

# 水素分子イオンの解離性再結合 断面積 III

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北里大 高木秀一

# 分子イオン・電子 データ

Molecular assisted recombination in divertor  
+ other processes

$H_2^+$ ,  $HeH^+/NeH^+$ ,  $CH^+$ ,  $H_3^+$ ,  
their isotopes **D, T**

日本原子力研究機構委託調査

CRP on Light Element Atom, Molecule and Radical Behaviour  
in the Divertor and Edge Plasma Regions by IAEA,

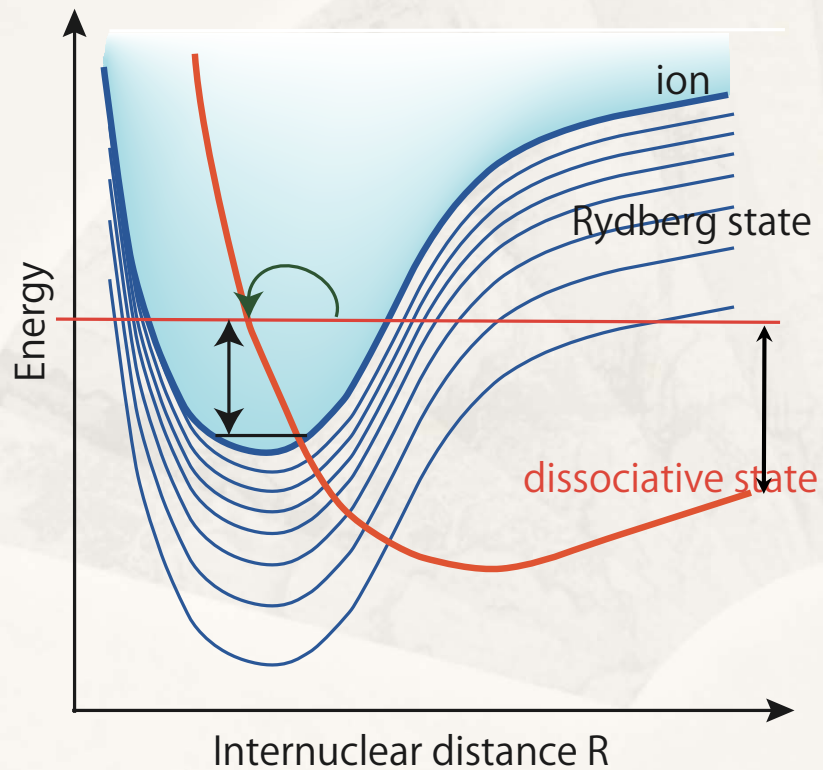
**データ作成, 収集**

# 2011の報告事項

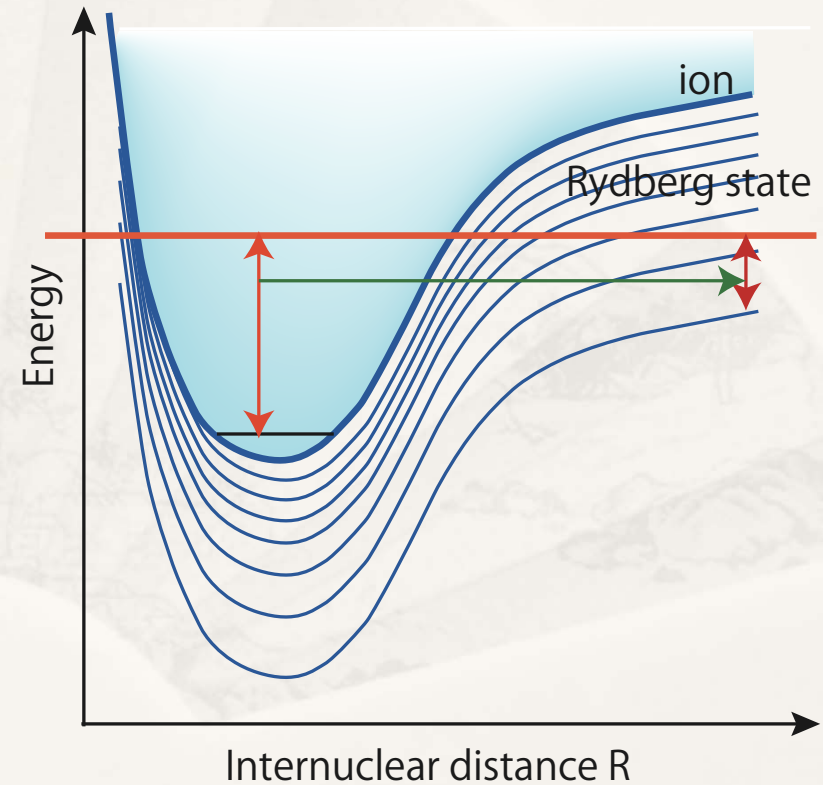
- \* 低エネルギー( $<1\text{eV}$ )  $\text{DT}^+(\nu, N)$  DR 訂正
- \* エネルギー 0.2-11 eV ( $\nu$ ):  
 $\text{H}_2^+$ ,  $\text{D}_2^+$ ,  $\text{T}_2^+$ ,  $\text{HD}^+$ ,  $\text{DT}^+$ . 間接過程を含む
- \* 低エネルギー( $<1\text{eV}$ )  $\text{HeH}^+(\nu, N)$
- \* 高エネルギー、高精度、開殻系電子状態、多原子分子への計算の拡張のための定式化

