Electron/H_2^+ (and isotopomers) collisions: theoretical cross sections and rates, and comparison with measured data

C. Argentin[1], A. Abdoulanziz[1], E. Djuissi[1], Y. Moulane[1,2,3], F. Iacob[4], N. Pop[5], M. D. Epée Epée[6], O. Motapon[6,7], K. Chakrabarti[8], J. Tennyson[9], V. Laporta[9,10], J. Zs Mezei[1,11], I. F. Schneider[1,12]

[1]LOMC, Univ. du Havre, [2]Univ. Cadi Ayyad, Marrakech, [3]Univ. De Liège, [4]West Univ. Timisoara, [5]Politehnica Univ. Timisoara, [6]Univ. of Douala, [7]Univ. of Maroua, [8]Scottish Church College, Calcutta, [9]University College London, [10]P.Las.Mi Lab CNR-Nanotec, Bari, [11]Inst. of Nuclear Res. of the Hungarian Acad. of Sciences, Debrecen, [12]Lab. Aimé Cotton, Univ. Paris-Saclay & ENS-Cachan.

$AB^+(N_i^+, v_i^+) + e^- \longrightarrow A + B$ Dissociative Recombination: DR

Ro-Vibrational (de)Excitation: RV(d)E $\longrightarrow AB^+(N_f^+, v_f^+) + e^-$

Dissociative Excitation: DE $\longrightarrow A + B^+ + e^-$

2019/06/06_Vienna_IAEA_CM

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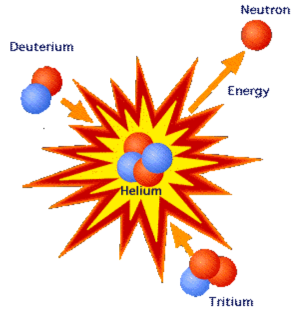
Eighth International Conference on Dissociative Recombination (DR2010) IOP Publishing
Journal of Physics: Conference Series **300** (2011) 012022 doi:10.1088/1742-6596/300/1/012022



Fusion edge plasma

Small Molecule Ion Chemistry in ITER

J. Brian A. Mitchell, S. Carles, J.L. LeGarrec

Institut de Physique de Rennes
UMR du CNRS No. 6251
Université de Rennes I
35042, Rennes, France

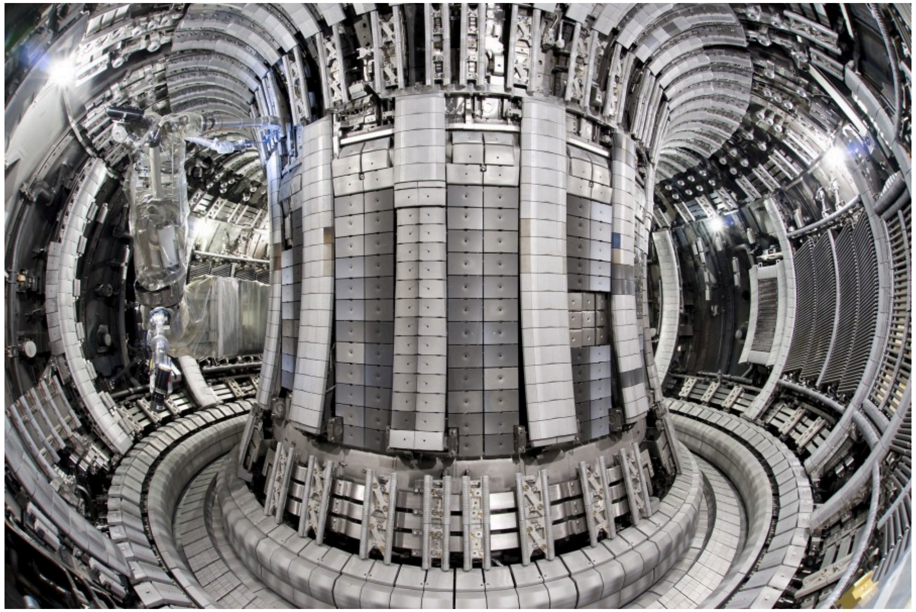


Table I: Primary species

–	H^+, He^+, He^{++}, Li^+, Li^{++}, Be^{z+} dominant boundary species
–	H^*, H^-, He, He*, $H_2(v)$
–	$H_2^+(v)$, $H_3^+(v)$, $He_2^+(v)$, $HeH^+(v)$, $HeH^{+*}(v)$, $LiH^+(v)$, $BeH^+(v)$
–	$NeH^+(v)$, $ArH^+(v)$, $HeNe^+(v)$

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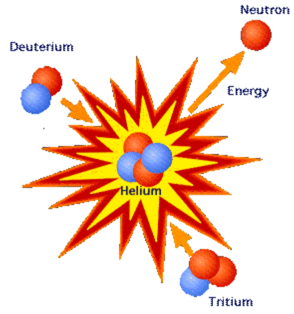

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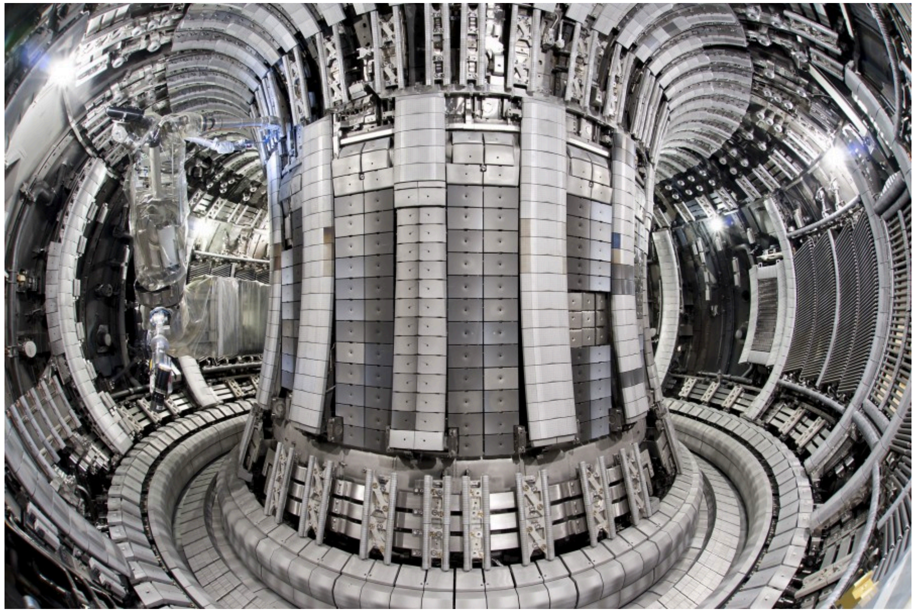

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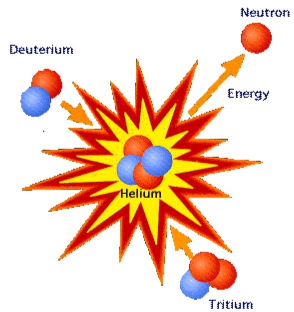
Vincenzo

4

Eighth International Conference on Dissociative Recombination (DR2010) IOP Publishing
Journal of Physics: Conference Series **300** (2011) 012022 doi:10.1088/1742-6596/300/1/012022



Fusion edge plasma

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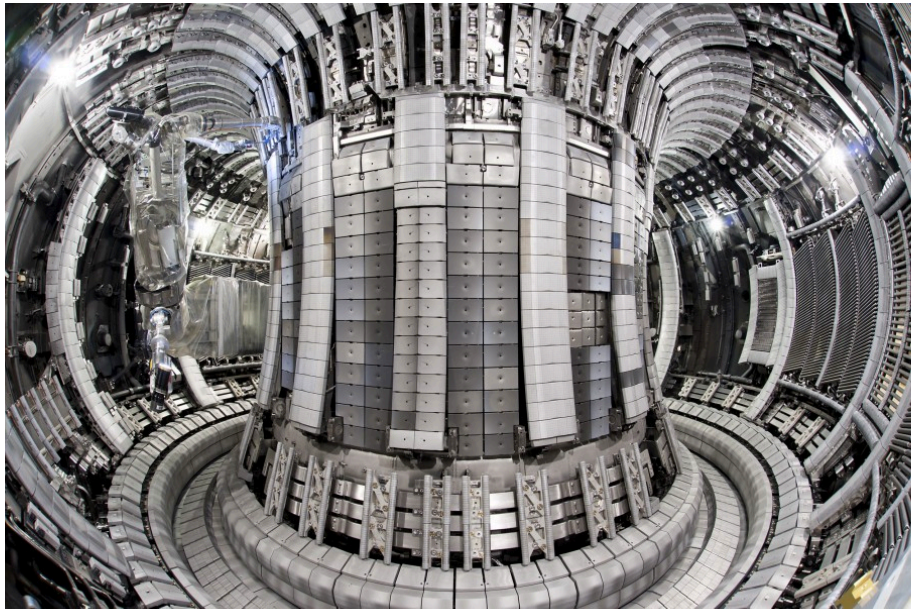

Table I: Primary species

Zsolt

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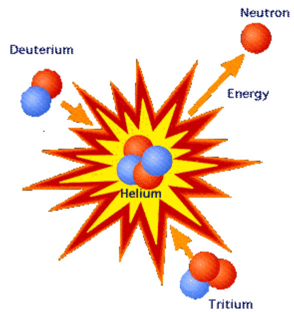

Fusion edge plasma

Small Molecule Ion Chemistry in ITER

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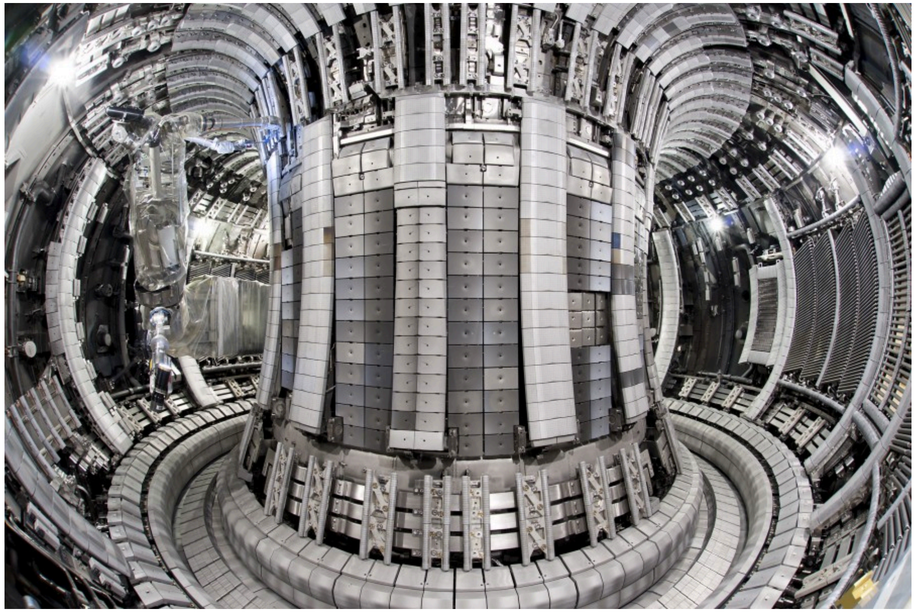

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- $H_2^+(v)$, $H_3^+(v)$, $He_2^+(v)$, $HeH^+(v)$, $HeH^{+*}(v)$, $LiH^+(v)$, $BeH^+(v)$
- $NeH^+(v)$, $ArH^+(v)$, $HeNe^+(v)$

Ioan → $H_2^+(v)$

. . .BUT !....

UNIONE EUROPEA

REGIONE PUGLIA

SMARTPUGLIA INTELLIGENTI DAL FUTURO

·a·r·t·i·
Agenzia regionale per la tecnologia e l'innovazione

Non-equilibrium chemistry of excited states of H_2 in the early Universe

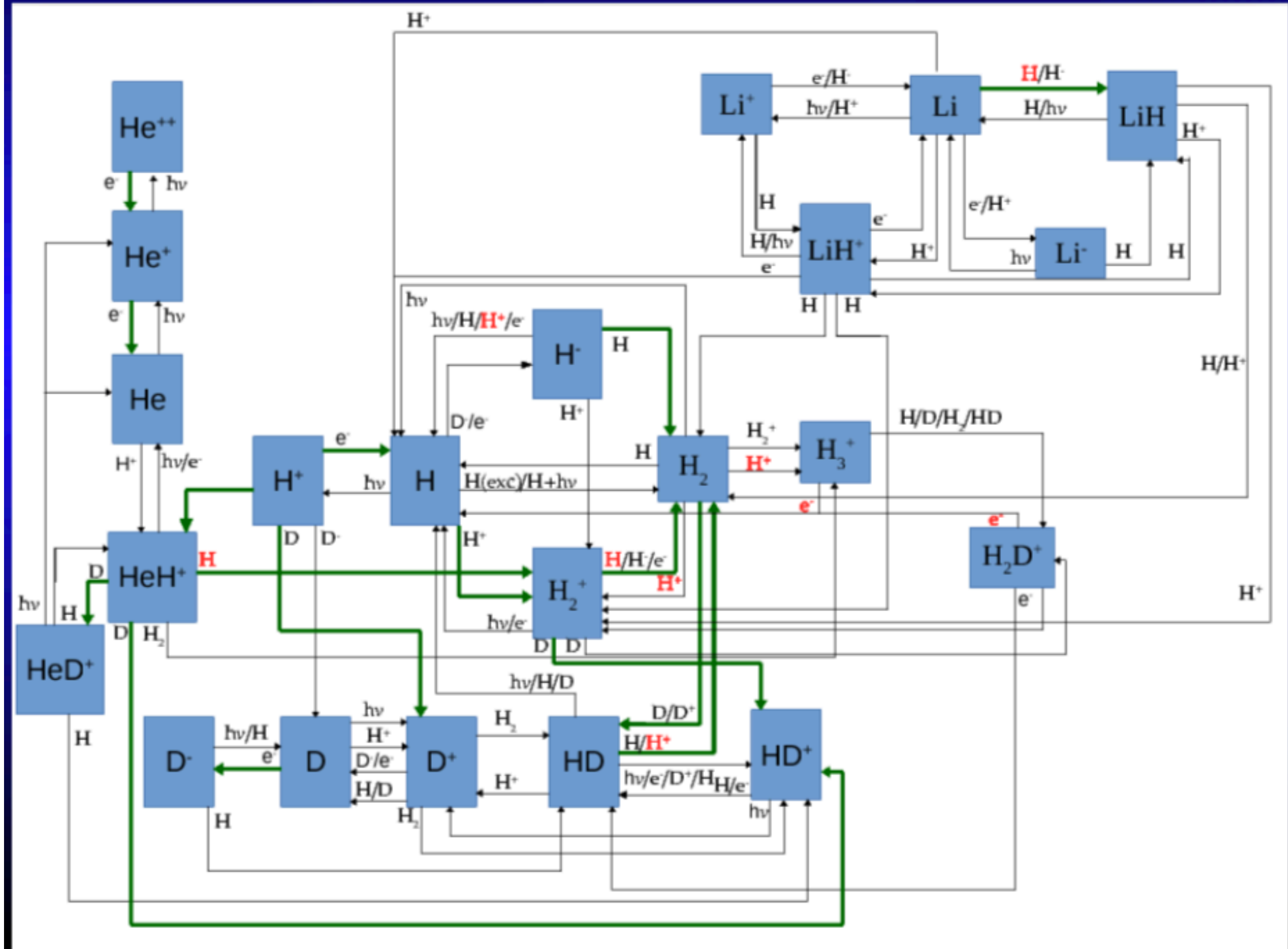
(work in progress: HD...)

Carla Maria Coppola

Università degli Studi "Aldo Moro" di Bari
Chemistry Department

INAF – Istituto Nazionale di Astrofisica
Osservatorio di Arcetri

KINETIC MODEL: CHEMICAL NETWORK



22 species
~ 200 reactions

state-to-state

~ 50 species
~ 2500 reactions

State-to-state chemistry HD (400 rovibrational levels)

1-2] $D + H_2(v, j) \leftrightarrow H + HD(v', j')$

3-4] $D^+ + H_2(v) \leftrightarrow H^+ + HD(v', j')$ (63)

5] $D + H^- \leftrightarrow HD(v, j) + e^-$ (67)

6] $D^- + H \leftrightarrow HD(v, j) + e^-$ (68)

7a] $H + D^* \leftrightarrow HD(v, j) + h\nu$ (116)

7b] $H^* + D \leftrightarrow HD(v, j) + h\nu$ (115)

8] $HD^+ + H \leftrightarrow HD + H^+$ (58)

9] $HD(v, j) + H \leftrightarrow HD(v', j') + H$

10] $HD(v, j) + He \leftrightarrow HD(v', j') + He$

11] $H^* + HD \rightarrow H_2D^+ + e^-$ (117)

$HD + e^- \leftrightarrow H + D + e^-$

$HD^+ + e^- \leftrightarrow HD^{+*} + e^-$

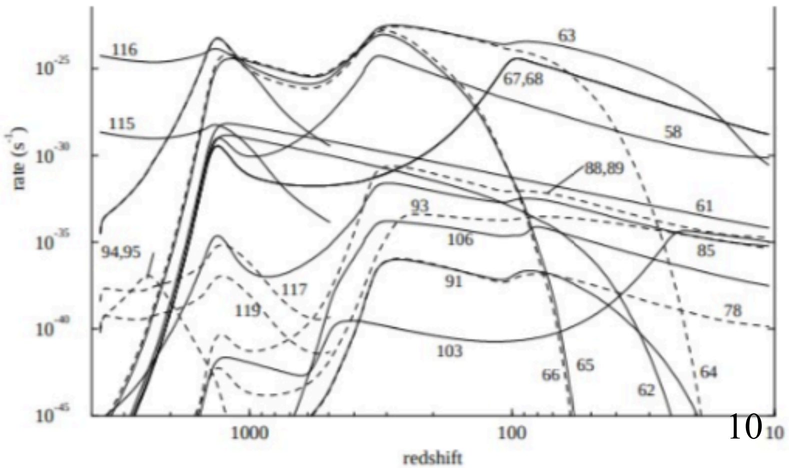
$HD^+ + e^- \leftrightarrow H + D$

$HD^+ + e^- \leftrightarrow H^+ + D + e^-$

THE DEUTERIUM CHEMISTRY OF THE EARLY UNIVERSE

P. C. Stancil,[1,2] S. Lepp,[3] and A. Dalgarno[4]

Received 1998 March 2; accepted 1998 July 16




Hidekazu TAKAGI,
1951-2016,
my «competitor»(?) & my brother in arms


DR2010 @ Lake Tahoe
Hidekazu TAKAGI,
1951-2016,
my «competitor»(?) & my brother in arms
Steve GUBERMAN

Physica Scripta. T96, 52–60, 2002

Dissociative Recombination and Excitation of H_2^+, HD^+, and D_2^+ with Electrons for Various Vibrational States

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Received May 4, 2001; accepted in revised form June 4, 2001

