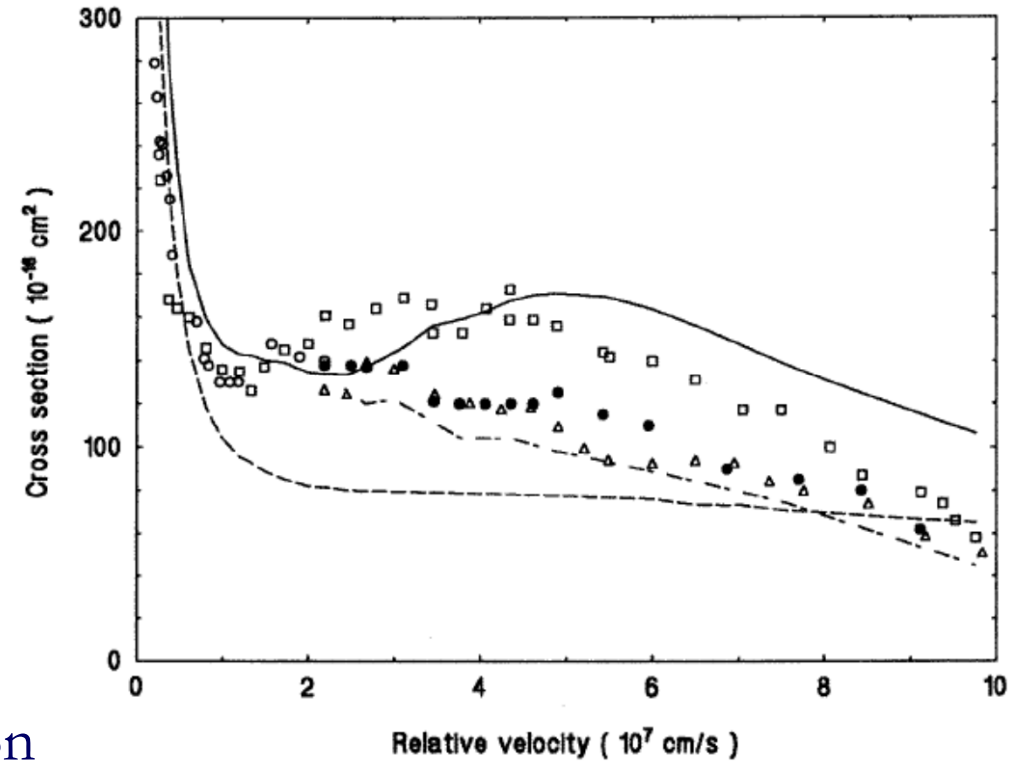
C. Strömholm et al., PRA 54 3086 (1996).

The HeH system

MN reaction

Previous experimental studies down to 0.6 eV [1]

Theory using either LZ or close-coupling calc. with classical nuclear motion [2].