# ポテンシャル交差の有無

Configuration Interaction



Non-adiabatic Interaction



# 量子欠損理論

\* 連続状態（電離状態）と束縛状態  
（リュードベリ状態）の統一

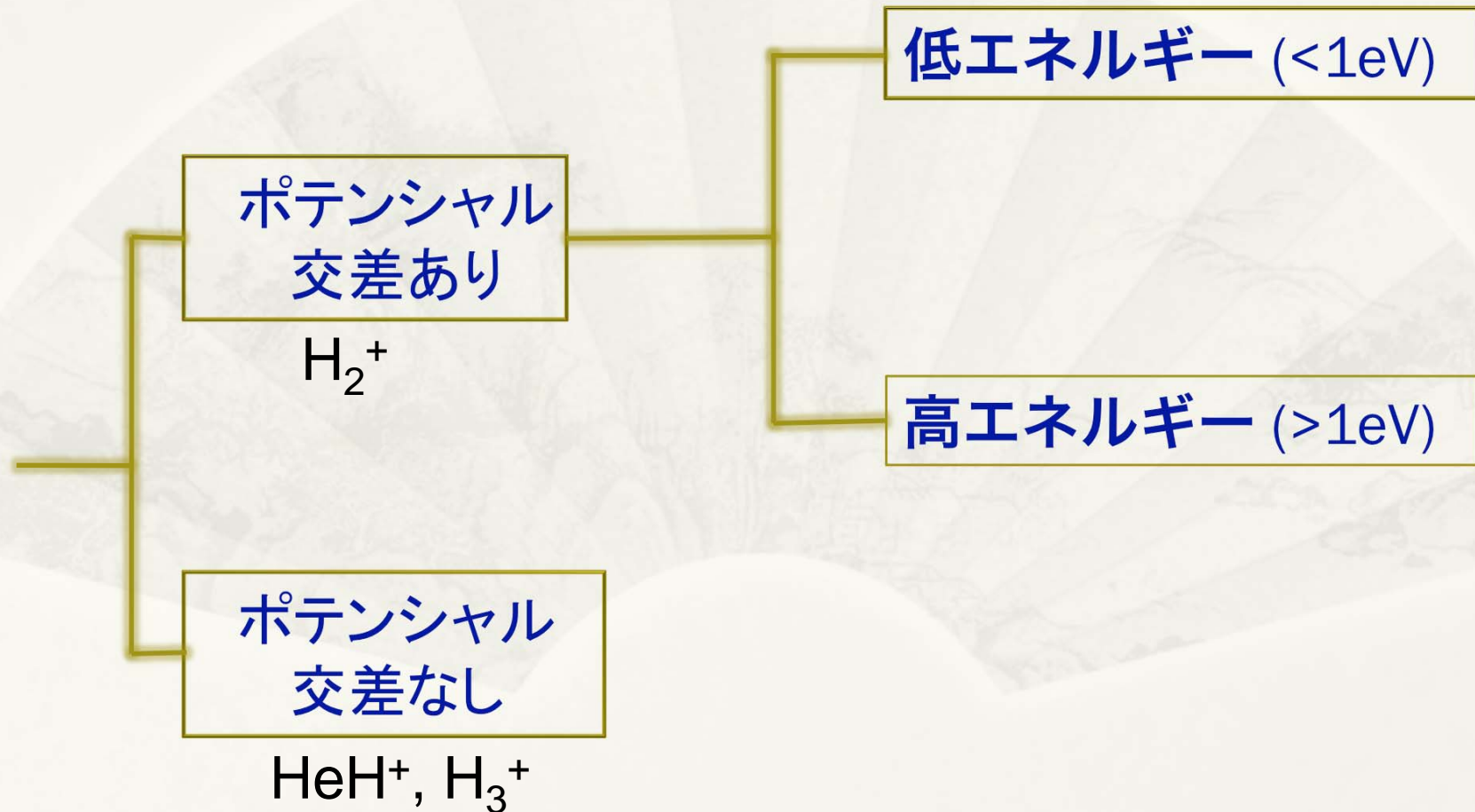
\* 強い非断熱結合の記述

振動回転励起してリュードベリ状態に一時再結合（間接過程）

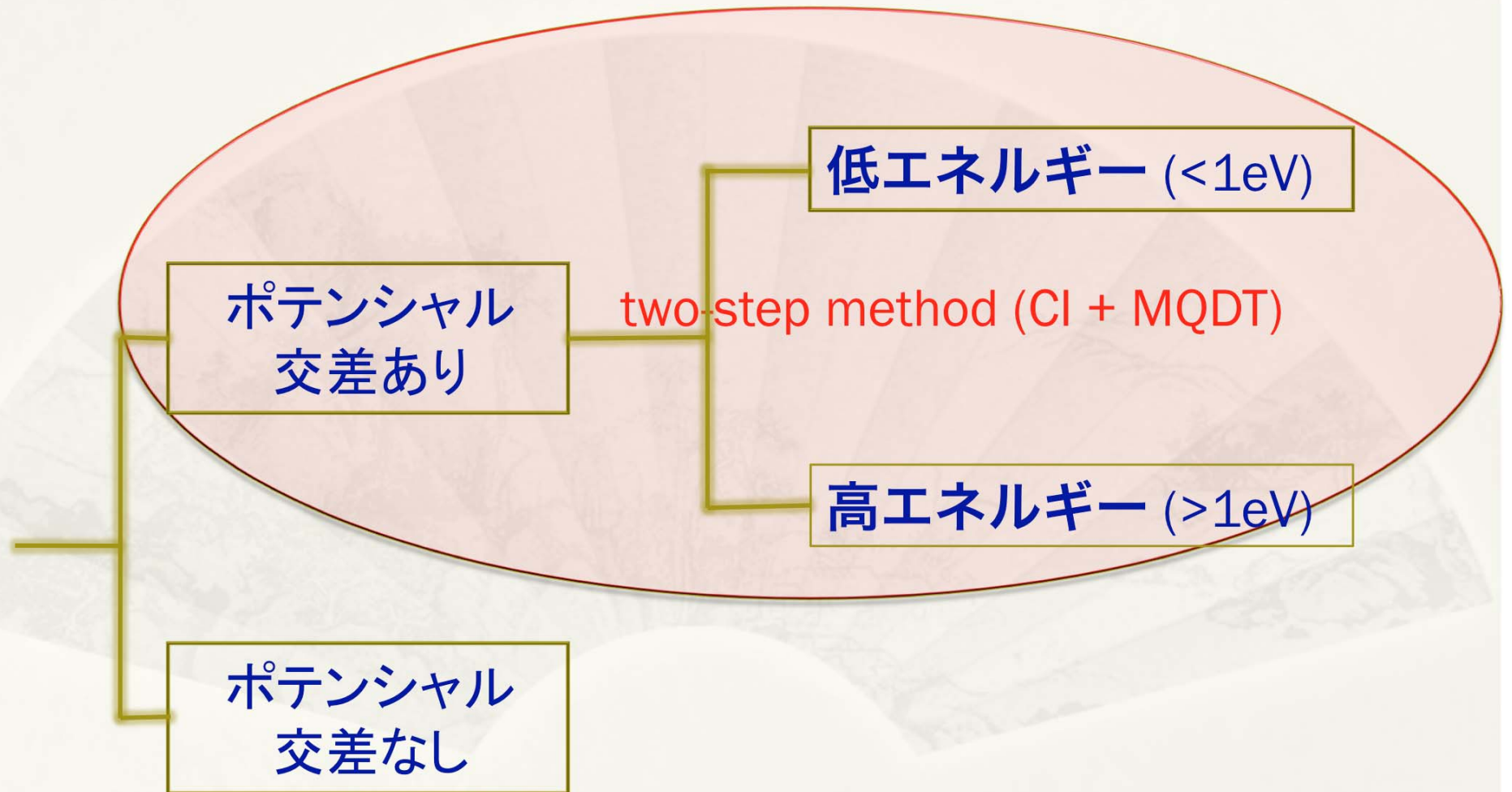
くっ付くか くっ付かないかは、 $\zeta$ と外で考える

Multi-channel Quantum Defect Theory

# 量子欠損理論に基づく計算

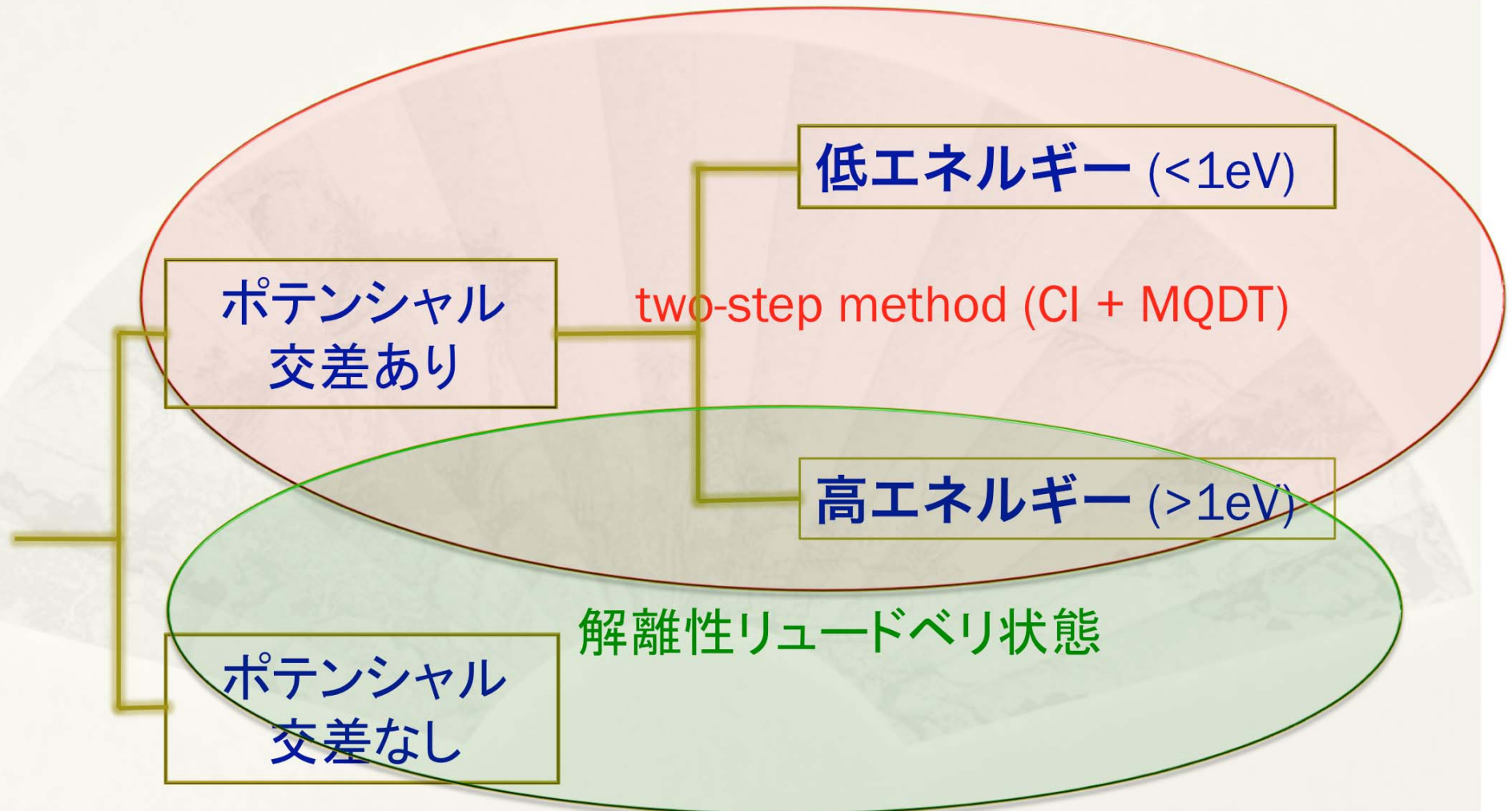


# 量子欠損理論に基づく計算



MQDT: リュードベリ状態との非断熱遷移

# 量子欠損理論に基づく計算

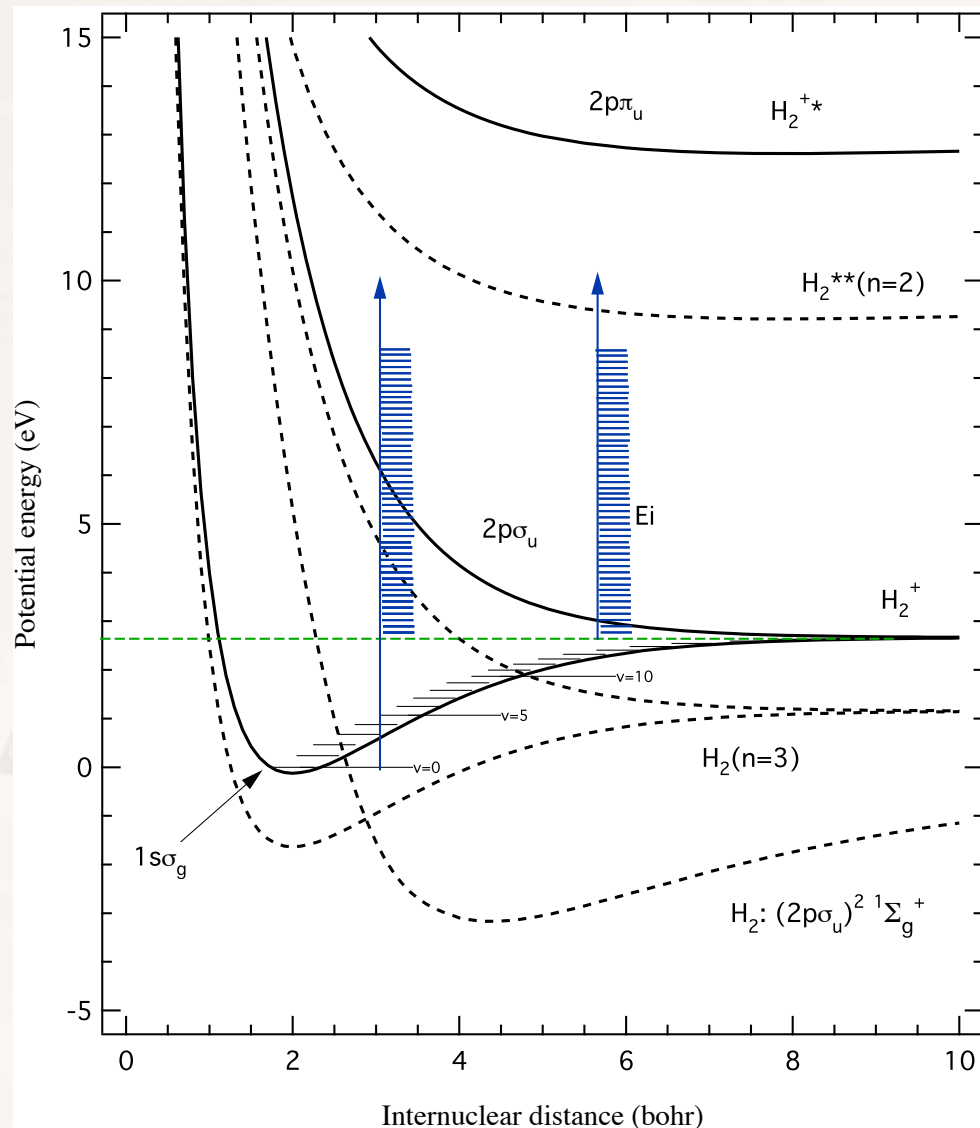


MQDT: リュードベリ状態との非断熱遷移



# 衝突エネルギー1 eV以上の記述

Fig. 1. Potential energy curves of  $H_2$ .



解離状態のエネルギー離散化 (状態規格化)

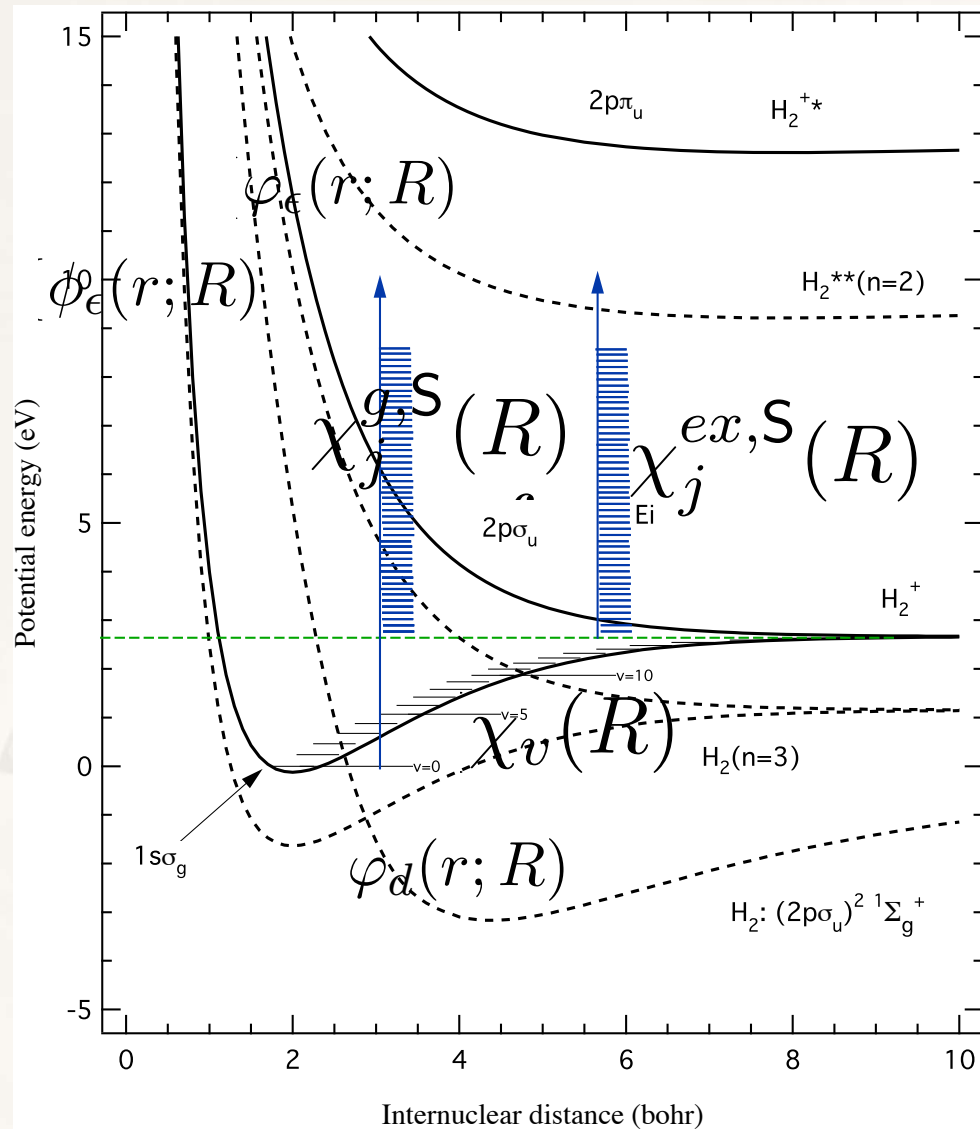
$E=0.3 \text{ --} 12 \text{ eV}$

$H_2^+, D_2^+, HD^+, DT^+, T_2^+$

Takagi 2002 Phys scripta

# Energies higher than 1 eV

Fig. 1. Potential energy curves of  $H_2$ .