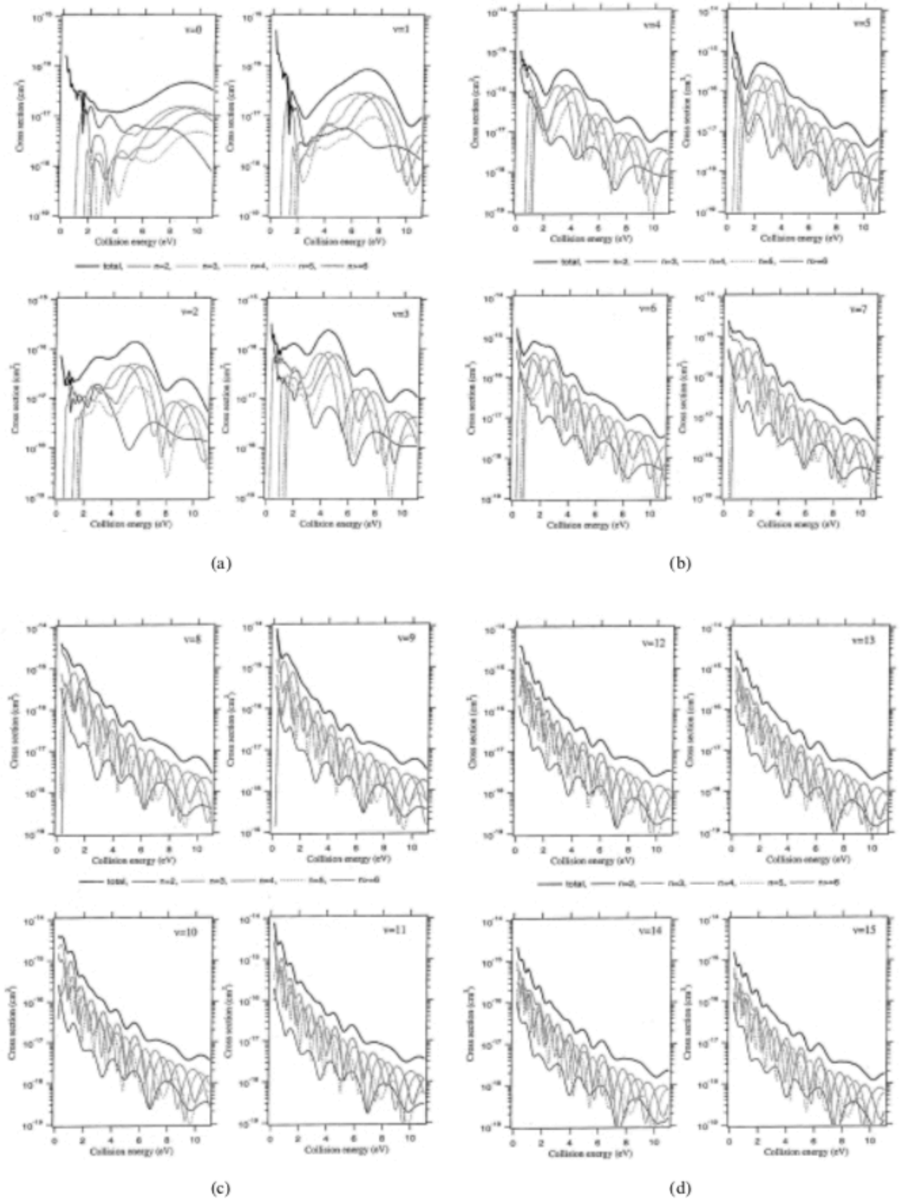


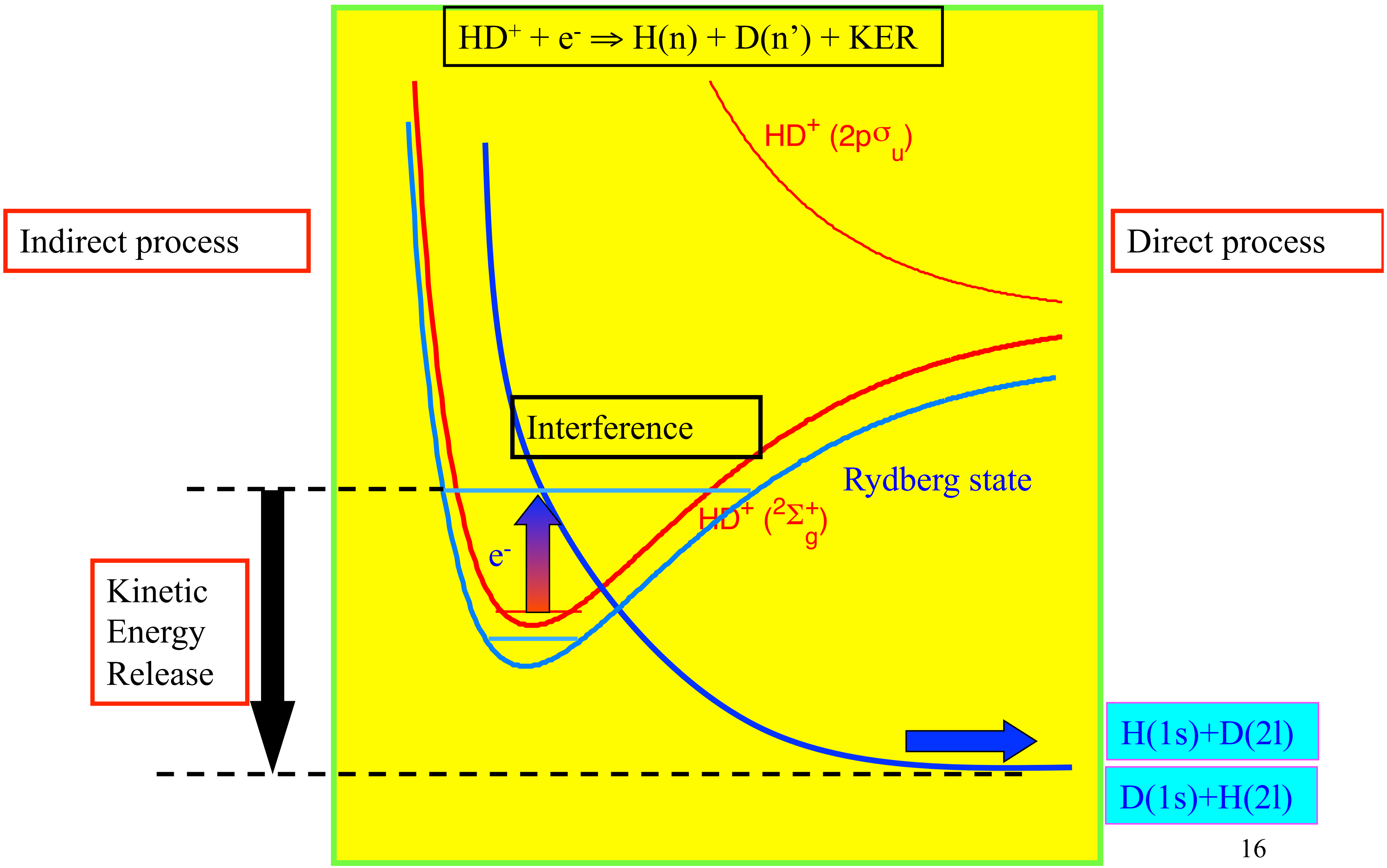
Fig. 4a–d. DR cross section of H_2^+ for each initial vibrational state *v*. The dark bold line indicates the total DR cross section. Other lines show the partial cross sections of producing the excited atoms of principle quantum number *n*, whose value is indicated in the figure. The symbol $n >= 6$ means $\infty \geq n \geq 6$.

$AB^{+}(N_i^{+}, v_i^{+}) + e^{-} \longrightarrow A + B$ Dissociative Recombination: DR

Ro-Vibrational (de)Excitation: RV(d)E $\longrightarrow AB^{+}(N_f^{+}, v_f^{+}) + e^{-}$

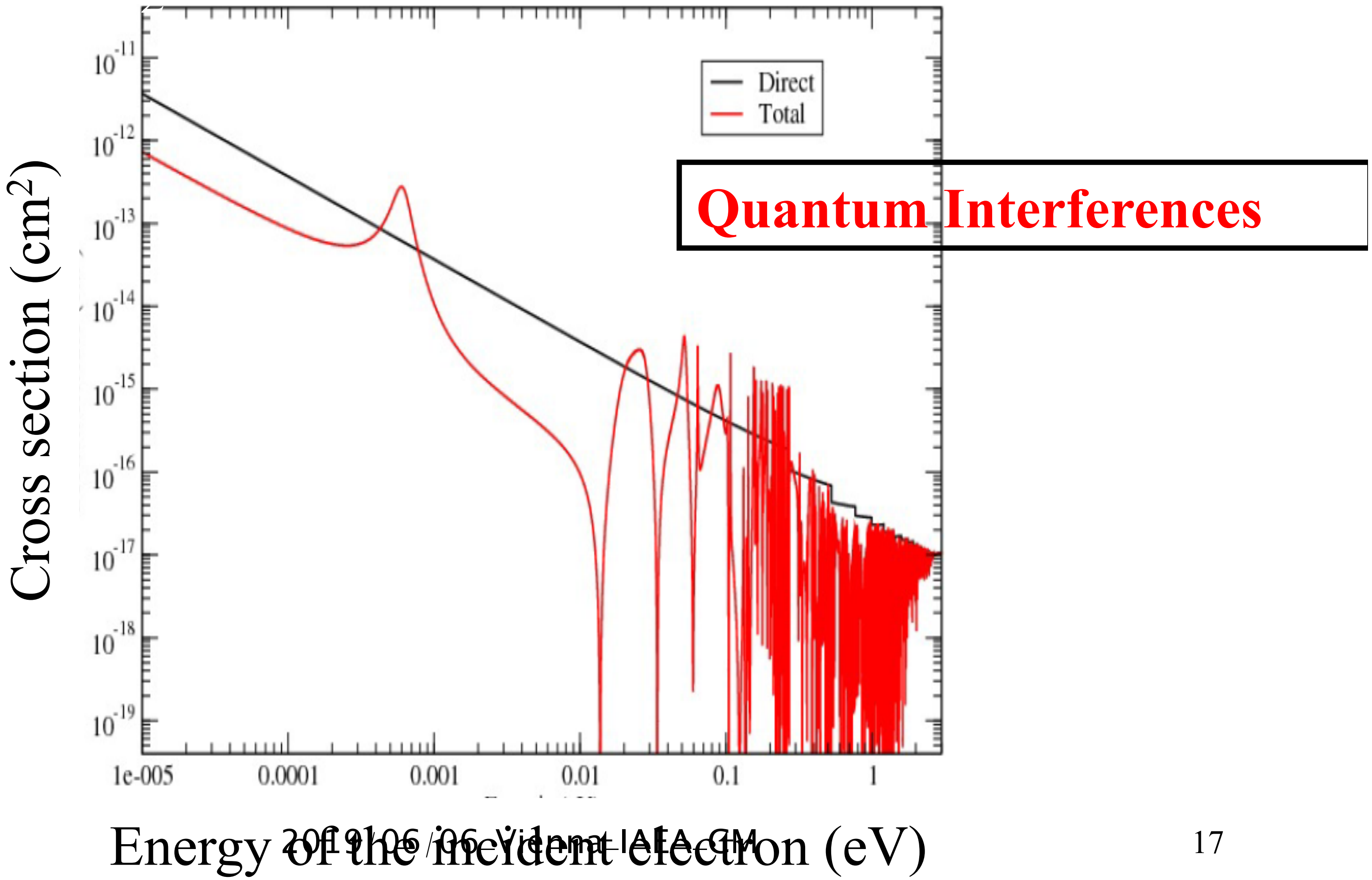
Dissociative Excitation: DE $\longrightarrow A + B^{+} + e^{-}$

Electron-cold molecular ion reaction: Dissociative Recombination



H_2^+: DR xs

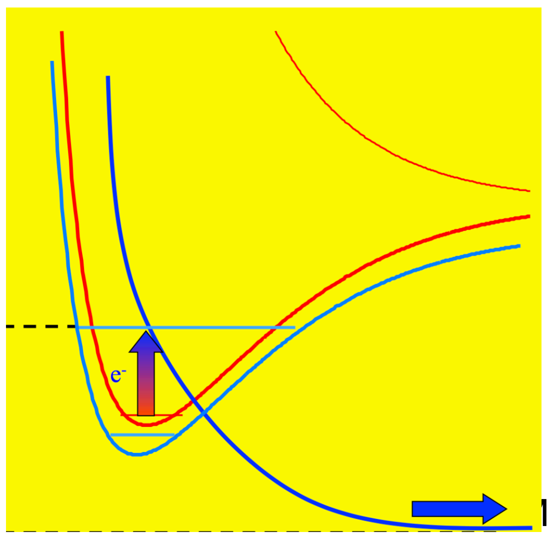
Total (direct & indirect) vs **direct** mechanisms



H_2^+ / HD^+ + e^-

The relevant

POTENTIAL ENERGY CURVES



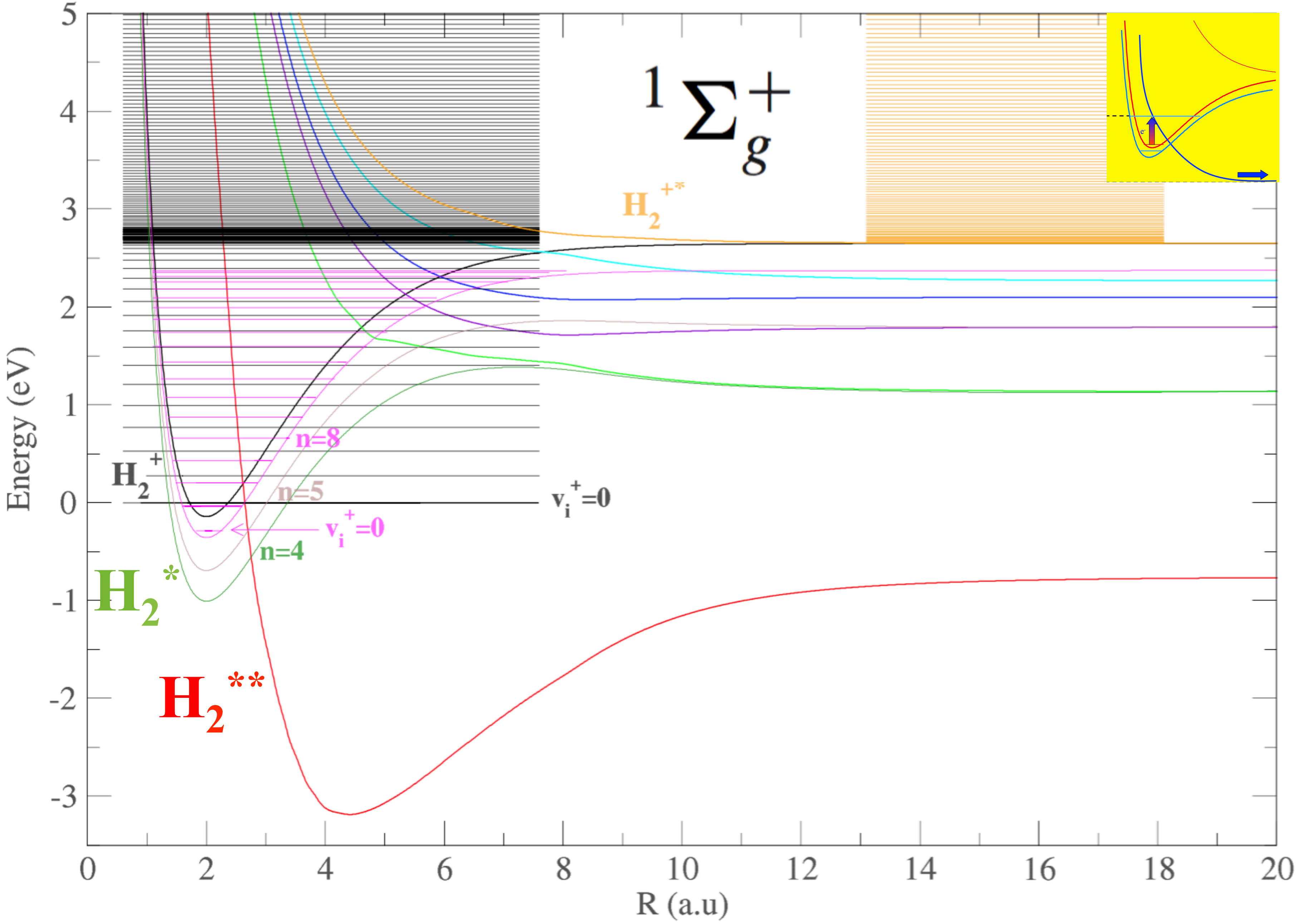
ATOMIC DATA AND NUCLEAR DATA TABLES **64,** 253–277 (1996)
ARTICLE NO. 0023

RESONANCE PARAMETERS AND QUANTUM DEFECTS FOR SUPEREXCITED H_2

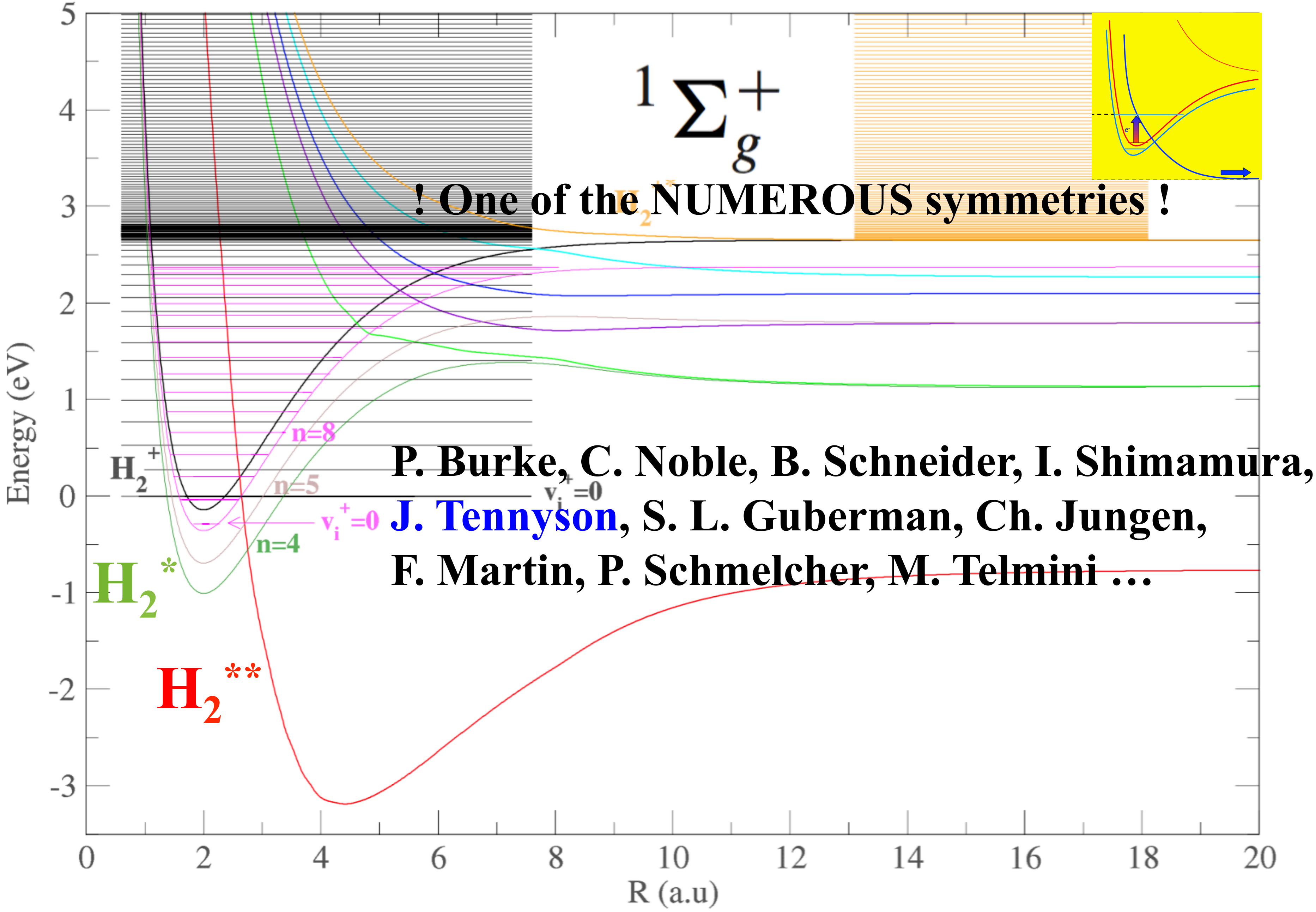
JONATHAN TENNYSON*

Institute for Theoretical Atomic and Molecular Physics
Harvard–Smithsonian Center for Astrophysics
60 Garden Street, Cambridge, Massachusetts 02138

