



Labex

EMC
ENERGY MATERIALS & CLEAN COMBUSTION CENTER



Fonds Européen de
développement Régional



IAEA
International Atomic Energy Agency
Atoms For Peace

Electron collisions with H_2^+ , HD^+ and D_2^+ : computation of cross sections and rate coefficients, and comparison with storage ring measurements

A. Abdoulanziz¹, E. Djuissi¹, J. Boffelli¹, Y. Moulane^{2,3}, F. Iacob⁴, N. Pop⁵,
M. D. Epée Epée⁶, O. Motapon^{6,7}, K. Chakrabarti⁸, J. Tennyson⁹,
V. Laporta^{9,10}, J. Zs Mezei¹¹, X. Urbain¹², I. F. Schneider^{1,13}

¹LOMC, Univ. Le Havre Normandie, ²Univ. Cadi Ayyad, Marrakech, ³Univ. De Liège, ⁴West Univ. Timisoara, ⁵Politehnica Univ. Timisoara, ⁶Univ. of Douala, ⁷Univ. of Maroua, ⁸Scottish Church College, Calcutta, ⁹University College London, ¹⁰Istituto per la Scienza e Tecnologia dei Plasmi, Bari, ¹¹Inst. for Nuclear Research, Debrecen, ¹²Inst. of Condensed Matter and Nanosciences, Univ. de Louvain, ¹³Lab. Aimé Cotton, Univ. Paris-Saclay.



Dissociative recombination (MAR)

Dissociative excitation (MAD)

of several molecular cations invoked in the previous talks

H₂⁺ and others (will be shown at the end)

Talks of:

Ivo CLASSEN,

Richard ENGELN,

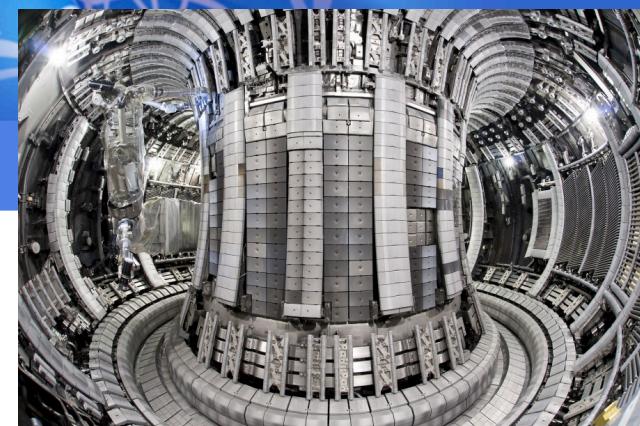
Dirk WÜNDERLICH,

Kevin VERHAEGH

Mathias GROTH,

Annarita LARICCHIUTA

“...”



Collision processes in low-temperature hydrogen plasmas

Janev, R.K.; Reiter, D.; Samm, U.

Forschungszentrum Juelich GmbH (Germany). Inst. fuer Plasmaphysik, EURATOM Association, Trilateral Euregio Cluster

Citation

Export

...

Abstract

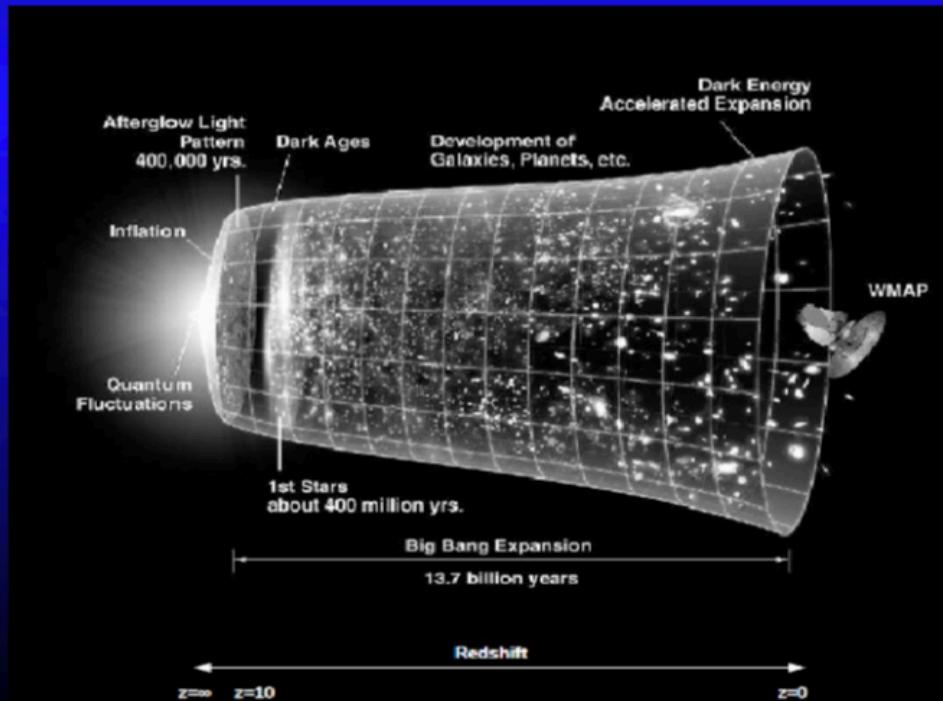
[en] Collision processes among the constituents of low-temperature hydrogen plasmas (e , H , H^+ , H^- , H_2 , H_2^+ , H_3^+) play a key role in technical plasma applications as well as in the boundary regions of magnetically confined fusion plasmas. In this work a review of the current knowledge on their cross sections is presented. Collision processes of electronically and vibrationally excited species are also included in the present review. The energy range in which these processes are considered extends from thermal energies to several hundreds electronvolts and to the keV region for some heavy-particle collision processes). The available experimental and theoretical cross section information is critically assessed and

on the collision processes taking place in hydrogen plasmas in the temperature range from 0.01 eV to several hundreds eV. This temperature range covers the typical temperature conditions of many astrophysical and laboratory plasmas in-

DENSITIES AND TEMPERATURE RANGES: PRIMORDIAL UNIVERSE CHEMISTRY

Densities $\sim 10^5 - 10^{-7} \text{ cm}^{-3}$
 $T \sim 30000 \text{ K} - 0.003 \text{ K}$

Coppola, Galli et
al, 2011-...



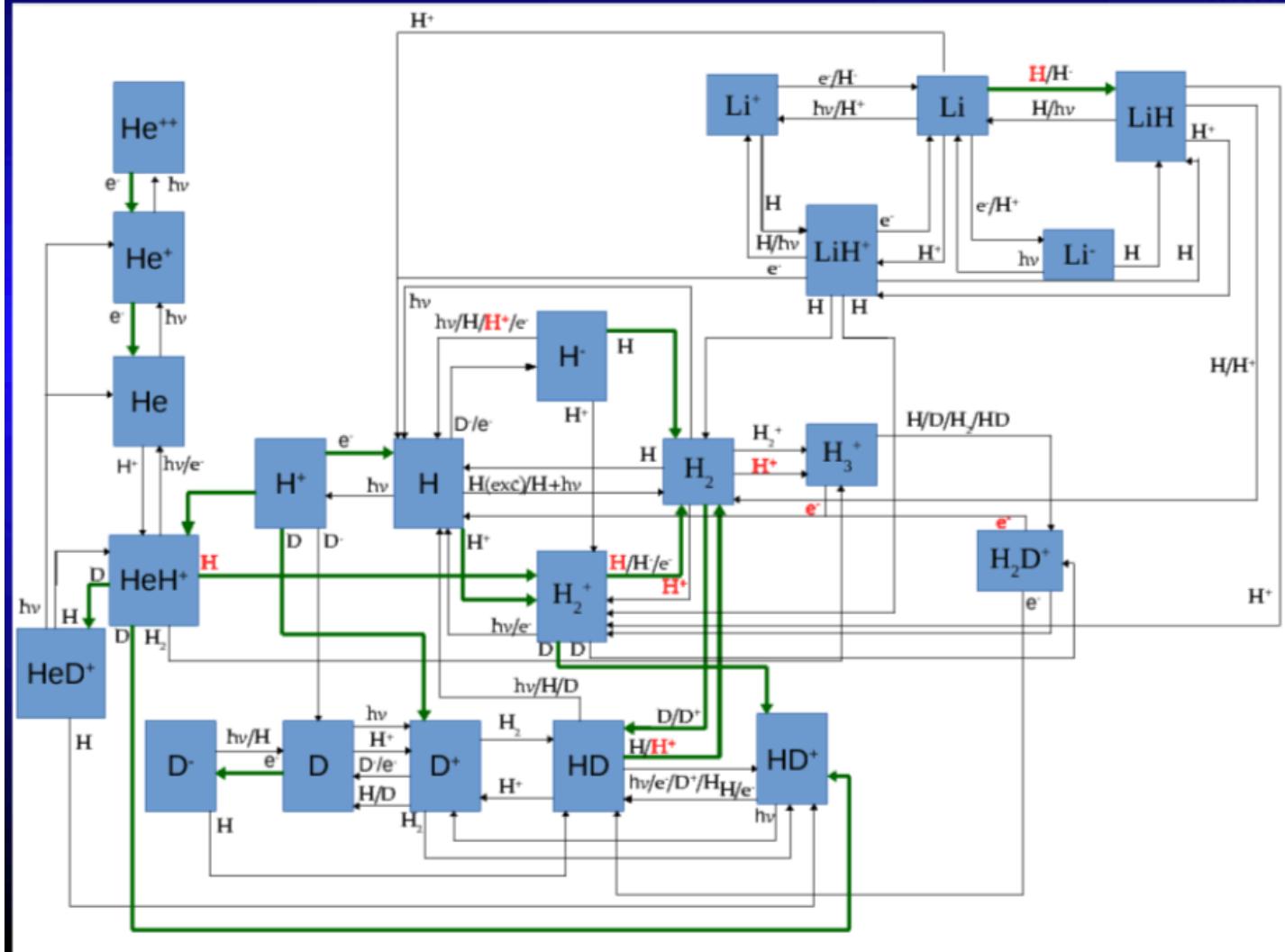
$$\frac{dn_i}{dt} = k_{form} n_j n_k - k_{dest} n_i + \dots$$

$$\frac{dn_i}{dz} = \frac{dt}{dz} \frac{dn_i}{dt}$$

$$n(z) = \Omega_b n_{cr} (1+z)^3$$

7/62

KINETIC MODEL: CHEMICAL NETWORK



Coppola, Galli et al, 2011-...

22 species
~ 200 reactions
state-to-state
↓
~ 50 species
~ 2500 reactions

Typical behaviour of e^-/H_2^+ (HD^+ , D_2^+) recombination

ALL 3 EUROPEAN storage rings:

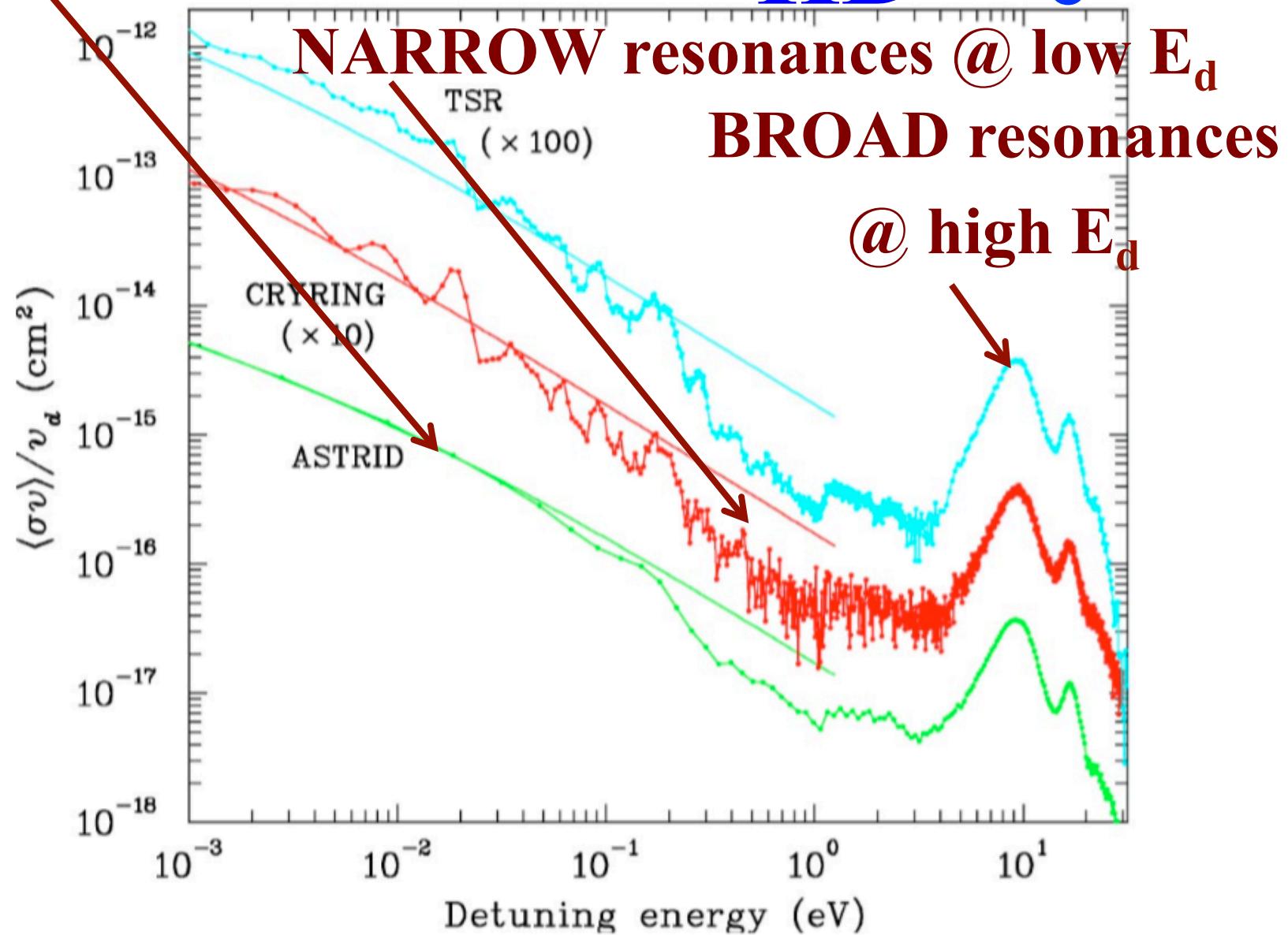
PHYSICAL REVIEW A **68**, 042702 (2003)

**Absolute high-resolution rate coefficients for dissociative recombination of electrons with HD⁺:
Comparison of results from three heavy-ion storage rings**

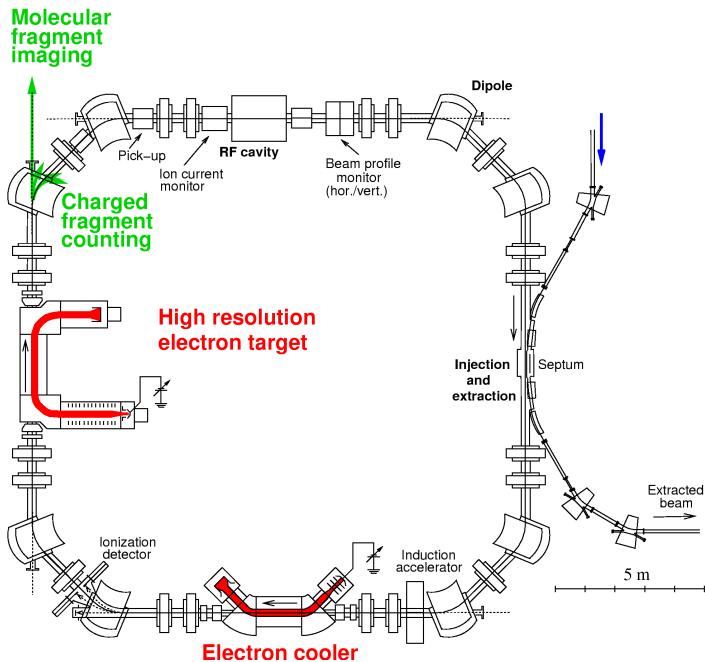
A. Al-Khalili,^{1,2} S. Rosén,¹ H. Danared,³ A. M. Derkatch,¹ A. Källberg,³ M. Larsson,¹ A. Le Padellec,^{1,4} A. Neau,¹ J. Semaniak,² R. Thomas,^{1,5} M. af Ugglas,³ L. Vikor,¹ W. Zong,¹ W. J. van der Zande,^{5,*} X. Urbain,^{6,†} M. J. Jensen,⁶ R. C. Bilodeau,⁶ O. Heber,⁷ H. B. Pedersen,⁶ C. P. Safvan,⁶ L. H. Andersen,⁶ M. Lange,^{8,‡} J. Levin,⁸ G. Gwinner,⁸ L. Knoll,⁸ M. Scheffel,⁸ D. Schwalm,⁸ R. Wester,⁸ D. Zajfman,^{7,8} and A. Wolf⁸

$1/E_d$ behaviour @ low E_d

$\text{HD}^+ + \text{e}^-$



How one measures ?



...+
**Convolution < 2012
 with
 ANISOTROPIC
 Maxwell
 Distribution:**

$$\alpha = \langle v\sigma \rangle = \iiint \sigma(v) v f(v_d, v) dv \quad (1)$$

$$f(v_d, v) = \frac{m}{2\pi k T_{e\perp}} \exp\left(-\frac{mv_\perp^2}{2k T_{e\perp}}\right) \sqrt{\frac{m}{2\pi k T_{e\parallel}}} \exp\left(-\frac{m(v_\parallel - v_d)^2}{2k T_{e\parallel}}\right) \quad (2)$$

Best parameters:

$$T_{\text{long}} = 20 \mu\text{eV} = 0,23 \text{ K} = 0,16 \text{ cm}^{-1}$$

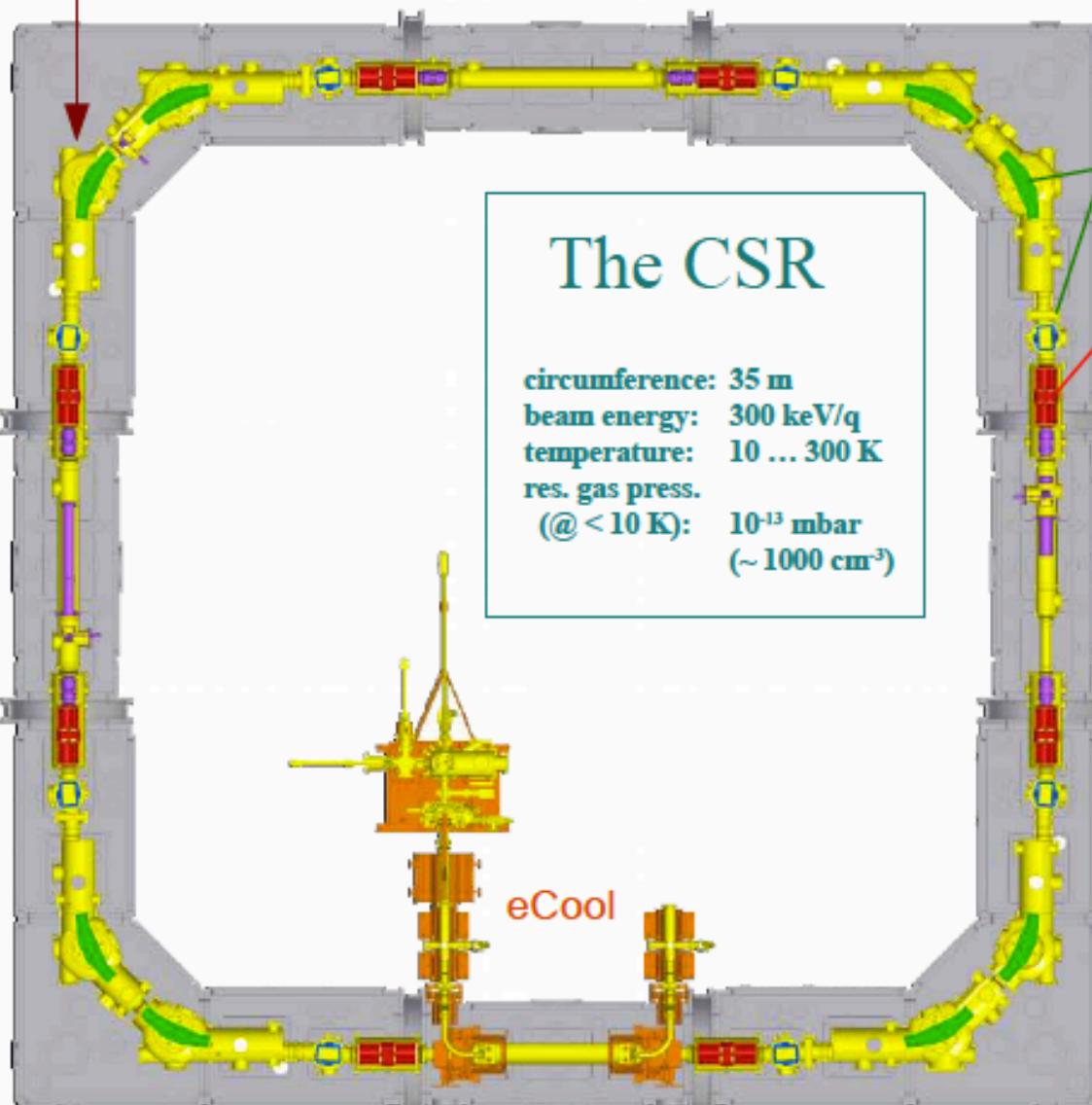
$$T_{\text{trans}} = 500 \mu\text{eV} = 5,80 \text{ K} = 4,03 \text{ cm}^{-1}$$



ion-neutral ex.

injection

> 2016



electrostatic benders
electrostatic quadrupoles
diagnostics:
Schottky, current, pos. pickups

2021/03/31-IAEA-FZJ-WH

**Towards STATE-to-STATE results,
i.e.
ROTATIONALLY &
VIBRATIONALLY
resolved xs & rates.**

On the theoretical side...