# 量子欠損理論に基づく計算

$$(\{\varphi_d(r; R)\} \otimes \{F_\varepsilon(R)\}) \cup (\{\phi_\varepsilon(r; R)\} \otimes \{\chi_v(R)\})$$

低エネルギー (<1eV)

ポテンシャル  
交差あり

$$(\{\varphi_d(r; R)\} \otimes \{F_\varepsilon(R)\}) \cup (\{\varphi_\varepsilon(r; R)\} \otimes \{\chi_j^{ex, S}(R)\})$$

$$\{\phi_\varepsilon(r; R)\} \otimes (\{\chi_v(R)\} \cup \{\chi_j^{g, S}(R)\})$$

高エネルギー (>1eV)

$$\{\phi_\varepsilon(r; R)\} \otimes (\{\chi_v(R)\} \cup \{\chi_j^S(R)\})$$

ポテンシャル  
交差なし

# Scattering by the CI

Lippman-Schwinger eqn. for K matrix

$$K = V + VG_0K$$

Perturbation (Born series): **not converge generally**

Algebraic method: **Chebyshev quadrature**

$$V_{v\epsilon,d\epsilon}^{NJ} = \langle \chi_v^N(R) | V_{\epsilon,d}(R) | F_\epsilon^J(R) \rangle_R,$$

vibration                      dissociation

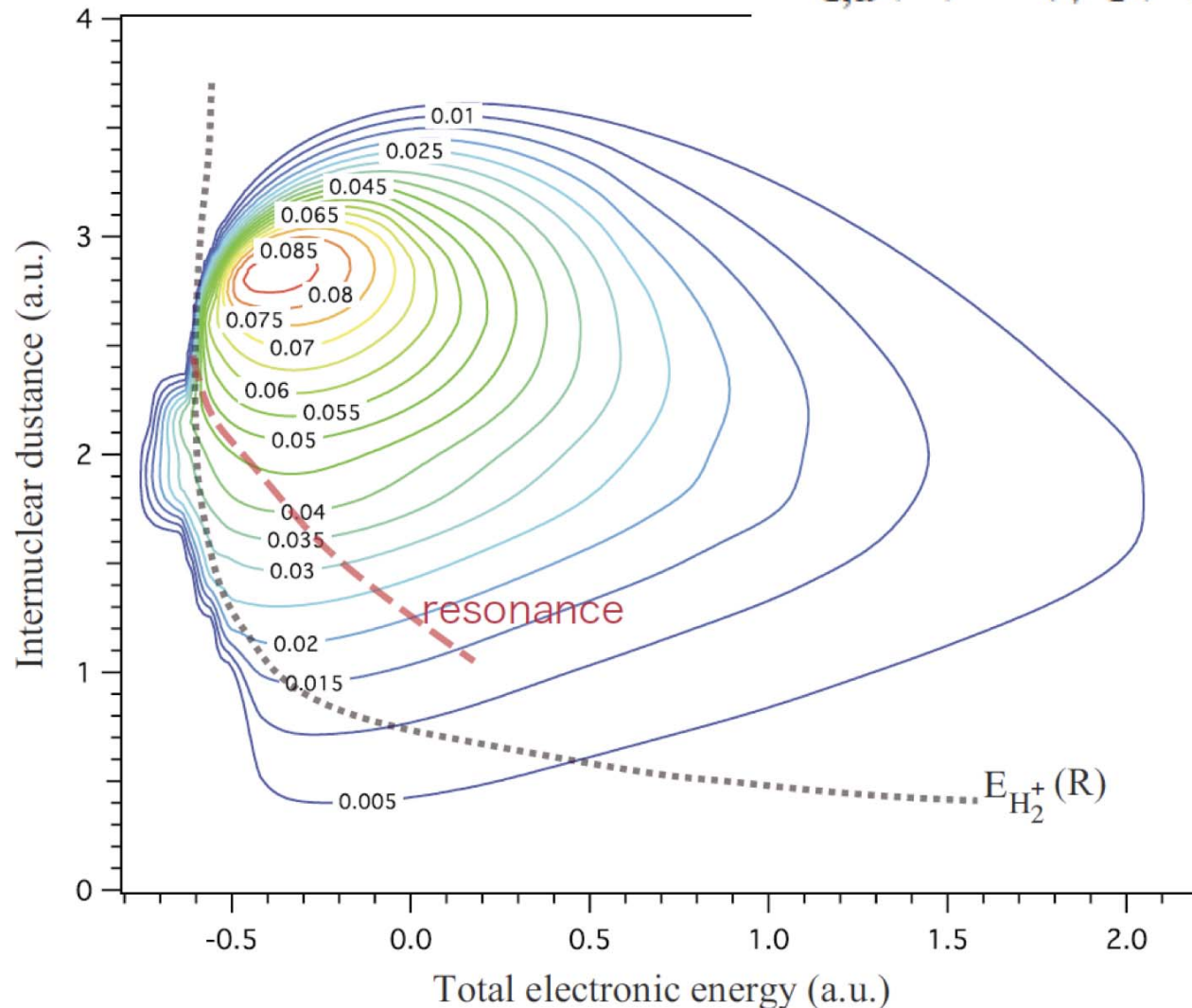
CI at R, Energy

$$V_{\epsilon,d}(R) = \langle \phi_\epsilon(r;R) | H^{ele}(r;R) | \phi_d(r;R) \rangle_r.$$

$$VG_0K = \sum_\gamma \rho_v \int_{-\infty}^{\infty} dE_\gamma \frac{V_{\beta\gamma}(E_\beta, E_\gamma)}{E_\alpha - E_\gamma} K_{\gamma\alpha}(E_\gamma, E_\alpha).$$

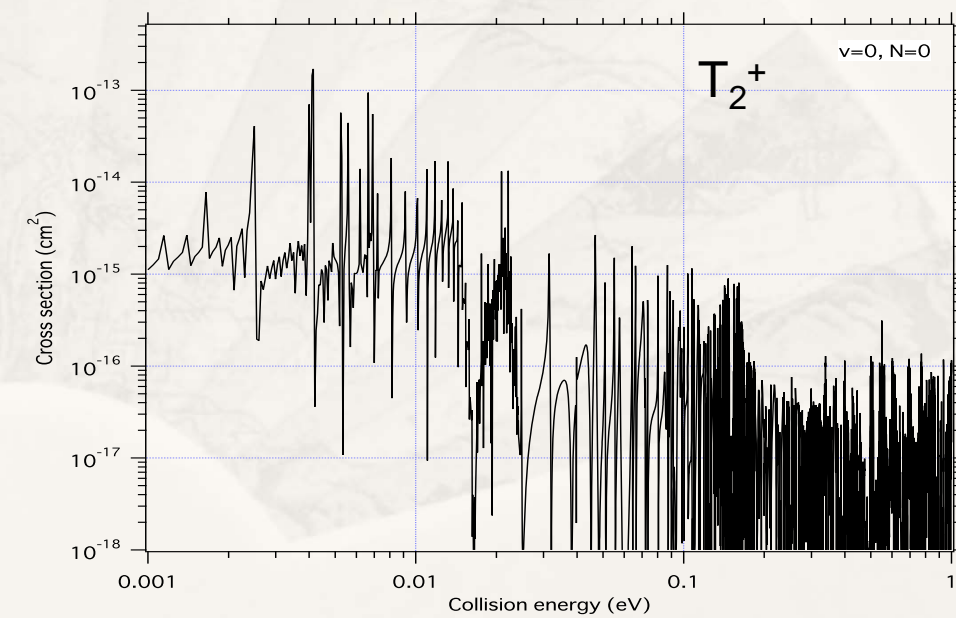
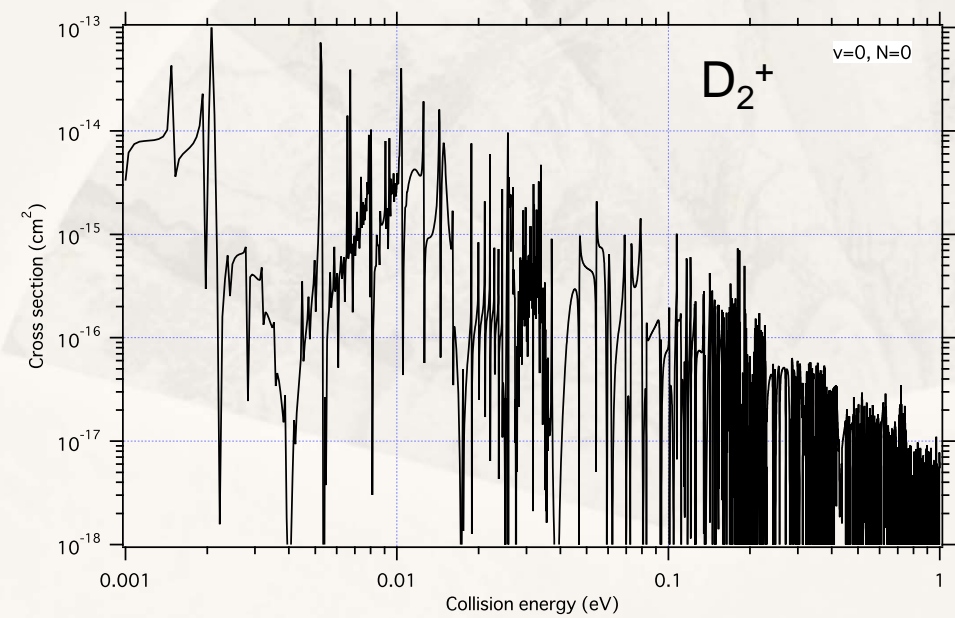
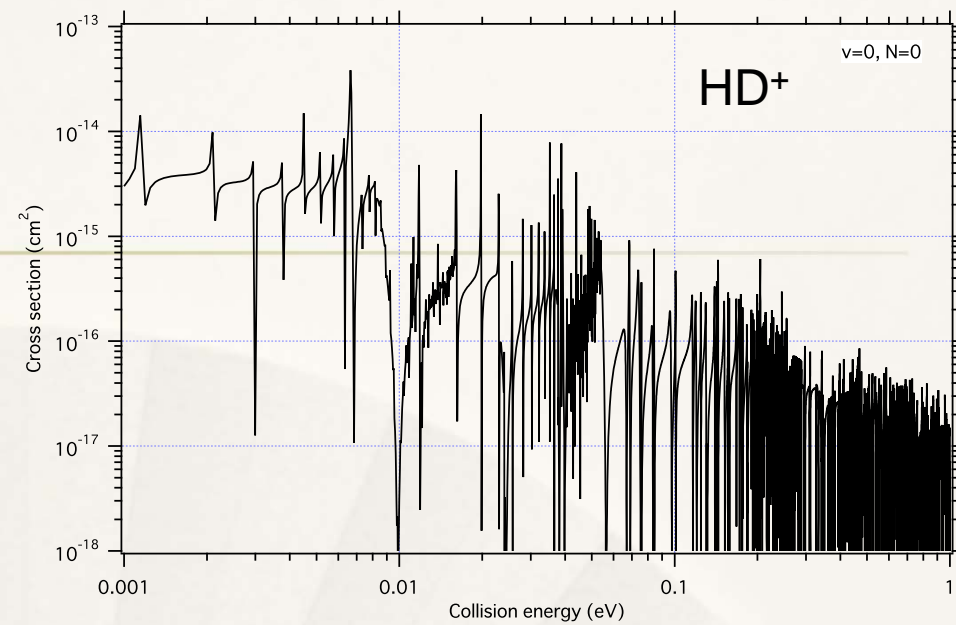
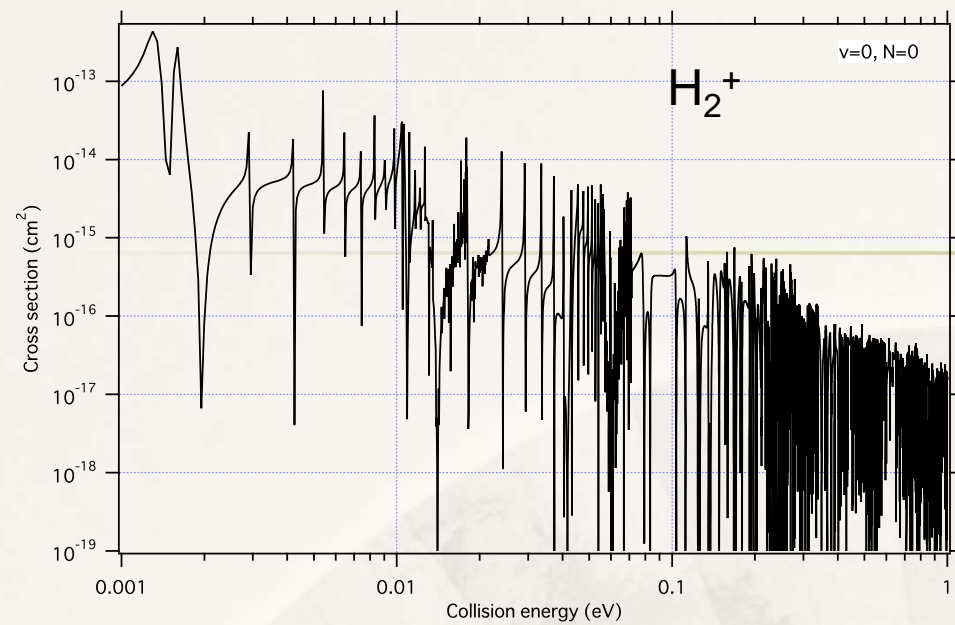
# CI as a function of R and E

$$V_{\epsilon,d}(R) = \langle \phi_{\epsilon}(r;R) | H^{ele}(r;R) | \phi_d(r;R) \rangle_r.$$