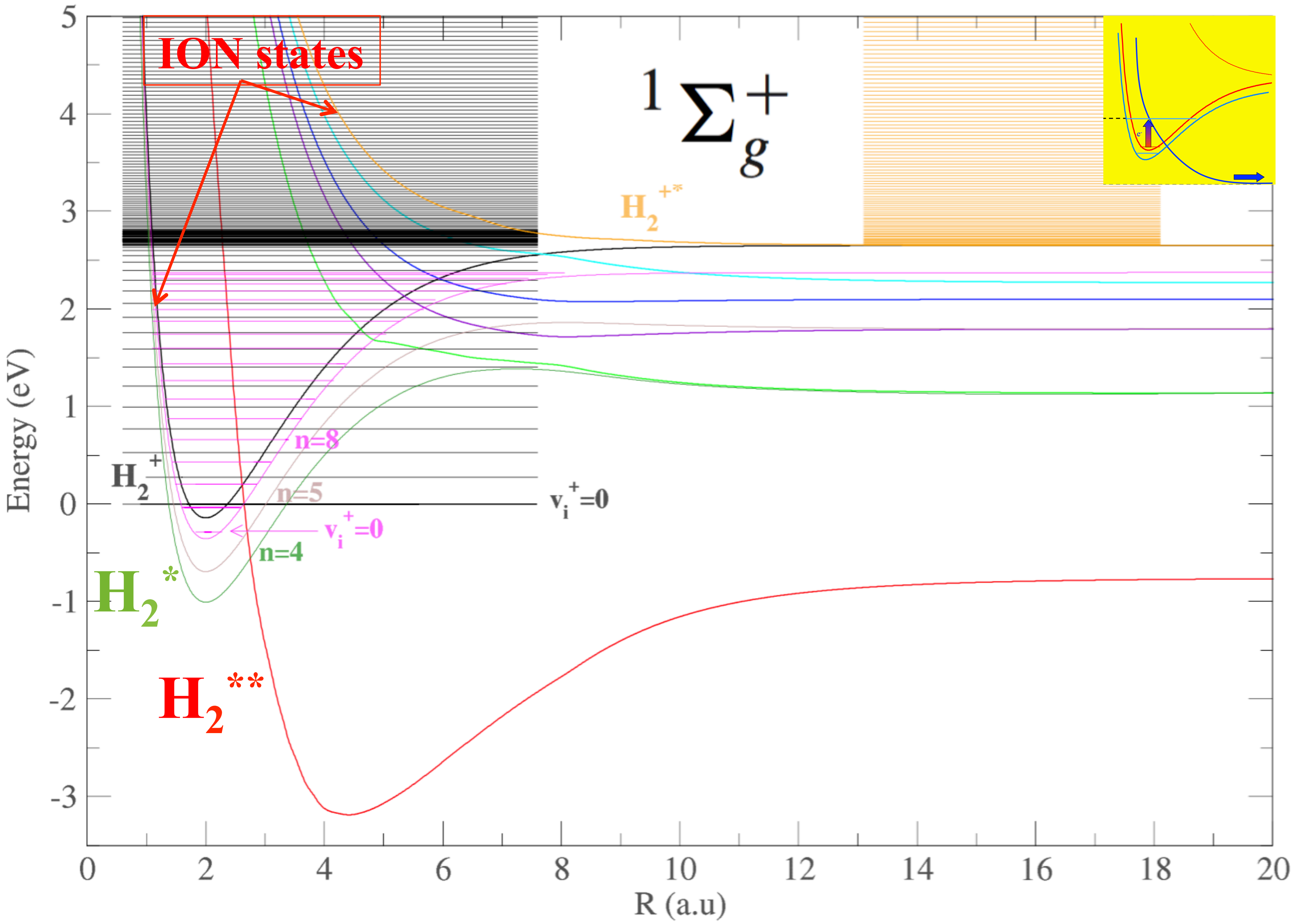
The results of R-matrix calculations on electron collisions with H_2^+ are presented. These calculations include the three lowest states of H_2^+ ($^2\Sigma_g^+$, $^2\Sigma_u^+$ and $^2\Pi_u$). Positions and widths of the Feshbach resonances converging to both the $^2\Sigma_u^+$ and $^2\Pi_u$ states are given, as are autoionization branching ratios for resonances lying above the $^2\Sigma_u^+$ state. Complex quantum defects, calculated by performing scattering calculations above threshold, are presented for all three states considered. Results are tabulated for 12 symmetries ($^1\Sigma_g^+$, $^1\Sigma_u^+$, $^1\Pi_u$, $^1\Pi_g$, $^1\Delta_g$, $^1\Delta_u$, $^3\Sigma_g^+$, $^3\Sigma_u^+$, $^3\Pi_u$, $^3\Pi_g$, $^3\Delta_g$, $^3\Delta_u$) and 13 internuclear separations from 1 to 4 a_0.



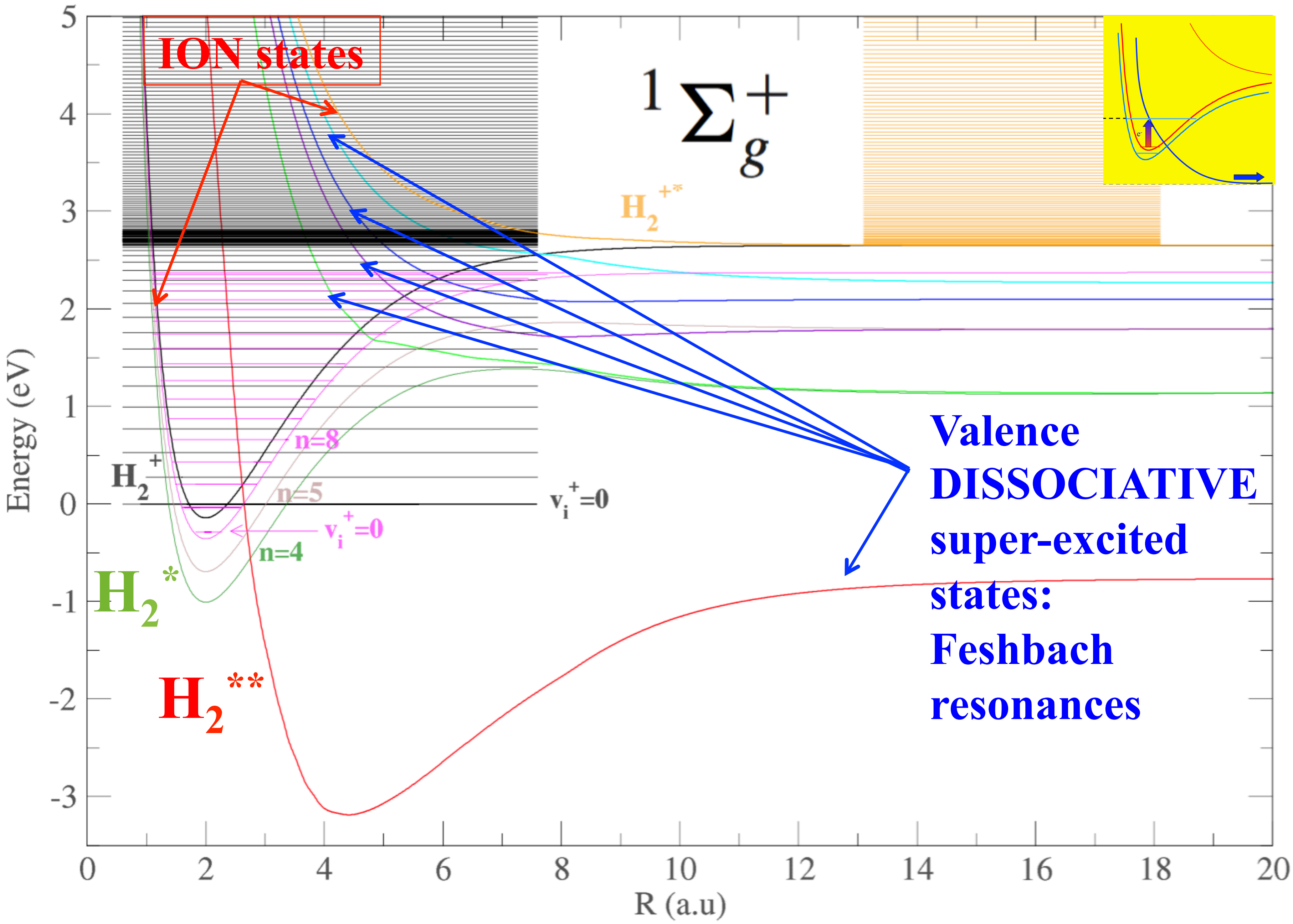
$^1\Sigma_g^+$
H_2^{+*}
H_2^+
$v_i^+=0$
n=8
n=5
$v_i^+=0$
n=4
H_2^*
H_2^{**}
Energy (eV)
R (a.u)



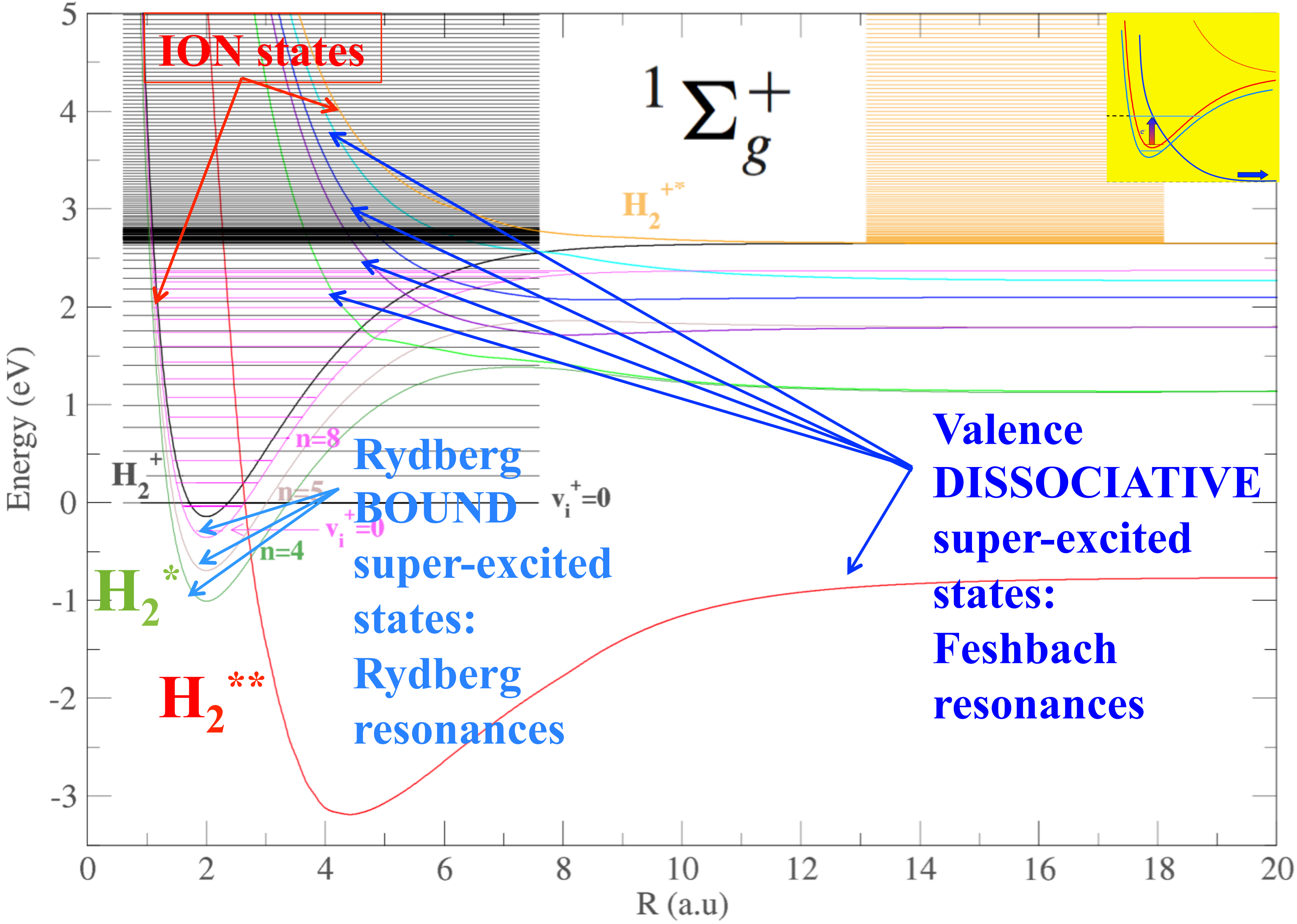
1Σg+
! One of the NUMEROUS symmetries !
P. Burke, C. Noble, B. Schneider, I. Shimamura,
J. Tennyson, S. L. Guberman, Ch. Jungen,
F. Martin, P. Schmelcher, M. Telmini …
H2+
H2*
H2**
n=8
n=5
n=4
vi+=0
Energy (eV)
R (a.u)



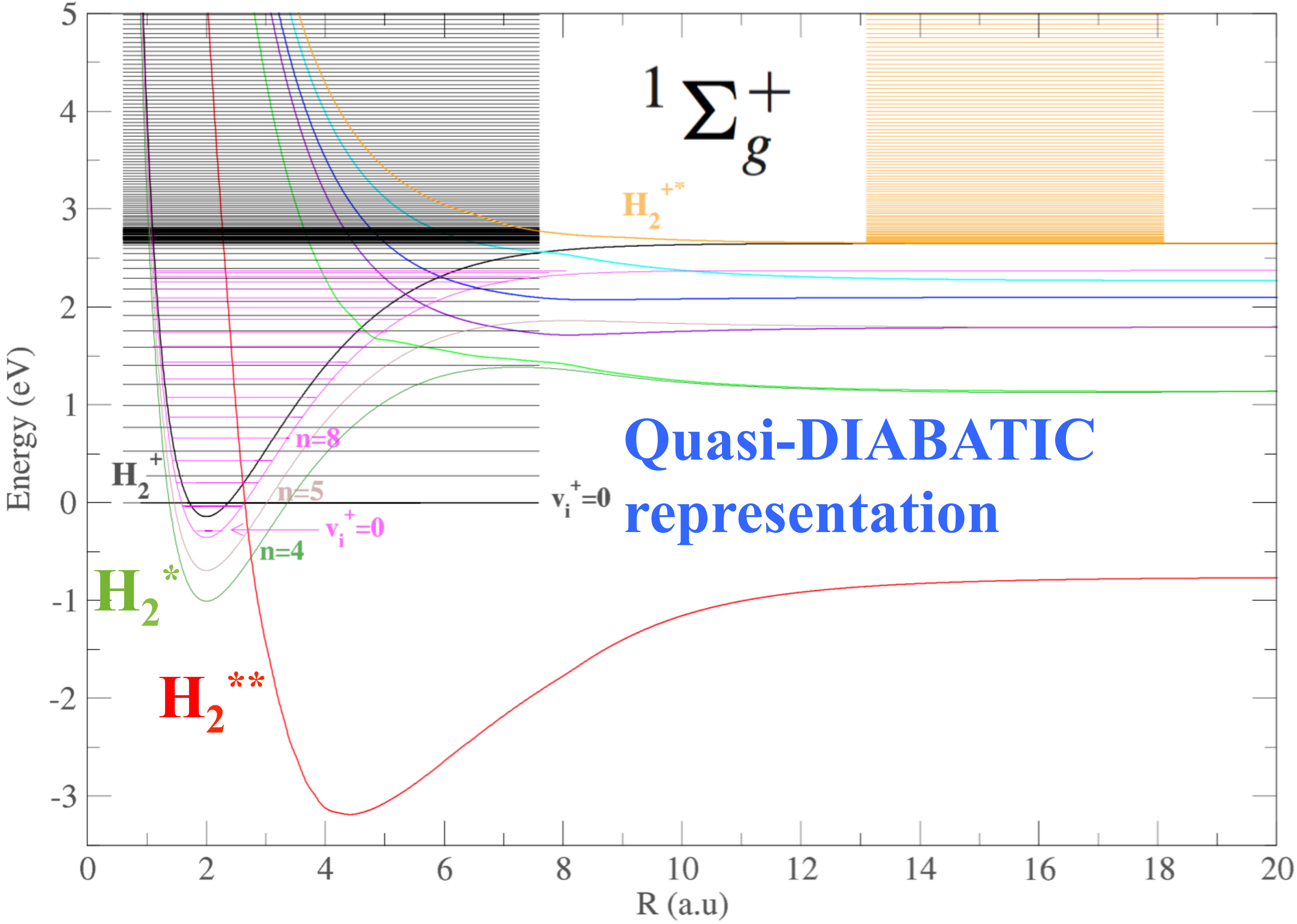
ION states
$^1\Sigma_g^+$
H_2^{+*}
H_2^+
$v_i^+=0$
n=8
n=5
n=4
H_2^*
H_2^{**}
Energy (eV)
R (a.u)