⇒ No quantum study

⇒ Include autoionization

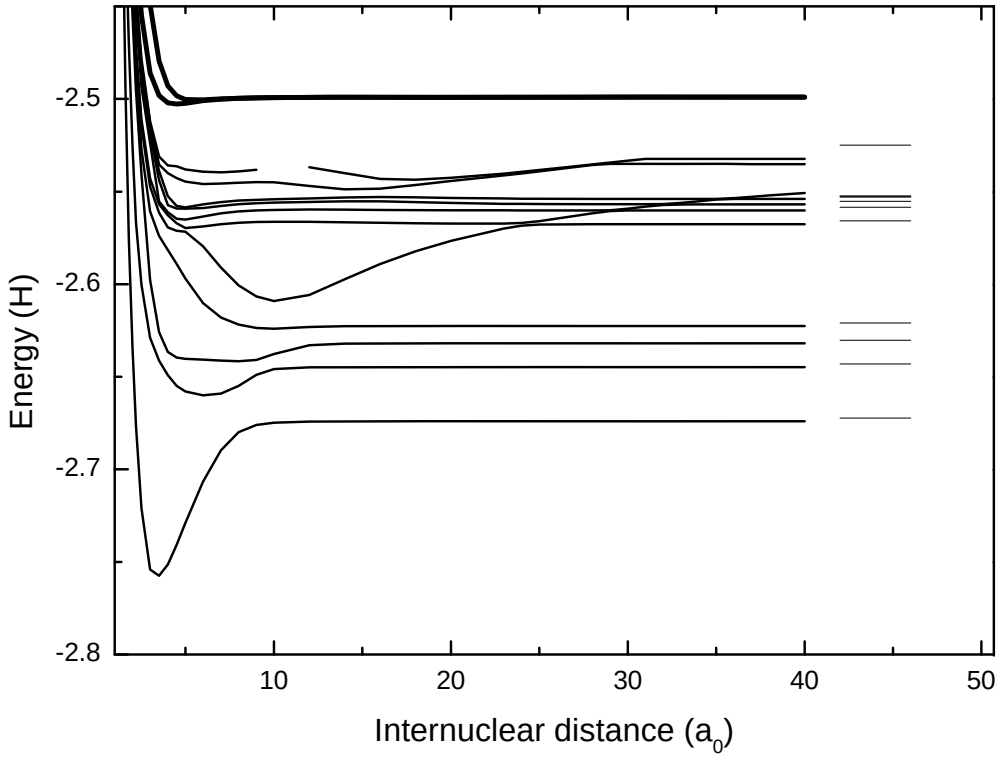
⇒ Good reaction for DESIREE

[1] B. Peart & D A Hayton, JPB, 27, 2551 (1994)

[2] Chibisov et al. JPB 30, 991 (1997)

The HeH system

MN reaction



Include 12 adiabatic states of $^2\Sigma^+$ symmetry

$\leq$ H + He(1s3lσ)

H + He(1s4lσ) states cross the ion-pair at R >100 a_0.

The HeH system

MN reaction

Previous study of $H^+ + H^-$ [1]

Strict diabatization: $\left[\mathbf{1}\frac{d}{dR} + \mathbf{f}\right]\mathbf{T} = \mathbf{0}$

⇒ Transform the complex adiabatic resonant states

Time-independent S.E. with partial wave expansion

⇒ Matrix Riccati-equation

⇒ Cross section

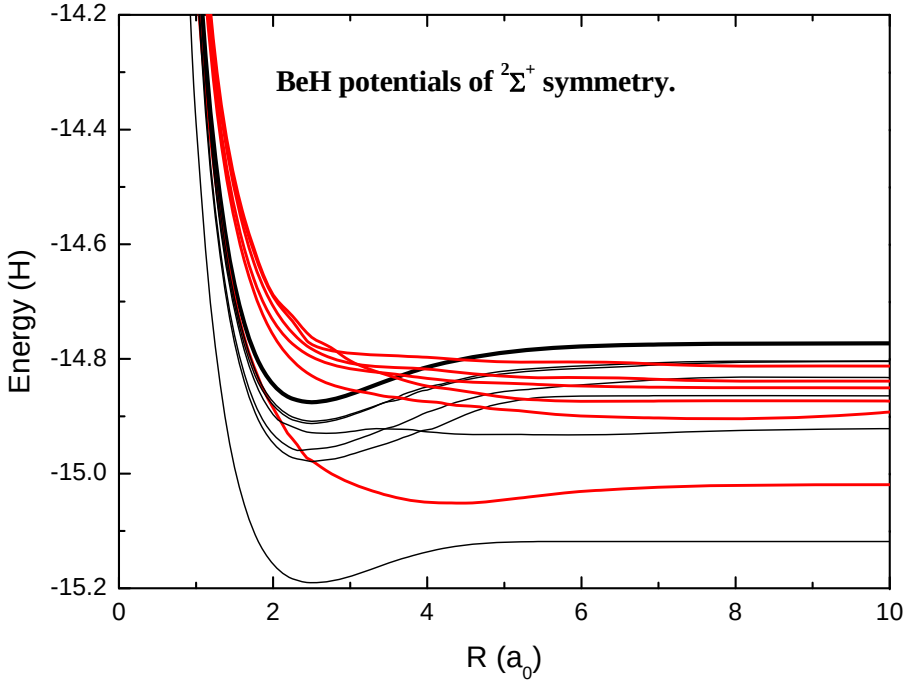
More to come…

Presently the non-adiabatic couplings are computed

[1] M. Stenrup et al. PRA, 79, 012713 (2009).