$H_2$  the lowest two-electron excited state  
Coupling with d partial wave

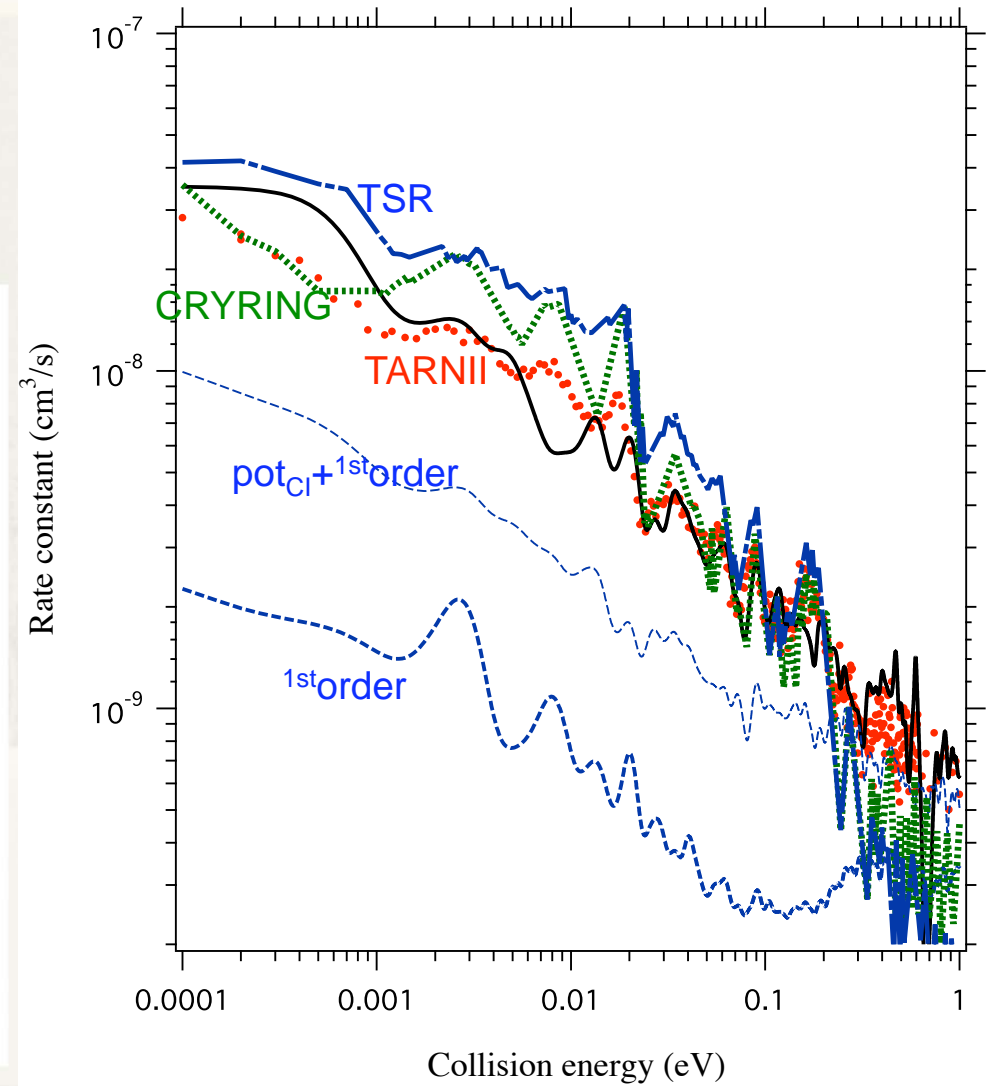
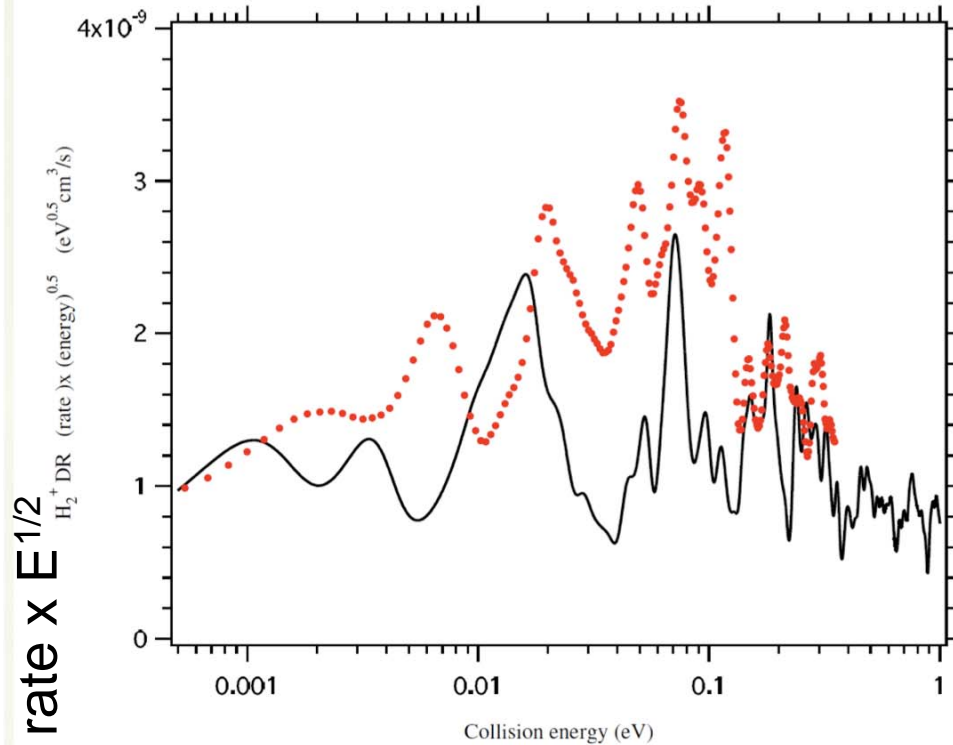
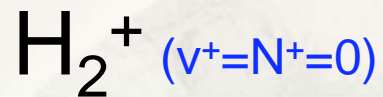
Takagi, Hara, Sato  
2009