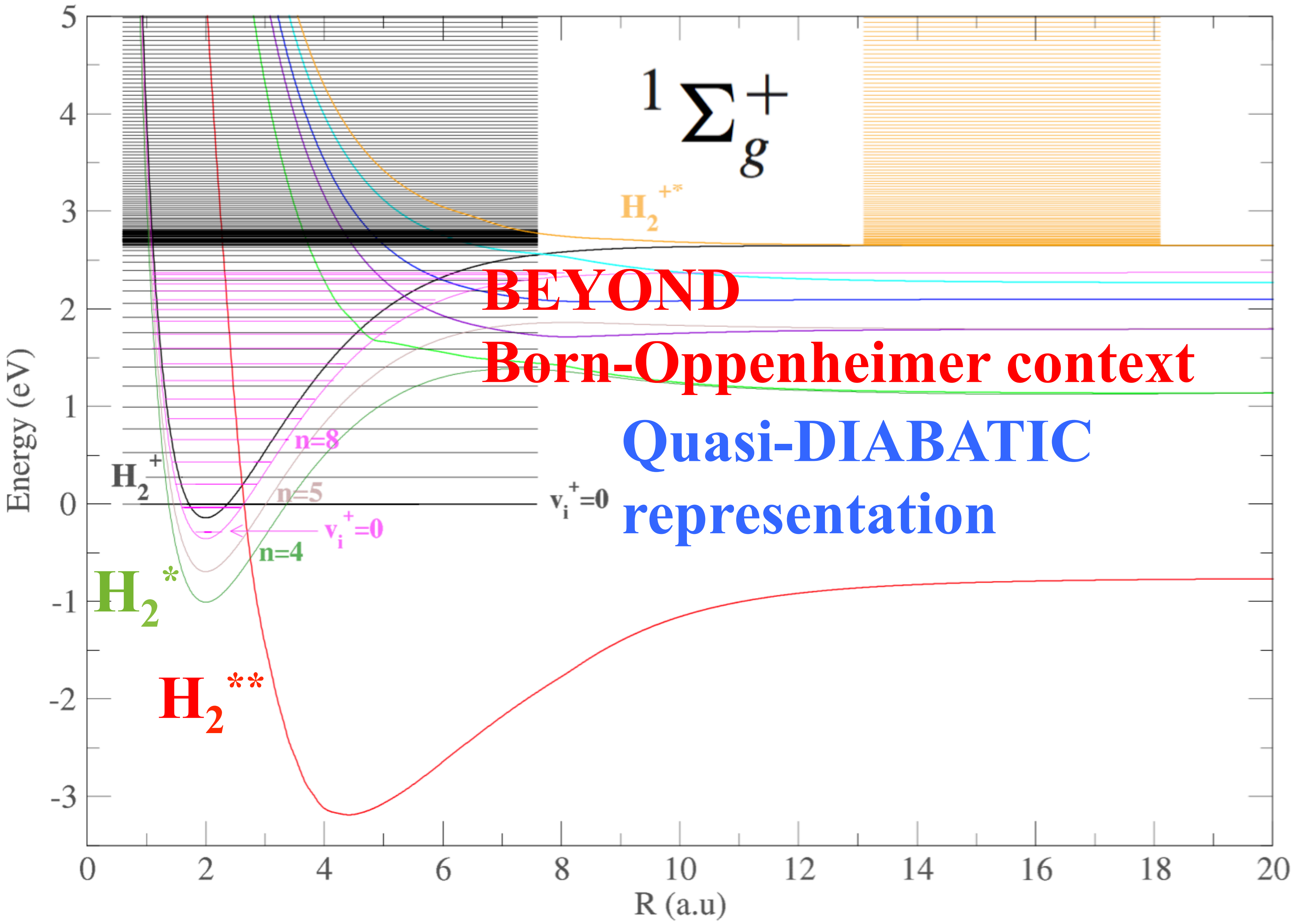
ION states
$^1\Sigma_g^+$
H_2^{+*}
H_2^+
$v_i^+=0$
n=8
n=5
n=4
H_2^*
H_2^{**}
Valence DISSOCIATIVE super-excited states: Feshbach resonances
Energy (eV)
R (a.u)



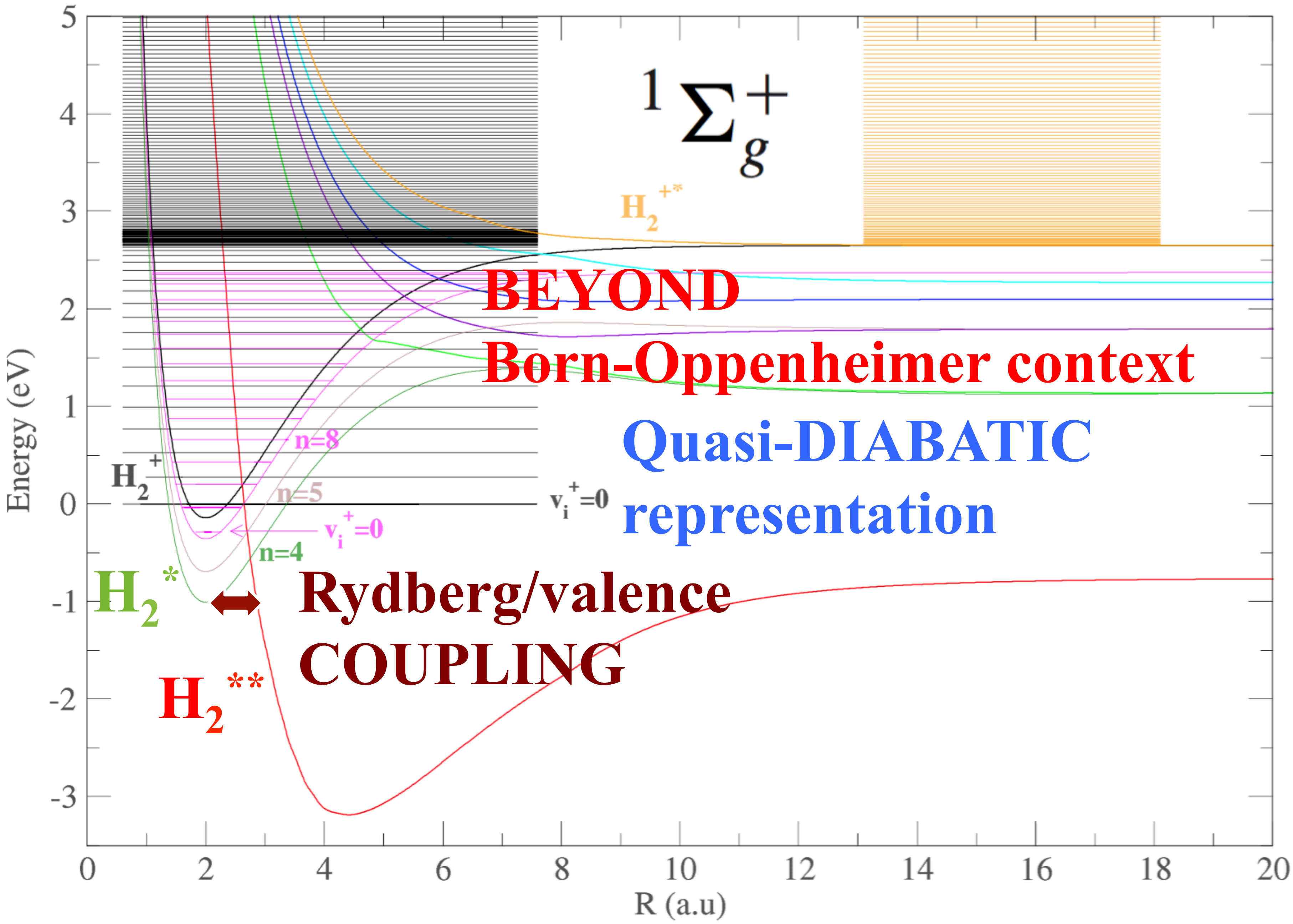
ION states
$^1\Sigma_g^+$
H_2^{+*}
H_2^+
$v_i^+=0$
n=8
n=5
n=4
H_2^*
H_2^{**}
Rydberg BOUND super-excited states: Rydberg resonances
Valence DISSOCIATIVE super-excited states: Feshbach resonances
Energy (eV)
R (a.u)



$^1\Sigma_g^+$
H_2^{+*}
Quasi-DIABATIC
representation
H_2^+
$v_i^+=0$
n=8
n=5
$v_i^+=0$
n=4
H_2^*
H_2^{**}
Energy (eV)
R (a.u)
5
4
3
2
1
0
-1
-2
-3
0
2
4
6
8
10
12
14
16
18
20



$^1\Sigma_g^+$
H_2^{+*}
BEYOND
Born-Oppenheimer context
Quasi-DIABATIC
representation
n=8
n=5
n=4
H_2^+
$v_i^+=0$
$v_i^+=0$
H_2^*
H_2^{**}
Energy (eV)
R (a.u)



Energy (eV)
R (a.u)
$^1\Sigma_g^+$
H_2^{+*}
BEYOND
Born-Oppenheimer context
Quasi-DIABATIC
representation
H_2^+
n=8
n=5
n=4
$v_i^+=0$
$v_i^+=0$
H_2^*
Rydberg/valence
COUPLING
H_2^{**}

Electron/molecular cation reactive collisions

Main THEORETICAL approach: MQDT

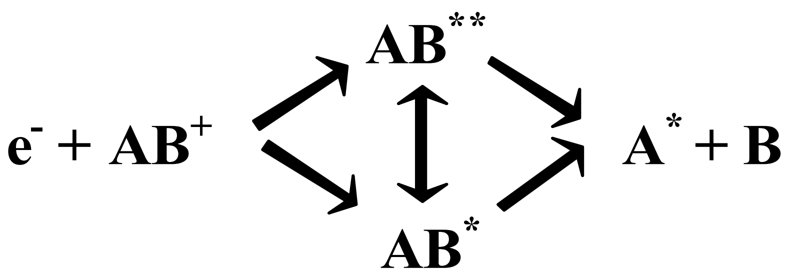
Multichannel Quantum Defect Theory

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

Quantum Interferences

DIRECT

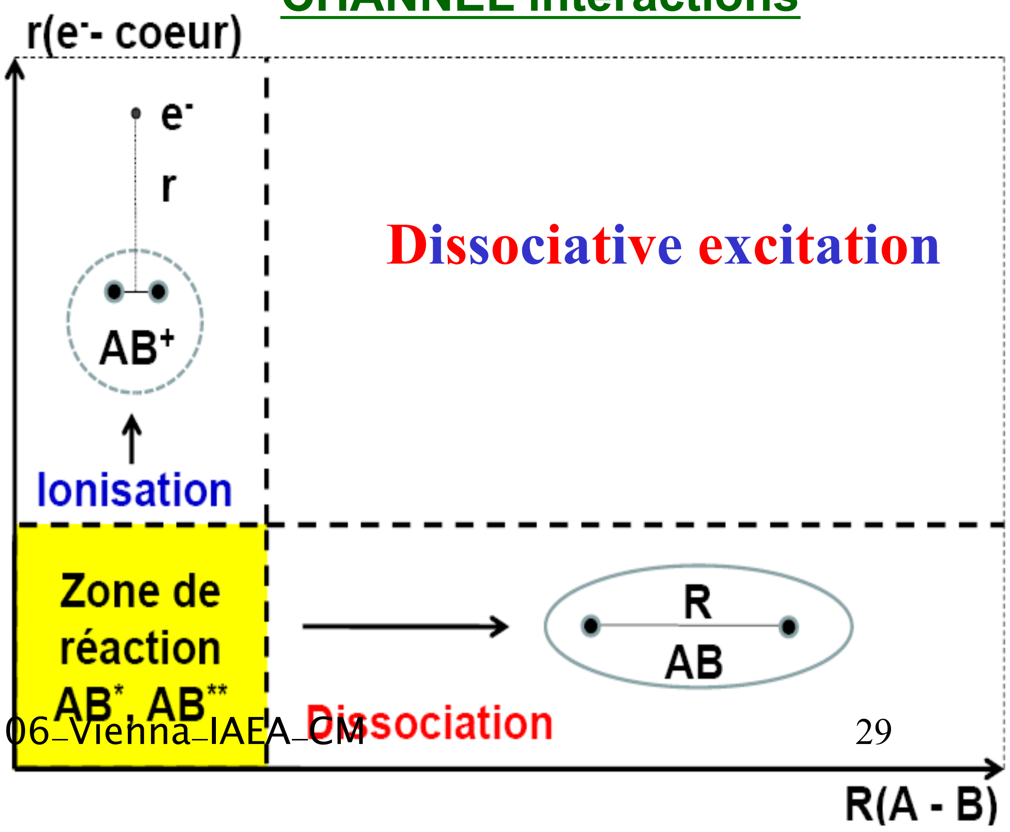
Dissociative state



Bound (Rydberg) state

INDIRECT

CHANNEL interactions



MULTICHANNEL QUANTUM DEFECT THEORY (MQDT):

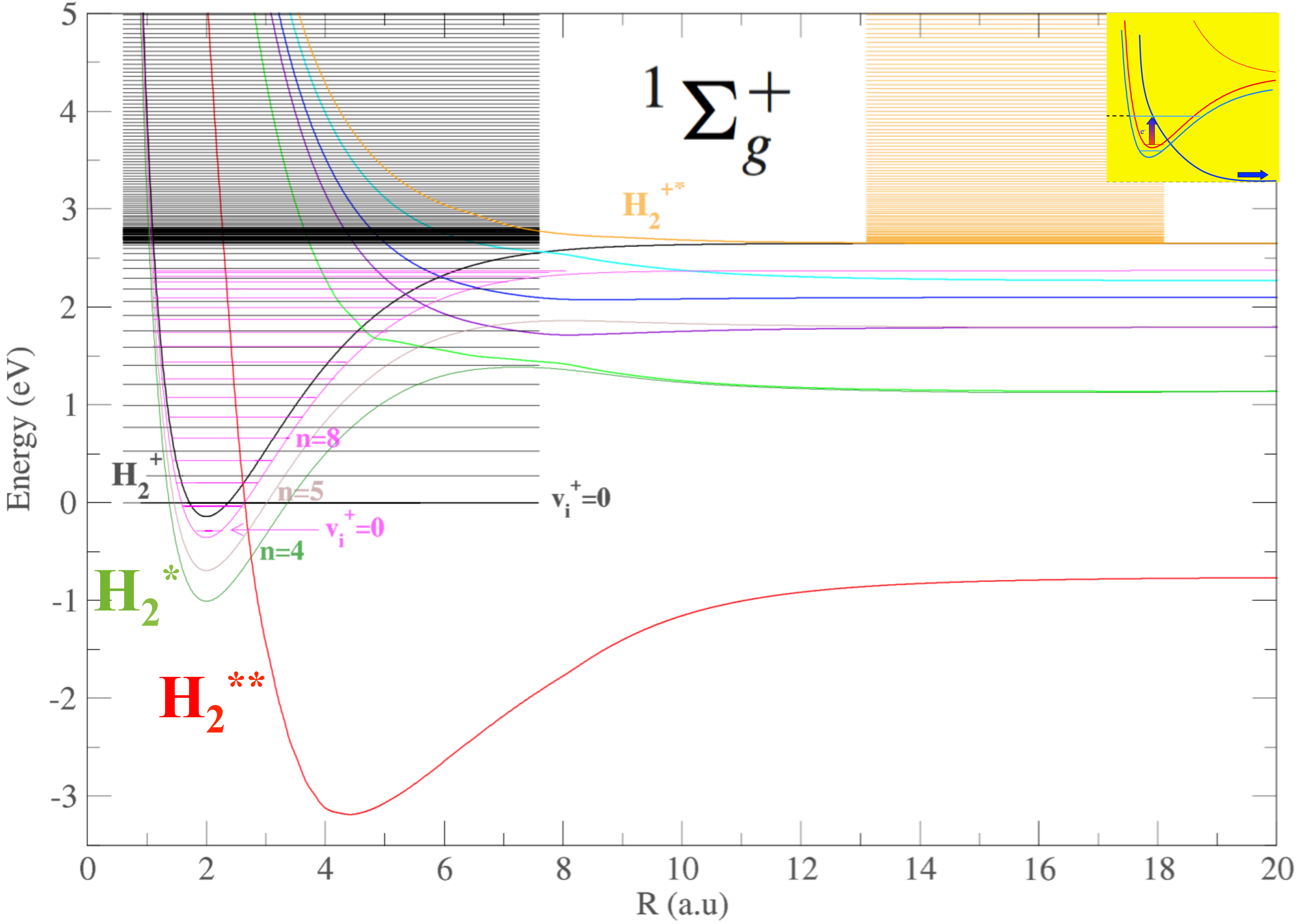
“Very” Low Energy:

ROTATION and Vibration,

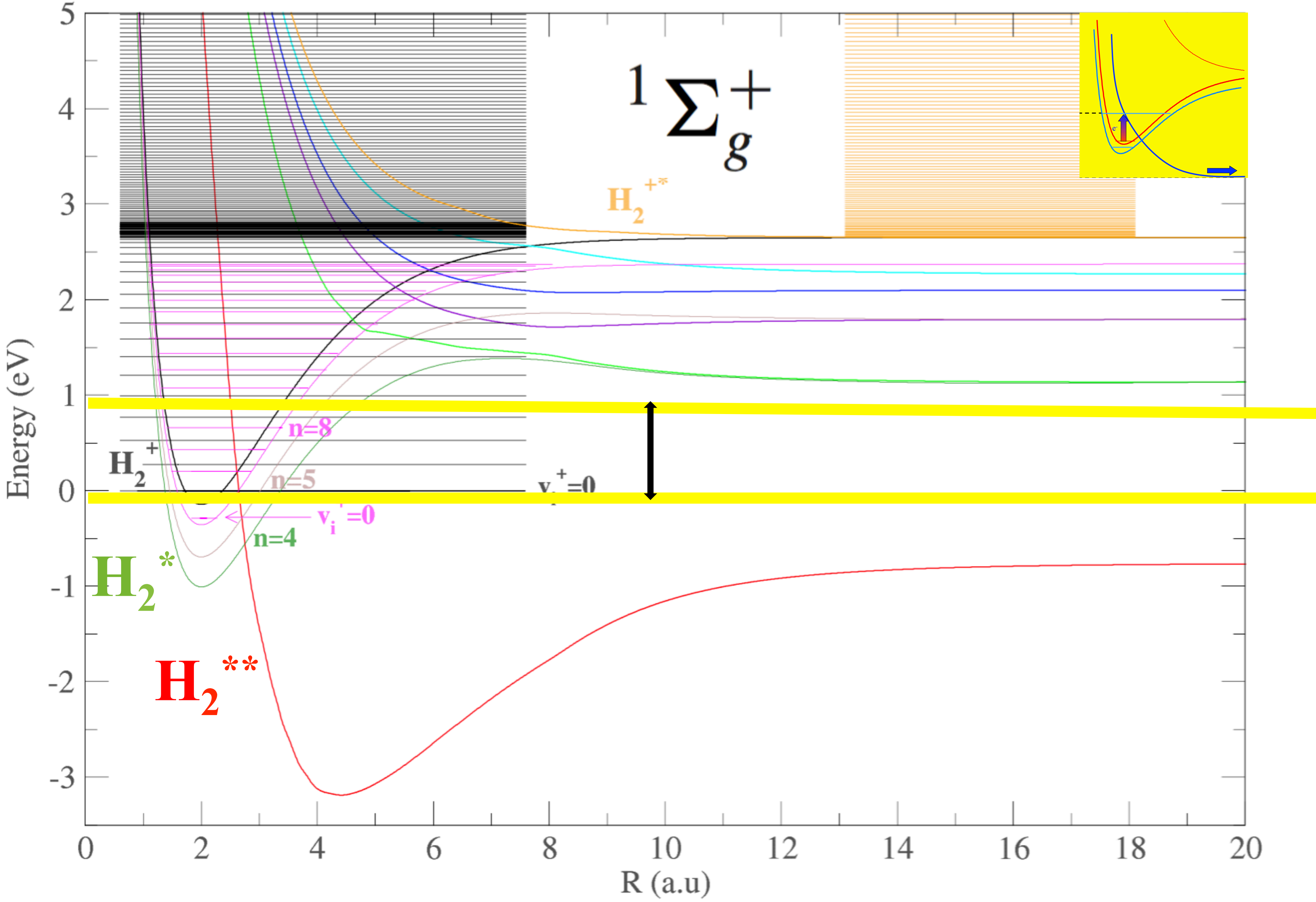
DISCRETE ro-vibrational spectrum,

“Fano”resonances,

maximum ACCURACY



$^1\Sigma_g^+$
H_2^{+*}
H_2^+
$v_i^+=0$
n=8
n=5
$v_i^+=0$
n=4
H_2^*
H_2^{**}
Energy (eV)
R (a.u)