Takagi: e⁻/H₂⁺ dynamics

Dissociative Recombination and Excitation of H₂⁺, HD⁺, and D₂⁺ with Electrons for Various Vibrational States

H. Takagi*

School of Medicine, Kitasato University, 1-15-1 Kitasato, Sagamihara, Kanagawa, 228-8555 Japan

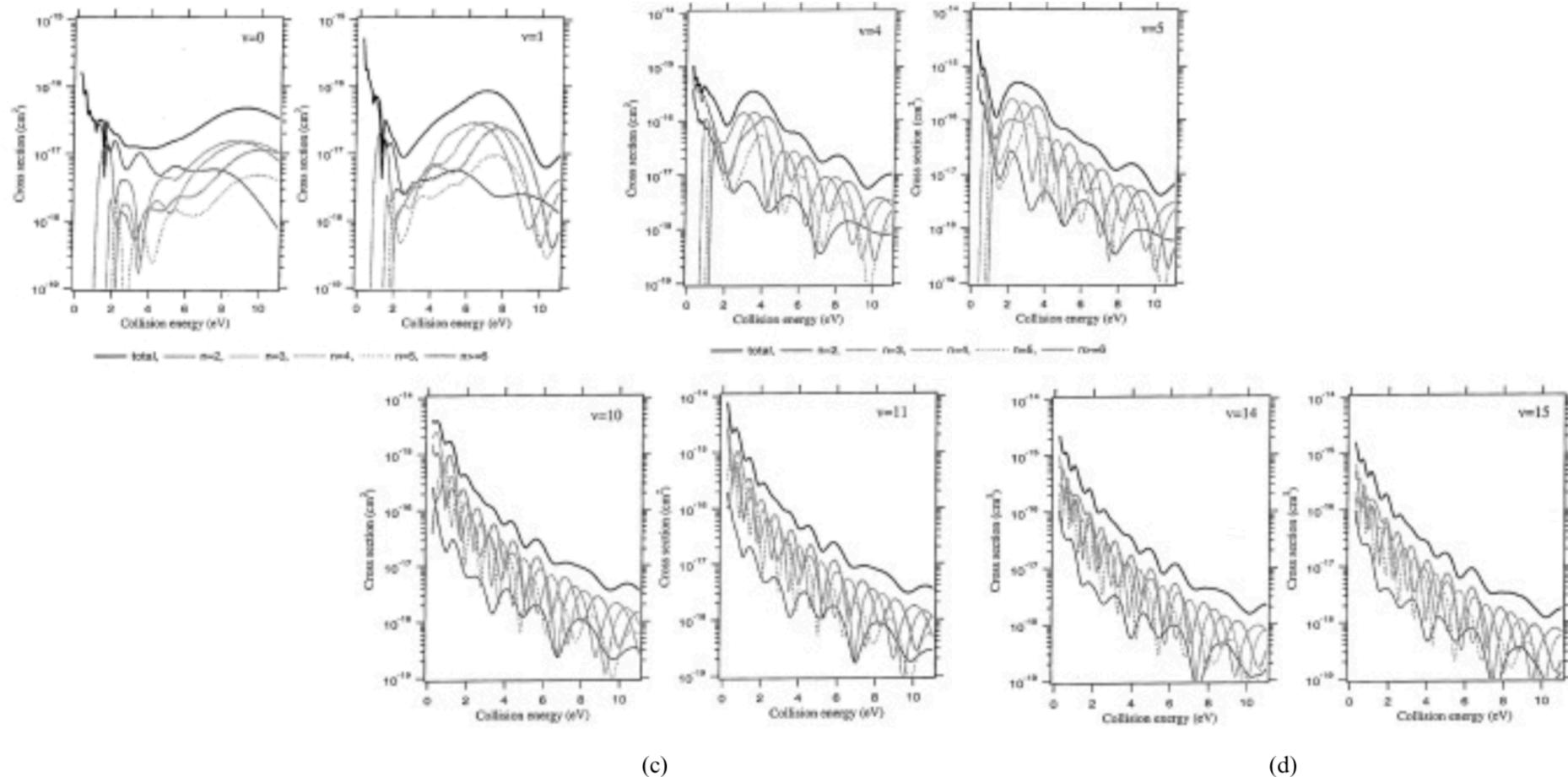


Fig. 4a–d. DR cross section of H₂⁺ for each initial vibrational state v . The dark bold line indicates the total DR cross section. Other lines show the partial cross sections of producing the excited atoms of principle quantum number n , whose value is indicated in the figure. The symbol $n \geq 6$ means $\infty \geq n \geq 6$.



Labex

EMC
ENERGY MATERIALS & CLEAN COMBUSTION CENTER





Labex

EMC
ENERGY MATERIALS & CLEAN COMBUSTION CENTER



WHY new calculations ?

- 1) Different - some updated - molecular structure data
- 2) Data on ro-vibrational transitions



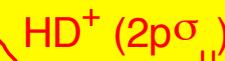
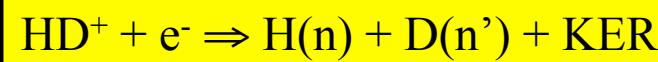
Electron-cold molecular ion reaction: Dissociative Recombination

D. Zajfman

Indirect process

Direct process

Kinetic Energy Release



Interference

Rydberg state



e^-

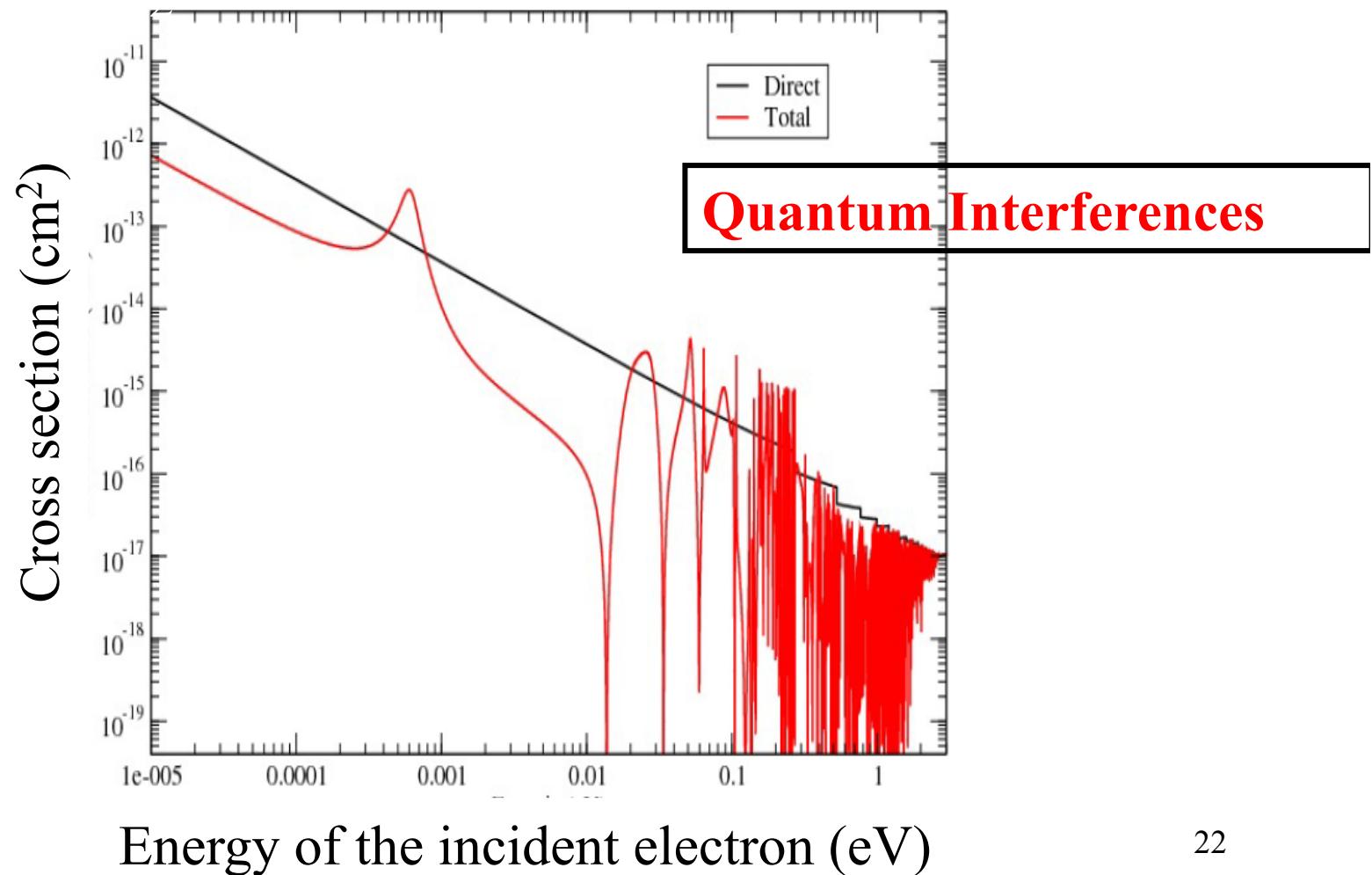
21

$\text{H}(1s) + \text{D}(2l)$

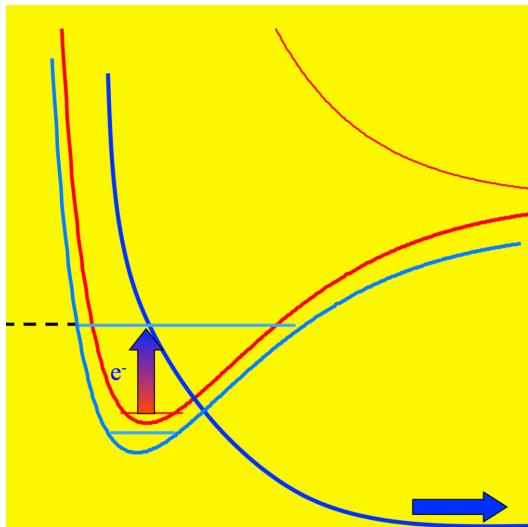
$\text{D}(1s) + \text{H}(2l)$

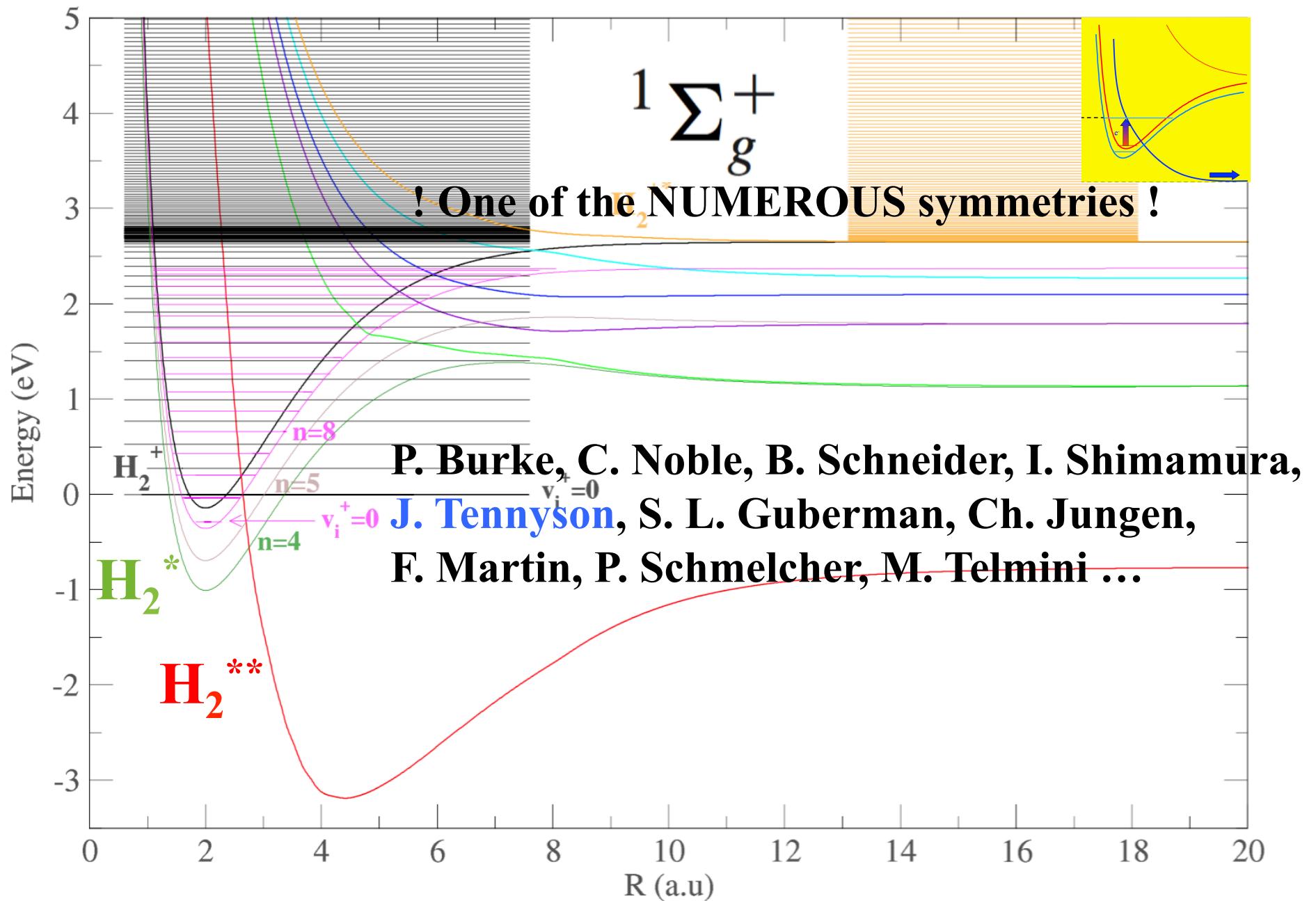
H_2^+ : DR xs

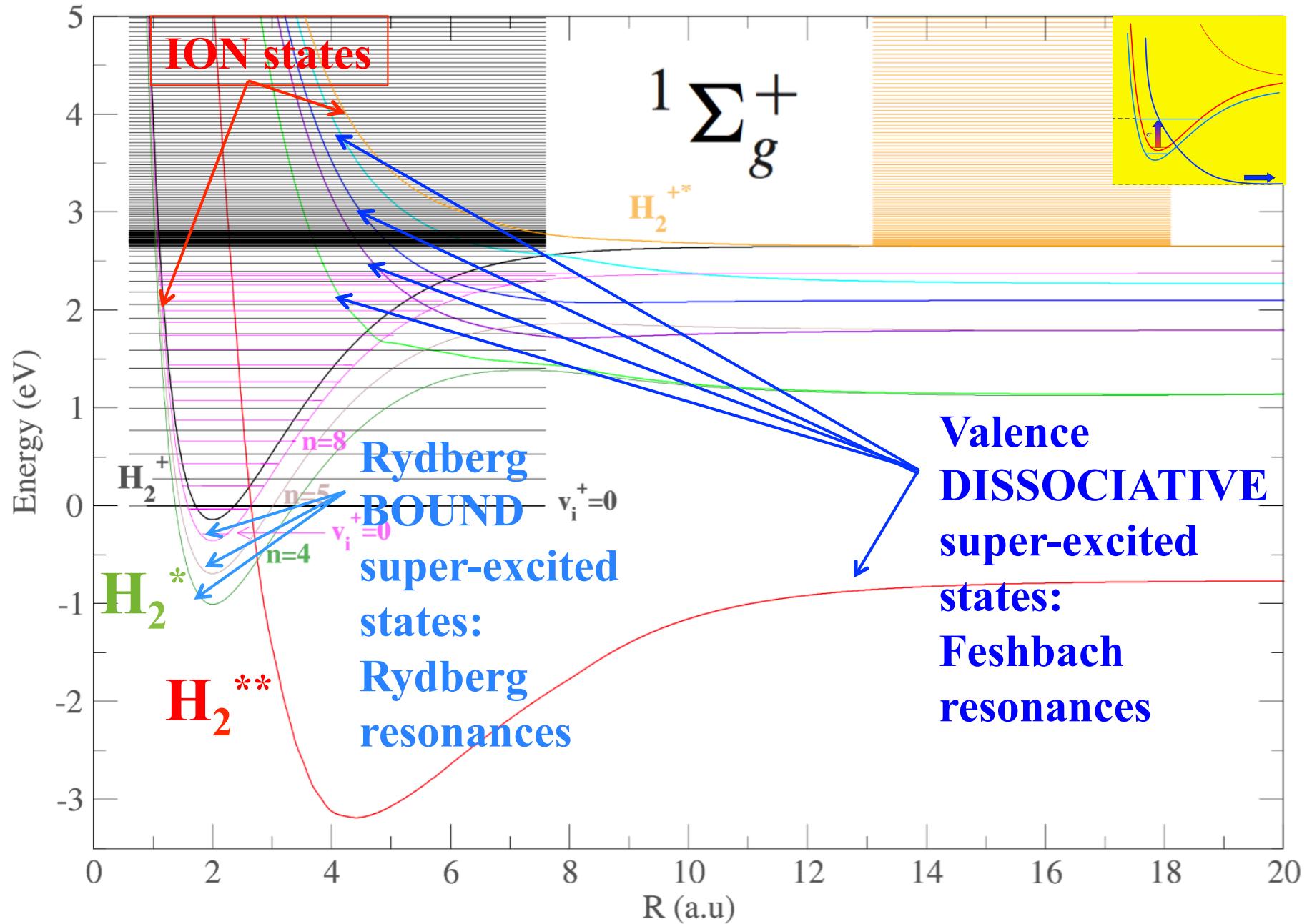
Total (direct & indirect) vs **direct** mechanisms

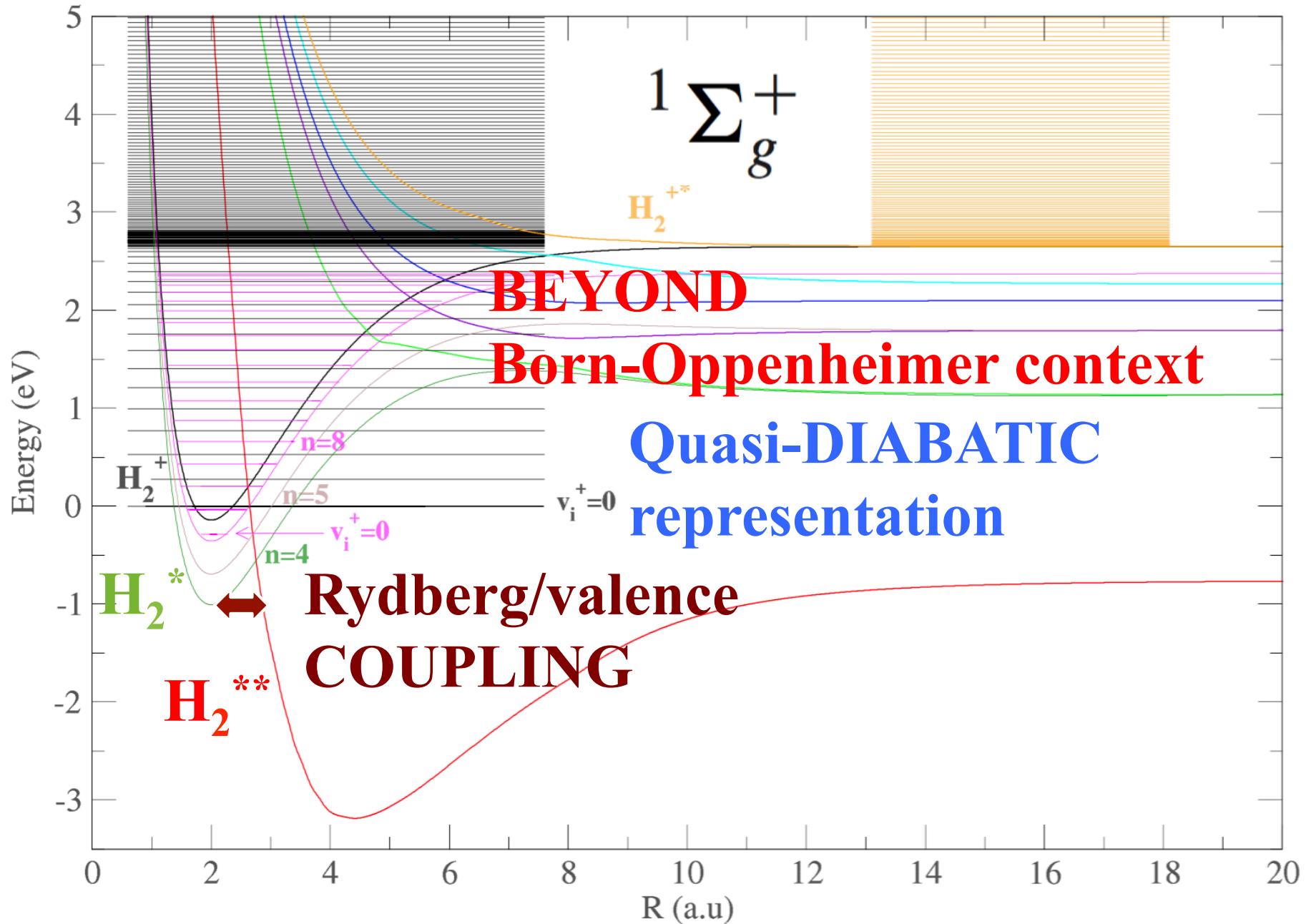


The relevant POTENTIAL ENERGY CURVES

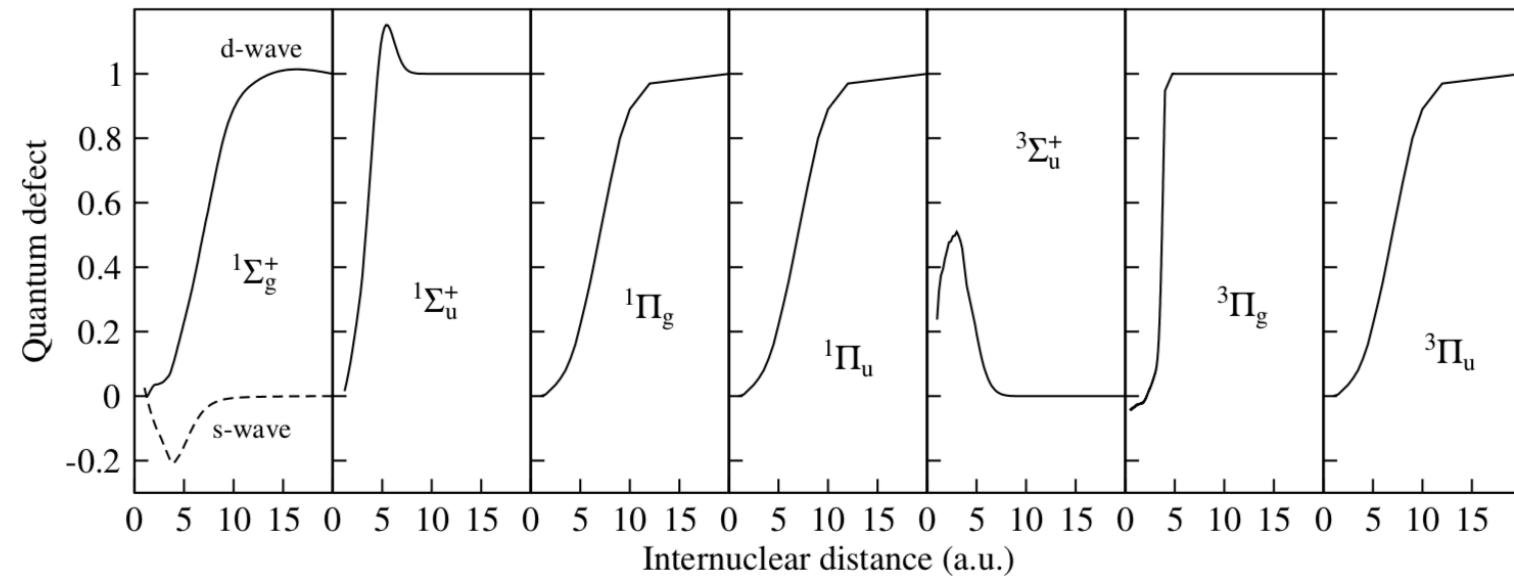
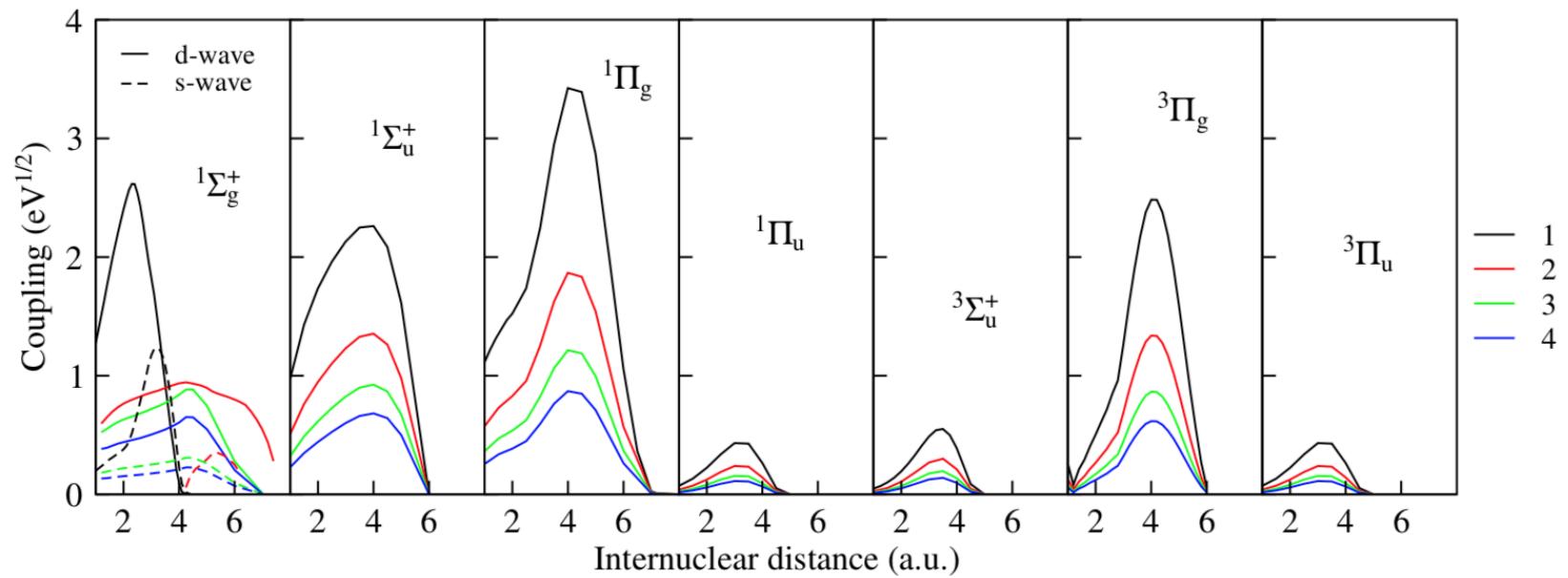