# Low energy DR

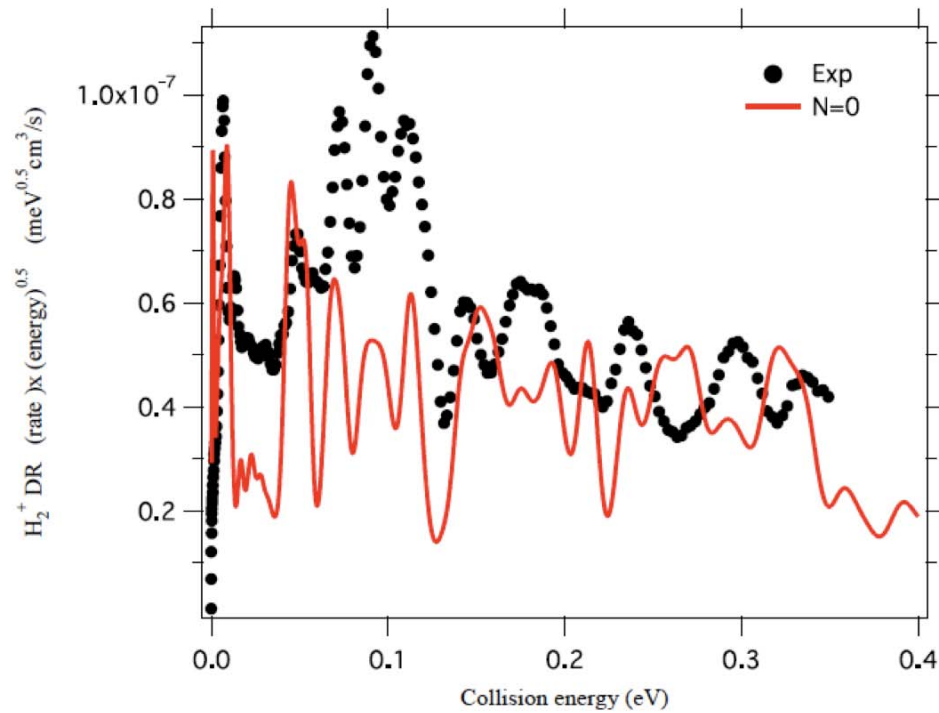
HD<sup>+</sup>

HD<sup>+</sup>(v=0) DR, 300K rotaional temperature

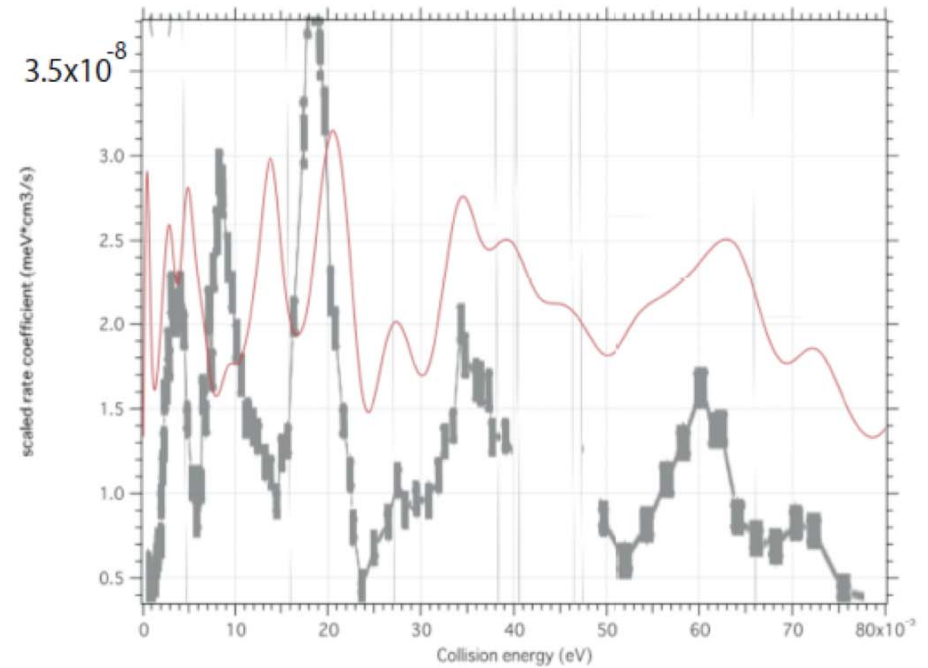


# State selective/ultra-cold experiments

$\text{H}_2^+$



$\text{HD}^+$



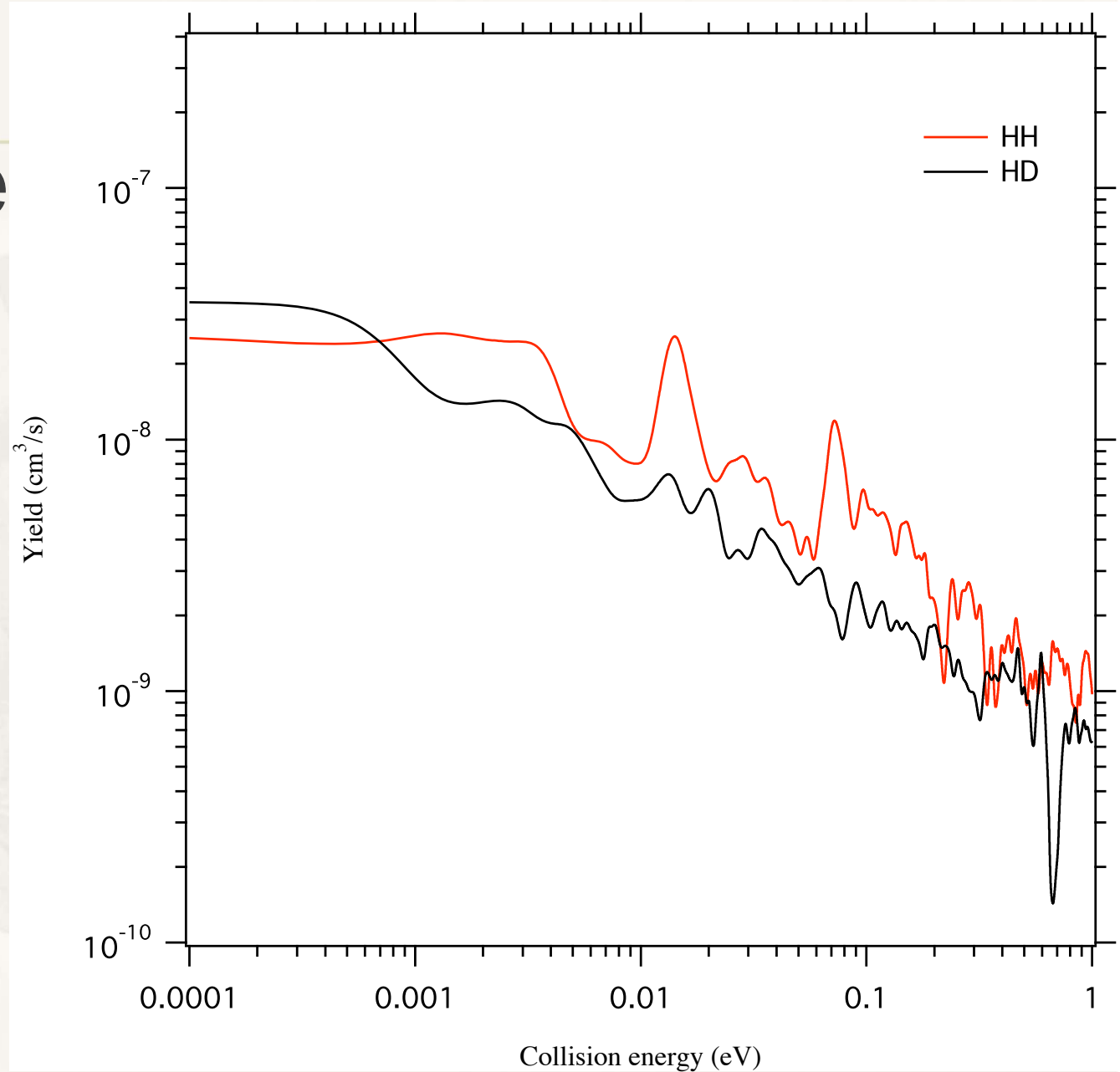


# Rotational temperature

## 300K

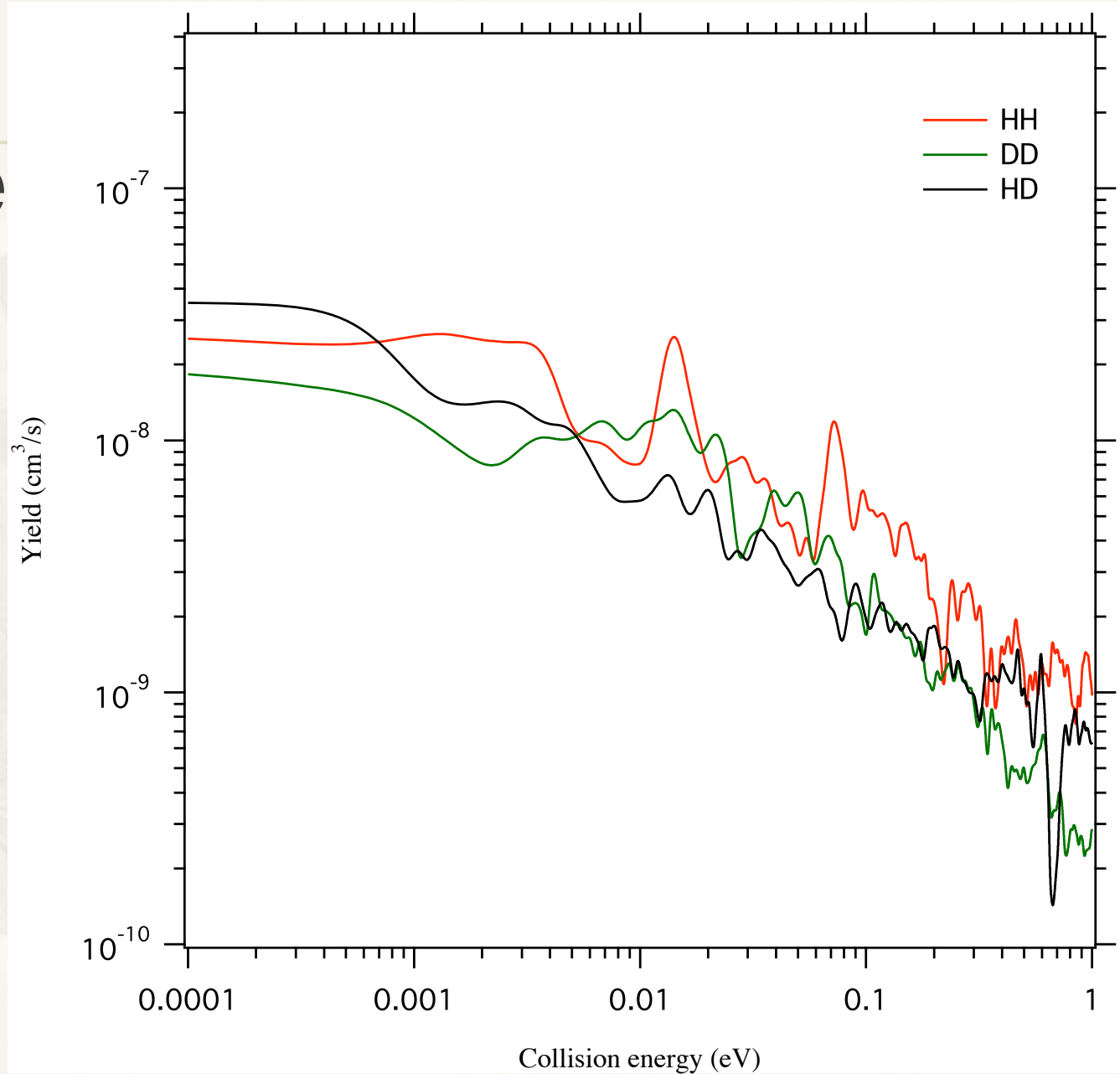
(transverse 1meV,  
logtudinal 0.5meV)

$$v = 0$$



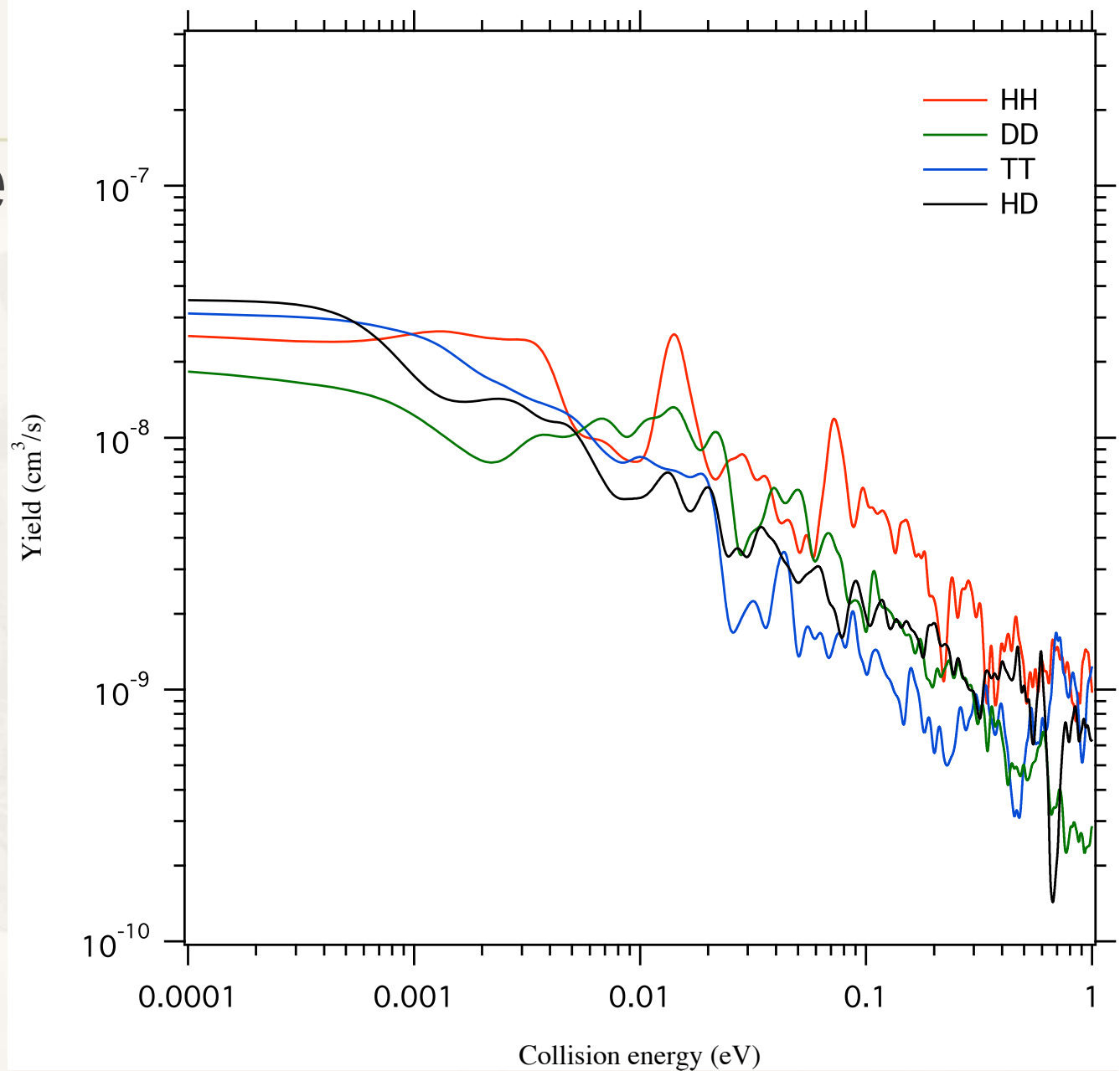
# Rotational temperature 300K

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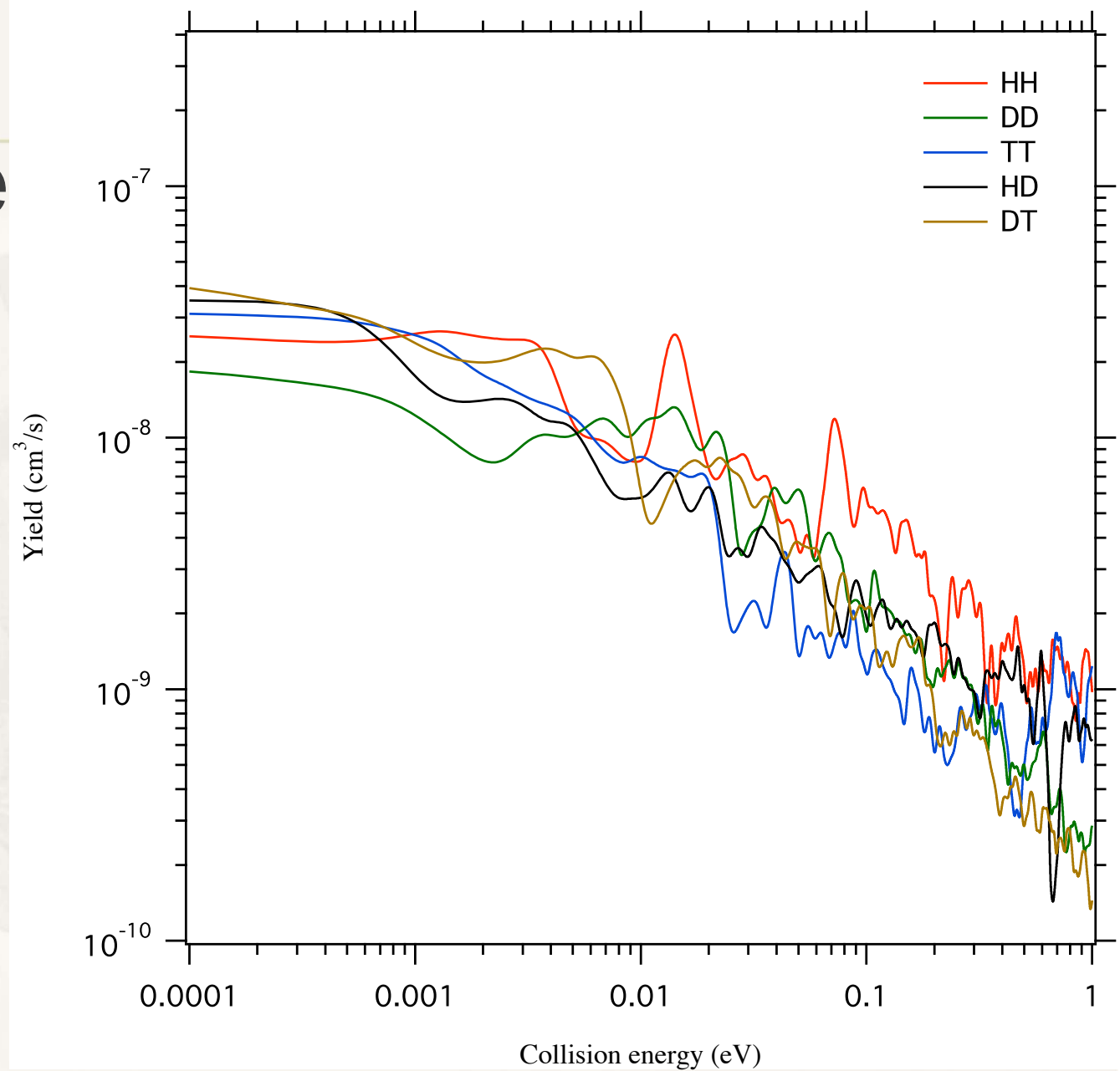


# Rotational temperature

## 300K

(transverse 1meV,  
logtudinal 0.5meV)

$$\nu = 0$$



# 非断熱相互作用（間接過程）

$$C_{j+l^+, \alpha}^{JN^+\Lambda} = \sum_{v\tilde{l}} \langle \chi_{j^+}^{SN^+\Lambda^+} | \cos(\pi \mu_{\tilde{l}\Lambda}(R) + \eta_{\alpha}^{J\Lambda}) M_{l+\tilde{l}}(R) | \chi_j^{SJ\Lambda} \rangle U_{v\tilde{l}, \alpha}^{J\Lambda}$$