The BeH system

DR $BeH^+ + e^- \rightarrow BeH^* \rightarrow Be + H$



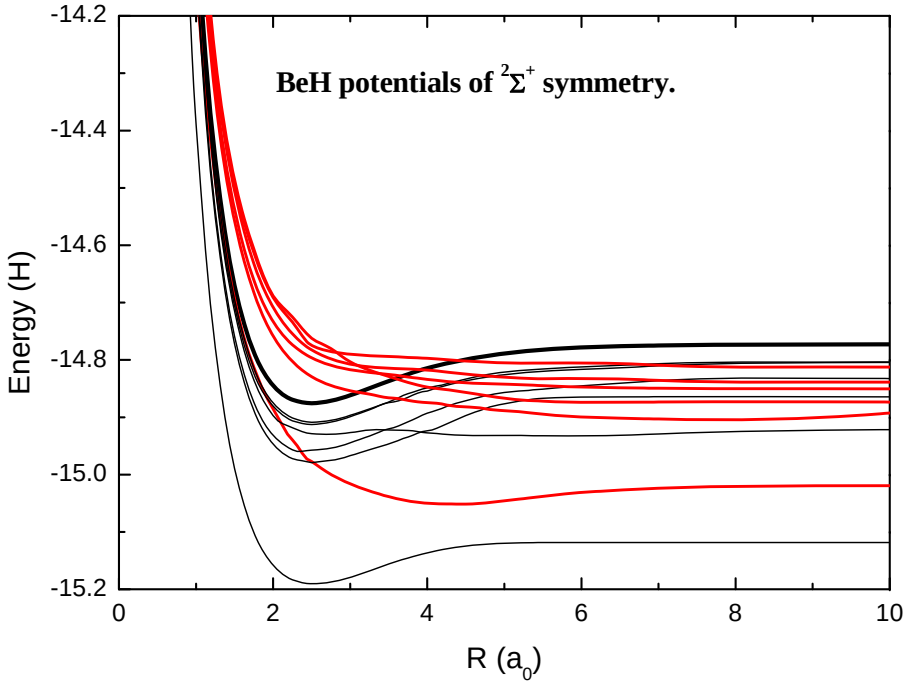
Previous study by us [1] where the electron was captured into the resonant states.

Couplings between the neutral states.

[1] J B Roos et al. PRA 80 012501 (2009)

The BeH system

DR $BeH^+ + e^- \rightarrow BeH^* \rightarrow Be + H$



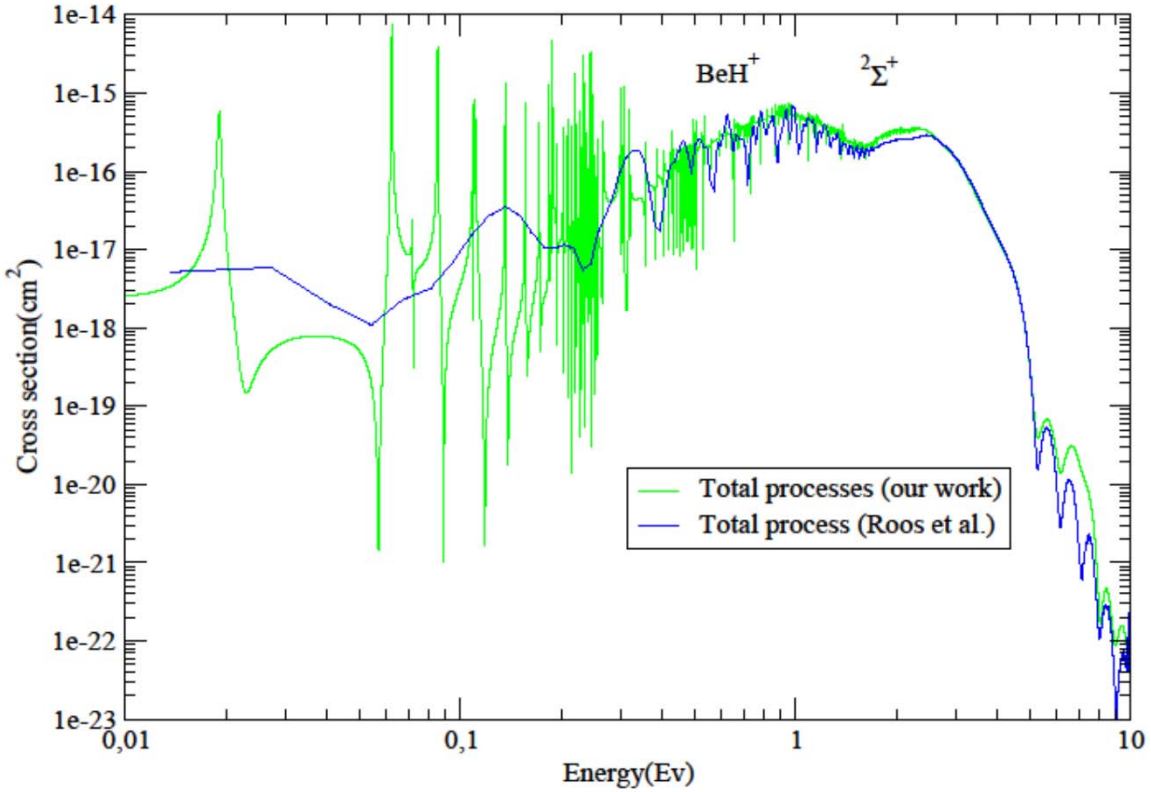
What about the indirect mechanism?