H₂



**How do we compute
electron-impact
recombination**

**and
excitation?**

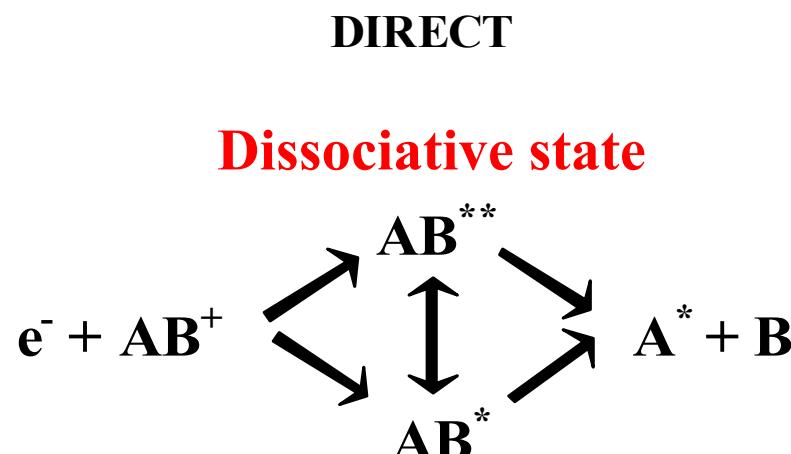
Electron/molecular cation reactive collisions

Main THEORETICAL approach: MQDT

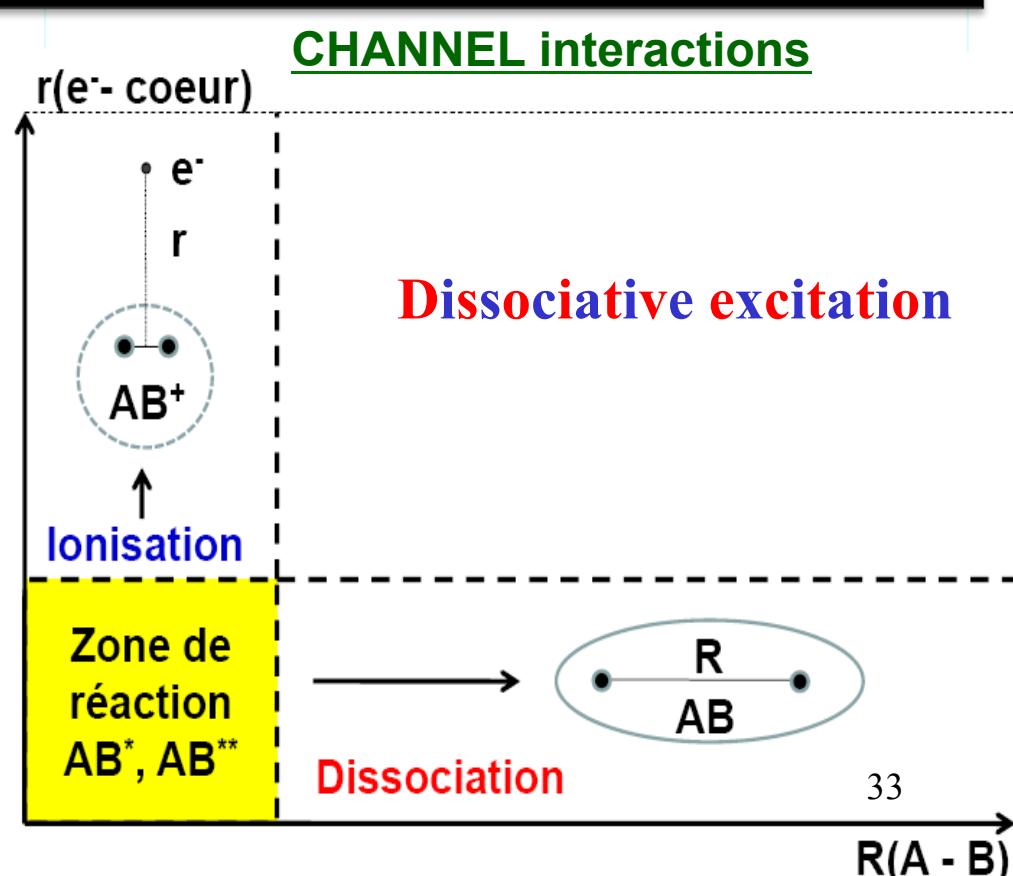
Multichannel Quantum Defect Theory

Seaton (1958-1983), Fano, Jungen, Greene, Giusti -Suzor (1970-...),...

Quantum Interferences

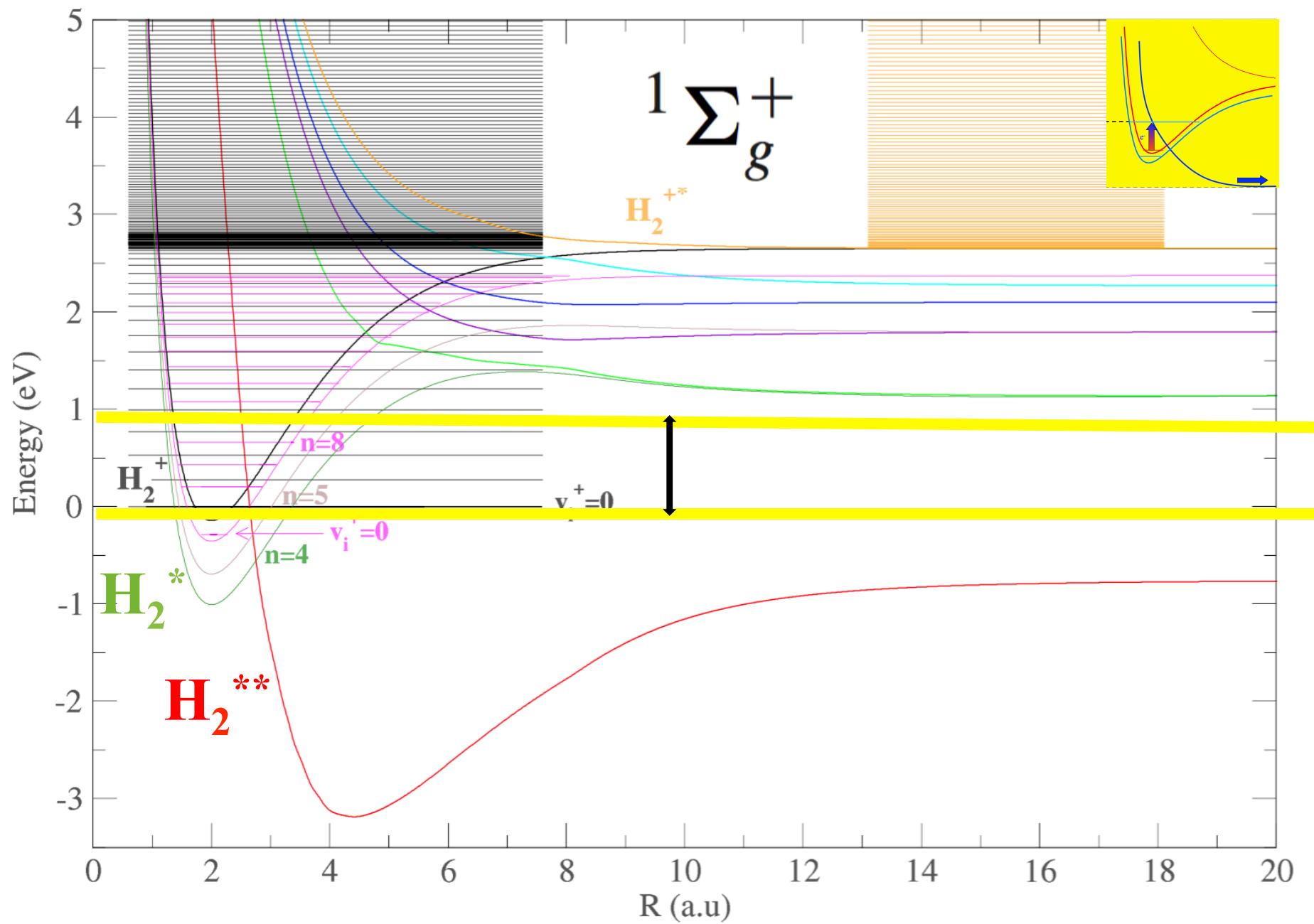


CHANNEL interactions



**The various mechanisms
which drive the DYNAMICS
depend on the
ENERGY:**

**“Very” Low Energy:
ROTATION and Vibration,
DISCRETE ro-vibrational spectrum,
“Fano”resonances,
maximum ACCURACY**



Rotational transitions induced by collisions of HD⁺ ions with low-energy electrons

O. Motapon,^{1,2} N. Pop,³ F. Argoubi,⁴ J. Zs Mezei,^{2,5,6} M. D. Epee Epee,¹ A. Faure,⁷ M. Telmini,⁴ J. Tennyson,⁸ and I. F. Schneider^{2,5}

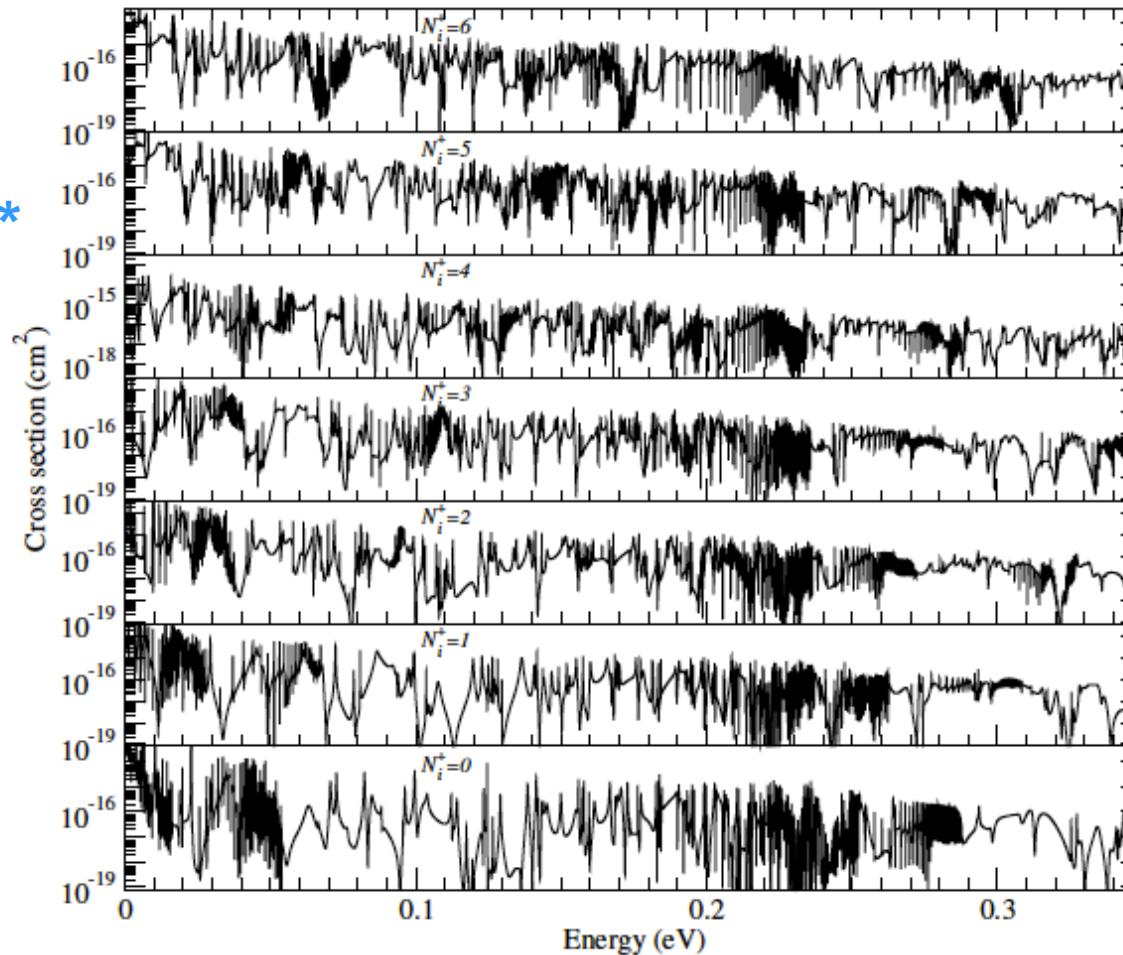
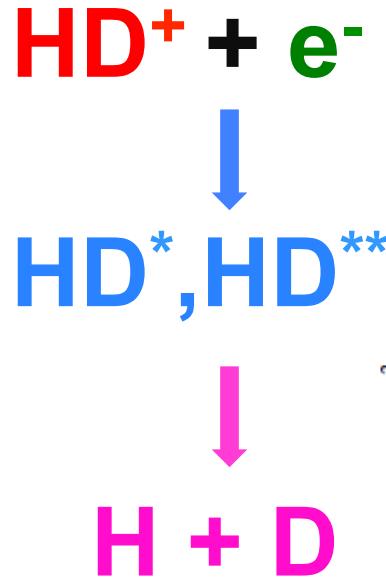
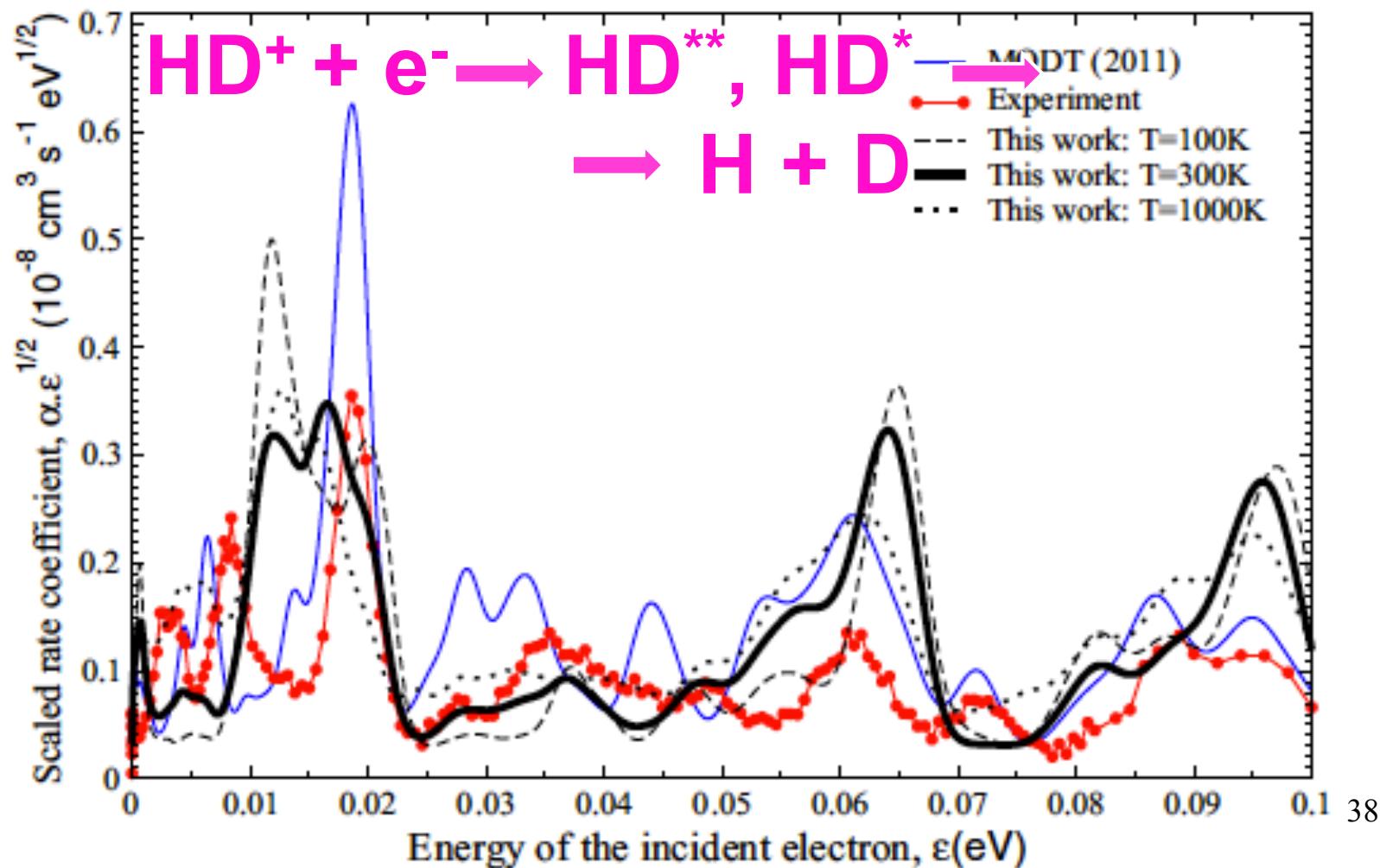


Figure 3. DR cross sections of HD⁺ initially in one of its lowest rotational level N_i^+ (vibrational ground state).

Rotational transitions induced by collisions of HD⁺ ions with low-energy electrons

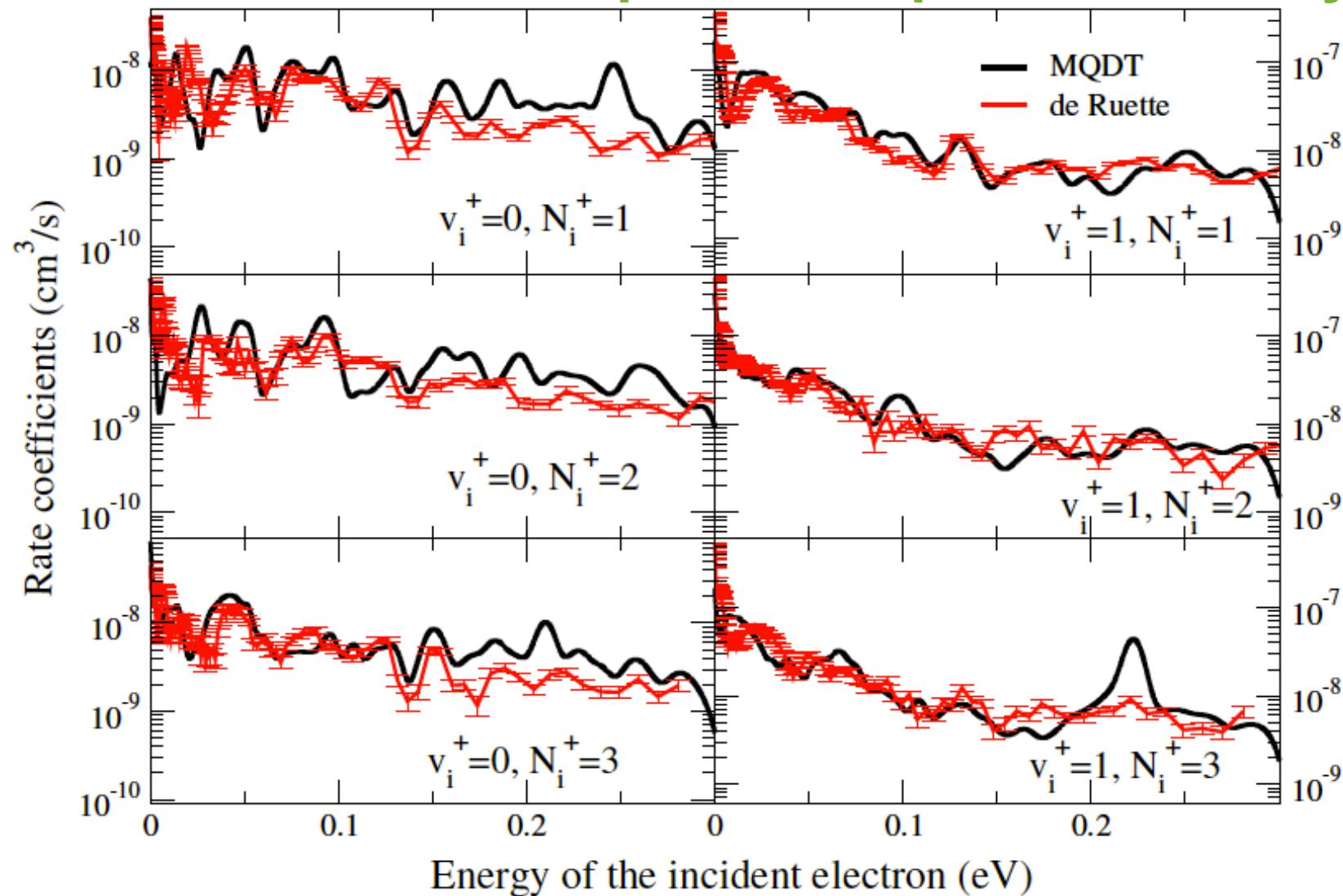
O. Motapon,^{1,2} N. Pop,³ F. Argoubi,⁴ J. Zs Mezei,^{2,5,6} M. D. Epee Epee,¹ A. Faure,⁷ M. Telmini,⁴ J. Tennyson,⁸ and I. F. Schneider^{2,5}



N. De Ruette, X. Urbain, O. Novotny, A. Wolf,... @ TSR vs MQDT



1st state-to-state comparison experiment/theory



How important is the target excitation ?