非断熱相互作用  
間接過程

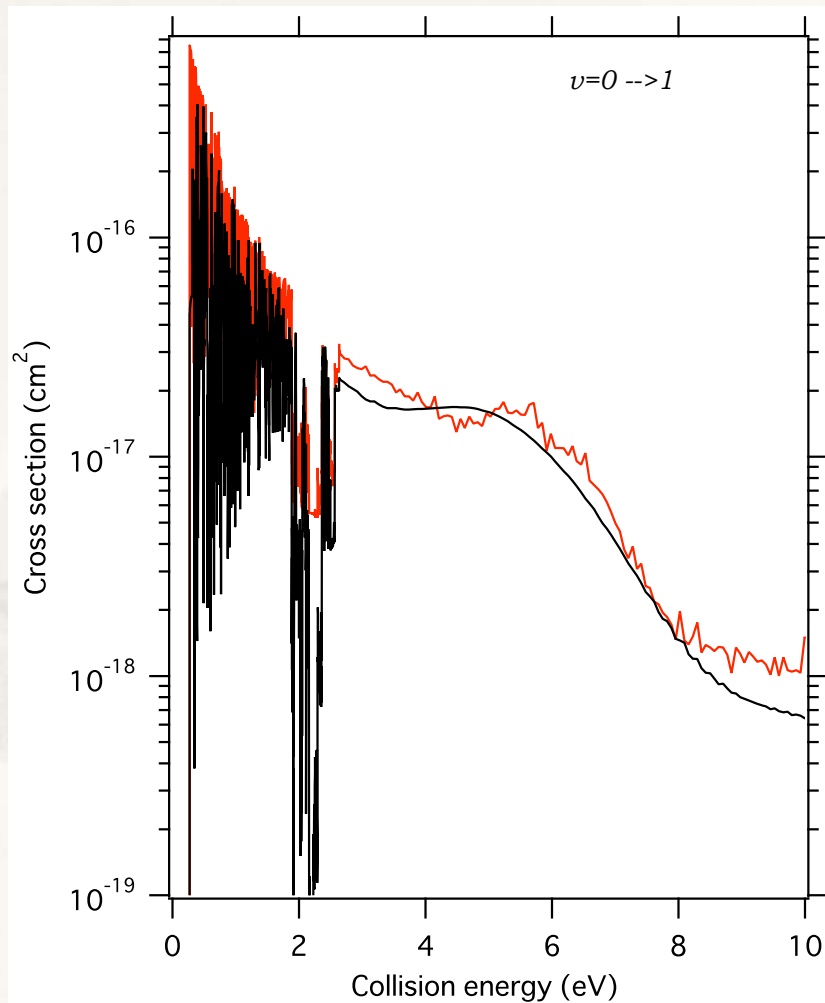
CI

直接過程

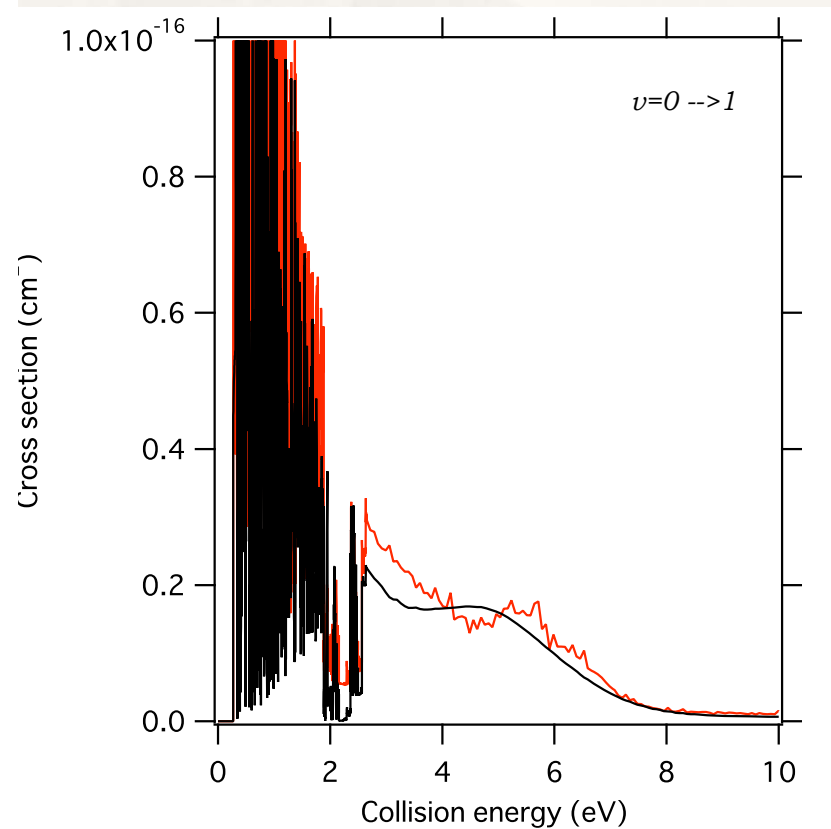
$S : \cos \longrightarrow \sin$

$$(\tilde{\mathcal{R}})_{\tilde{i}', \tilde{i}}^J = \sum_{\Lambda} G(\tilde{i}J\Lambda) (SC^{-1})_{\tilde{i}', \tilde{i}}^{J\Lambda} G(\tilde{i}J\Lambda)$$