Best described using MQDT

(collaboration with I. Schneider and co-workers at Univ. Le Havre, France)

The BeH system

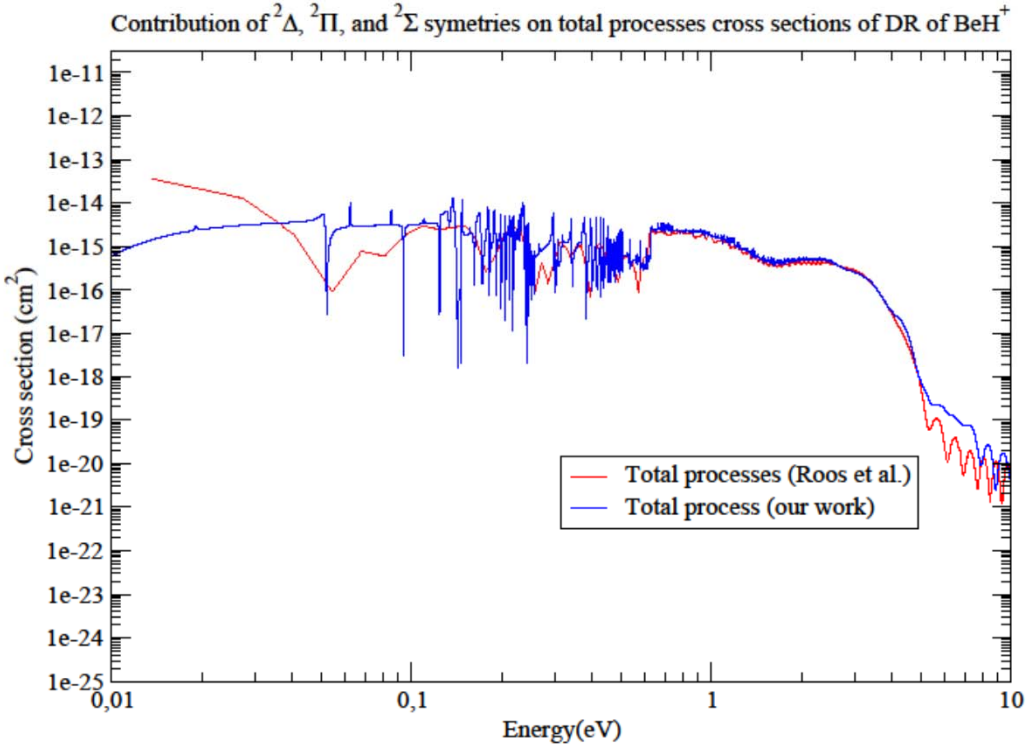
DR



⇨ Narrow resonant structures