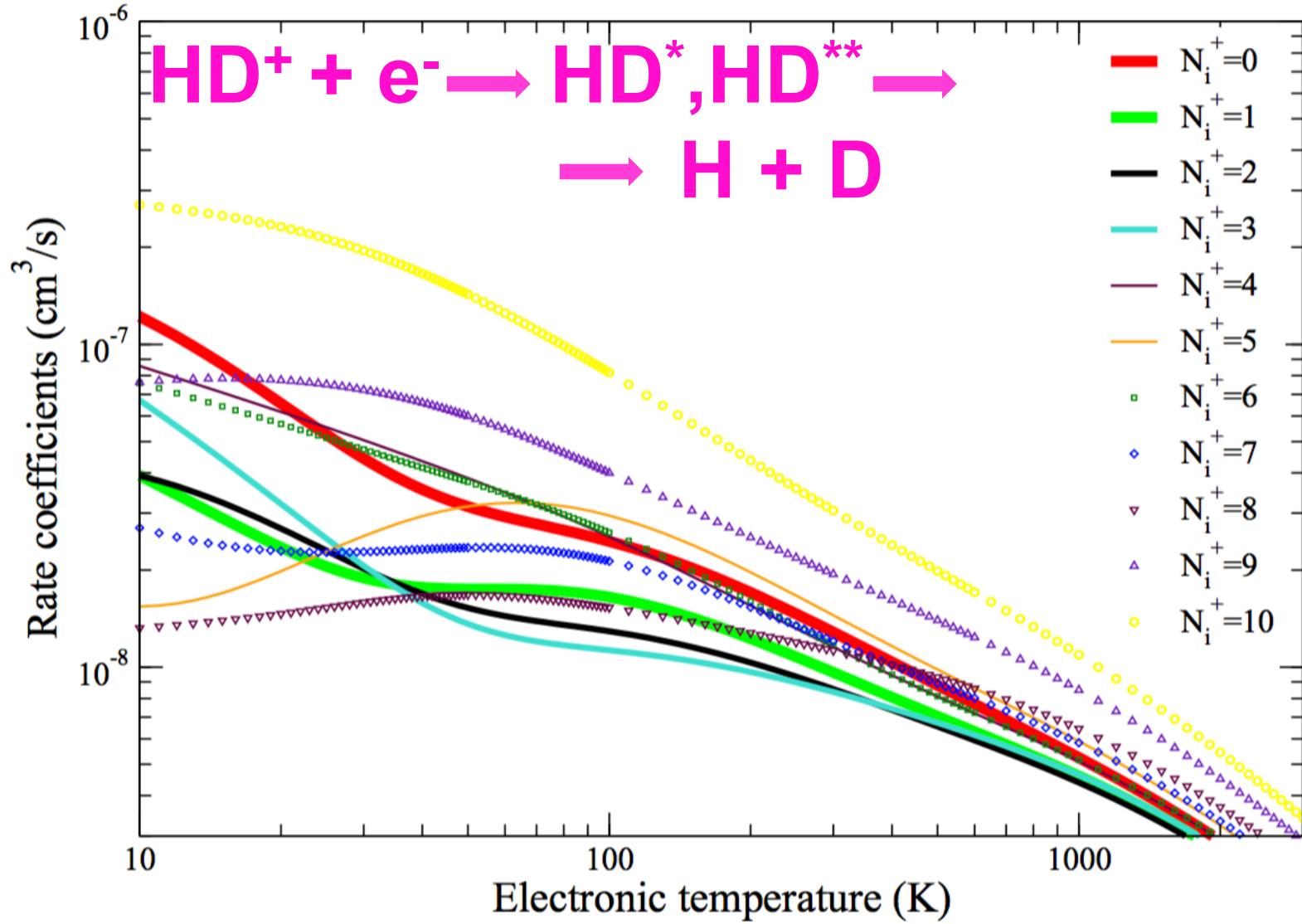
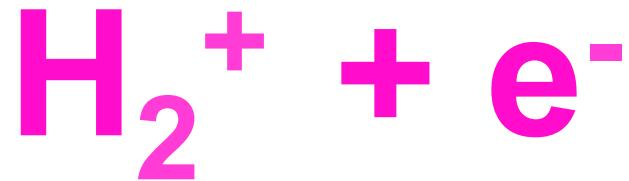


FIG. 9. (Color online) Maxwell isotropic rate coefficients for the dissociative recombination $\text{HD}^+(X^2\Sigma_g^+)$ with $v_i^+ = 0$ as a function of initial rotational level, $N_i^+ = 0$ to 10.



Monthly Notices
of the
ROYAL ASTRONOMICAL SOCIETY
MNRAS 455, 276–281 (2015)



Reactive collisions of very low-energy electrons with H_2^+ : rotational transitions and dissociative recombination

M. D. Epée Epée,¹ J. Zs Mezei,^{2,3,4} O. Motapon,^{1,5★} N. Pop⁶ and I. F. Schneider^{2,3★}

¹LPF, UFD Mathématiques, Informatique Appliquée et Physique Fondamentale, University of Douala, P. O. Box 24157, Douala, Cameroon

²Laboratoire Ondes et Milieux Complexes, UMR 6294 CNRS and Université du Havre, 25, rue Philippe Lebon, BP 540, F-76058 Le Havre, France

³Laboratoire Aimé Cotton CNRS-UPR-3321, Université Paris-Sud, Orsay F-91405, France

⁴Laboratoire des Sciences des Procédés et des Matériaux, UPR 3407 CNRS and Univ. Paris 13, 99 avenue Jean-Baptiste Clément, F-93430 Villetaneuse, France

⁵Faculty of Science, University of Maroua, PO Box 814 Maroua, Cameroon

⁶Department of Physical Foundation of Engineering, University Politehnica of Timisoara, Bv Vasile Parvan No 2, 300223, Timisoara, Romania

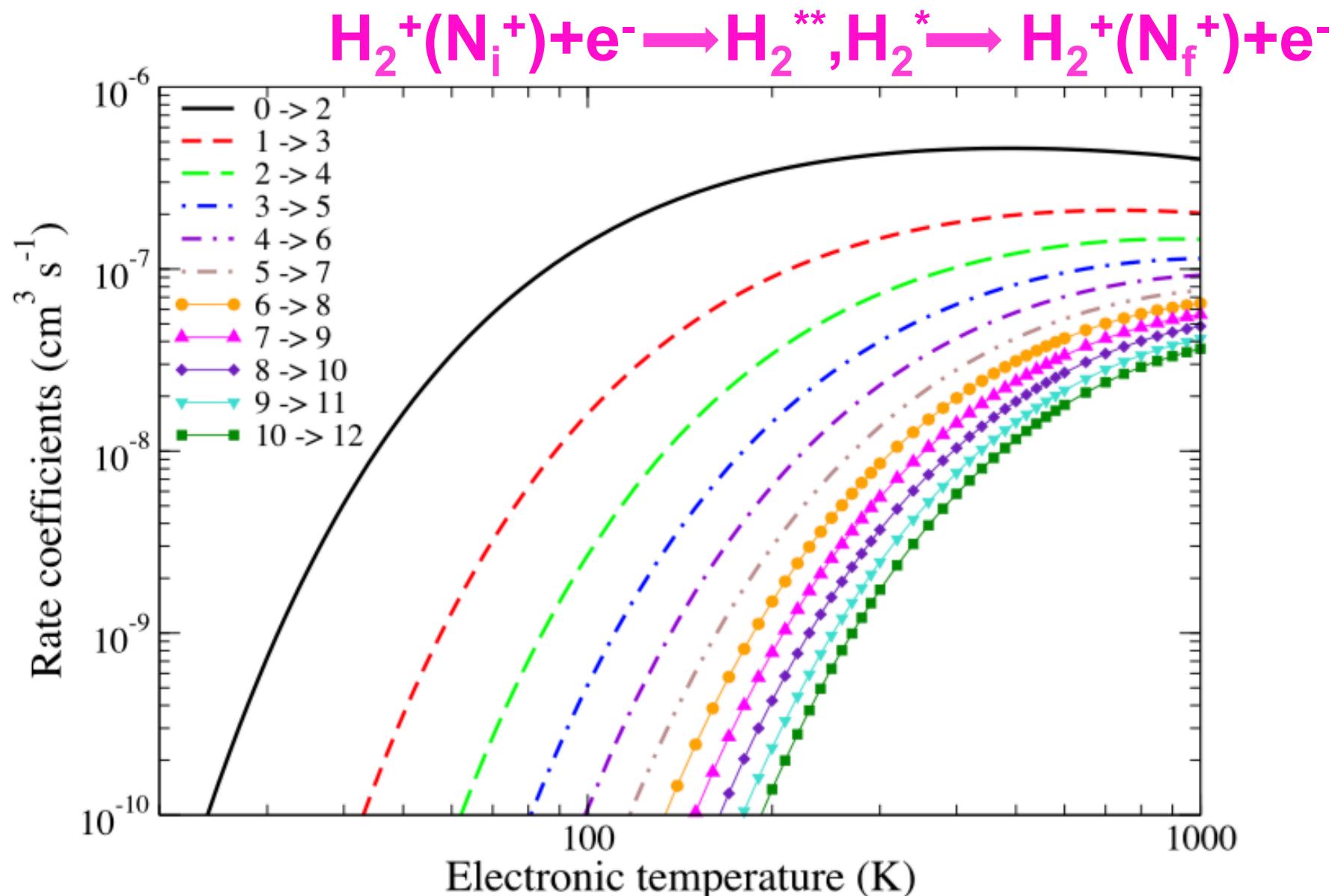
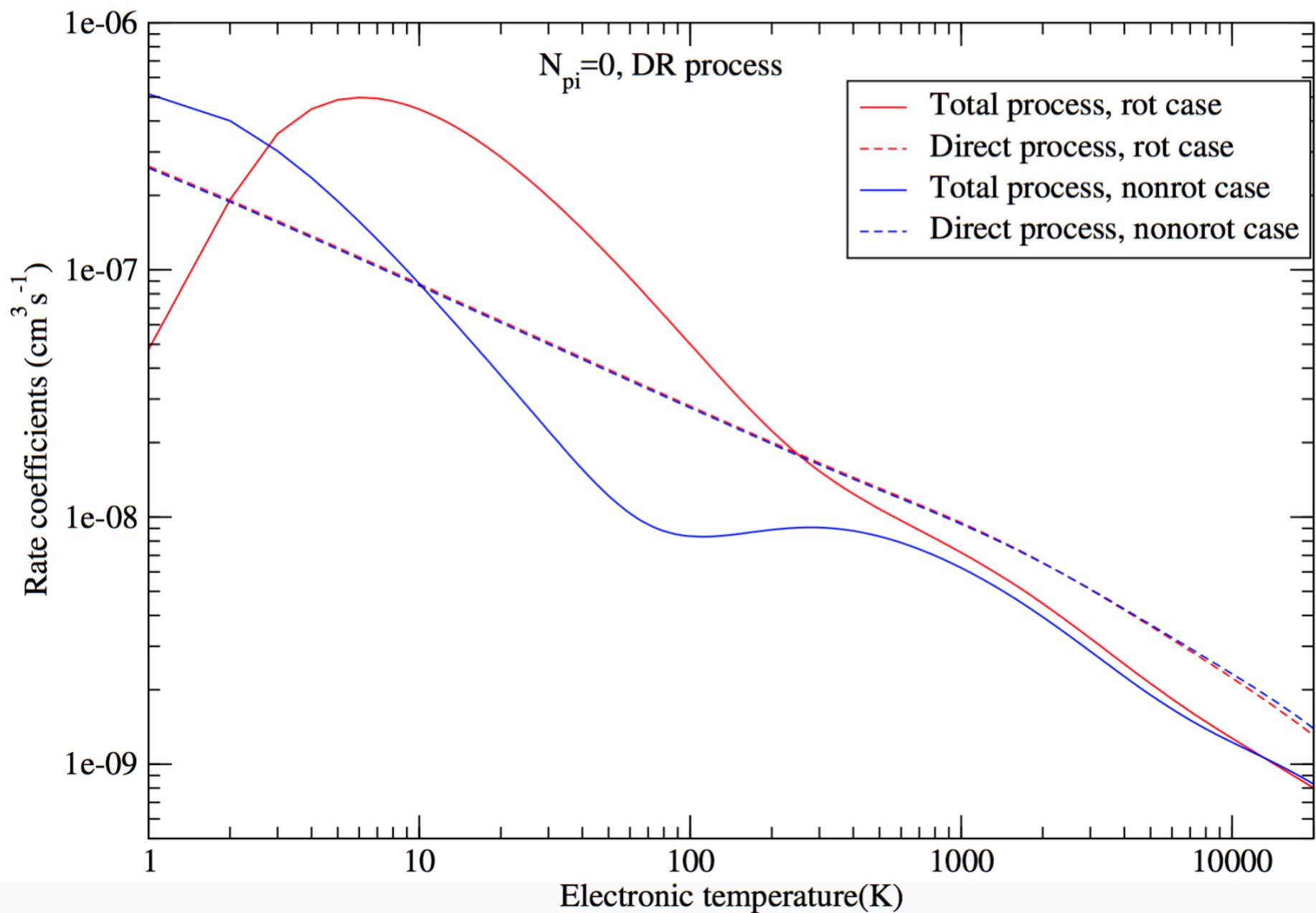
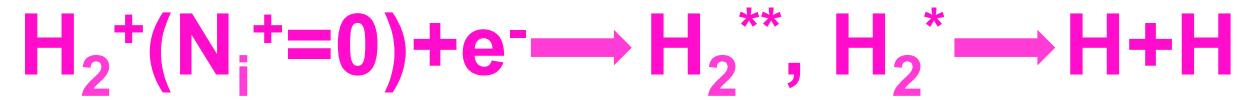


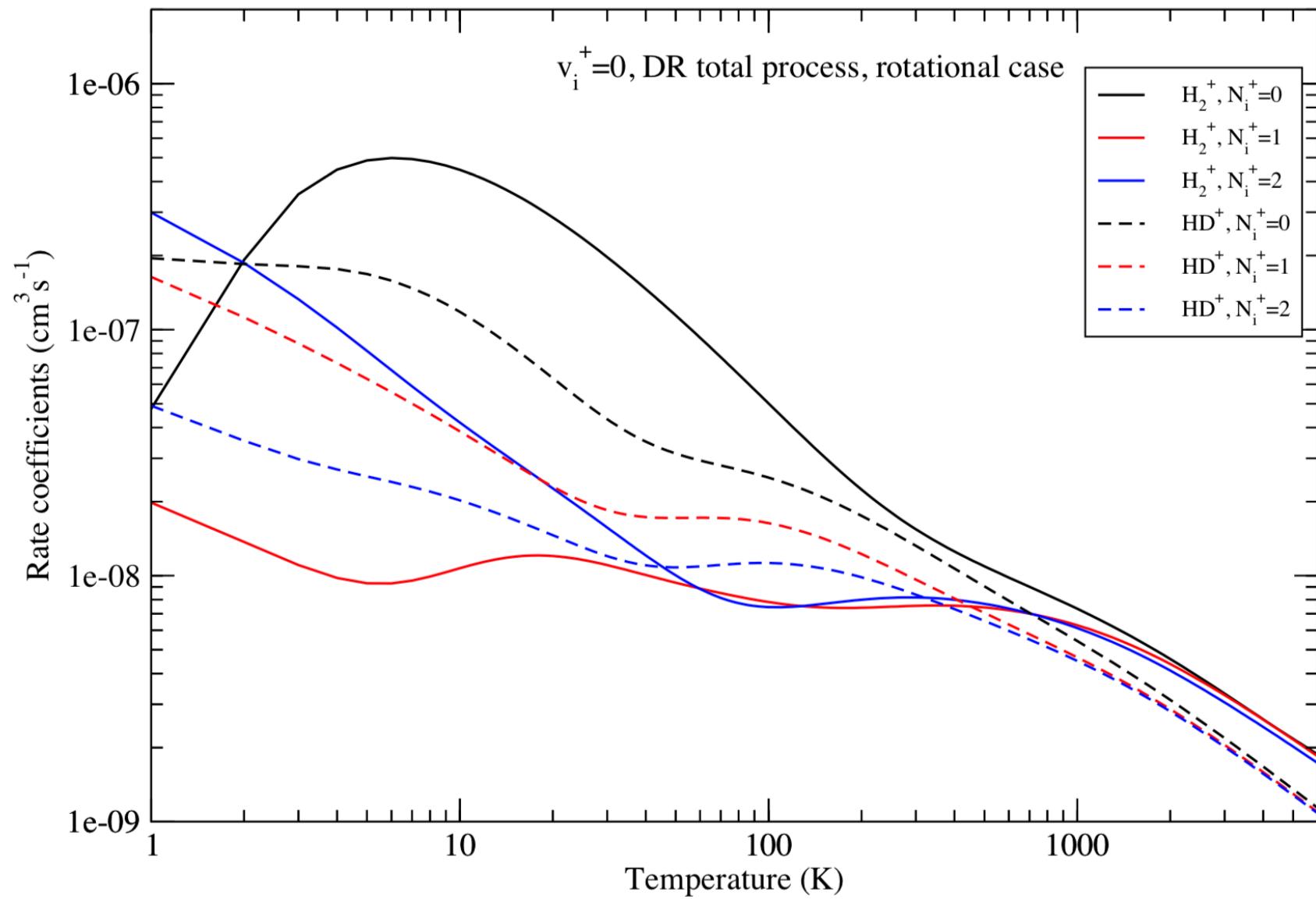
Figure 3. Maxwell rate coefficients for rotational excitation $\text{N}_i^+ \rightarrow \text{N}_i^+ + {}_{44}^2$, with $\text{N}_i^+ = 0$ to 10 of $\text{H}_2^+(X^2\Sigma_g^+)$ on its ground vibrational level $v_i^+ = 0$.

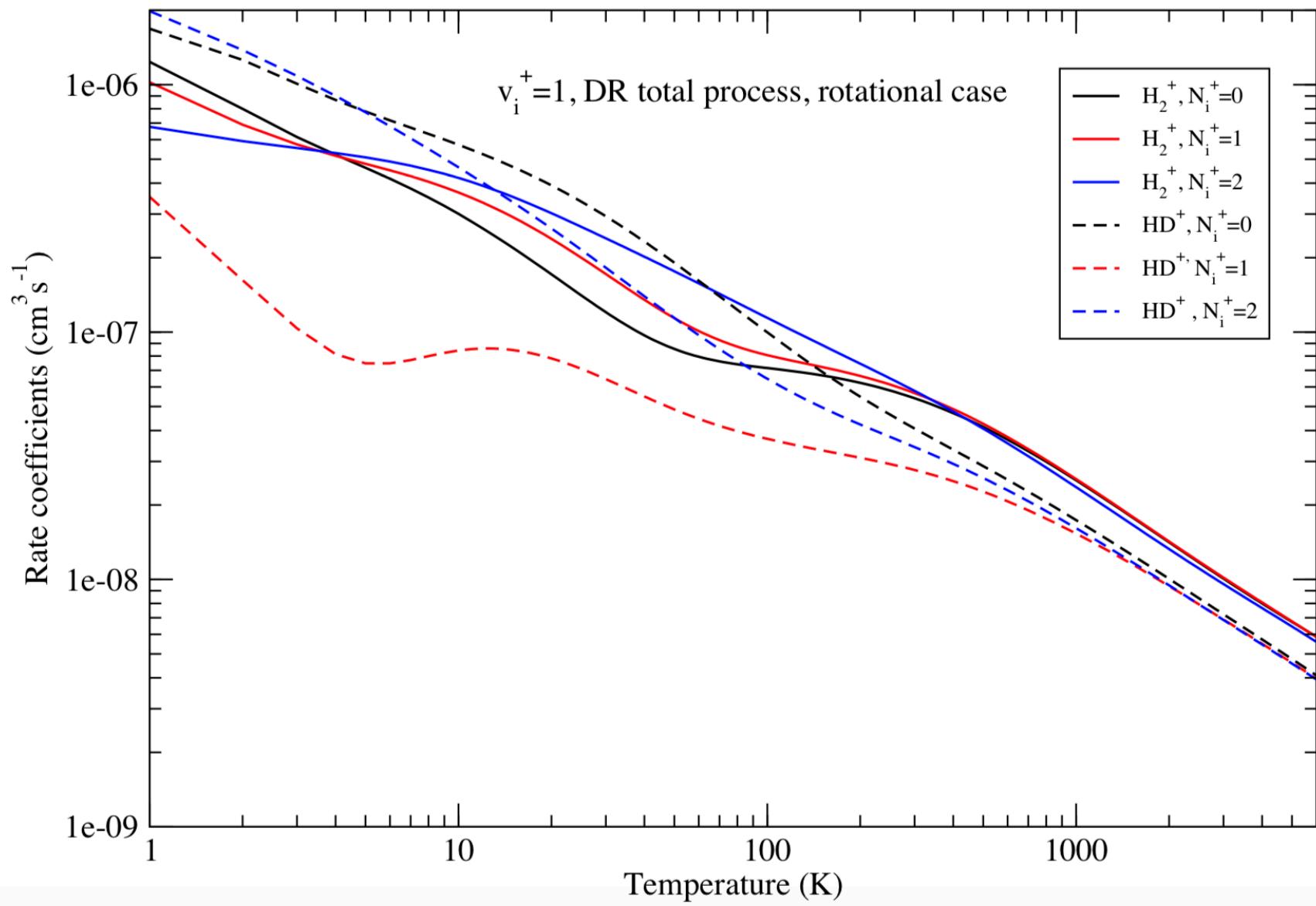
**How important are the
RESONANCES ?**

**How important are the
ROTATIONAL effects ?**



Focus on ISOTOPIC effects





HD⁺ DR & rovibrational transitions for « ALL » the rovibrational levels

Table 1. The energy of the first 30 ro-vibrational levels of HD⁺ $X^1\Sigma_g^+$ electronic state relative to the ground $(N_i^+, v_i^+) = (0, 0)$ level.

no	(N_i^+, v_i^+)	energy(eV)	no	(N_i^+, v_i^+)	energy(eV)
1	(0,0)	0.0000	16	(4,1)	0.289
2	(1,0)	0.0054	17	(5,1)	0.314
3	(2,0)	0.0163	18	(11,0)	0.337
4	(3,0)	0.0325	19	(6,1)	0.344
5	(4,0)	0.0539	20	(7,1)	0.379
6	(5,0)	0.0804	21	(12,0)	0.394
7	(6,0)	0.112	22	(8,1)	0.418
8	(7,0)	0.148	23	(13,0)	0.455
9	(8,0)	0.189	24	(9,1)	0.461
10	(9,0)	0.234	25	(0,2)	0.462
11	(0,1)	0.237	26	(1,2)	0.467
12	(1,1)	0.242	27	(2,2)	0.477
13	(2,1)	0.253	28	(3,2)	0.492
14	(3,1)	0.268	29	(10,1)	0.508
15	(10,0)	0.284	30	(4,2)	0.511

HD^+ DR & rovibrational transitions for « ALL » the rovibrational levels

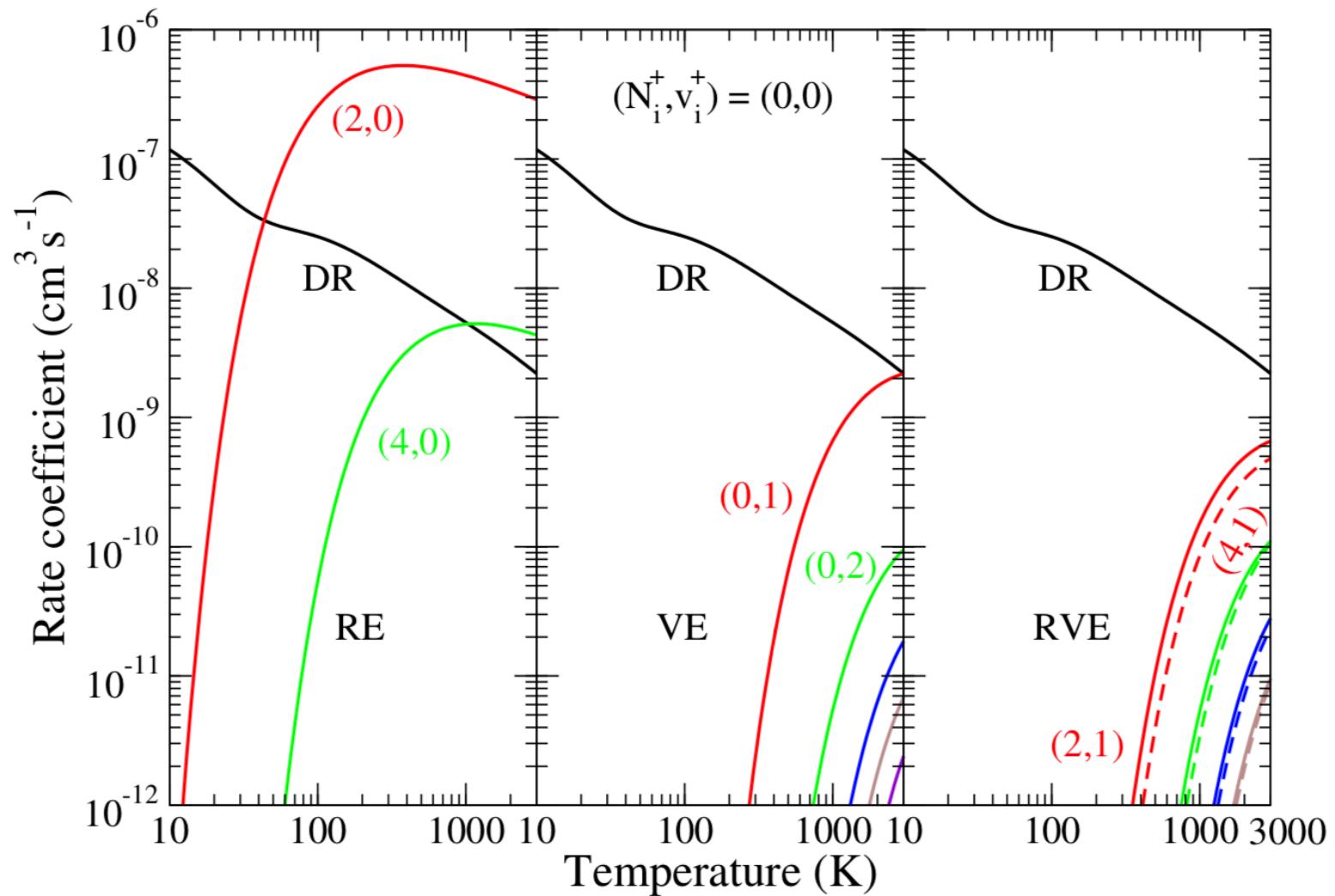


Figure 1. Maxwell rate coefficients of the ground $\text{HD}^+(X^2\Sigma_g^+)$ molecular target for Dissociative Recombination (DR) and Rotational Excitation (RE) in the left, DR and Vibrational Excitation (VE) in the middle and DR and mixed Ro-Vibrational Excitations (RVE) in the right panels.