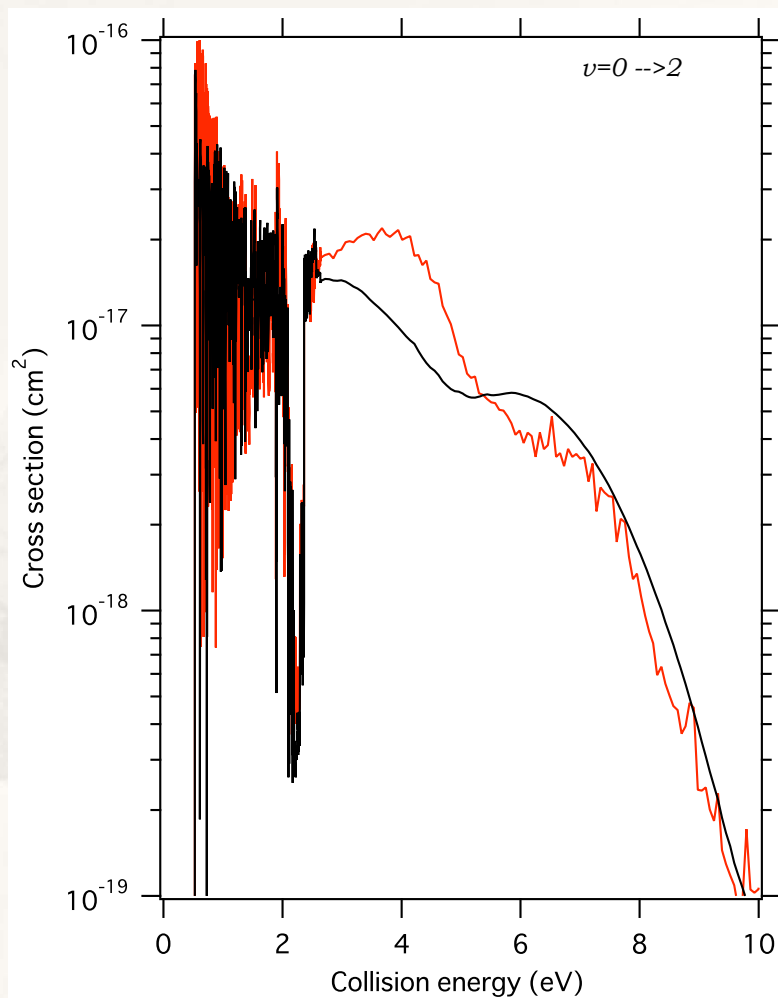
# H<sub>2</sub><sup>+</sup>振動遷移



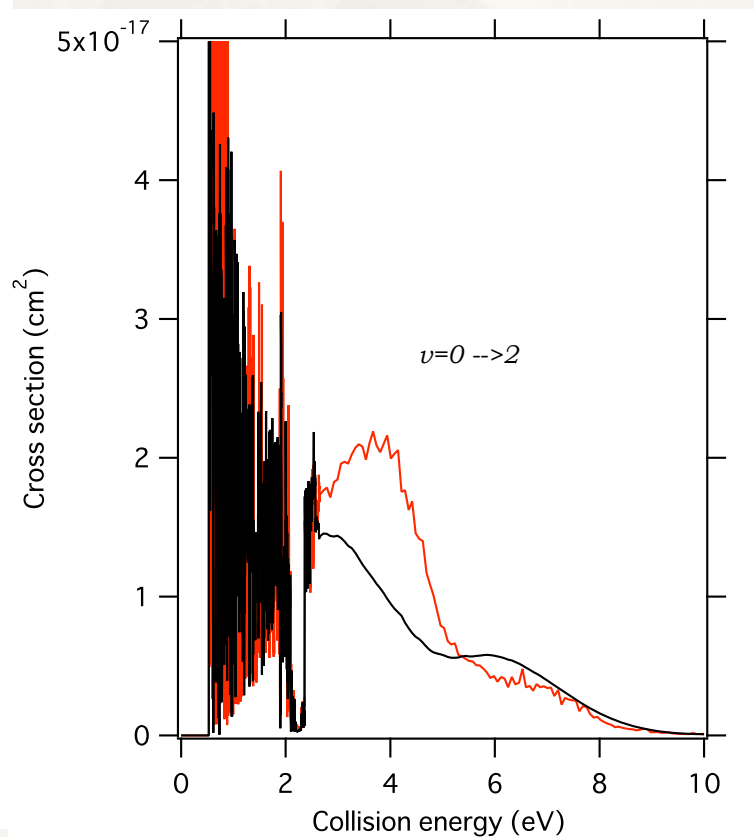
間接過程含む  
直接過程



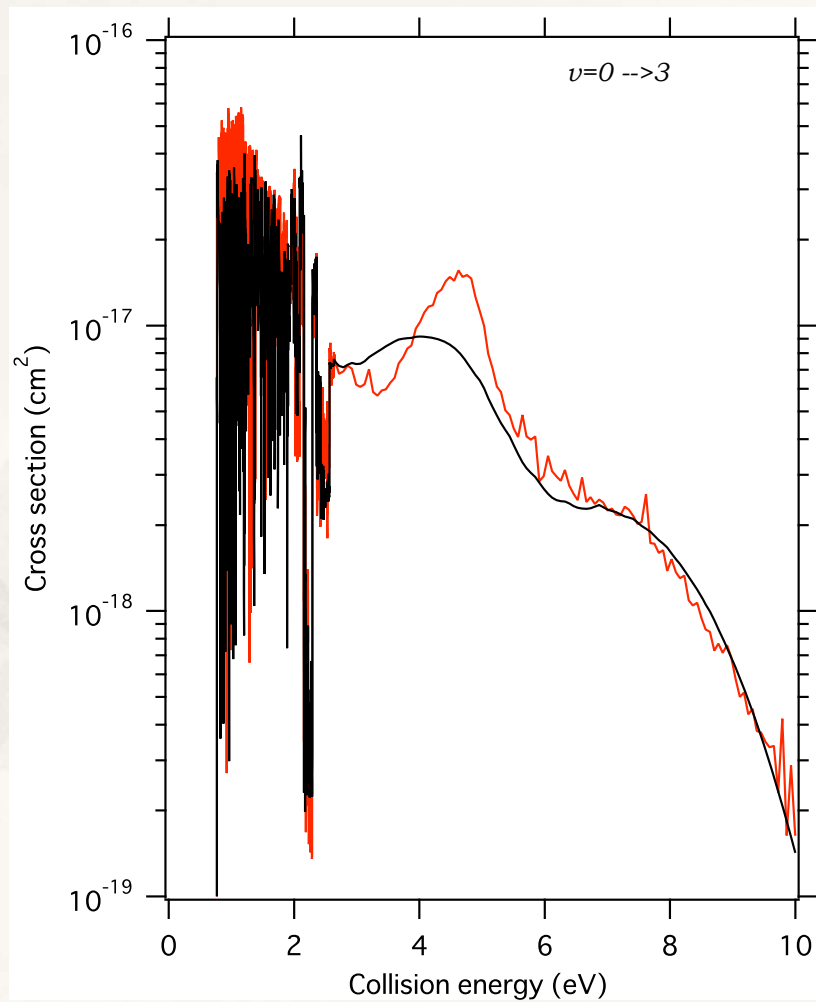
# H<sub>2</sub><sup>+</sup>振動遷移



間接過程含む  
直接過程



# H<sub>2</sub><sup>+</sup>振動遷移



間接過程含む  
直接過程

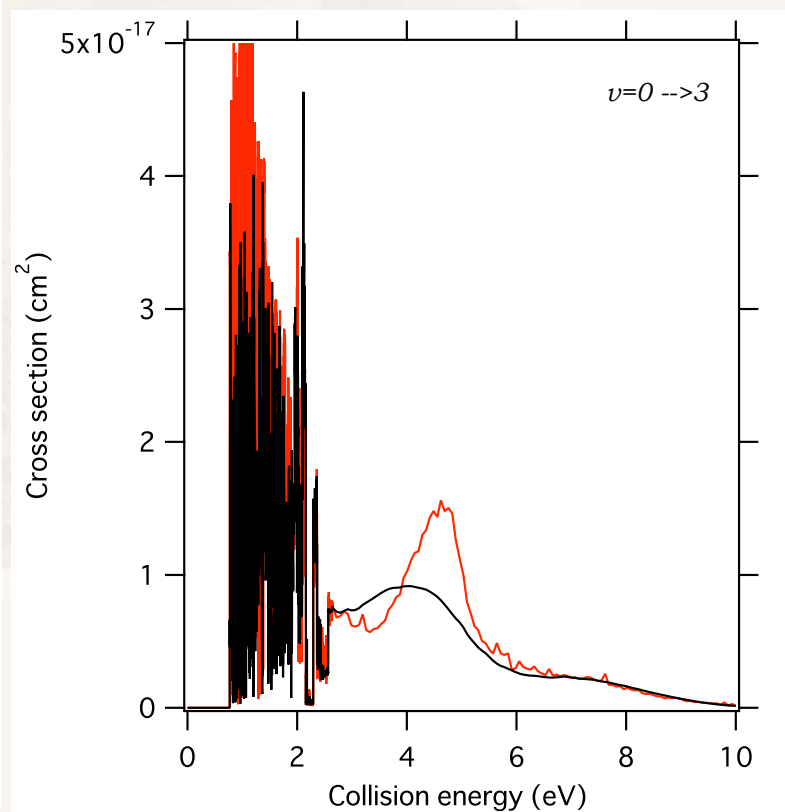
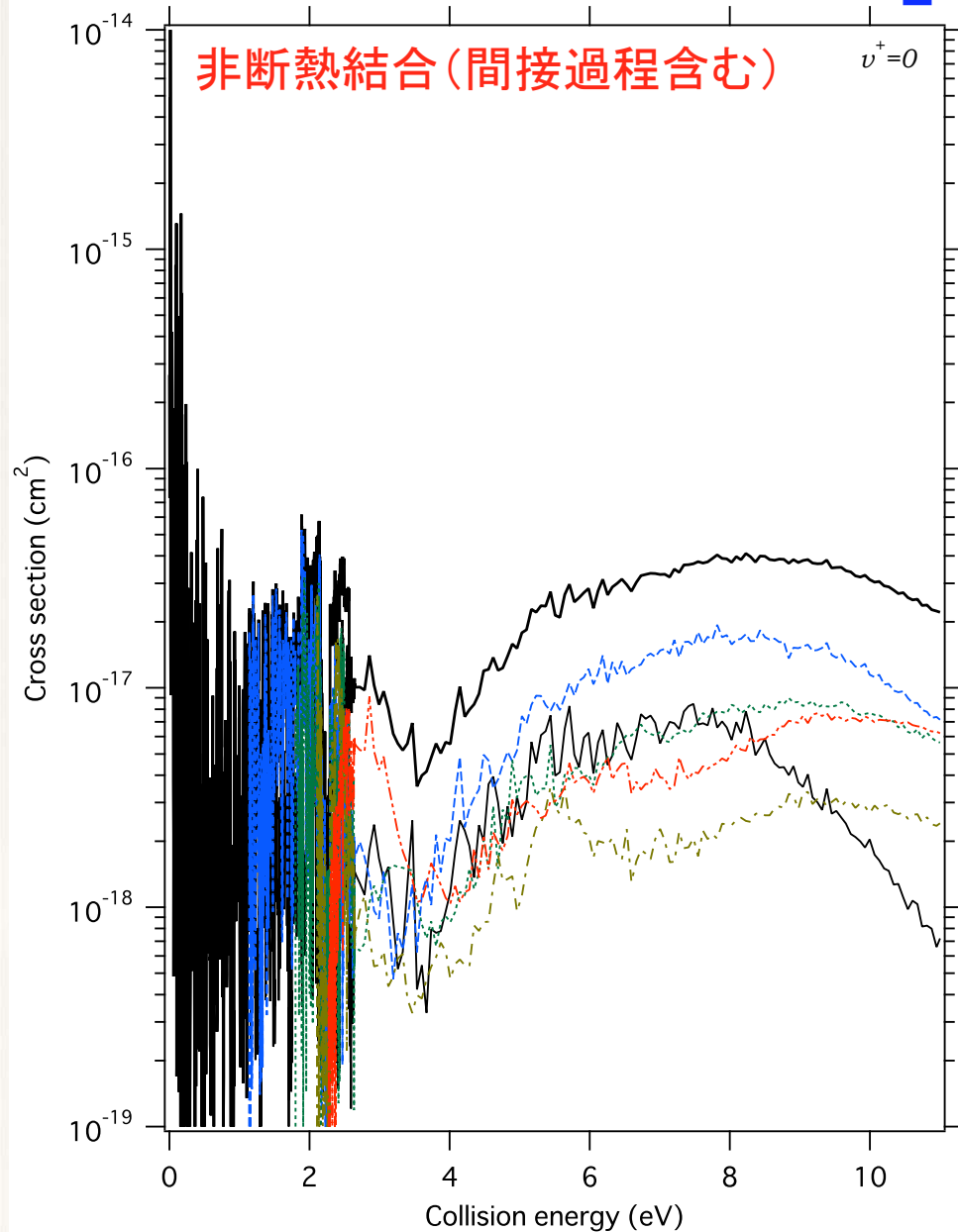
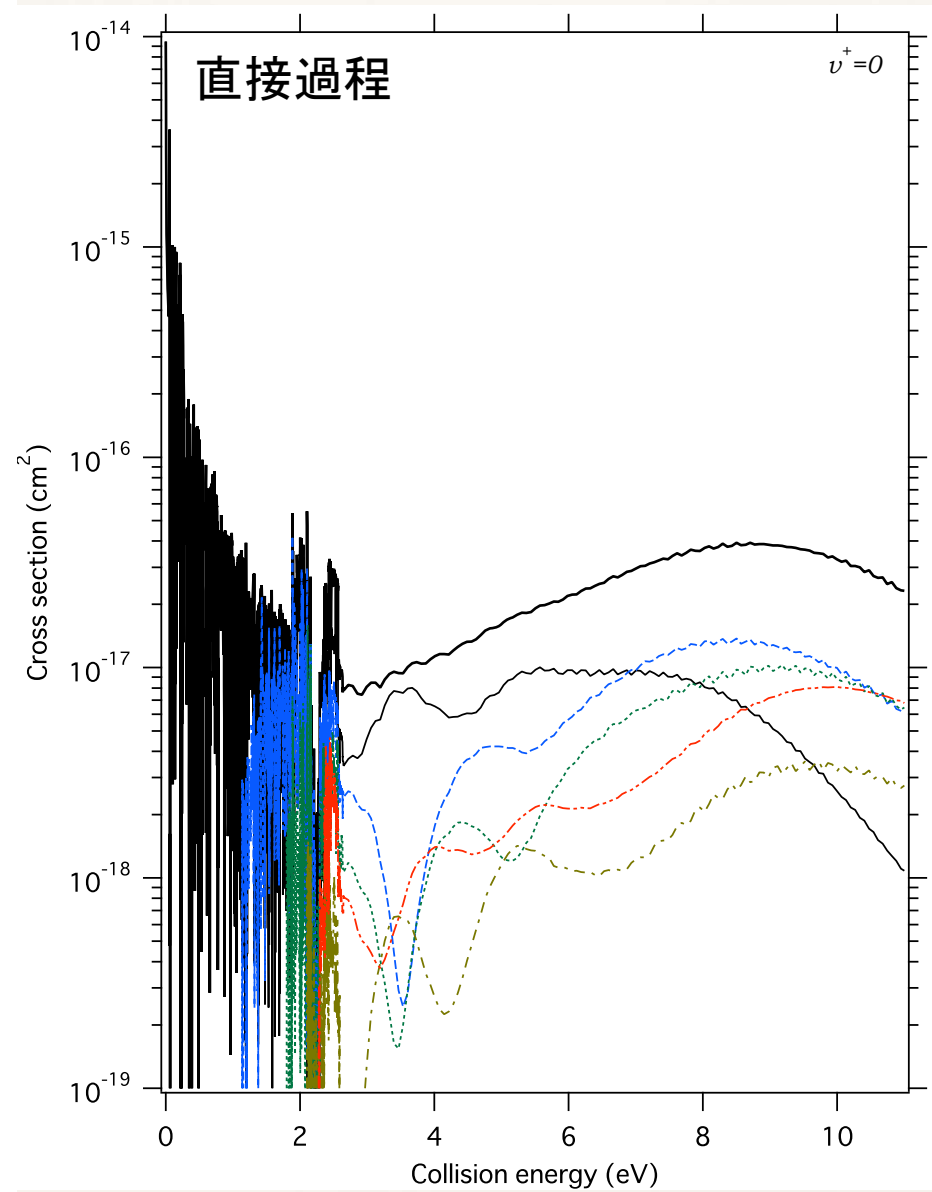




Fig. 034 n-distribution in  $H_2^+(v^+) + e \rightarrow H + H(n)$   $H_2^+(v=0)$  解離性再結合