5
4
3
2
1
0
-1
-2
-3
Energy (eV)
0
2
4
6
8
10
12
14
16
18
20
R (a.u)
$^1\Sigma_g^+$
H_2^{+*}
H_2^+
n=8
n=5
n=4
$v_i^+=0$
$v_i^+=0$
H_2^*
H_2^{**}

PHYSICAL REVIEW A **90**, 012706 (2014)

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]

$HD^+ + e^-$

↓

HD^*, HD^{**}

↓

$H + D$

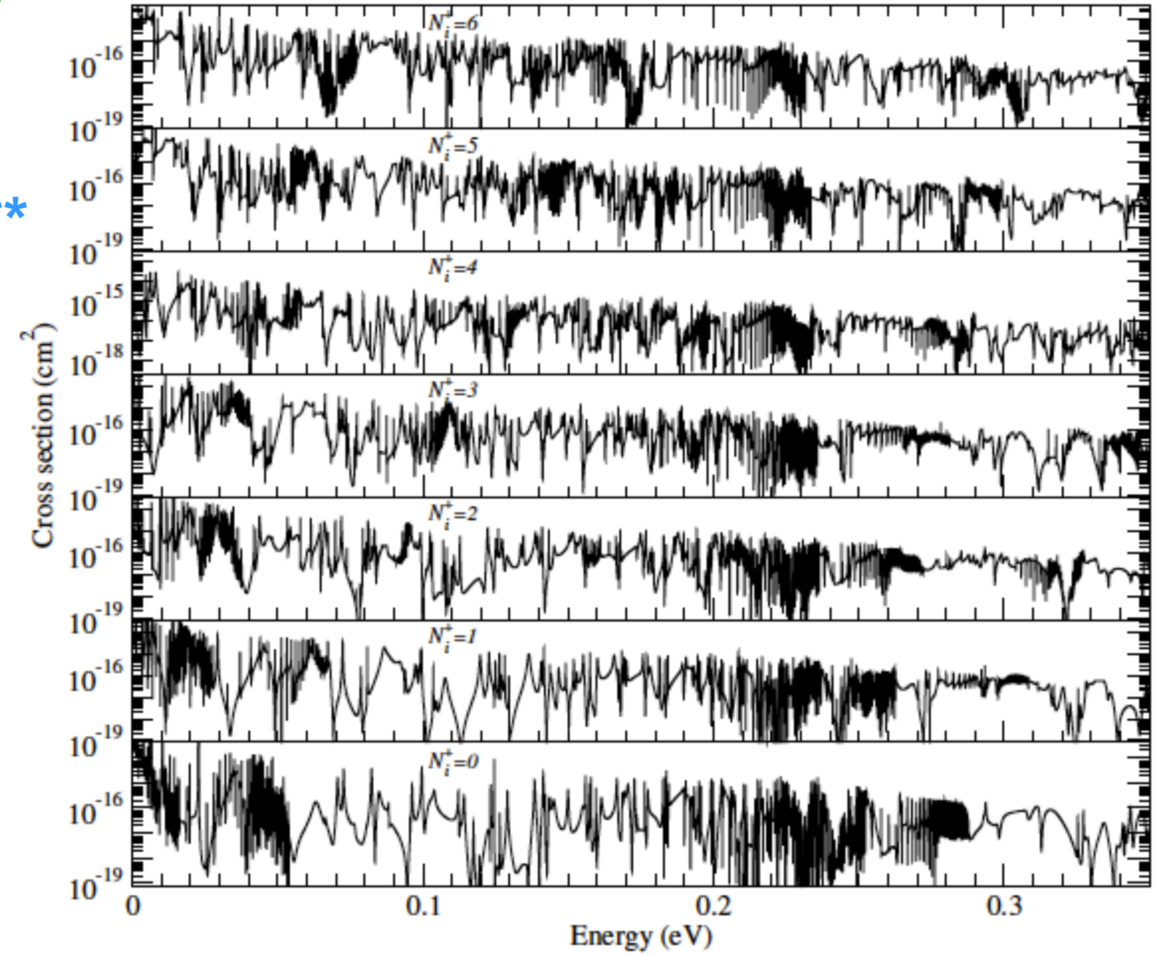
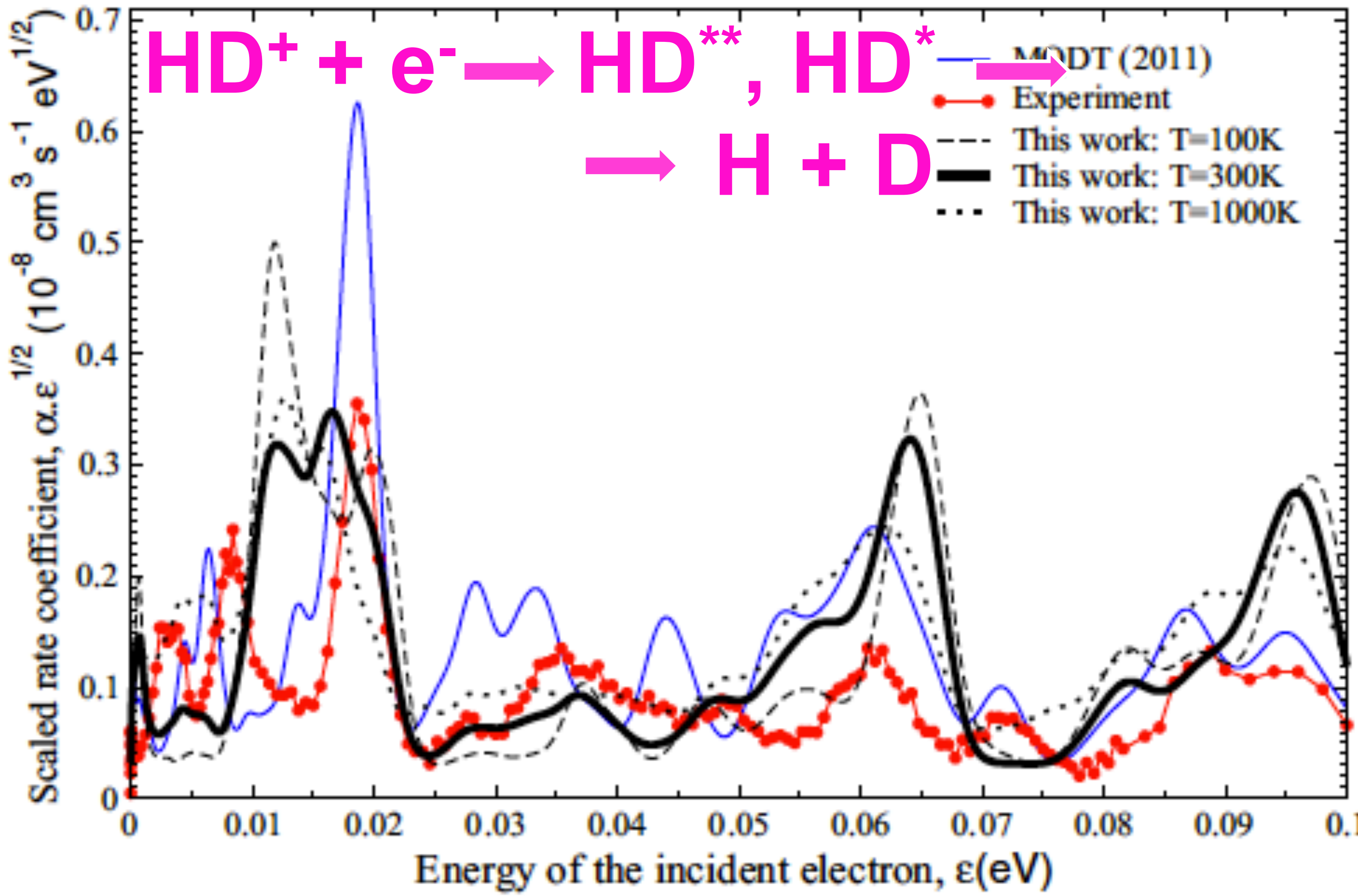


Figure 3. DR cross sections of HD^+ initially in one of its lowest rotational level N_i^+ (vibrational ground state).

PHYSICAL REVIEW A **90**, 012706 (2014)

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]



How important is the target excitation ?

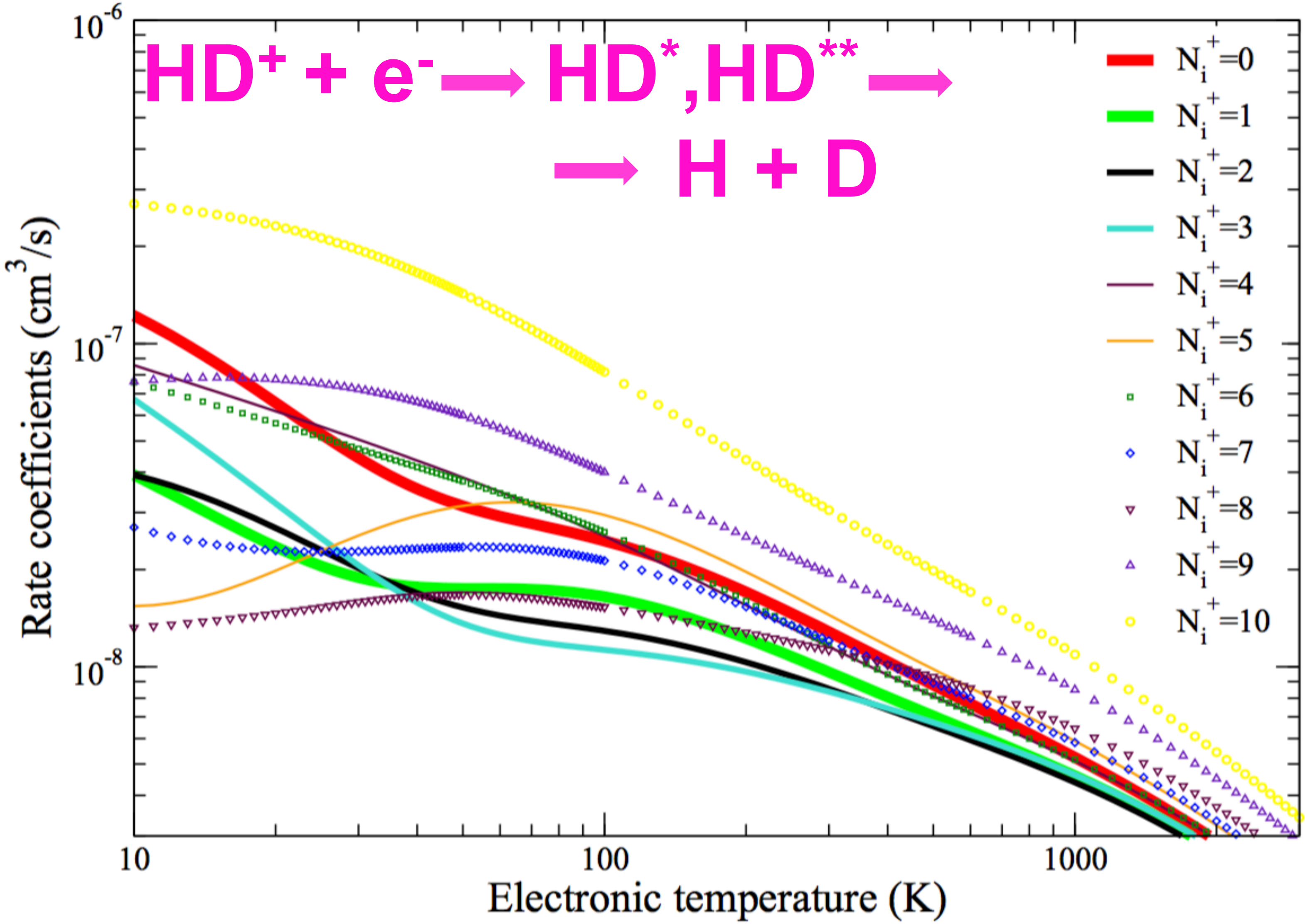


FIG. 9. (Color online) Maxwell isotropic rate coefficients for the dissociative recombination $HD^+(X\,^2\Sigma_g^+)$ with $v_i^+ = 0$ as a function of initial rotational level, $N_i^+ = 0$ to 10 .

EPJ Web of Conferences **84**, 01001 (2015)
DOI: 10.1051/epjconf/20158401001

The HD^+ dissociative recombination rate coefficient at low temperature

A. Wolf[1,a], O. Novotný[2], H. Buhr[2], C. Krantz[2], I.F. Schneider[3], O. Motapon[4] and J.Zs. Mezei[3,5]

[1] Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany
[2] Columbia Astrophysics Laboratory, Columbia University, New York, NY 10027, USA
[3] Laboratoire Ondes et Milieux Complexes UMR-6294 CNRS and Université du Havre, 25, rue Philippe Lebon, BP. 540, 76058 Le Havre, France
[4] LPF, UFD Mathémathiques, Informatique Appliquée et Physique Fondamentale, University of Douala, PO Box 24157, Douala, Cameroun
[5] Laboratoire Aimé Coton, CNRS-UPR-3321, Univ. Paris-Sud et Ecole Normale Supérieure de Cachan, 91405 Orsay, France

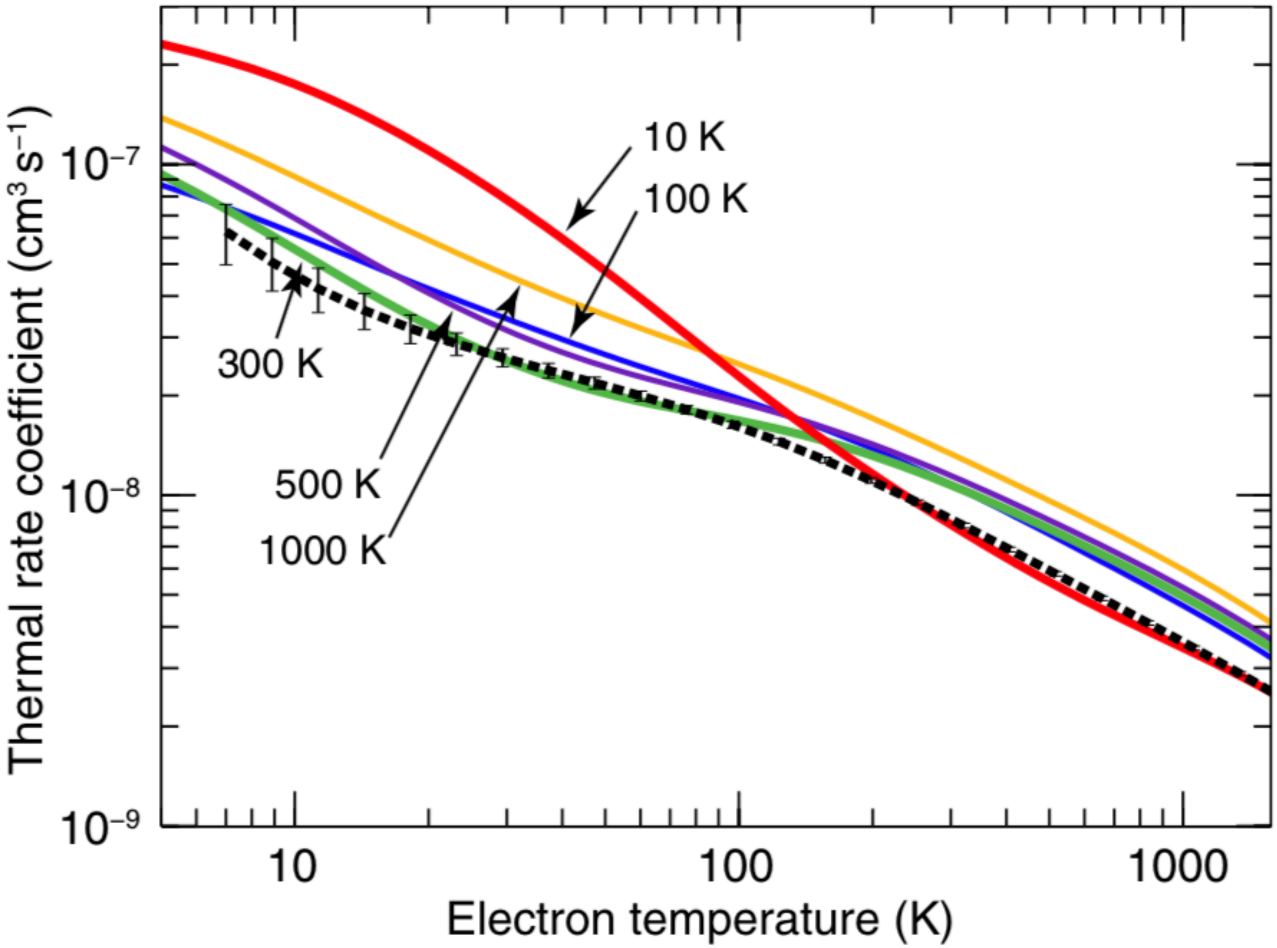
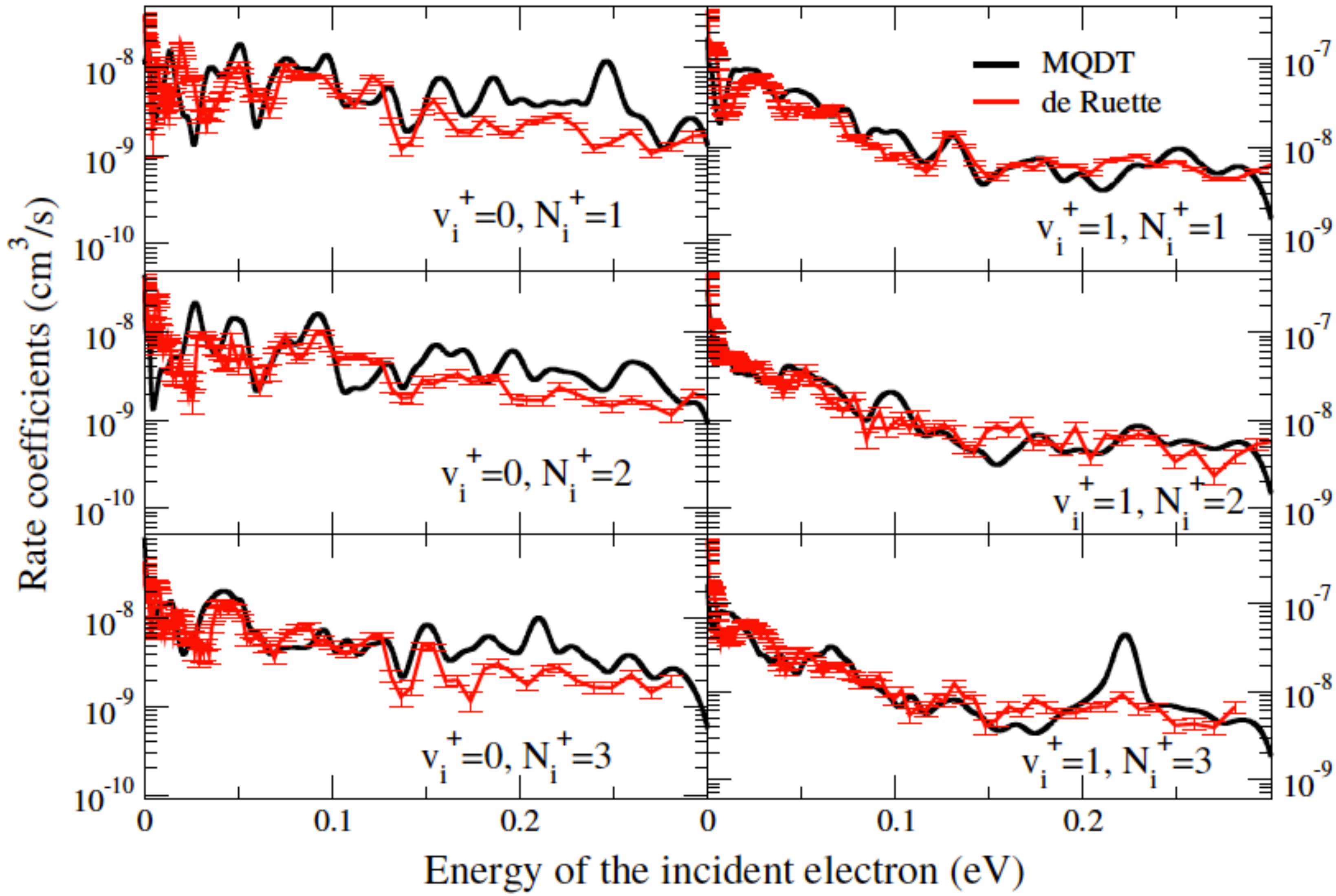