HD^+ DR & rovibrational transitions for « ALL » the rovibrational levels

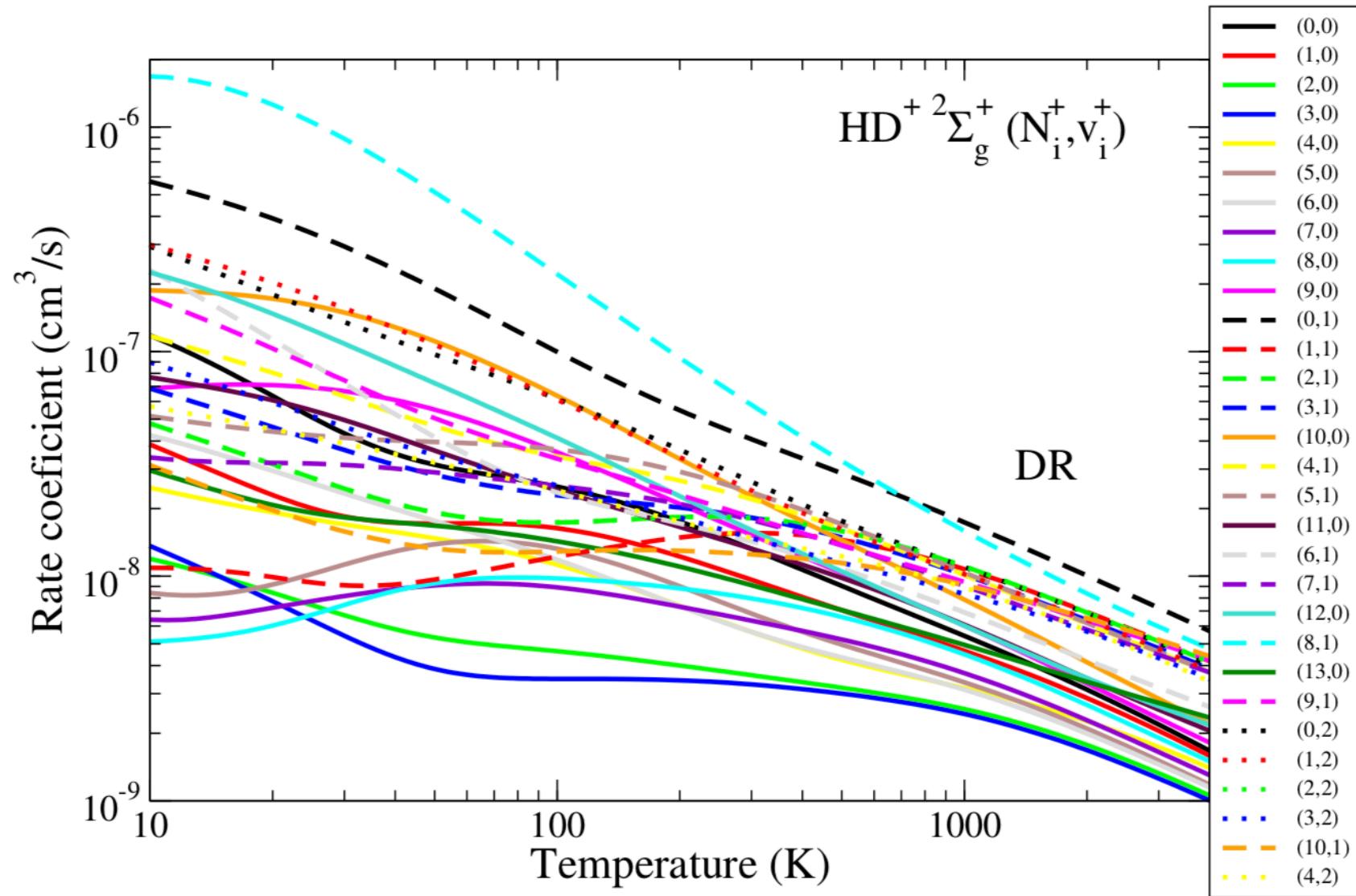


Figure 2. DR Maxwell rate coefficients for the lowest 30 ro-vibrational levels of $\text{HD}^+(\text{X}^2\Sigma_g^+)$ molecular target.

HD⁺ DR & rovibrational transitions for « ALL » the rovibrational levels

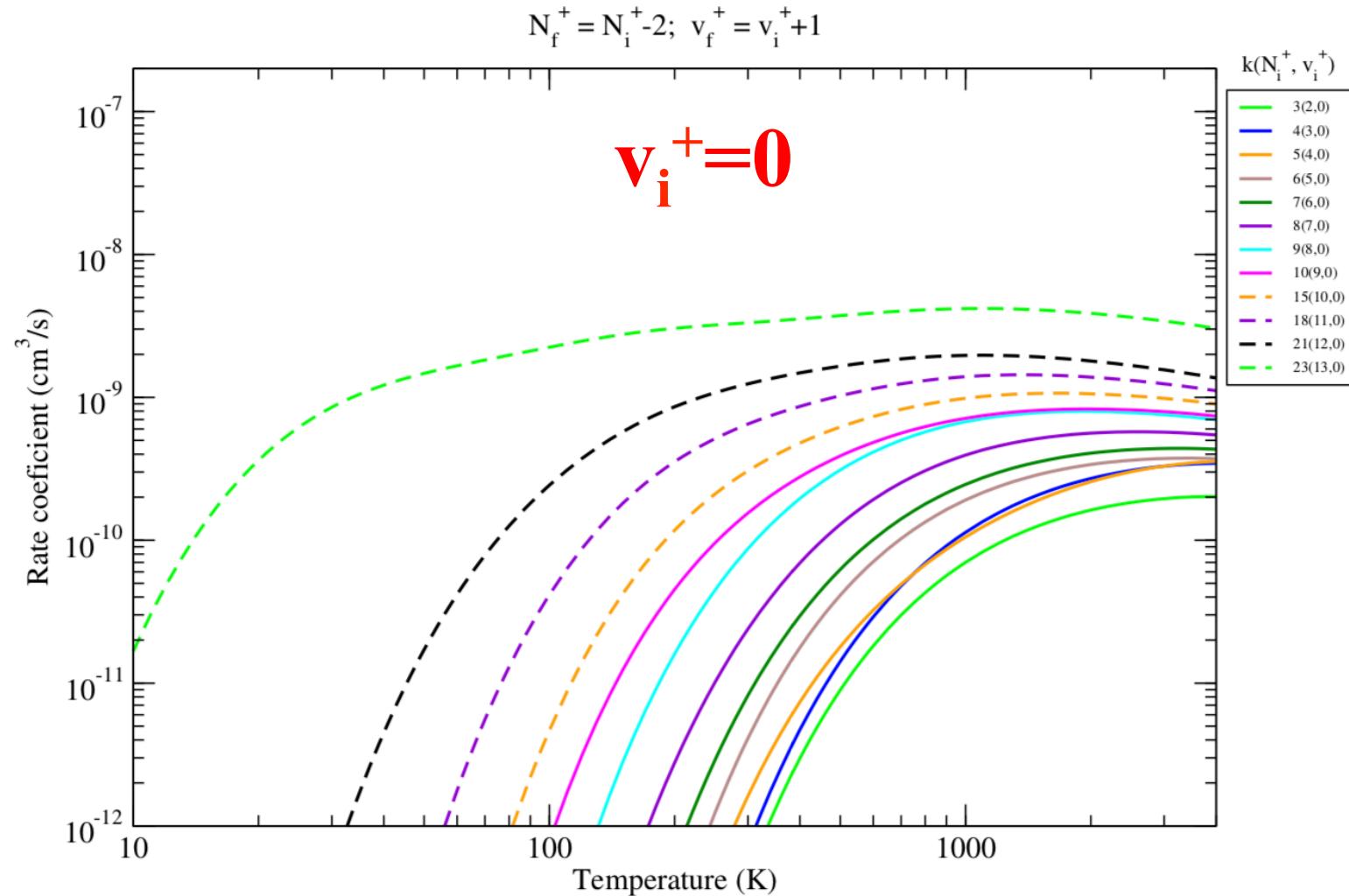


Figure 22. Electron-impact rotational de-excitation ($\Delta N^+ = -2$) and vibrational excitation ($\Delta v^+ = 1$) of HD⁺ [$[2\Sigma_g^+ (N_i^+, v_i^+ = 0)]$:

HD⁺ DR & rovibrational transitions for « ALL » the rovibrational levels

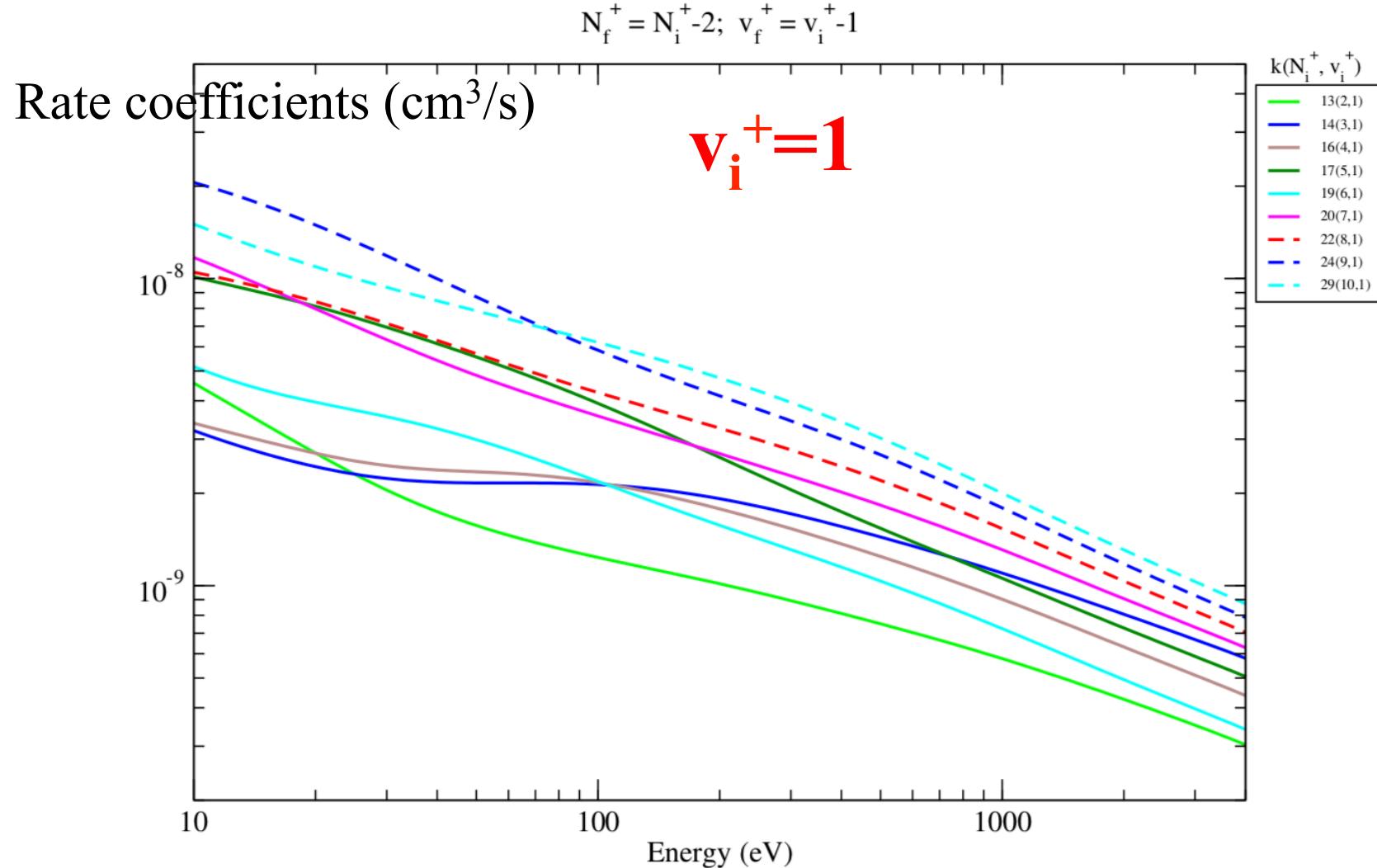


Figure 25. Electron-impact rotational and vibrational de-excitation ($\Delta N_i^+ = -2, \Delta v_i^+ = -1$) of HD⁺ [${}^2\Sigma_g^+$ ($N_i^+, v_i^+ = 1$)]: The effect of the ro-vibrational excitation of the target.

D_2^+ DR & rotational transitions for vibrationally relaxed states

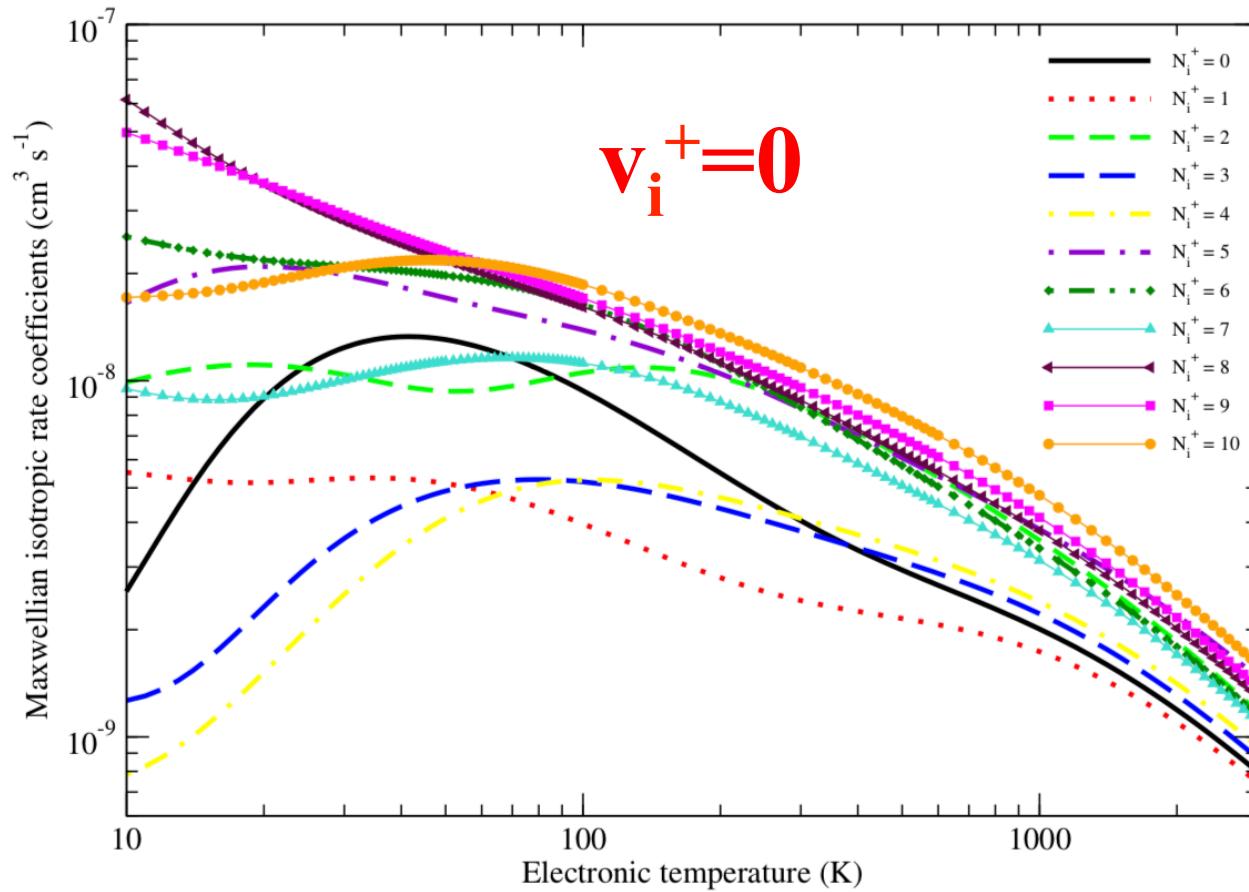
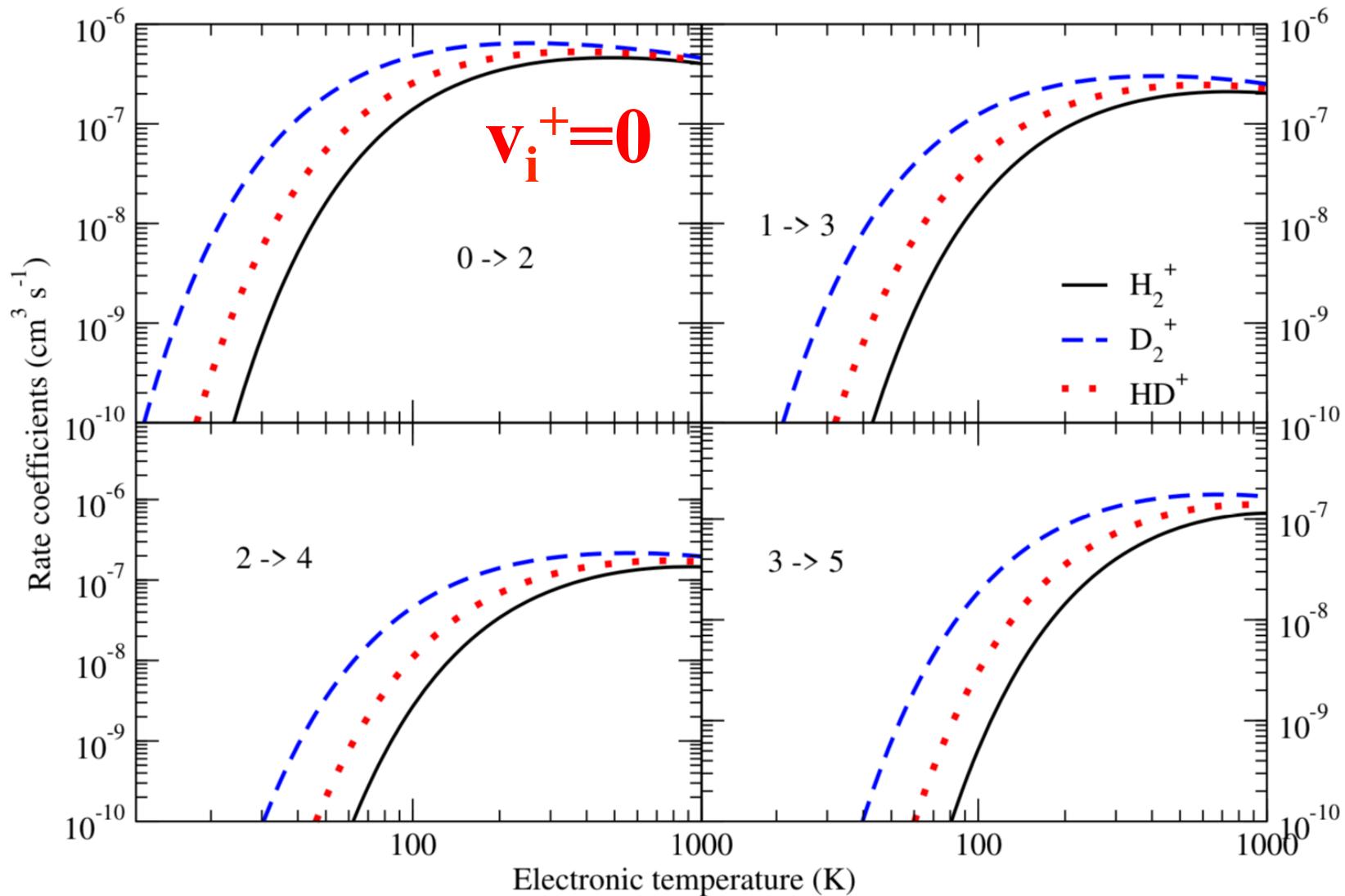
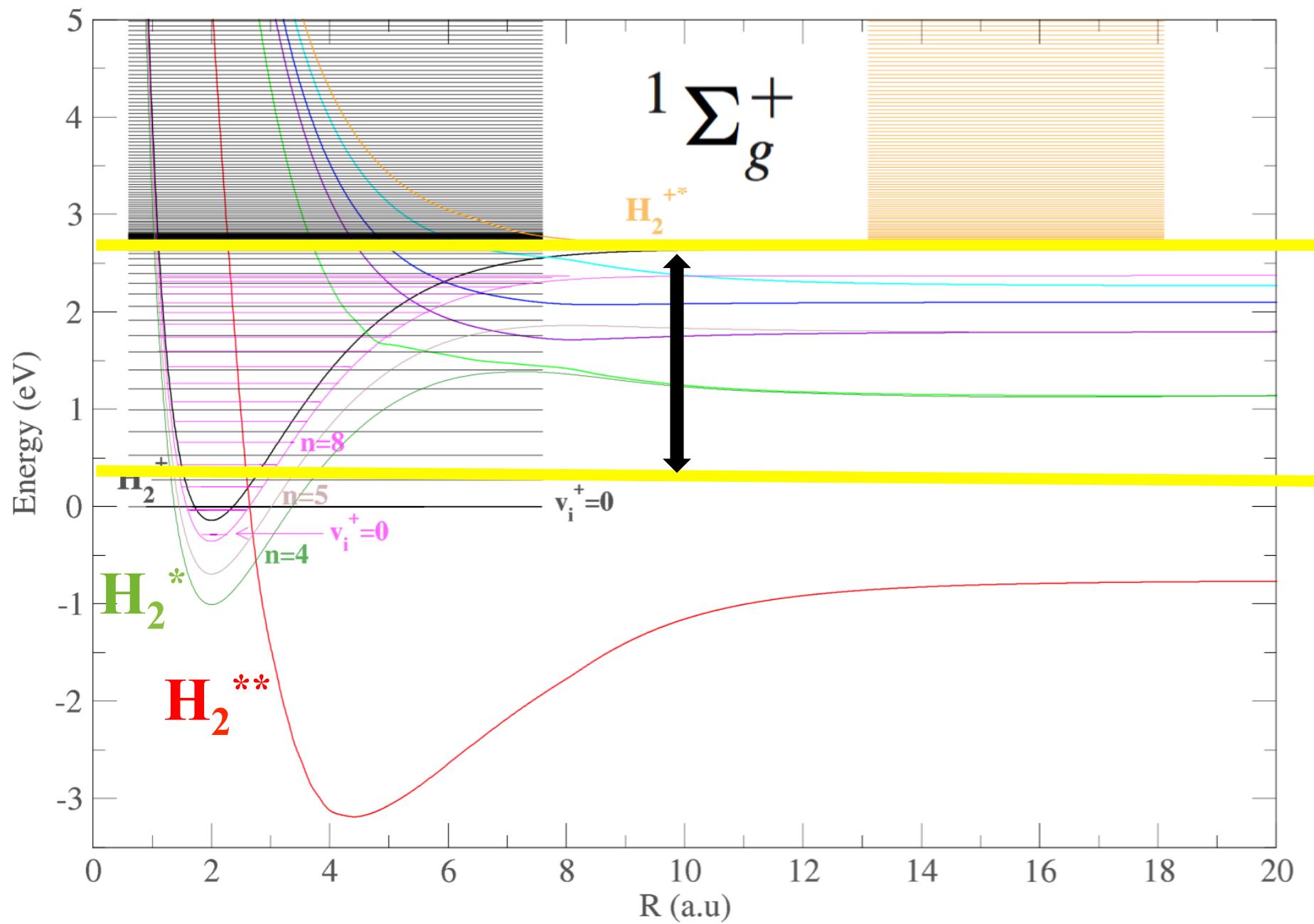


Figure 2. Maxwell rate coefficients for the dissociative recombination of $D_2^+(X^2\Sigma_g^+)$ on its ground vibrational level $v_i^+ = 0$, as a function of its initial rotational level, $N_i^+ = 0$ to 10.