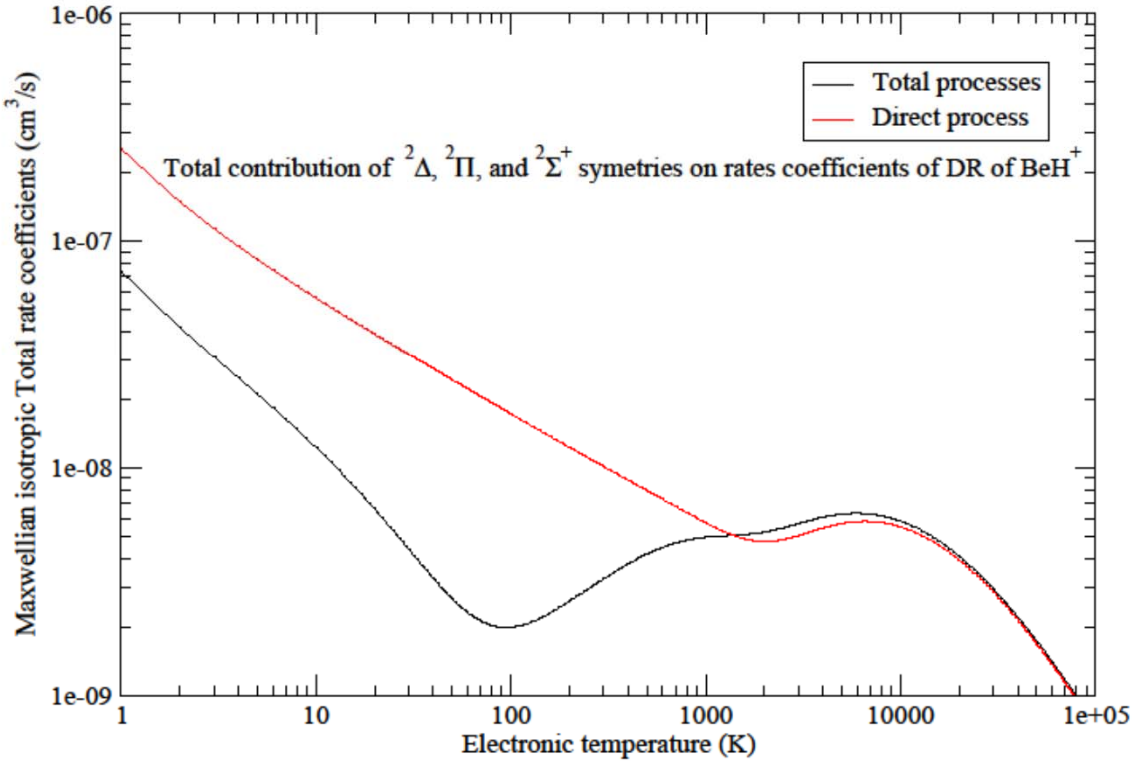
The BeH system

DR Total cross section for v = 0



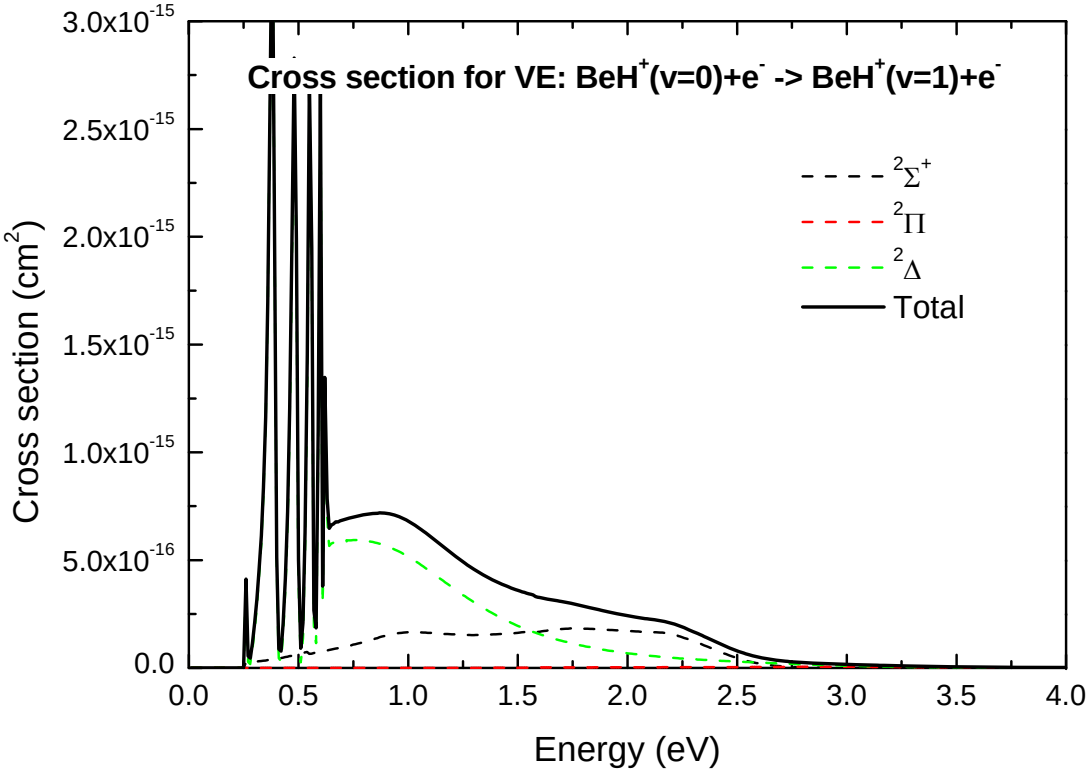
The BeH system

DR Thermal rate coefficient



The BeH system

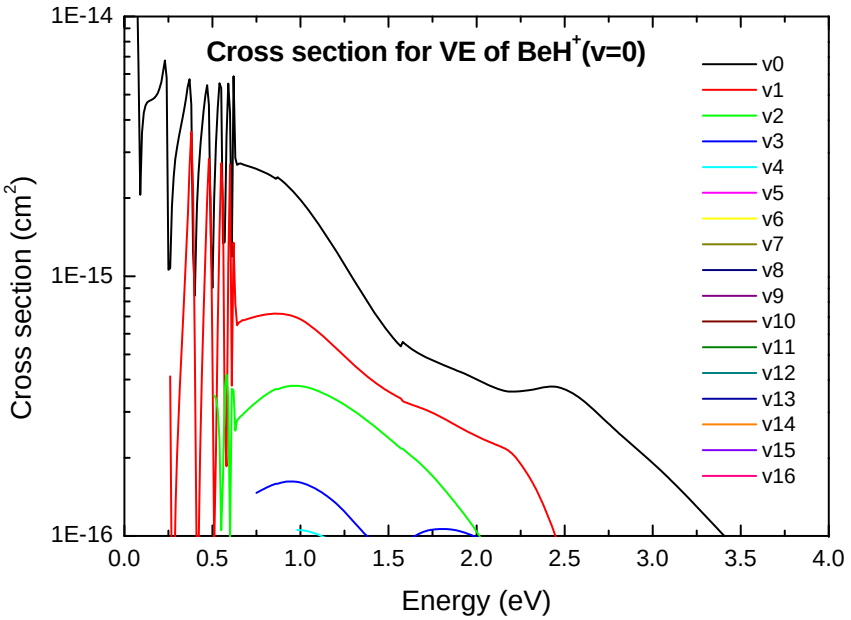