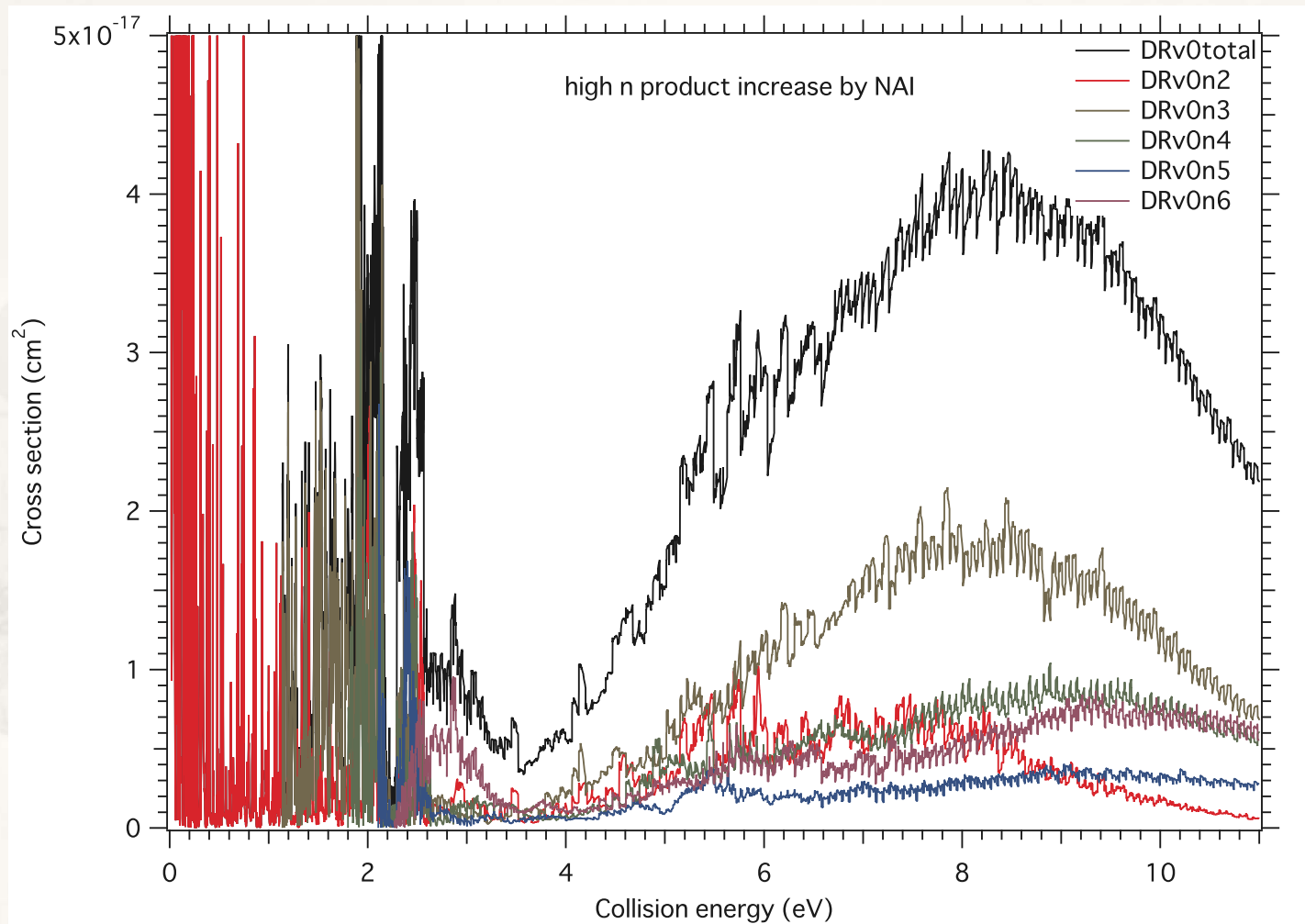


— total  
 — n2, - - - n3, ···· n4  
 - · - n5, - - - n>=6



— total  
 — n2, - - - n3, ···· n4  
 - · - n5, - - - n>=6

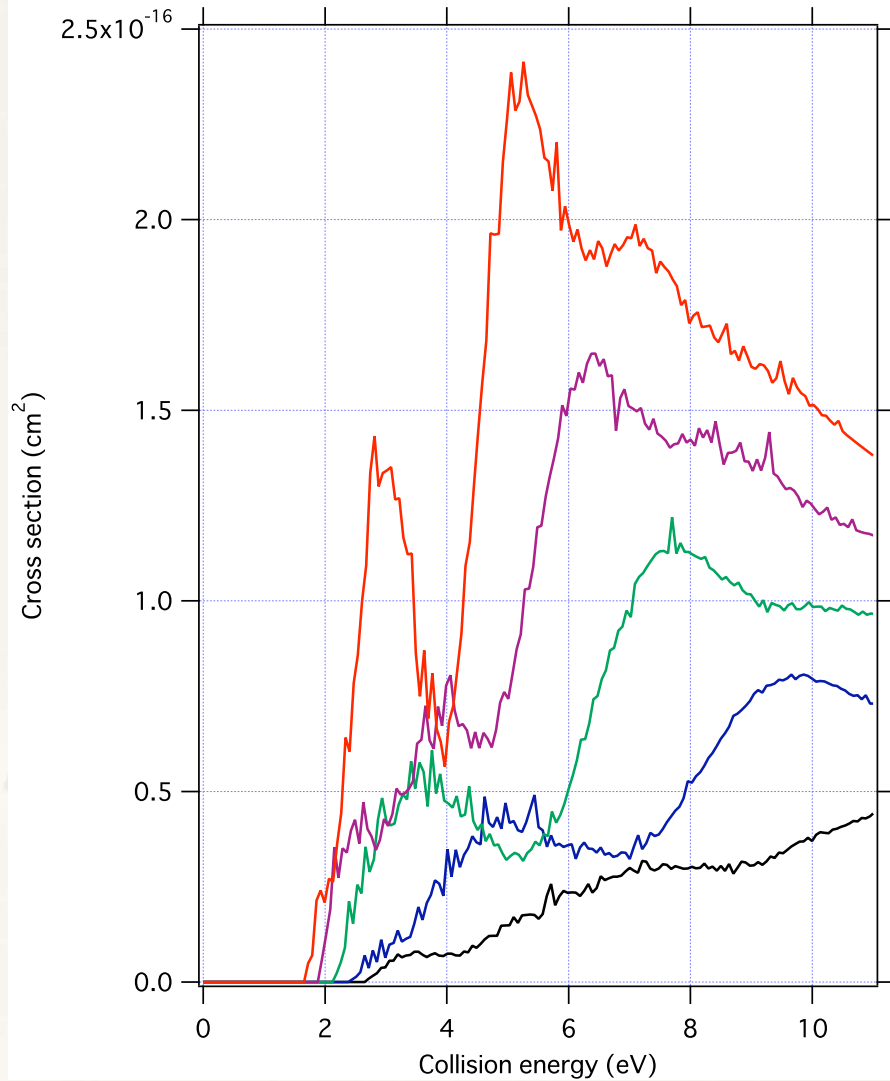
# 微細な構造



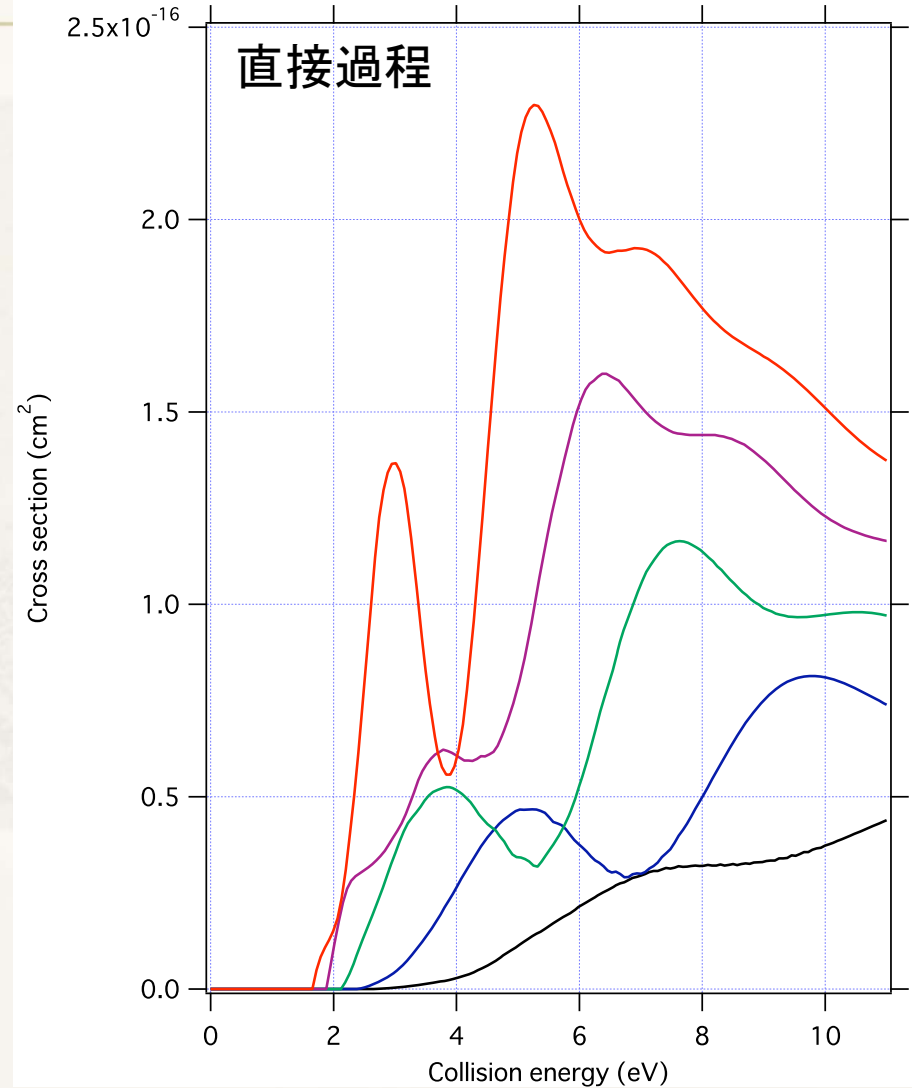
# $H_2^+(v=0-4)$ 解離性励起

Fig. 053 n-distribution in  $H_2^+(v^+) + e \rightarrow H + H(n)$

Dessociative excitation cross section of  $H_2^+$



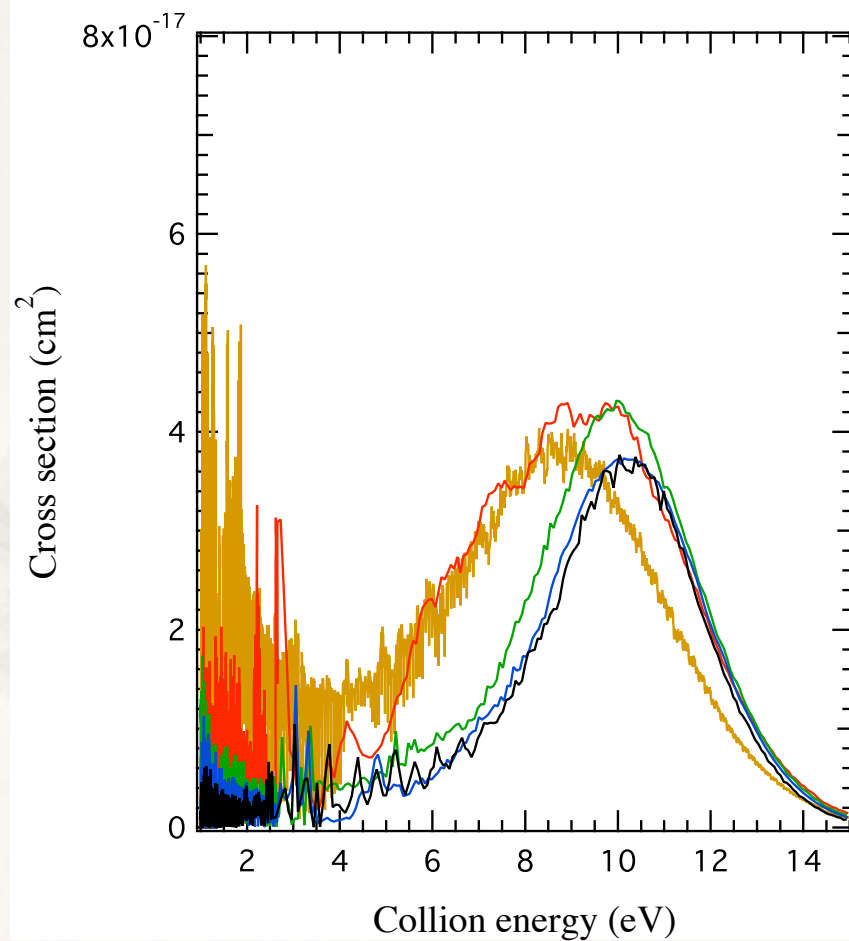
— v=0, — v=1, — v=2  
— v=3, — v=4



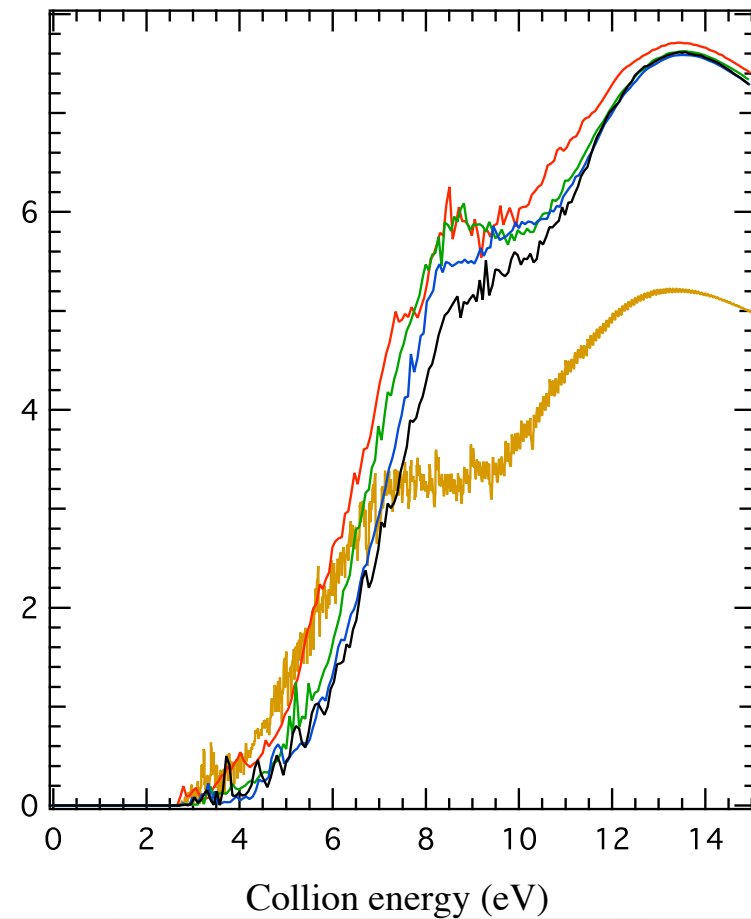
— v=0, — v=1, — v=2  
— v=3, — v=4

# 同位体( $v=0$ ) 解離性再結合 / 解離性励起

(a) dissociative recombination



(b) dissociative excitation



$\text{H}_2^+$ ,  $\text{D}_2^+$ ,  $\text{T}_2^+$ ,  $\text{HD}^+$ ,  $\text{TD}^+$

# 量子欠損理論に基づく計算

$$(\{\varphi_d(r; R)\} \otimes \{F_\epsilon(R)\}) \cup (\{\phi_\epsilon(r; R)\} \otimes \{\chi_v(R)\})$$

低エネルギー (<1eV)

ポテンシャル  
交差あり

$$(\{\varphi_d(r; R)\} \otimes \{F_\epsilon(R)\}) \cup (\{\varphi_\epsilon(r; R)\} \otimes \{\chi_j^{ex,S}(R)\})$$
$$\{\phi_\epsilon(r; R)\} \otimes (\{\chi_v(R)\} \cup \{\chi_j^{g,S}(R)\})$$

高エネルギー (>1eV)

$$\{\phi_\epsilon(r; R)\} \otimes (\{\chi_v(R)\} \cup \{\chi_j^S(R)\})$$

ポテンシャル  
交差なし

# 量子欠損理論に基づく計算

$$(\{\varphi_d(r; R)\} \otimes \{F_\varepsilon(R)\}) \cup (\{\phi_\varepsilon(r; R)\} \otimes \{\chi_v(R)\})$$

低エネルギー (<1eV)

ポテンシャル  
交差あり

$$\begin{aligned} & (\{\varphi_d(r; R)\} \otimes \{F_\varepsilon(R)\}) \cup (\{\varphi_\varepsilon(r; R)\} \otimes \{\chi_j^{ex,S}(R)\}) \\ & \{\phi_\varepsilon(r; R)\} \otimes (\{\chi_v(R)\} \cup \{\chi_j^{g,S}(R)\}) \end{aligned}$$

高エネルギー (>1eV)

$$\{\phi_\varepsilon(r; R)\} \otimes (\{\chi_v(R)\} \cup \{\chi_j^S(R)\})$$

ポテンシャル  
交差なし

新方法(非断熱強結合)

$$(\{\varphi_\varepsilon(r; R)\} \cup \{\phi_\varepsilon(r; R)\}) \otimes (\{\chi_v(R)\} \cup \{\chi_j^{ex,S}(R)\} \cup \{\chi_j^{g,S}(R)\})$$

# (近い) 将来計画

$$\mathcal{R}_{i'j'N'l'+,ijNl+}^{\epsilon J} = \sum_{\Lambda} \langle N' | \Lambda \rangle^{Jl'+\Lambda+} \sum_{\tilde{l}} \langle \chi_{j'}^{i'N'\Lambda+S} | K_{i'l'+,il+}^{\Lambda\tilde{l}}(R, \epsilon) | \chi_j^{iN\Lambda+S} \rangle \langle \Lambda | N \rangle^{Jl'+\Lambda+}$$

$i, i'$ : 非弾性散乱チャンネルを含む

断熱的電子散乱状態が解ければ動的過程が解ける

従来と比較

$$\mathcal{R}_{k'N'l'+,kNl+}^{\epsilon J} = \sum_{\Lambda} \langle N' | \Lambda \rangle^{Jl'+\Lambda+} \sum_{\alpha\tilde{l}} U_{k',\alpha}^{J\Lambda} \langle \chi_{v'}^{N'\Lambda+} | K_{k'l'+,kl+}^{\alpha\Lambda\tilde{l}}(R) | \chi_v^{N\Lambda+} \rangle U_{\alpha,k}^{J\Lambda} \langle \Lambda | N \rangle^{Jl'+\Lambda+}$$

# 分子イオン・電子 データ

Molecular assisted recombination in divertor  
+ other processes

$H_2^+$ ,  $HeH^+/NeH^+$ ,  $CH^+$ ,  $H_3^+$ ,  
their isotopes **D, T**

日本原子力研究機構委託調査

CRP on Light Element Atom, Molecule and Radical Behaviour  
in the Divertor and Edge Plasma Regions by IAEA,

**データ作成, 収集**



# 有効性 つなげるために

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原子分子データ

プラズマ解析

ダイバータの設計・診断