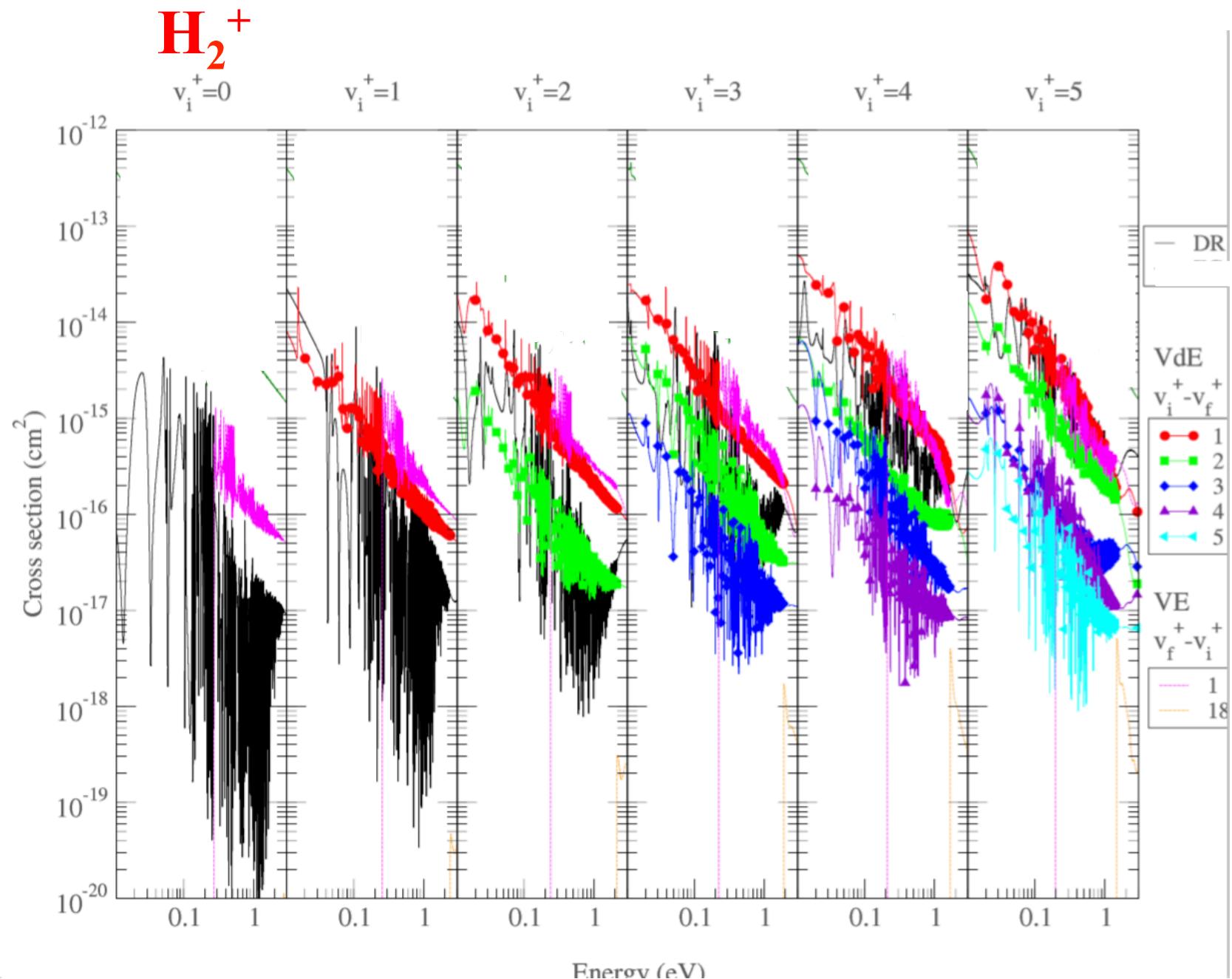
D_2^+ vs HD^+ vs H_2^+ : rotational transitions for vibrationally relaxed states



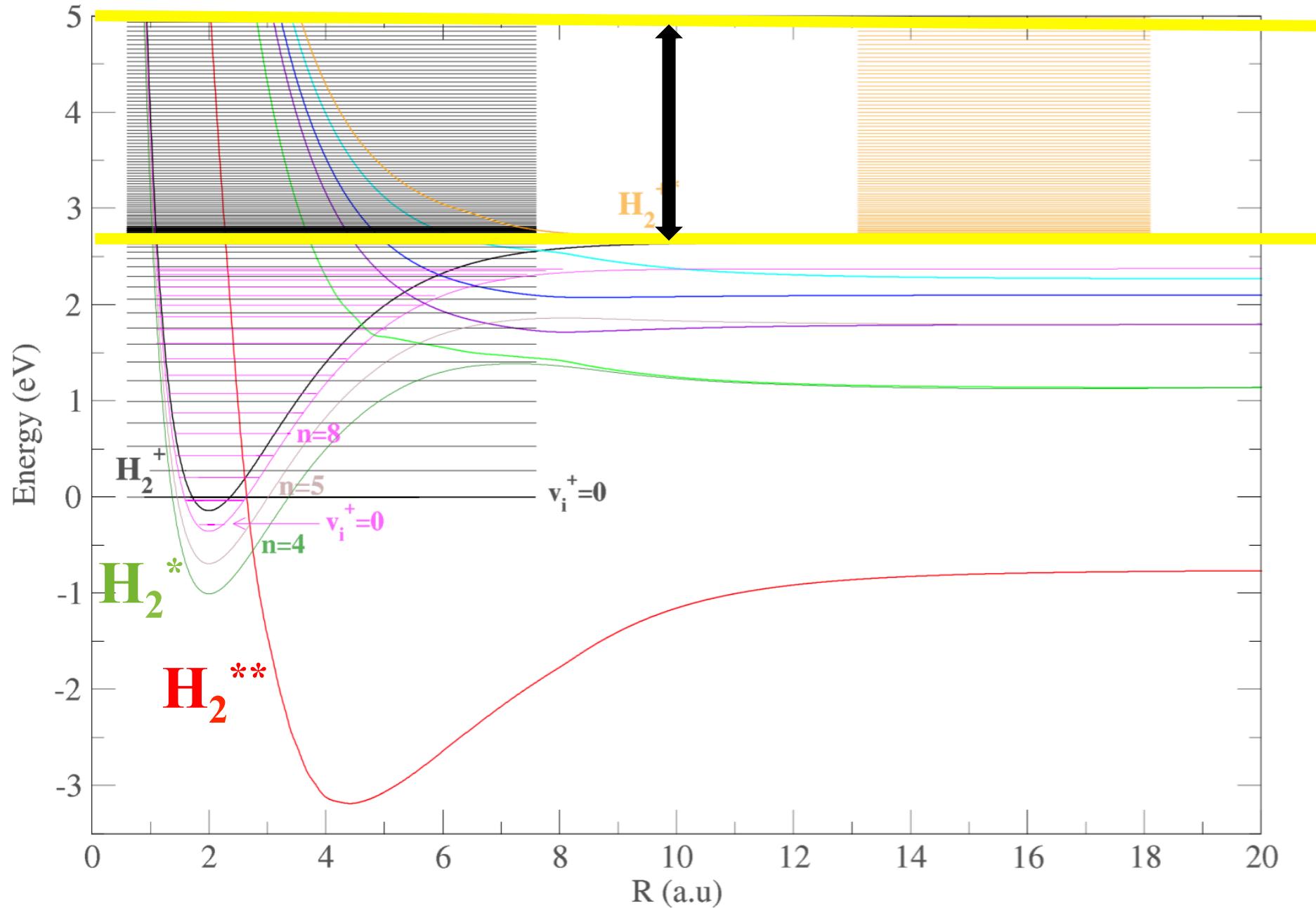
**“Moderately” Low Energy:
“NO rotation”,
DISCRETE vibrational spectrum,
“Fano” RESONANCES**

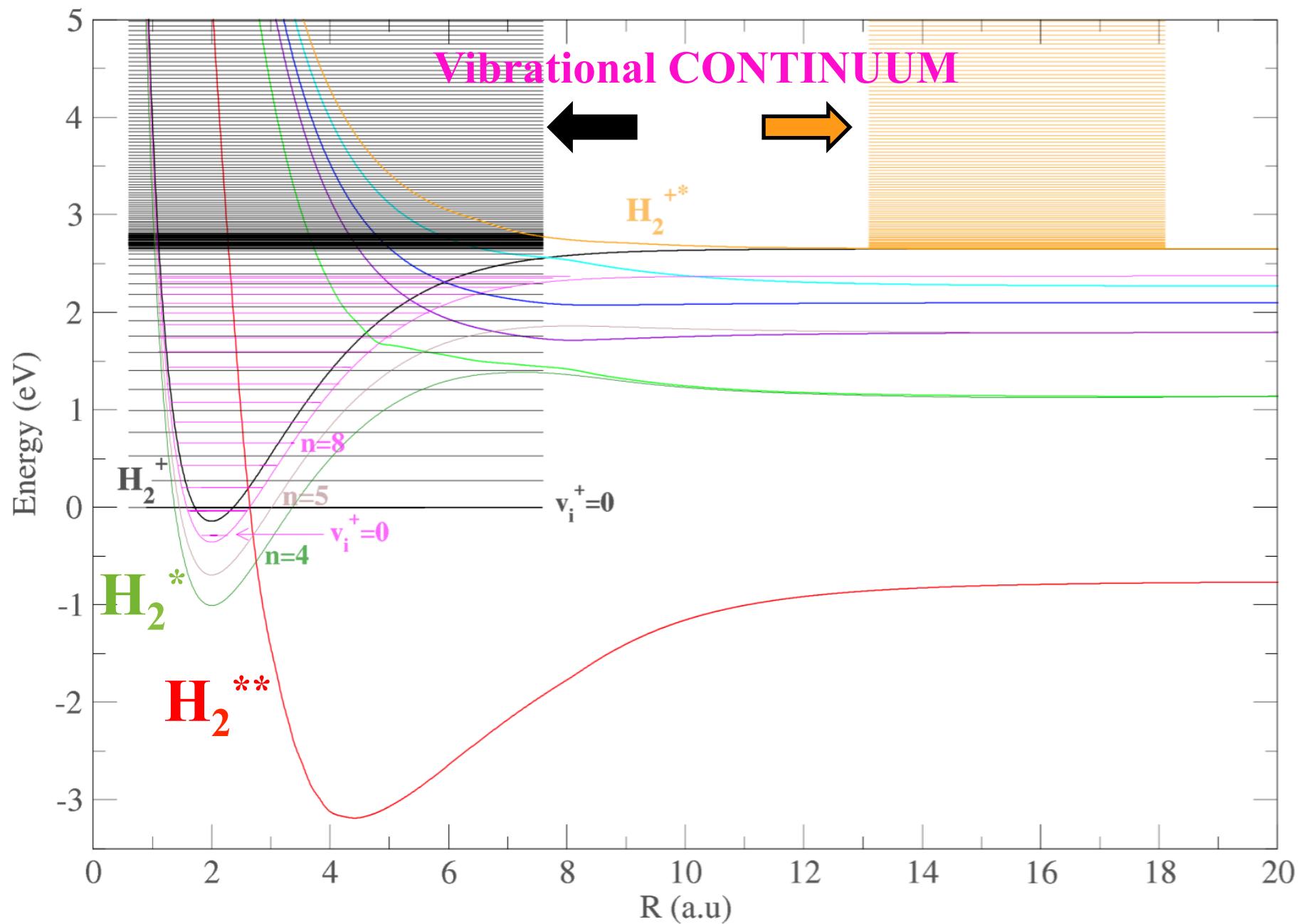


Moulane 2017, Colboc 2016



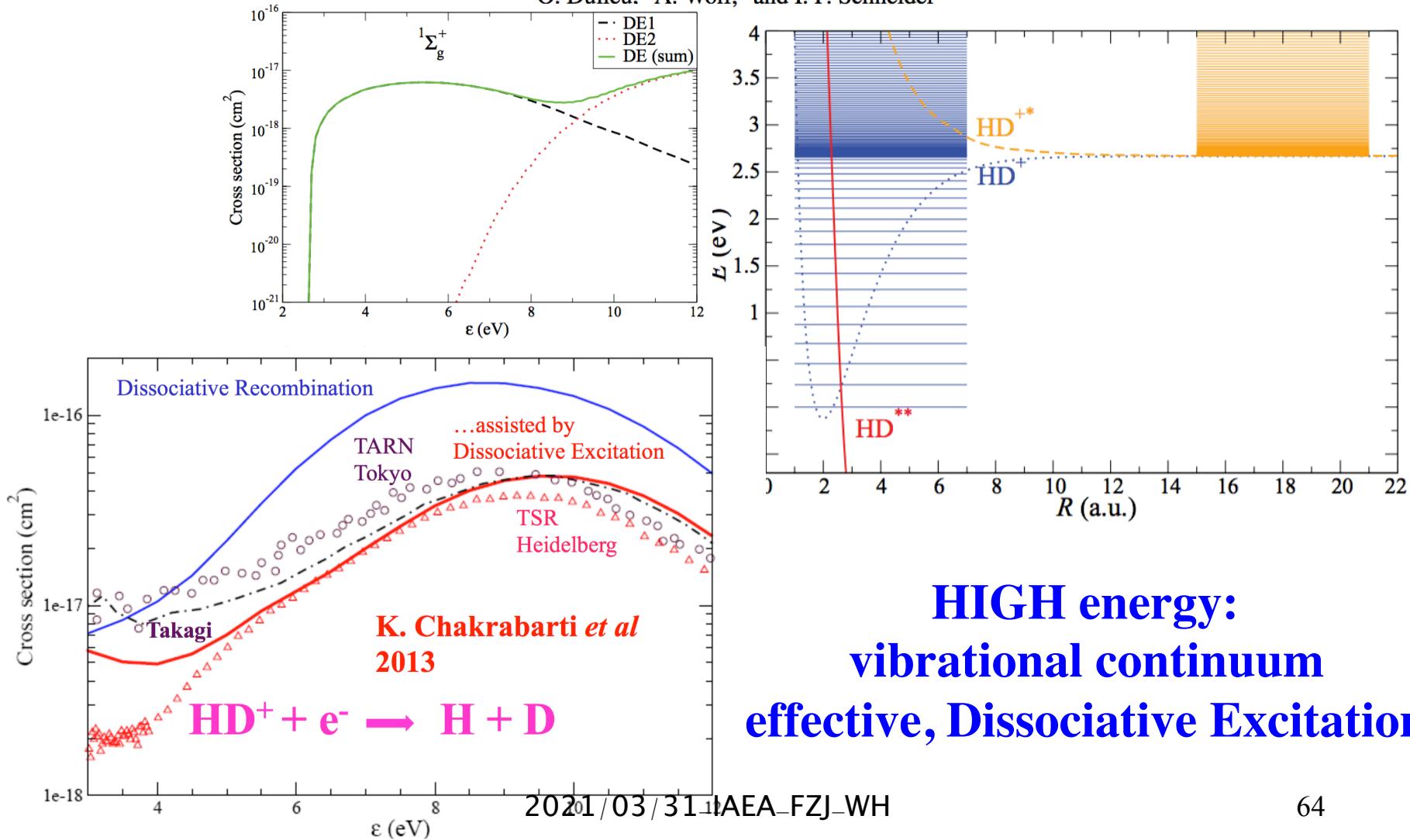
**High Energy:
“NO rotation”,
DISCRETE & CONTINUUM
vibrational spectrum,
NO “Fano” RESONANCES**





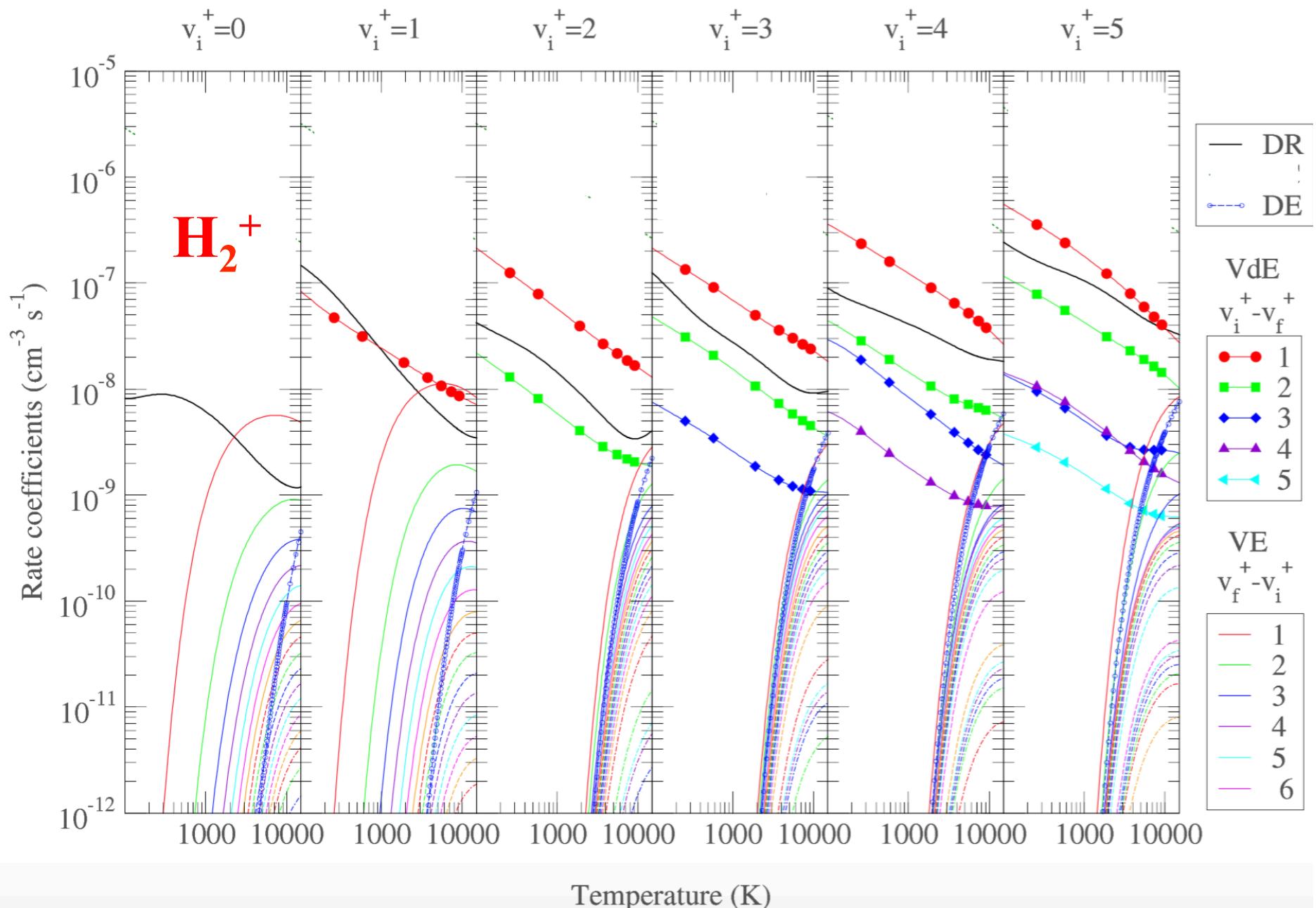
Dissociative recombination of electrons with diatomic molecular cations above dissociation threshold: Application to H_2^+ and HD^+

K. Chakrabarti,^{1,2} D. R. Backodissa-Kiminou,¹ N. Pop,³ J. Zs. Mezei,^{1,4,5} O. Motapon,⁶ F. Lique,¹
O. Dulieu,⁴ A. Wolf,⁷ and I. F. Schneider¹