VE: $BeH^+(v) + e^- \rightarrow BeH^* \rightarrow BeH^+(v') + e^-$

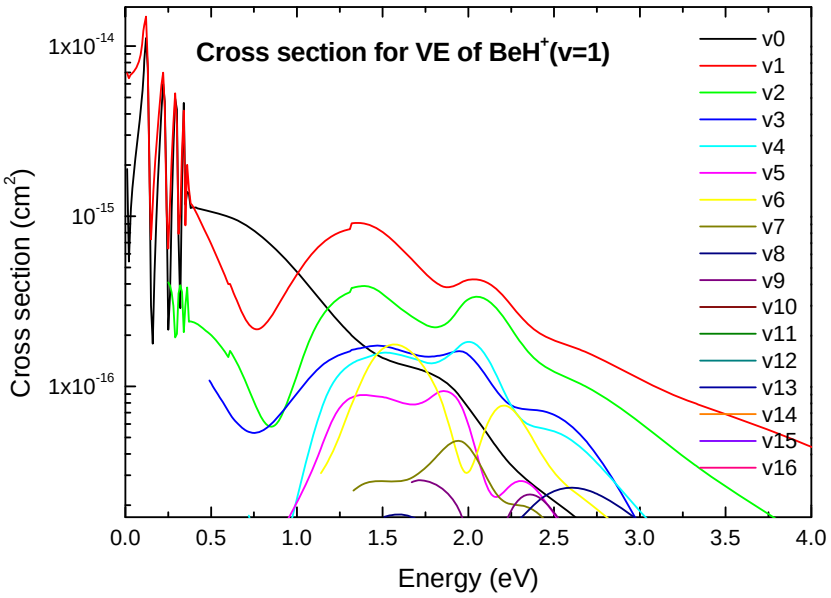


- Important at lower collision energies.
- Resonant structures due to bound vibrational states.