Figure 2. Thermal rate coefficient for HD^+ DR as a function of the electron temperature. Experiment is given by a the thick dashed line; 1σ estimated experimental errors due to uncertainties in the electron beam temperatures are also indicated. Theory is obtained for the given rotational temperatures.

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

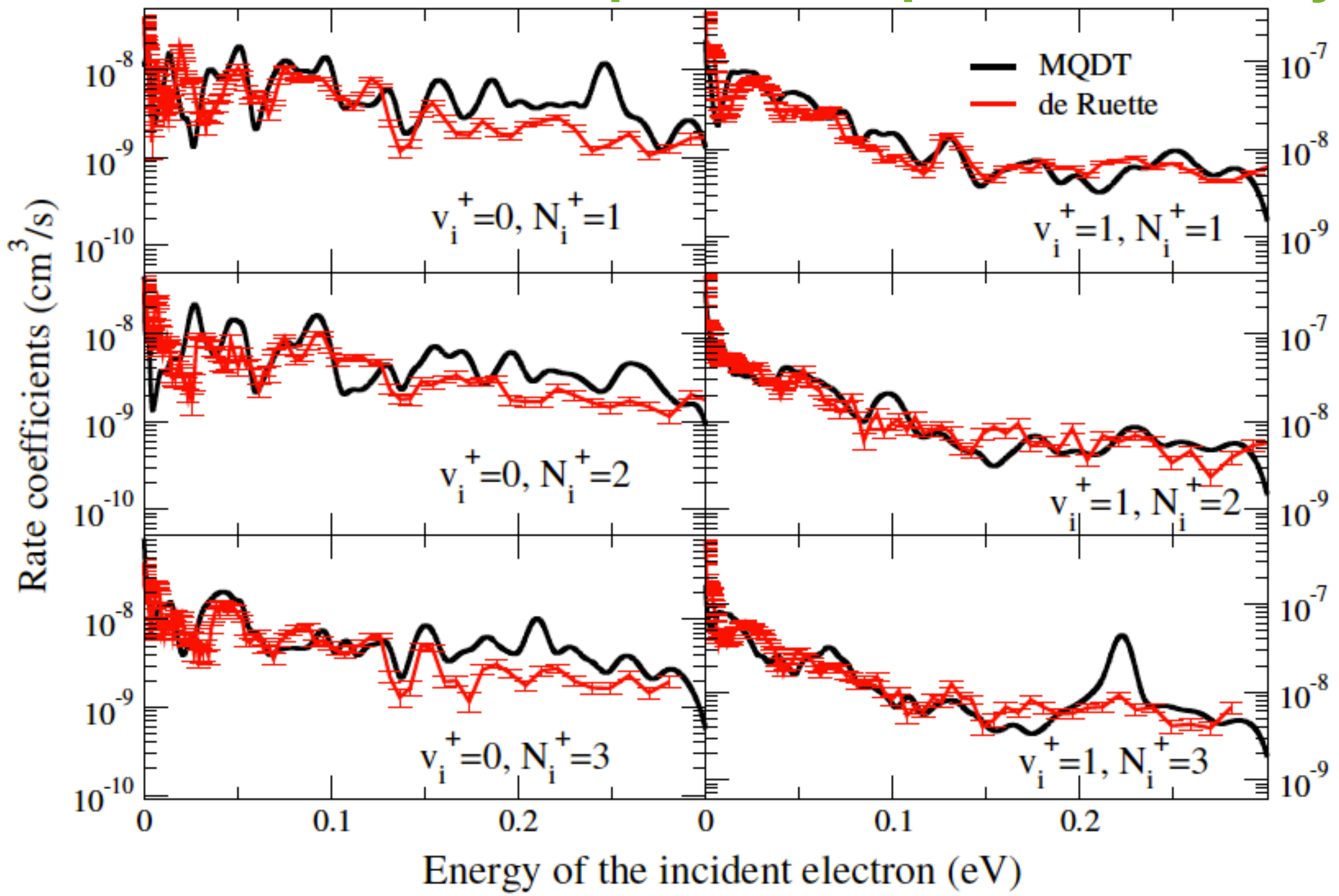
$H_2^+(N_i^+, v_i^+) + e^- \longrightarrow H + H$



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

$H_2^+(N_i^+, v_i^+) + e^- \rightarrow H + H$

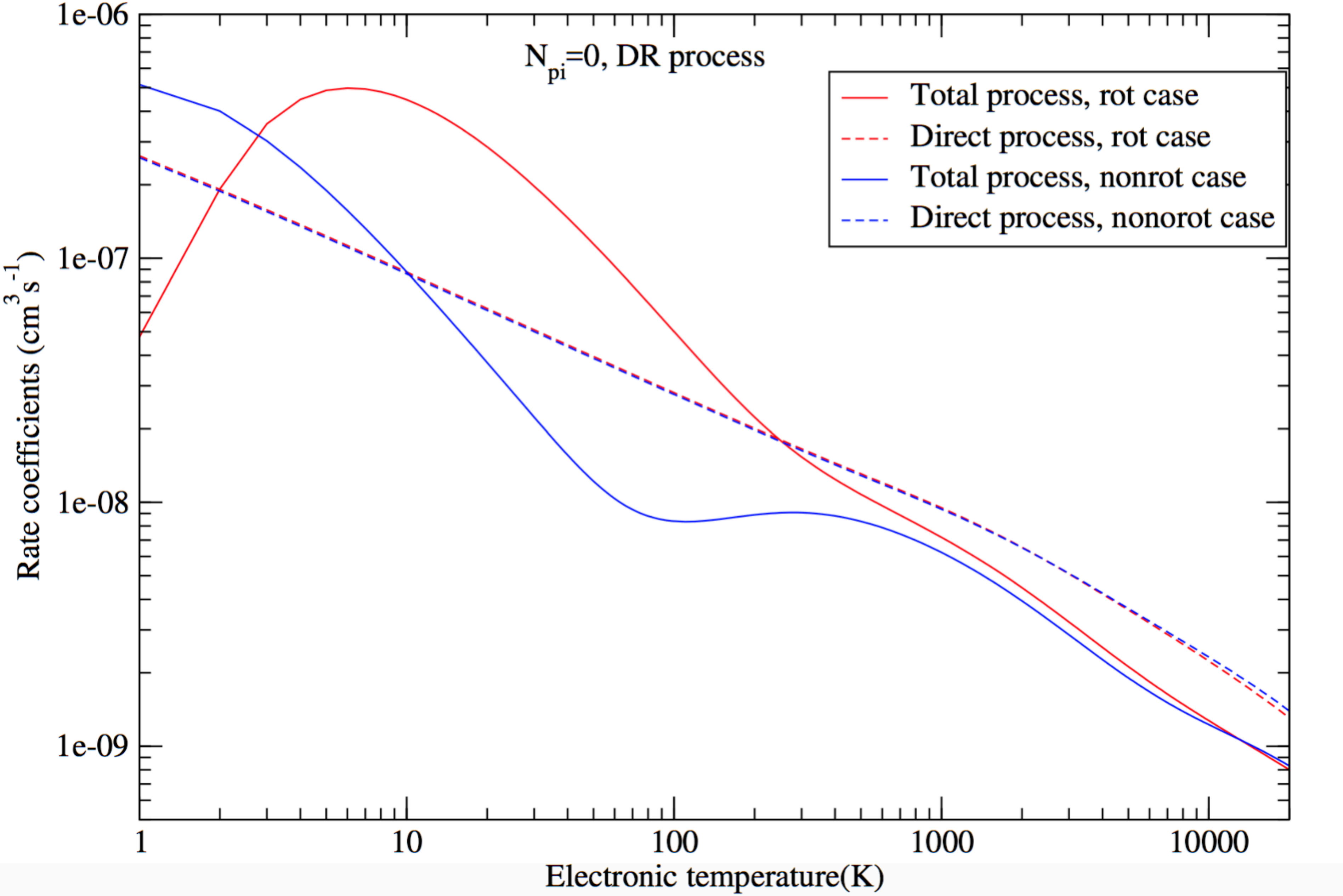
1st state-to-state comparison experiment/theory



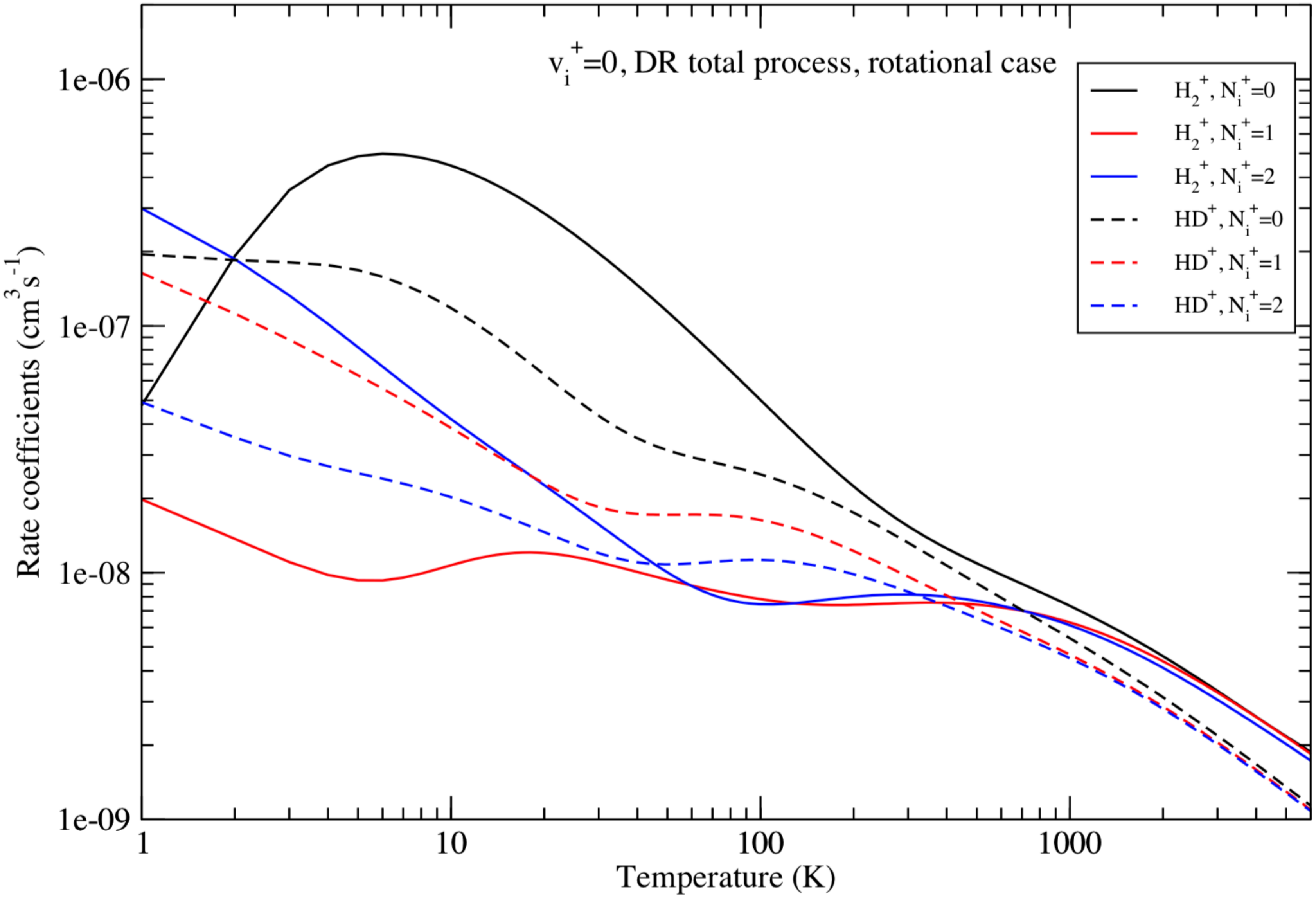
How important are the RESONANCES ?

How important are the ROTATIONAL effects ?

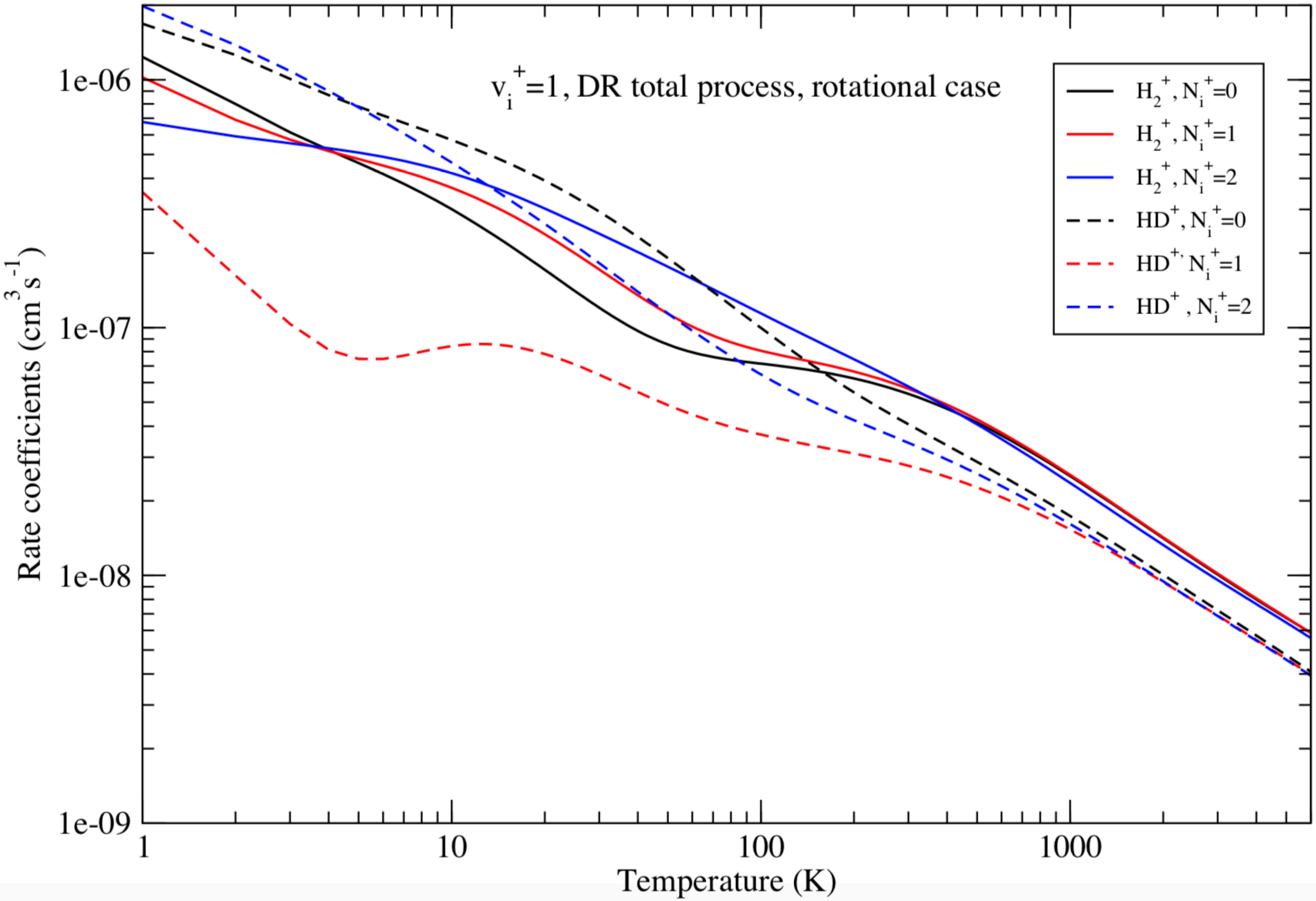
$H_2^+(N_i^+=0)+e^- \longrightarrow H_2^{**}, H_2^* \longrightarrow H+H$