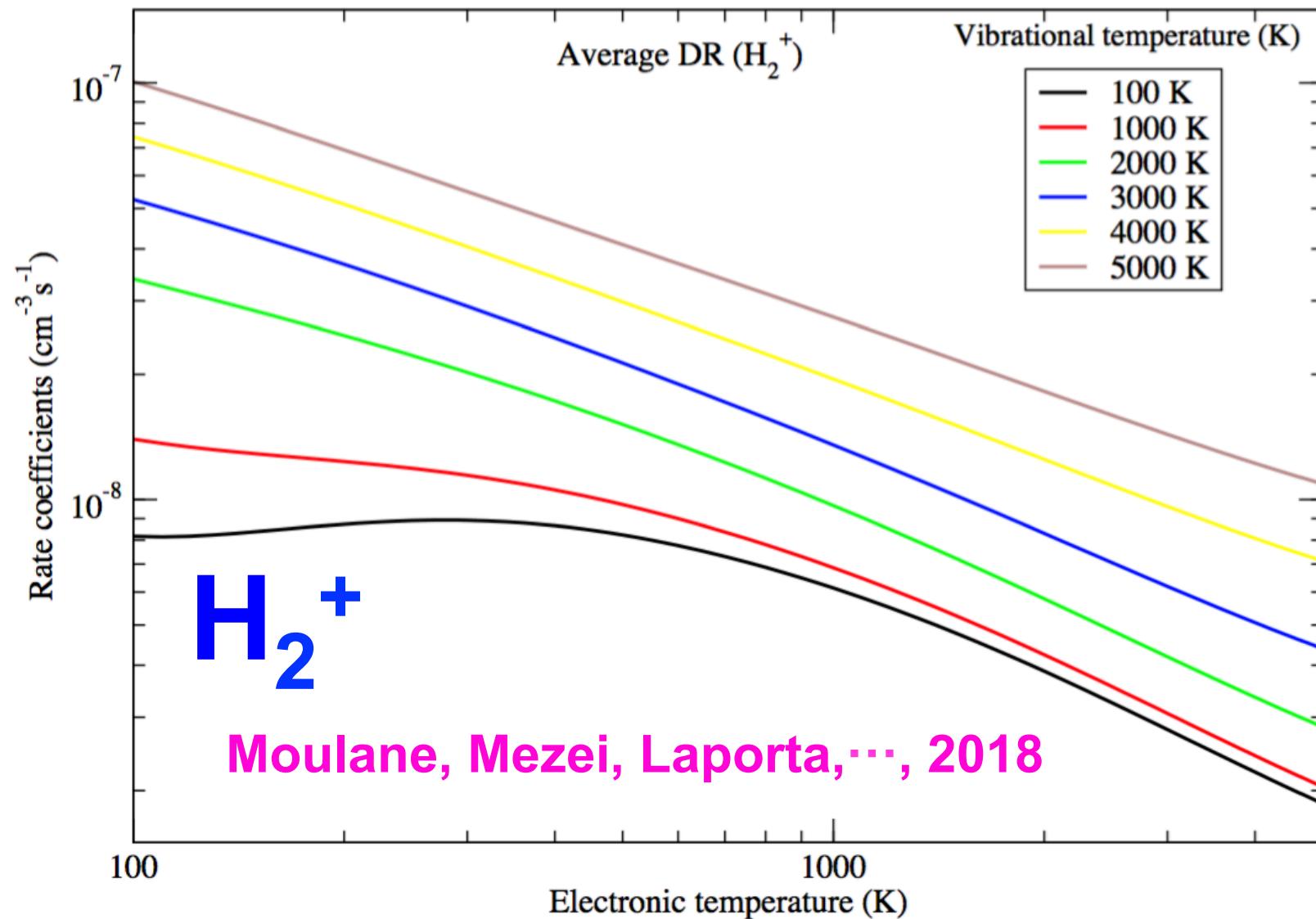


**HIGH energy:
vibrational continuum
effective, Dissociative Excitation**

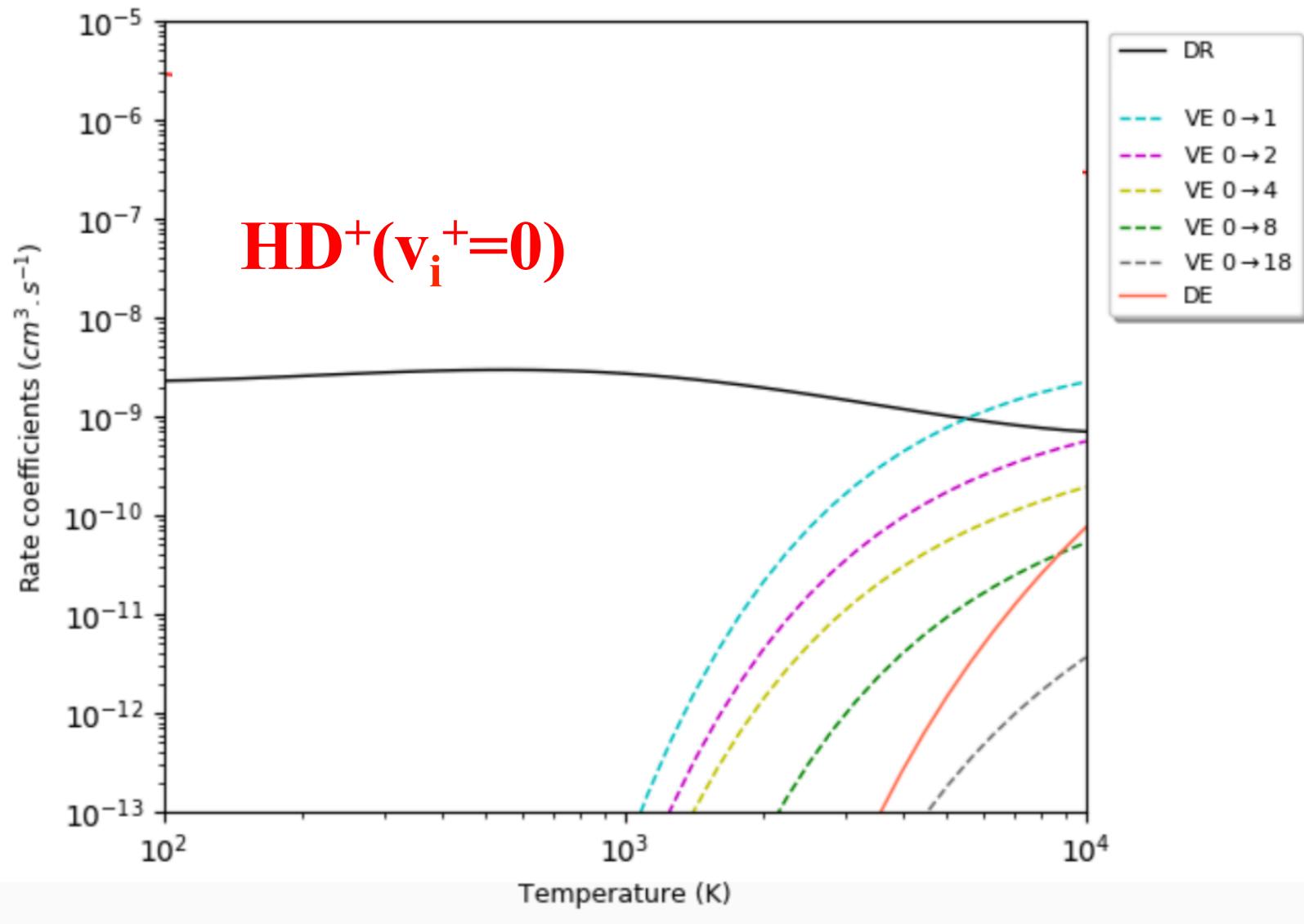
Moulane 2017



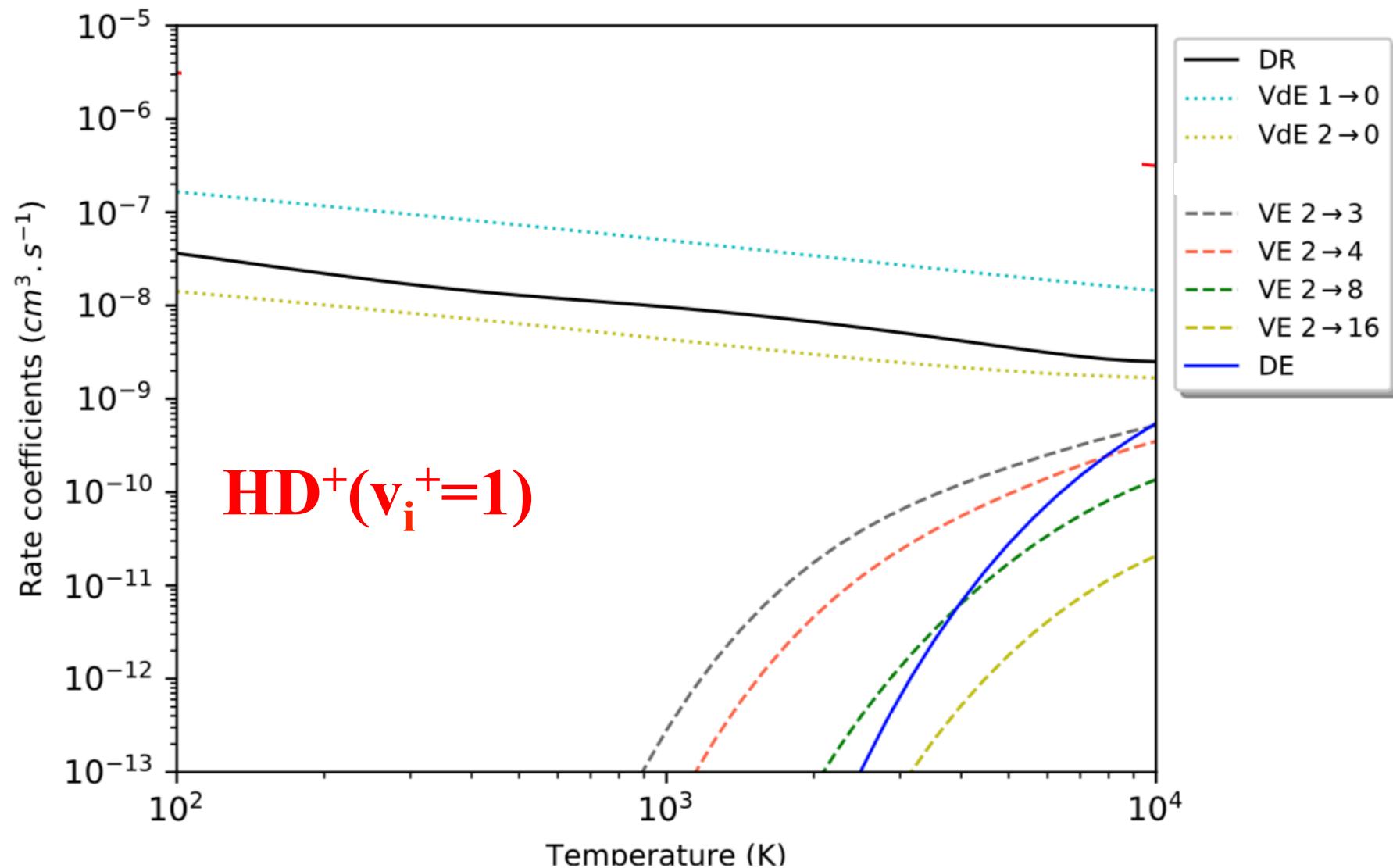
Rate coefficients depending on T_e and T_v



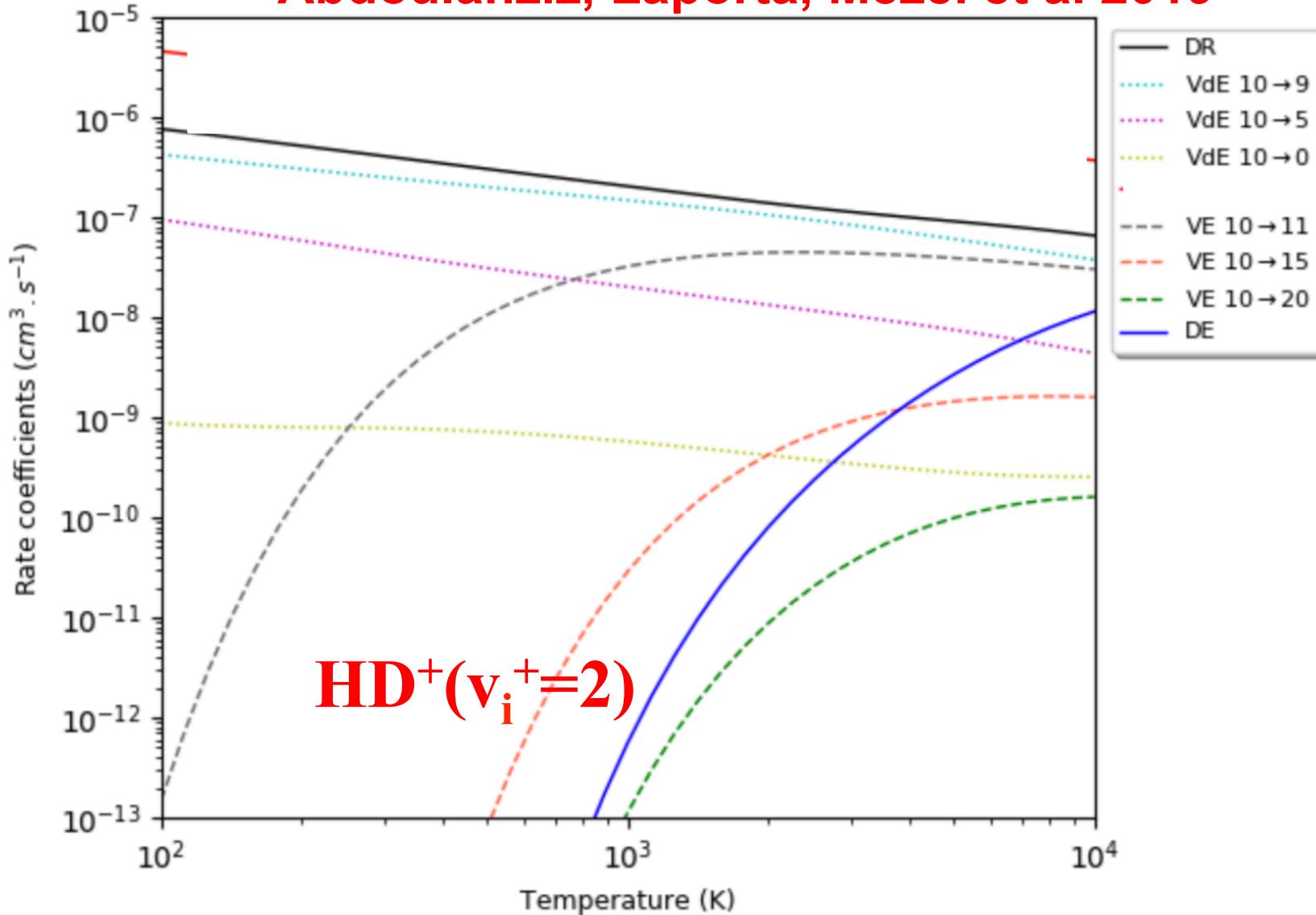
Abdoulanziz, Laporta, Mezei et al 2019



Abdoulanziz, Laporta, Mezei et al 2019

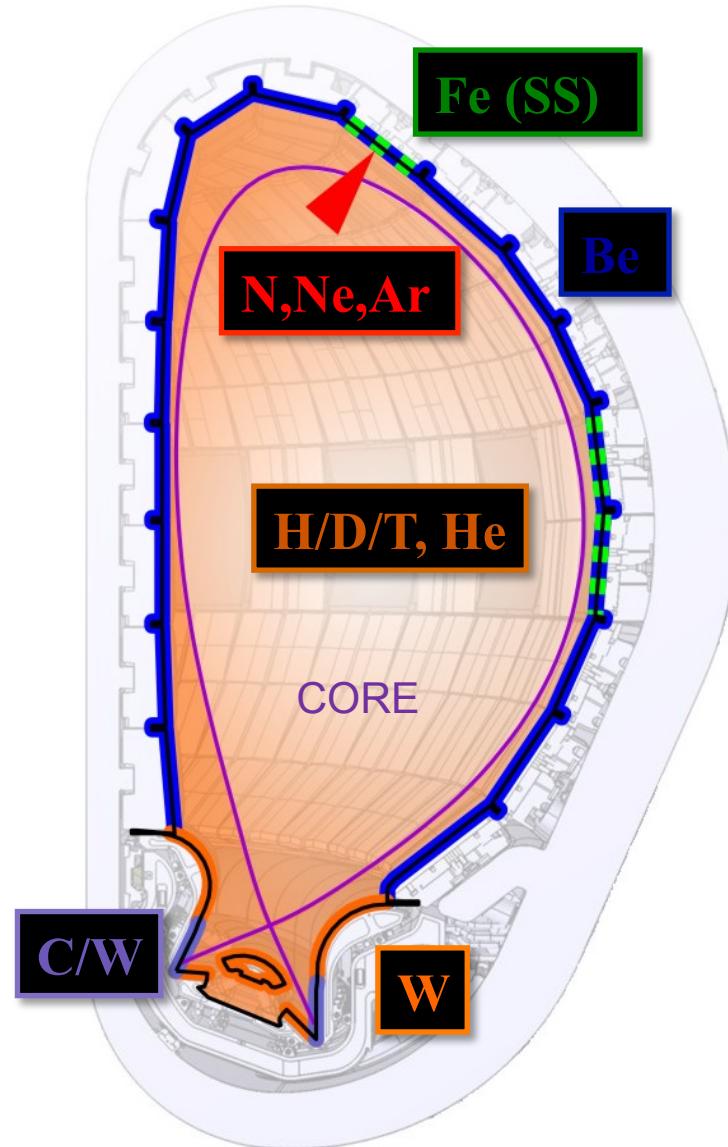


Abdoulanziz, Laporta, Mezei et al 2019



HYDRIDES !

List of the main elements relevant to the ITER plasma (D. Reiter)

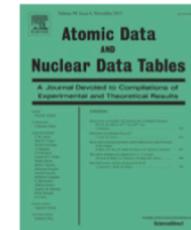




Contents lists available at ScienceDirect

Atomic Data and Nuclear Data Tables

journal homepage: www.elsevier.com/locate/adt



2017

Low-energy collisions between electrons and BeH⁺: Cross sections and rate coefficients for all the vibrational states of the ion



S. Niyonzima ^{a,b}, S. Ilie ^{a,c}, N. Pop ^{a,c}, J. Zs. Mezei ^{a,d,e,f}, K. Chakrabarti ^g, V. Morel ^h, B. Peres ^h, D.A. Little ⁱ, K. Hassouni ^d, Å. Larson ^j, A.E. Orel ^k, D. Benredjem ^e, A. Bultel ^h, J. Tennyson ⁱ, D. Reiter ^l, I.F. Schneider ^{a,e,*}

IOP Publishing

Plasma Physics and Controlled Fusion

Plasma Phys. Control. Fusion 59 (2017) 045008 (10pp)

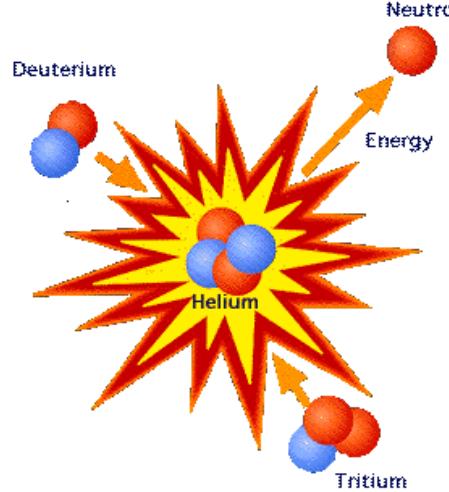
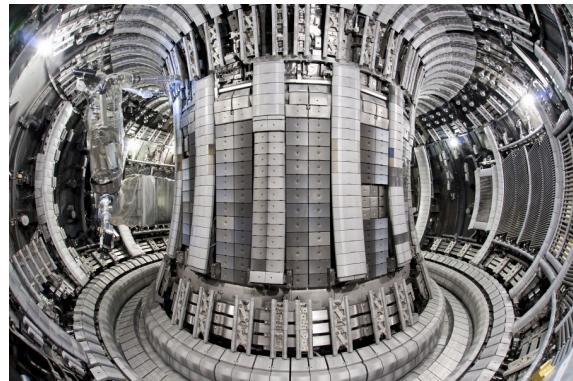
<https://doi.org/10.1088/1361-6587/aa5c56>

2017

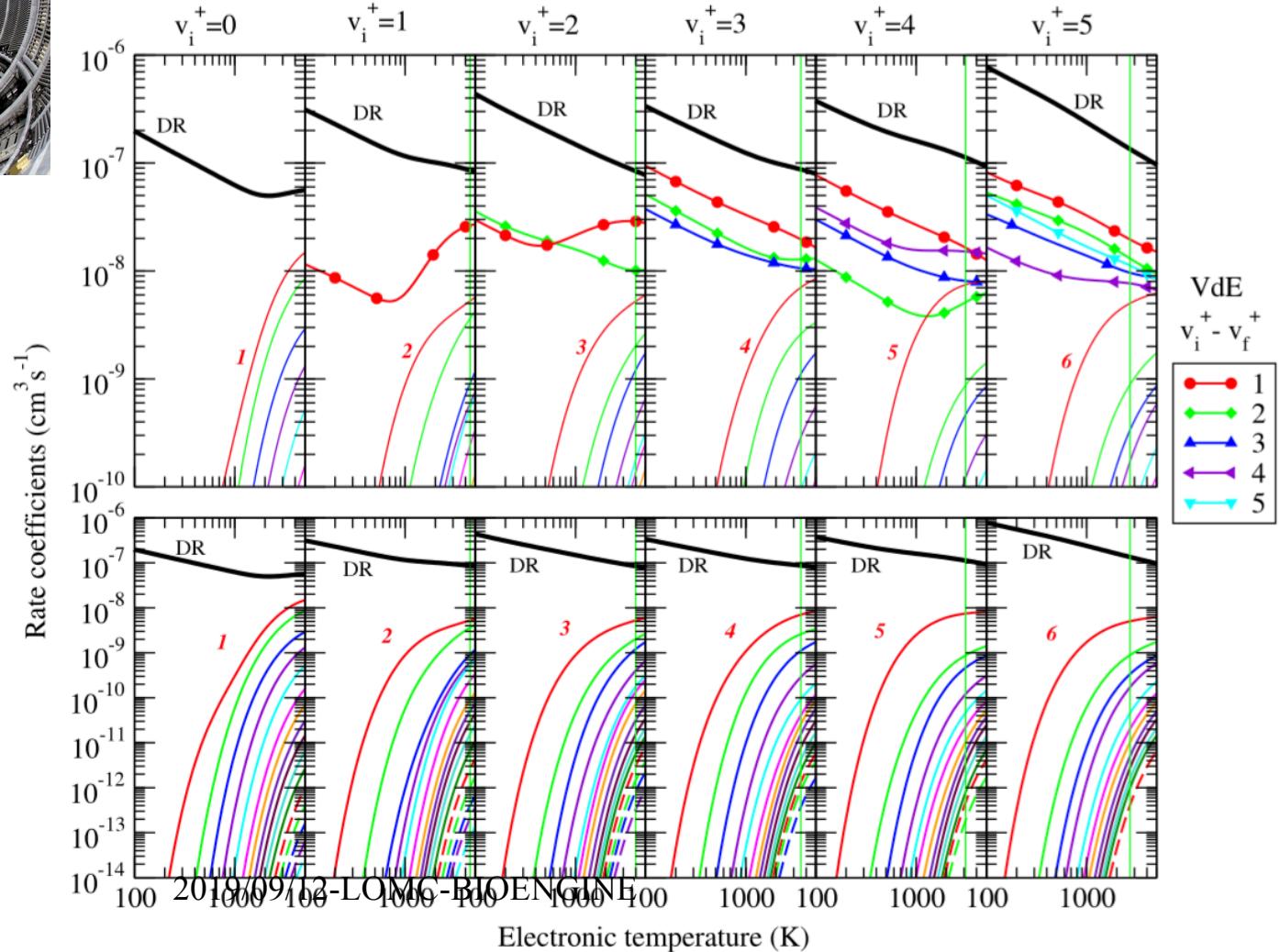
Theoretical resonant electron-impact
vibrational excitation, dissociative
recombination and dissociative excitation
cross sections of ro-vibrationally excited
BeH⁺ ion