The BeH system

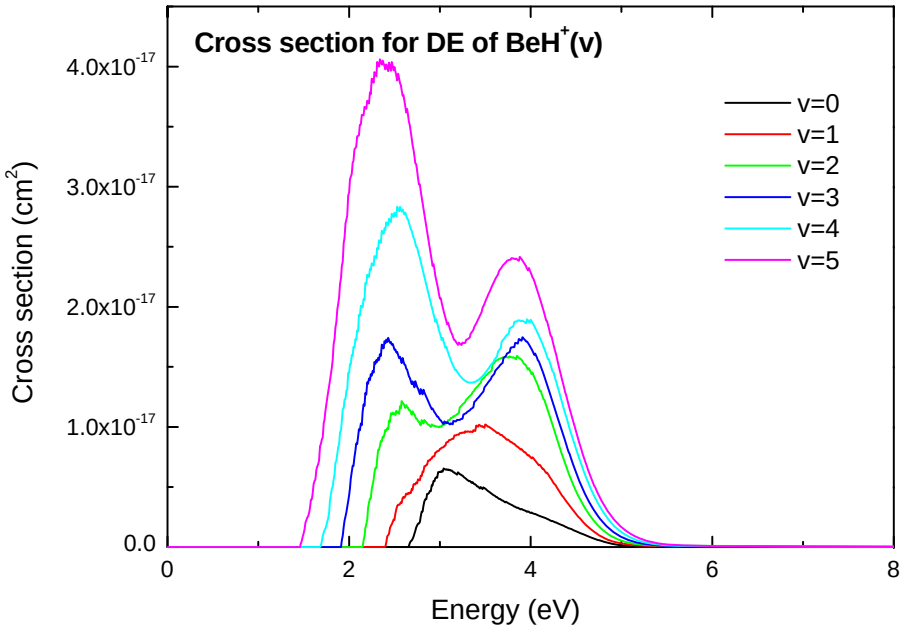
VE: $BeH^+(v) + e^- \rightarrow BeH^* \rightarrow BeH^+(v') + e^-$





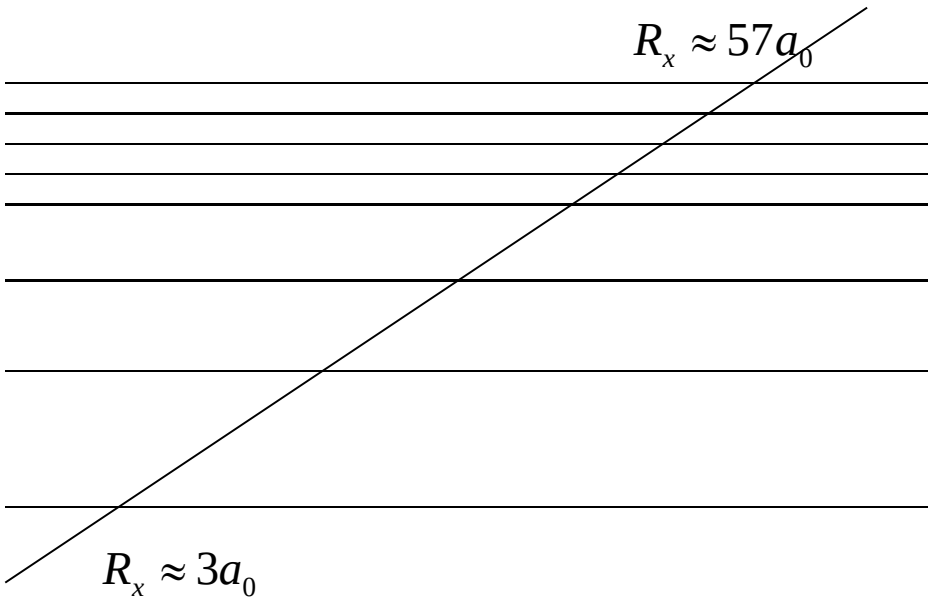
The BeH system

DE: $BeH^+(v) + e^- \rightarrow BeH^* \rightarrow Be^+ + H + e^-$



The BeH system

What about MN? $Be^+ + H^- \rightarrow BeH^* \rightarrow Be^* + H$



$Be^+ + H^-$

$Be(2s4s,^1S) + H$

- 12 states of
- $^2\Sigma^+$ symmetry

$Be(2s2p,^3P) + H$

⇨ Not possible with present MRCI calculation!

Summary

HeH

- recalculation of resonant states
- study of VE and DE
- calculation on non-adiabatic interactions
- will study MN and maybe DR and RIP.

BeH

- Inclusion of the indirect mechanism in DR using MQDT
- VE and DE
- The MN reaction demands a full CI.

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