V Laporta ^{1,2}, K Chakrabarti ³, R Celiberto ^{1,4}, R K Janev ⁵, J Zs Mezei ^{6,7,8,9},
S Niyonzima ^{6,10}, J Tennyson ² and I F Schneider ^{6,8}

BeH⁺ + e⁻



2017



BeD⁺ + e⁻

2018

N. Pop, S. Niyonzima, J. Zs. Mezei, ...

Plasma Sources Sci. Technol. **27** (2018) 025015 (10pp)

<https://doi.org/10.1088/1361-6595/aaabef>

Low-energy collisions between electrons and BeD⁺

S Niyonzima^{1,2}, N Pop³, F Iacob⁴, Å Larson⁵, A E Orel⁶, J Zs Mezei^{2,7,8},
K Chakrabarti⁹, V Laporta^{2,10} , K Hassouni⁷, D Benredjem¹¹, A Bultel¹²,
J Tennyson¹⁰ , D Reiter¹³ and I F Schneider^{2,11}

BeT⁺ + e⁻

2021

ARTICLE IN PRESS

Atomic Data and Nuclear Data Tables xxx (xxxx) xxx

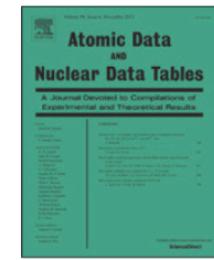


ELSEVIER

Contents lists available at ScienceDirect

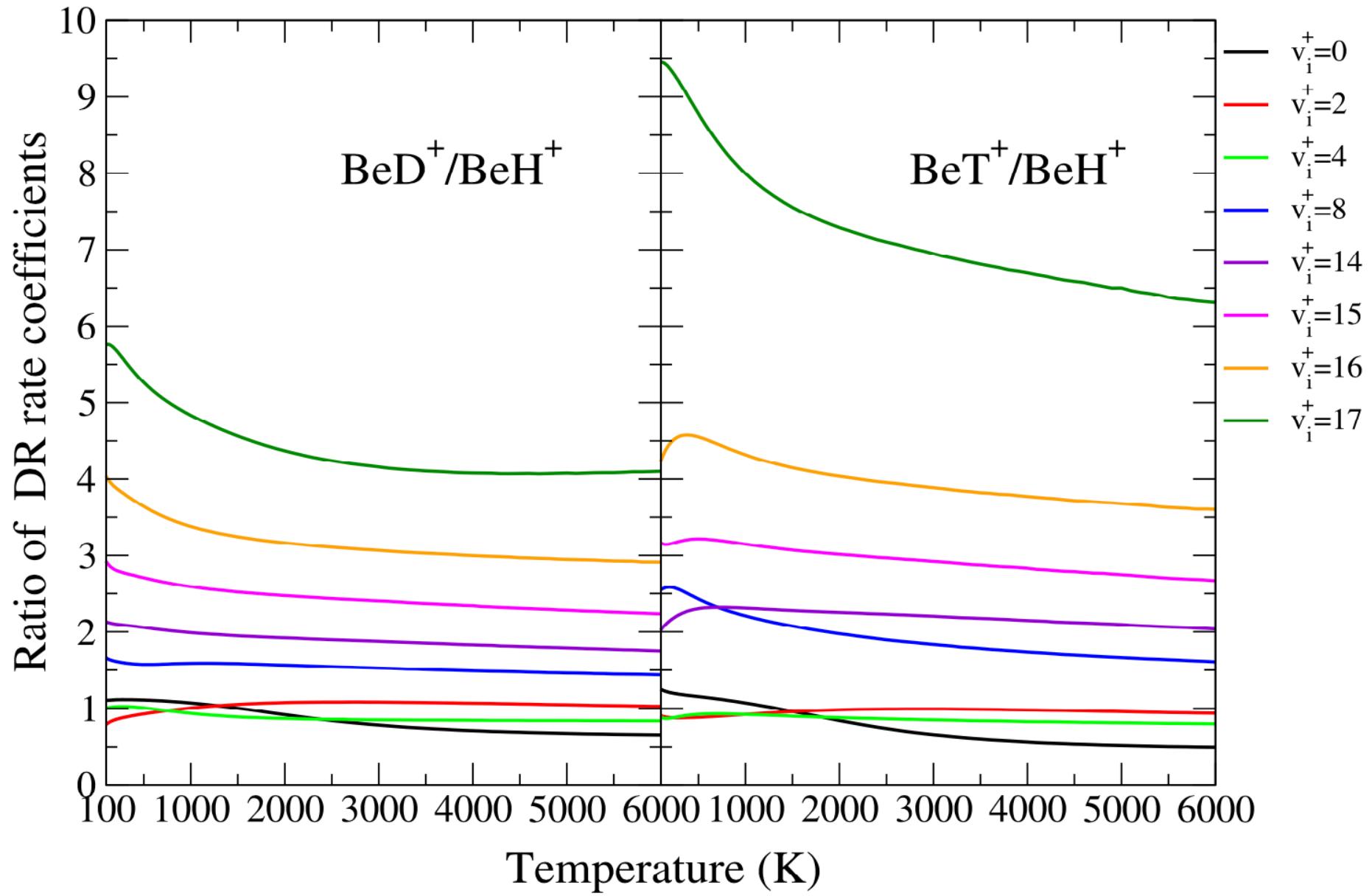
Atomic Data and Nuclear Data Tables

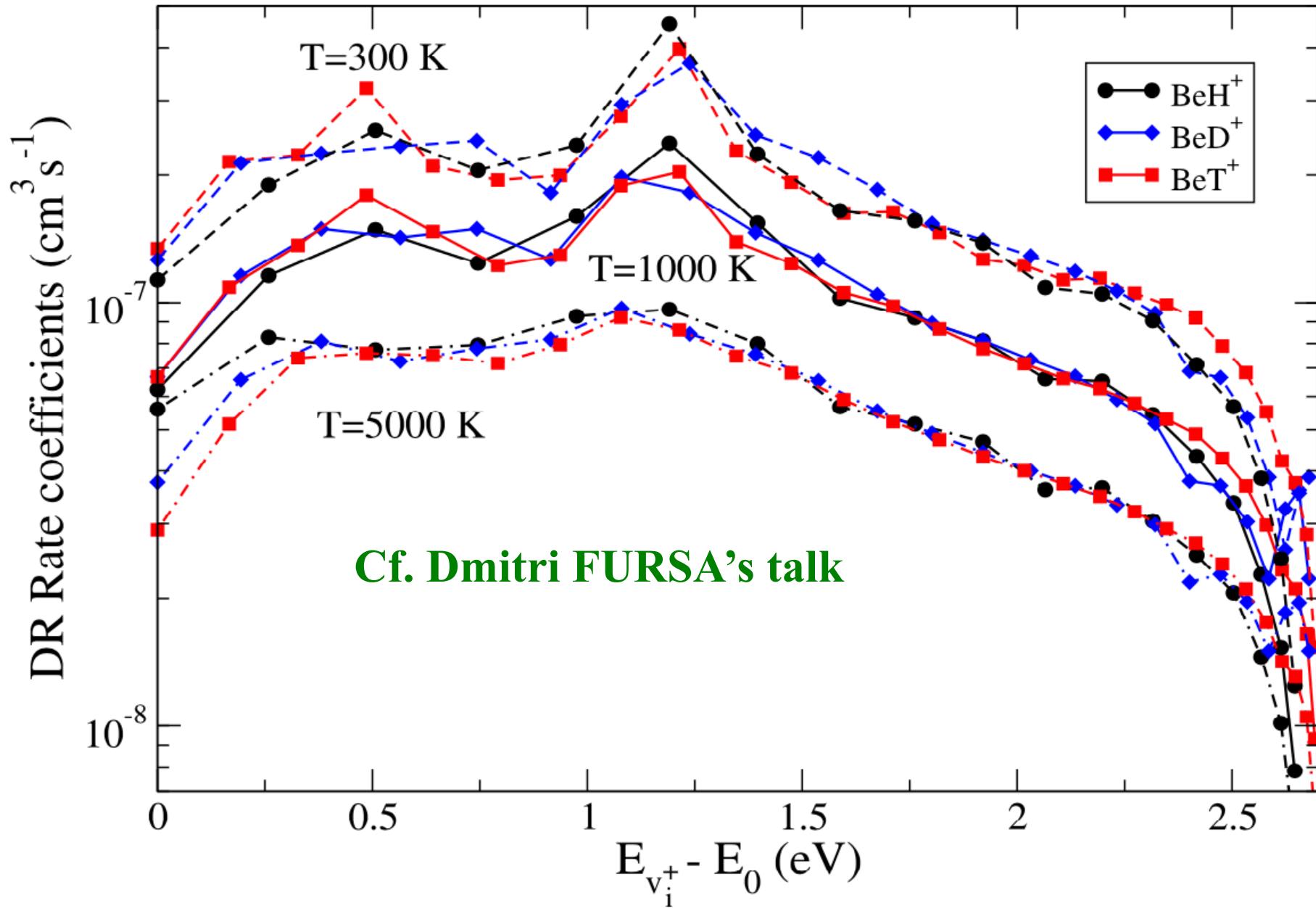
journal homepage: www.elsevier.com/locate/adt



Reactive collisions between electrons and BeT⁺: Complete set of thermal rate coefficients up to 5000 K

N. Pop ^a, F. Iacob ^{b,*}, S. Niyonzima ^c, A. Abdoulanziz ^d, V. Laporta ^e, D. Reiter ^f,
I.F. Schneider ^{d,g}, J.Zs. Mezei ^{d,h}



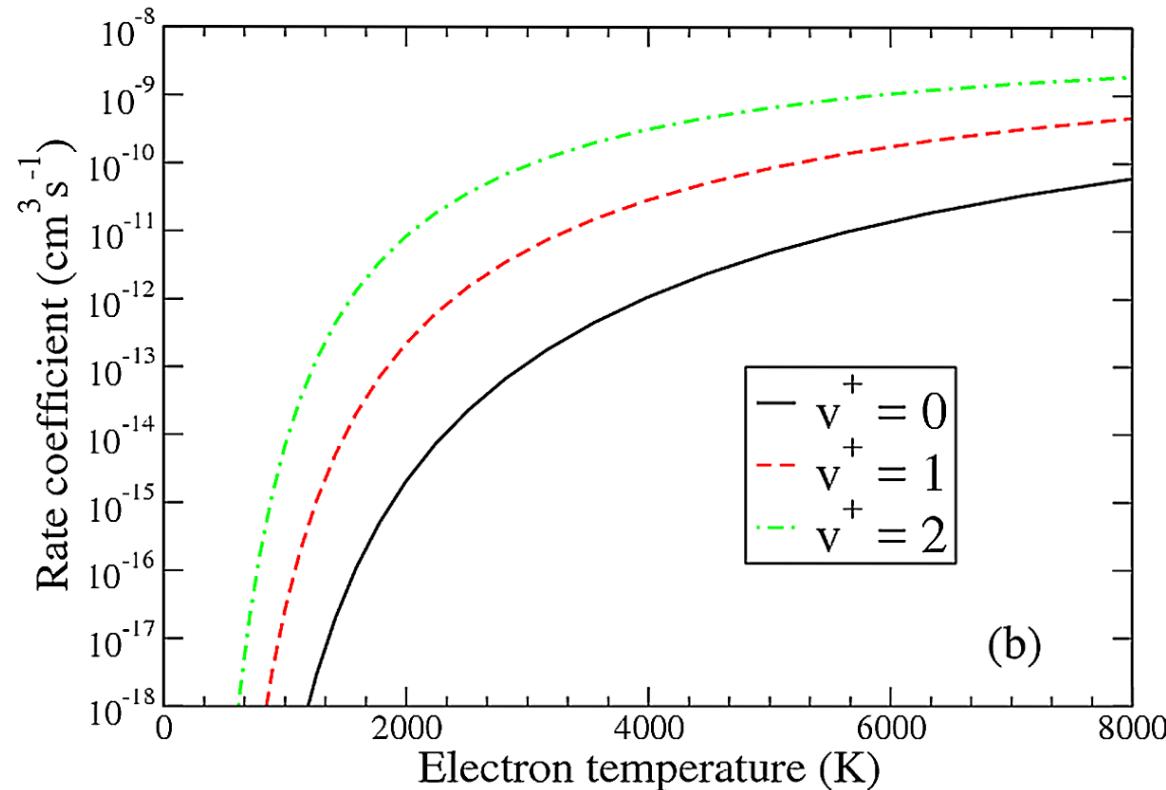




**V. Laporta, A. Abdoulanziz,
 E. Roueff, ...**

Theoretical study of ArH^+ dissociative recombination and electron-impact vibrational excitation

A. Abdoulanziz,¹ F. Colboc,¹ D. A. Little,² Y. Moulane,^{3,4} J. Zs. Mezei,^{1,5,6} E. Roueff,⁷ J. Tennyson,² I. F. Schneider^{1,8} and V. Laporta^{1,2★}



ArH⁺ + e⁻
2018

E. Djuissi, V. Laporta, et al
2019-2021 ArH⁺ + e⁻

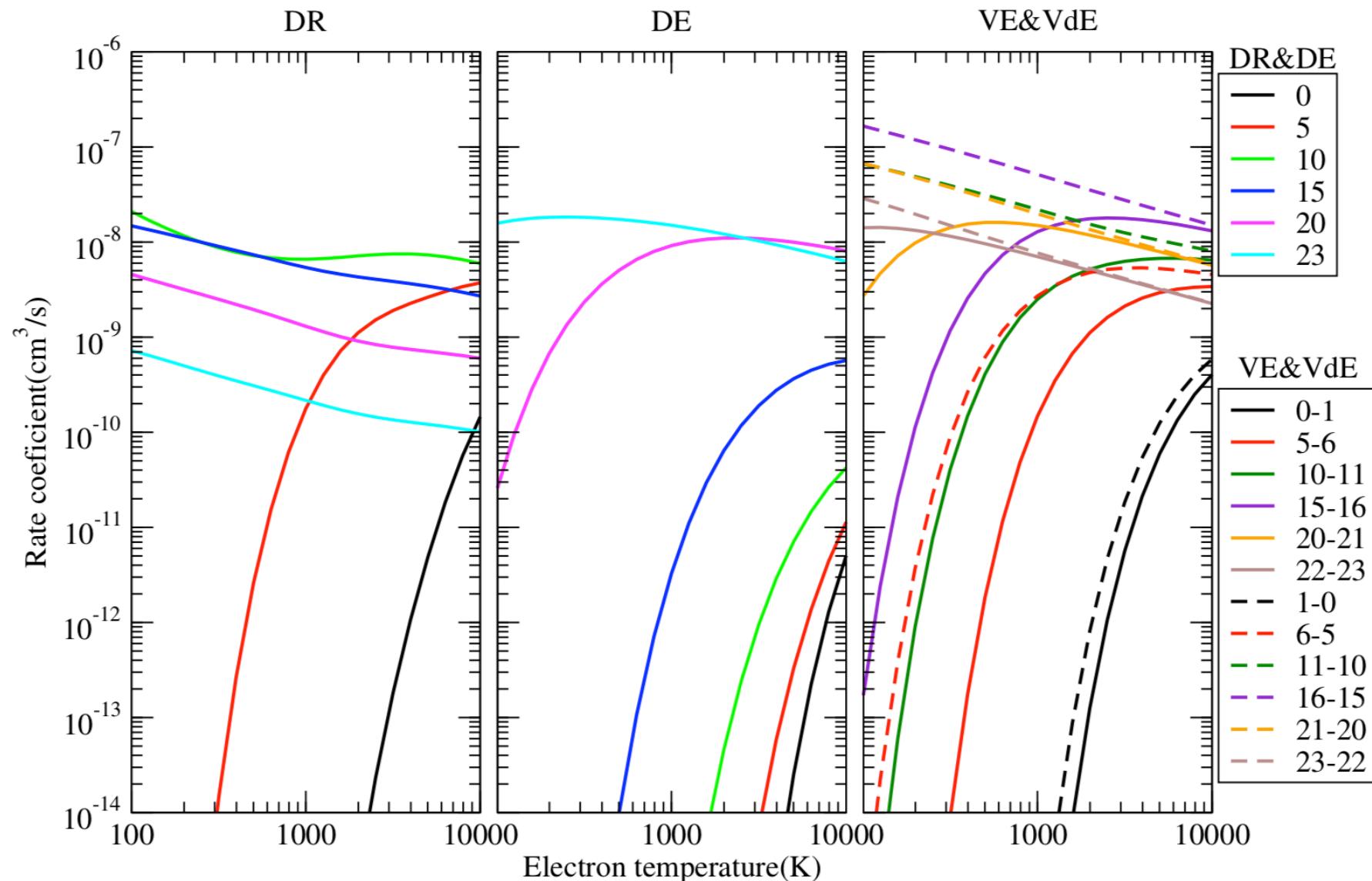
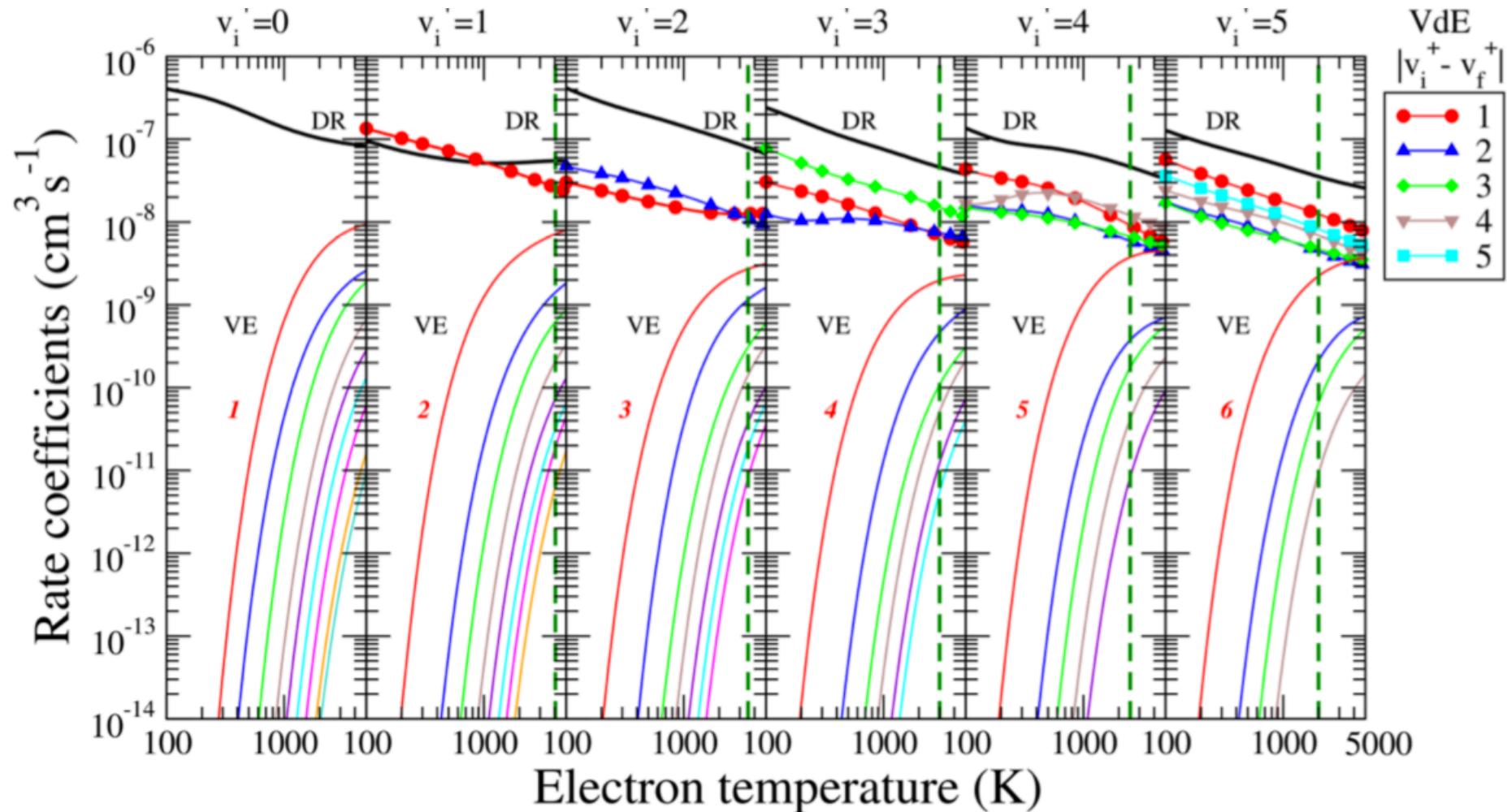


FIG. 3: Rate coefficient curves of the dissociative recombination and the competitive process (DE, EC, VE and VdE)



**What about
 WH^+ ? $W_m X_n^+$?**

CONCLUSIONS

**Temporary captures into super-excited states:
HUGE RESONANT EFFECTS**

**Dependence of the cross section and
rate coefficients on the
INITIAL ro-vibrational level:
STRONG**

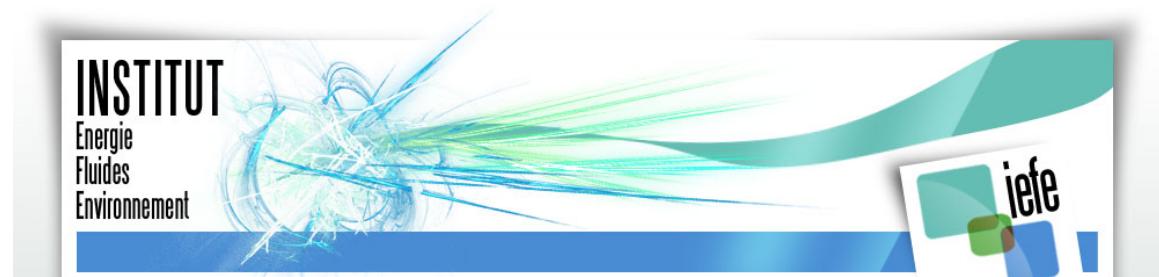
**We provide STATE-TO-STATE
cross sections & rate coefficients**

SUPPORT



ADAS

Atomic Data and Analysis Structure



Fédération de Recherche
Fusion par Confinement Magnétique - ITER

Financement

Labex



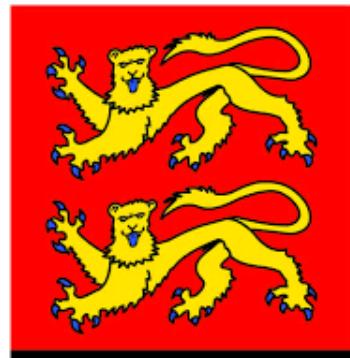
PicoLIBS (2014-2018)



Union européenne

Fonds européen de développement régional

EMoPlaf (2017-2019)



REGION NORMANDIE



RIN-VIRIDIS-CO2 (2018-2019)

PCMI/INSU (2018-2020)



Thank you for your attention