Focus on ISOTOPIC effects

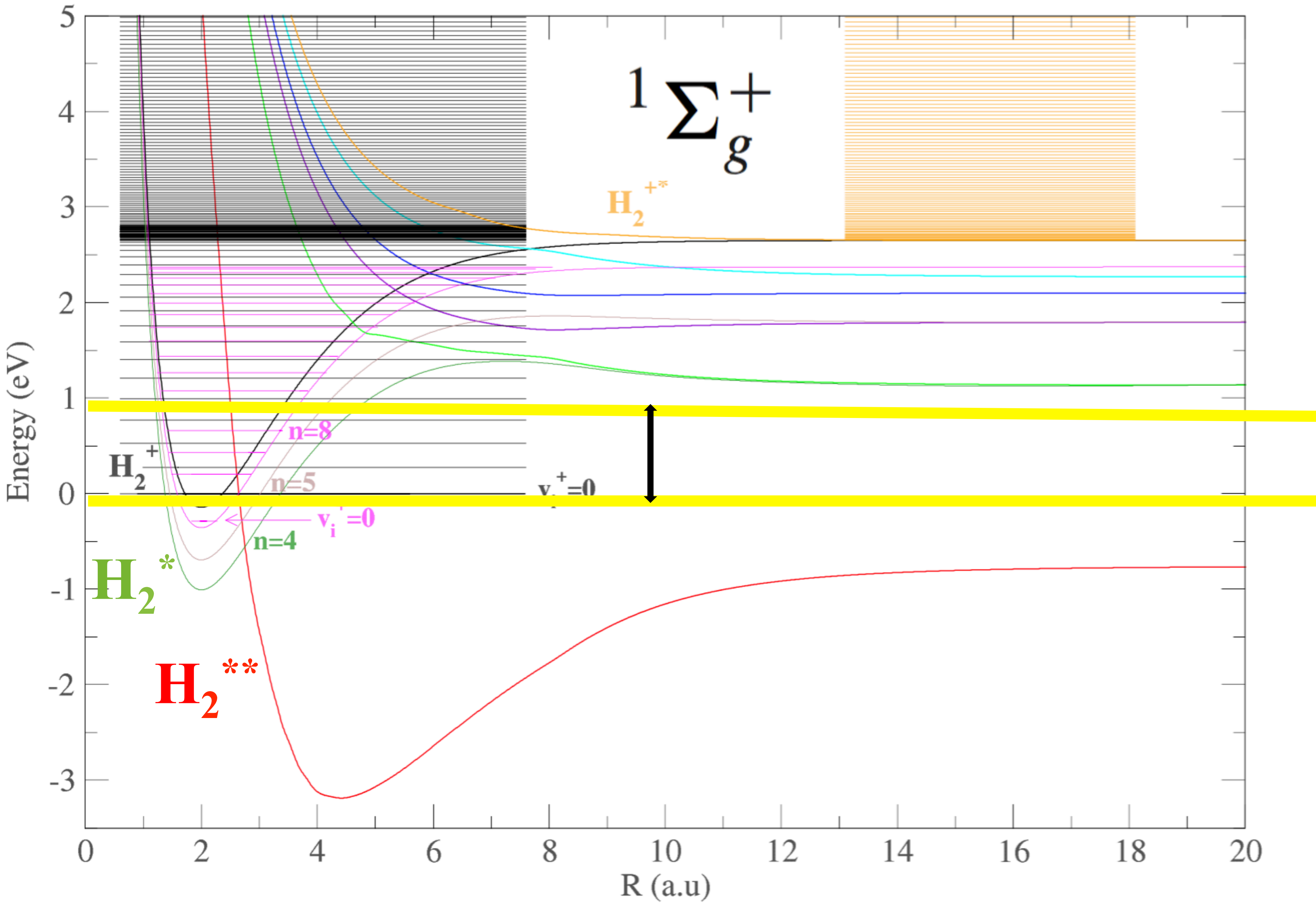


v_i^+=0, DR total process, rotational case
H_2^+, N_i^+=0
H_2^+, N_i^+=1
H_2^+, N_i^+=2
HD^+, N_i^+=0
HD^+, N_i^+=1
HD^+, N_i^+=2
Rate coefficients ($cm^3 s^{-1}$)
1e-06
1e-07
1e-08
1e-09
1
10
100
1000
Temperature (K)

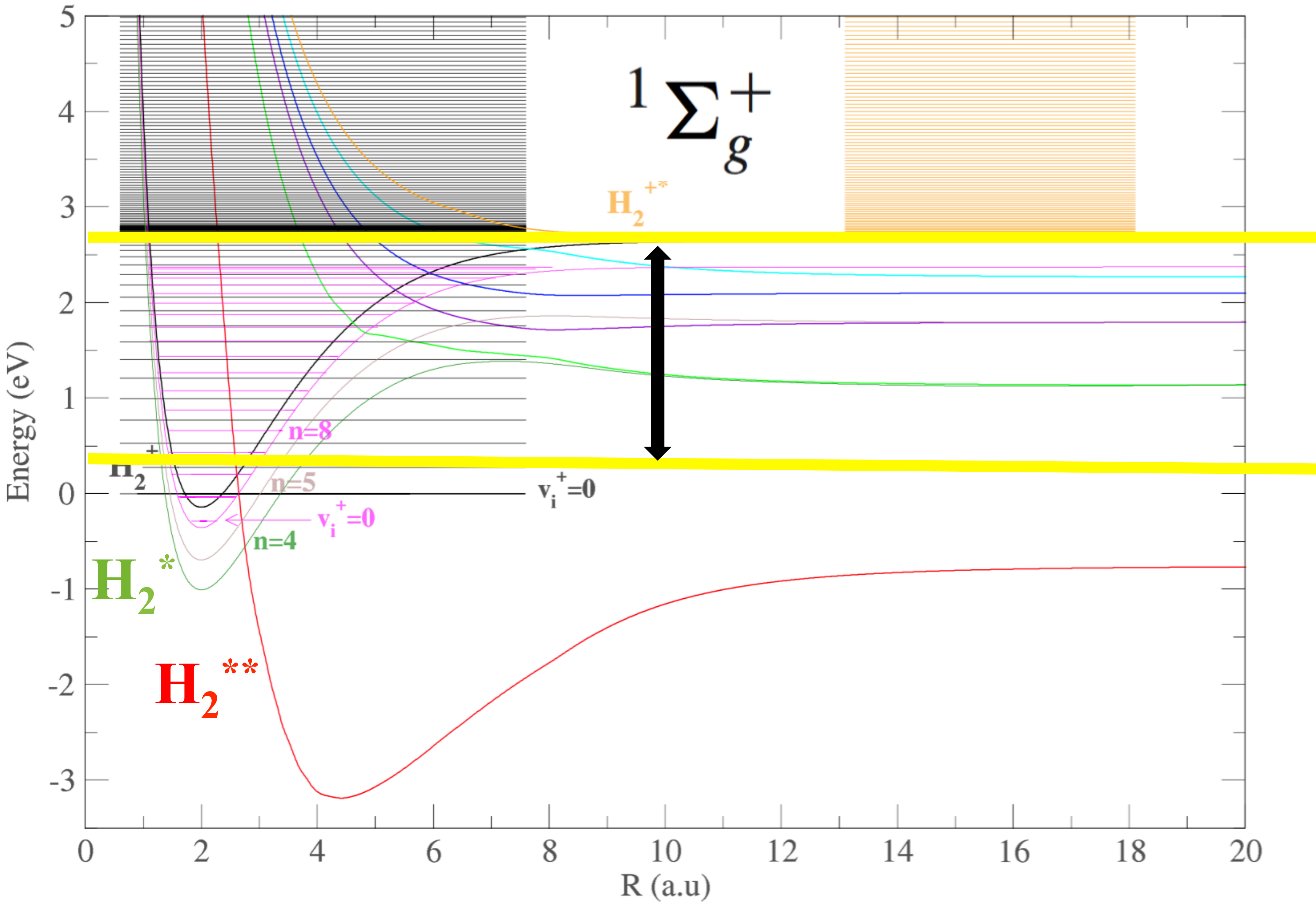


v_i^+=1, DR total process, rotational case
H_2^+, N_i^+=0
H_2^+, N_i^+=1
H_2^+, N_i^+=2
HD^+, N_i^+=0
HD^+, N_i^+=1
HD^+, N_i^+=2
Rate coefficients ($cm^3 s^{-1}$)
1e-06
1e-07
1e-08
1e-09
1
10
100
1000
Temperature (K)

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

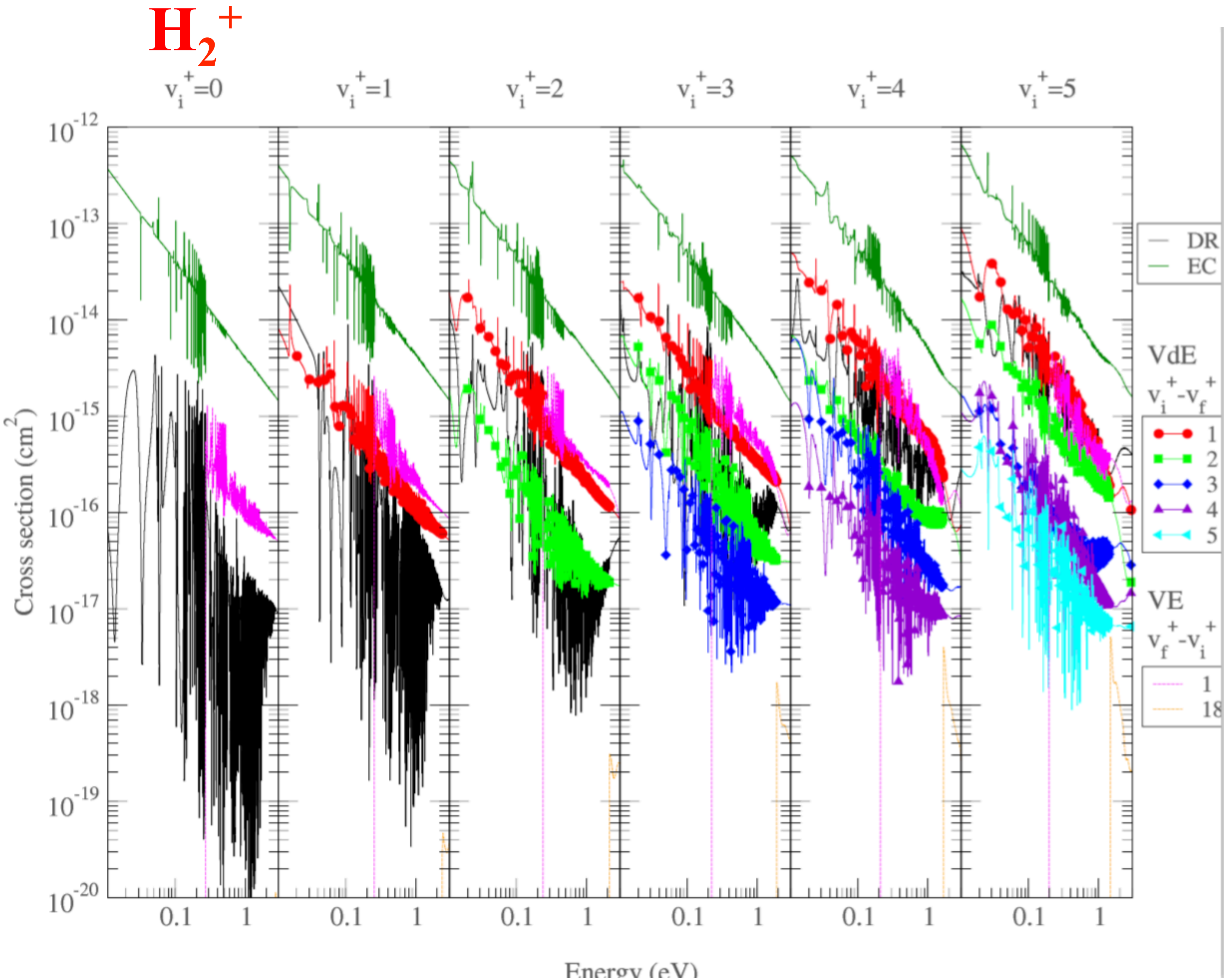


$^1\Sigma_g^+$
H_2^{+*}
H_2^+
n=8
n=5
$v_i^+=0$
$v_i^+=0$
n=4
H_2^*
H_2^{**}
Energy (eV)
R (a.u)



Energy (eV)
R (a.u)
$^1\Sigma_g^+$
H_2^{+*}
H_2^+
n=8
n=5
n=4
$v_i^+=0$
$v_i^+=0$
H_2^*
H_2^{**}

Moulane 2017, Colboc 2016



High Energy:

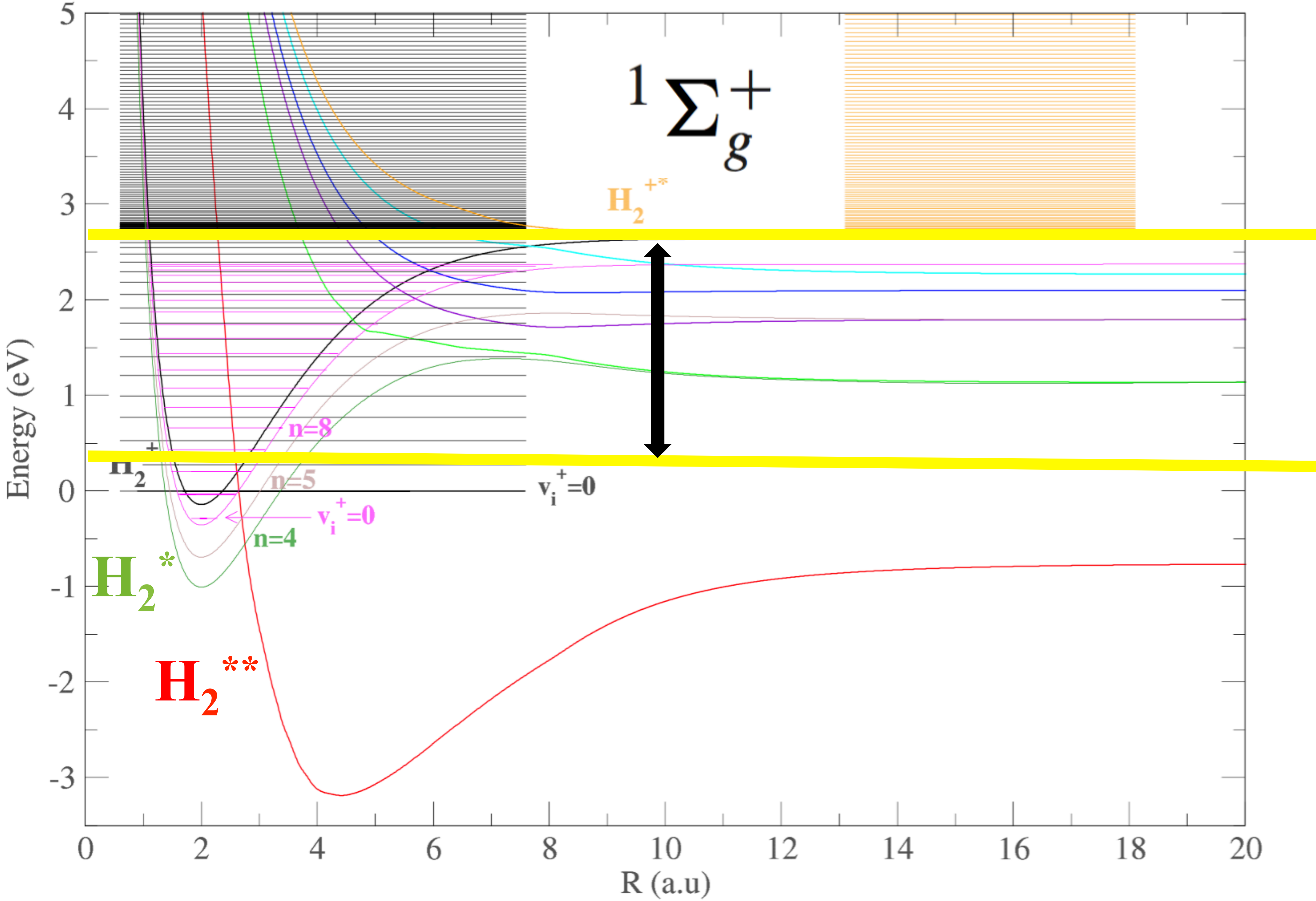
“NO rotation”,

DISCRETE & CONTINUUM

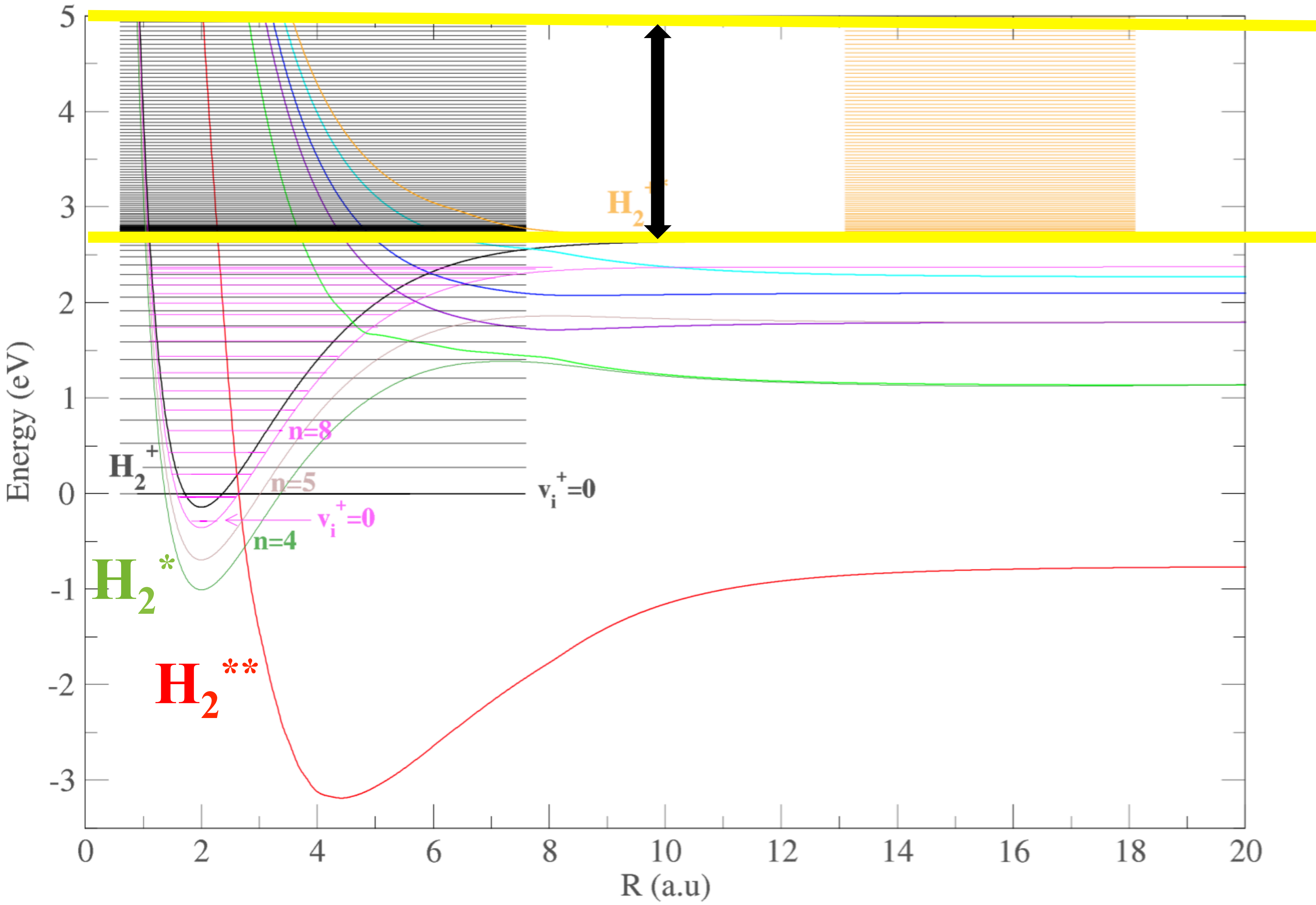
vibrational spectrum,

NO “Fano” RESONANCES

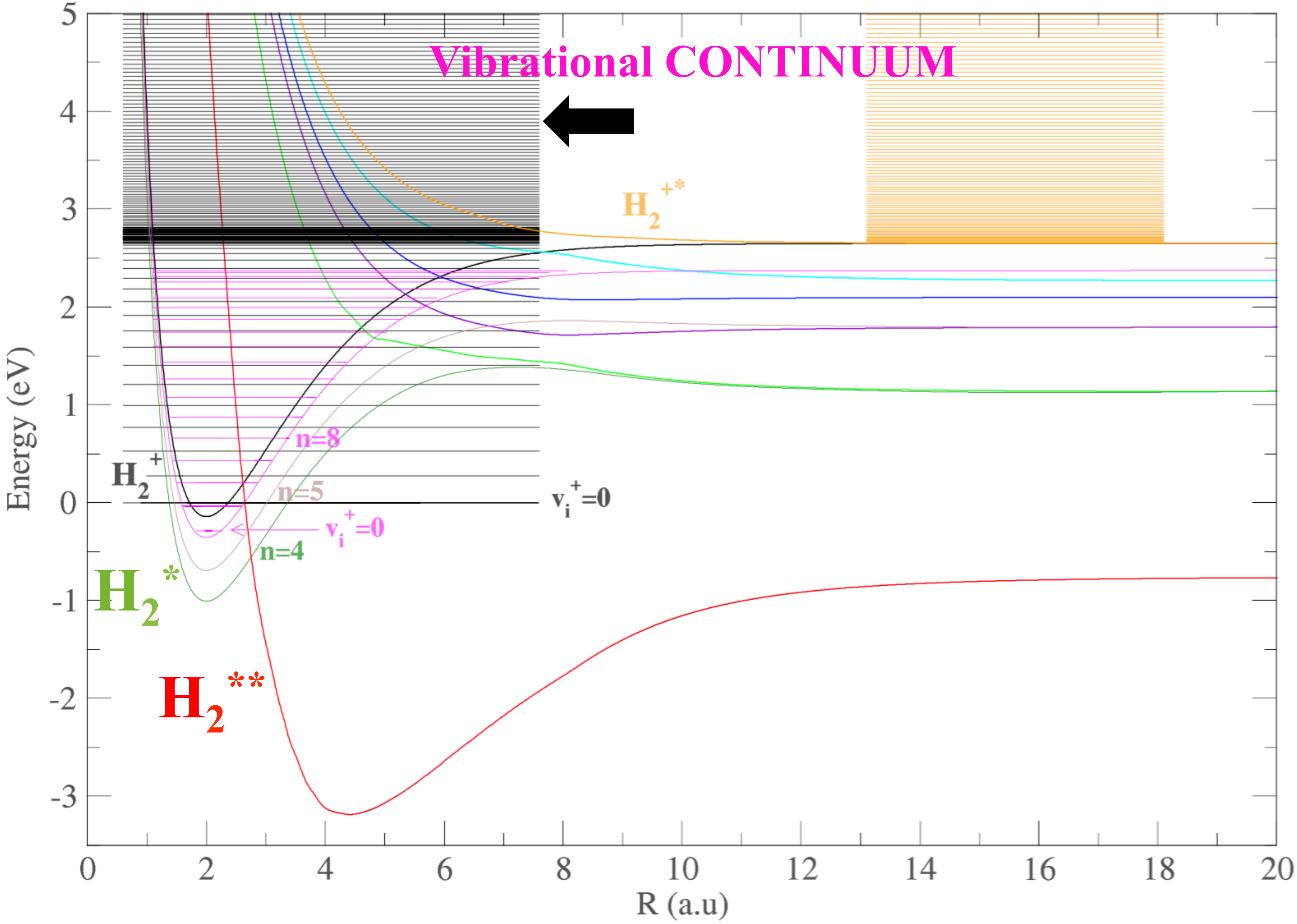
High Energy:



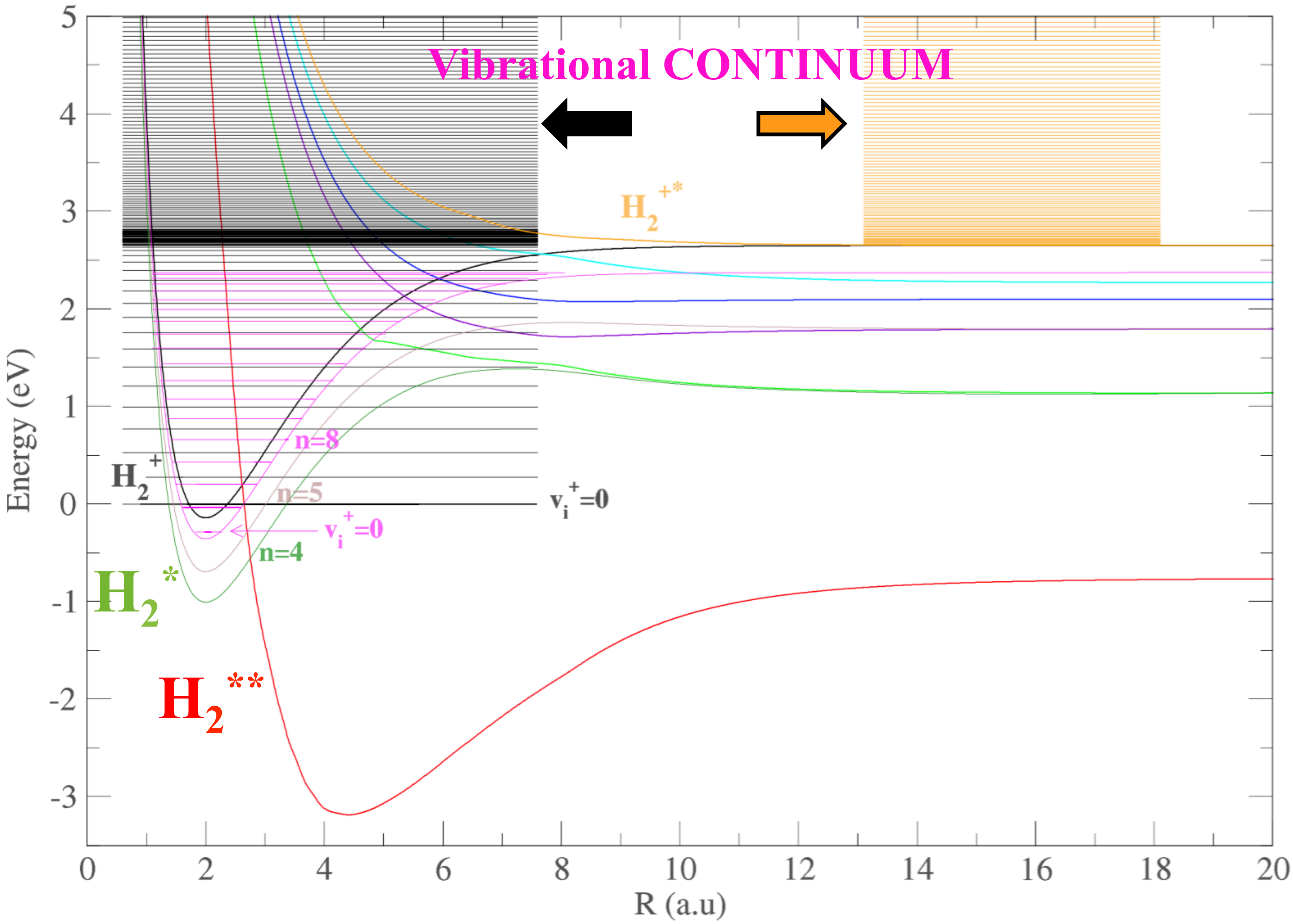
Energy (eV)
R (a.u)
$^1\Sigma_g^+$
H_2^{+*}
H_2^+
n=8
n=5
n=4
$v_i^+=0$
$v_i^+=0$
H_2^*
H_2^{**}



Energy (eV)
R (a.u)
H$_2^+$
v_i^+=0
n=8
n=5
n=4
H$_2^*$
H$_2^{**}$
H$_2^{+*}$



Vibrational CONTINUUM
H_2^{+*}
H_2^+
$v_i^+=0$
n=8
n=5
$v_i^+=0$
n=4
H_2^*
H_2^{**}
Energy (eV)
R (a.u)
5
4
3
2
1
0
-1
-2
-3
0
2
4
6
8
10
12
14
16
18
20

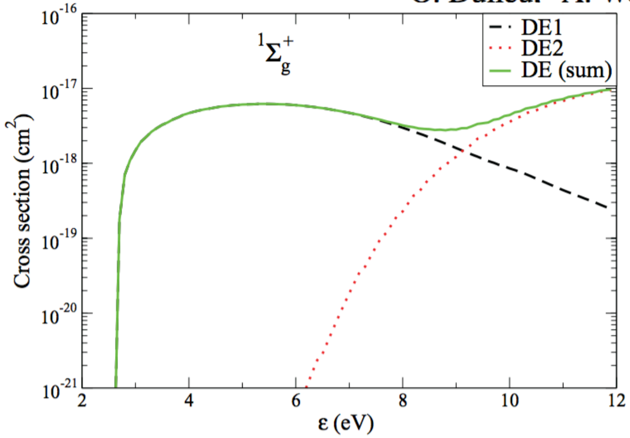


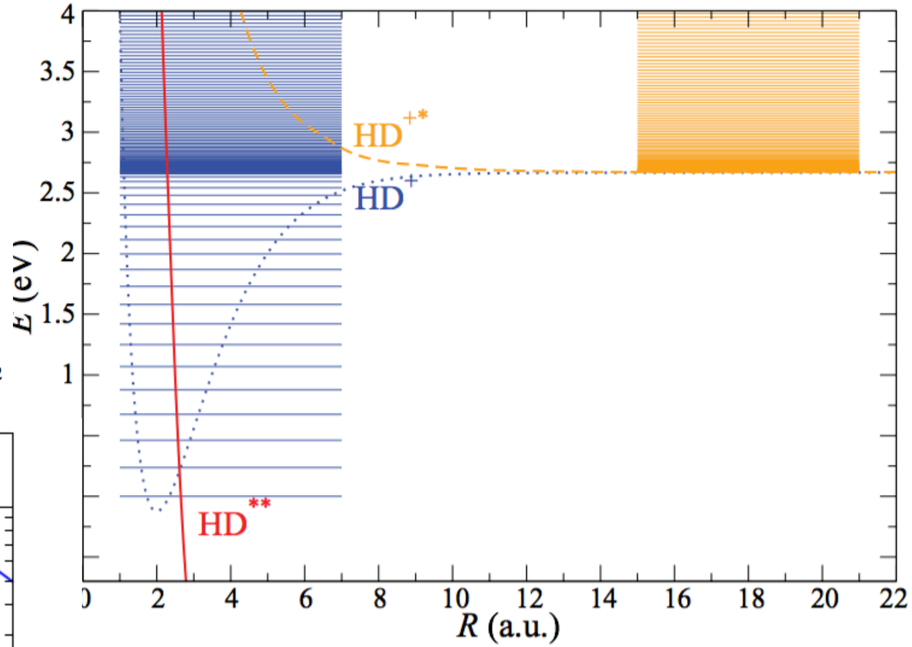
Vibrational CONTINUUM
Energy (eV)
R (a.u)
H_2^{+*}
H_2^{+}
$v_i^{+}=0$
n=8
n=5
$v_i^{+}=0$
n=4
H_2^{*}
H_2^{**}
5
4
3
2
1
0
-1
-2
-3
0
2
4
6
8
10
12
14
16
18
20

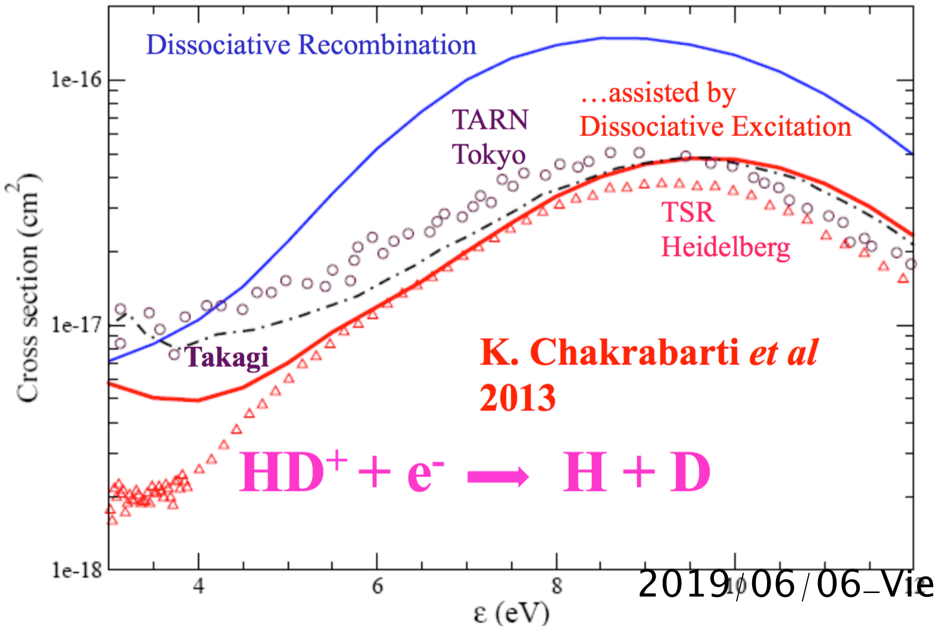
PHYSICAL REVIEW A **87**, 022702 (2013)

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. Schneider[1]

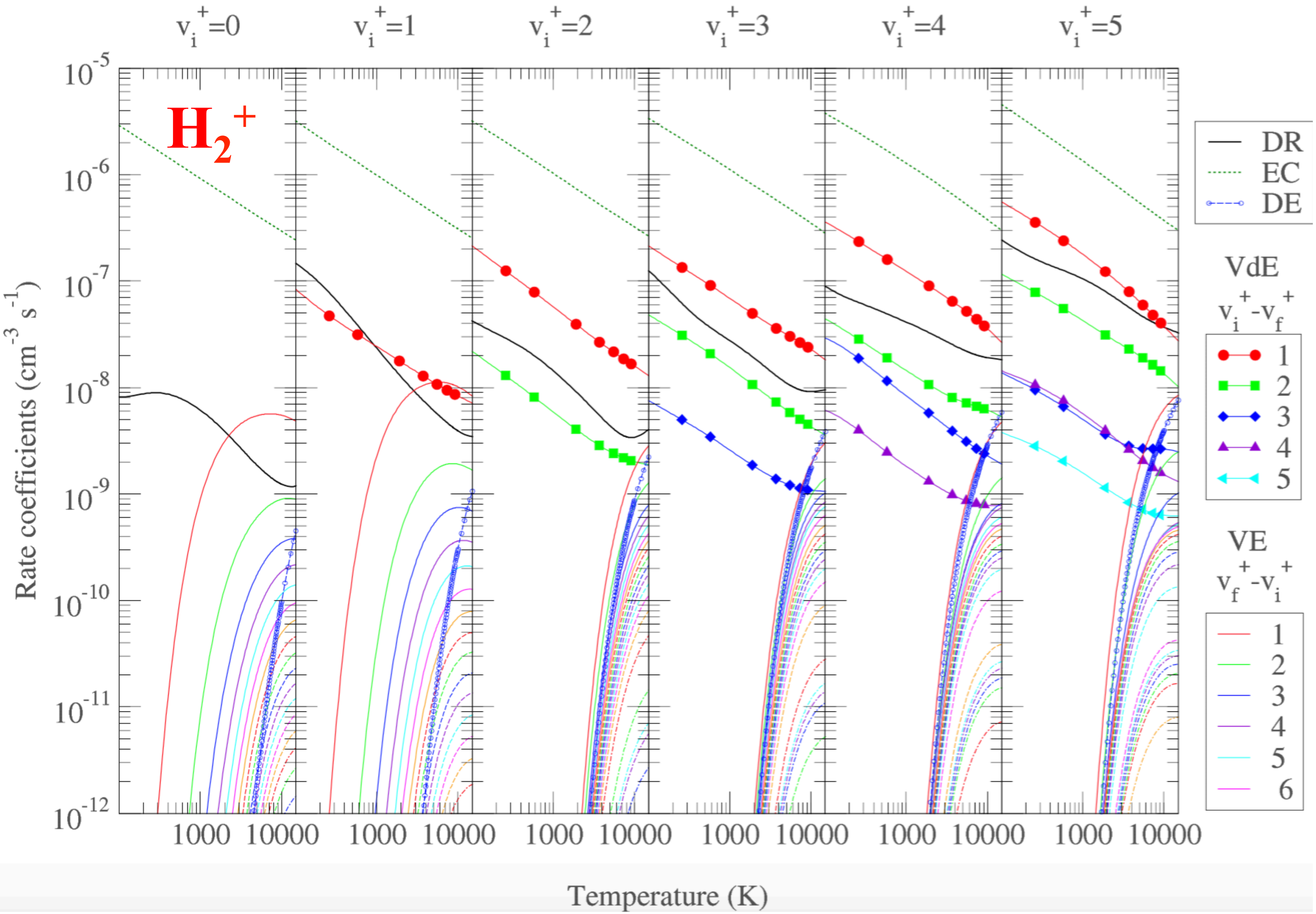






HIGH energy:
vibrational continuum
effective, Dissociative Excitation

Moulane 2017



Draft version March 30, 2019
Typeset using LaTeX default style in AASTeX62

Electron-driven H_2^+/H_2^* dynamics: a broad energy-range state-to-state study

V. Laporta,[1,2,3] Y. Moulane,[4] N. Pop,[1] F. Colboc,[1] M.D. Epée Epée,[5] F. Iacob,[6] J.Zs. Mezei,[1] K. Chakrabarti,[7] O. Motapon,[8] N. Deruette,[1] X. Urbain,[9] A. Wolf,[1] and I.F. Schneider[1,10]

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[9] *Institute of Condensed Matter and Nanosciences, PAMO - Louvain-la-Neuve, Belgium*
[10] *Laboratoire Aimé-Cotton CNRS-UPR-3321, Université Paris-Sud, F-91405 Orsay, France*

(Received January 1, 2018; Revised January 7, 2018; Accepted March 30, 2019)

Submitted to ApJ

ABSTRACT

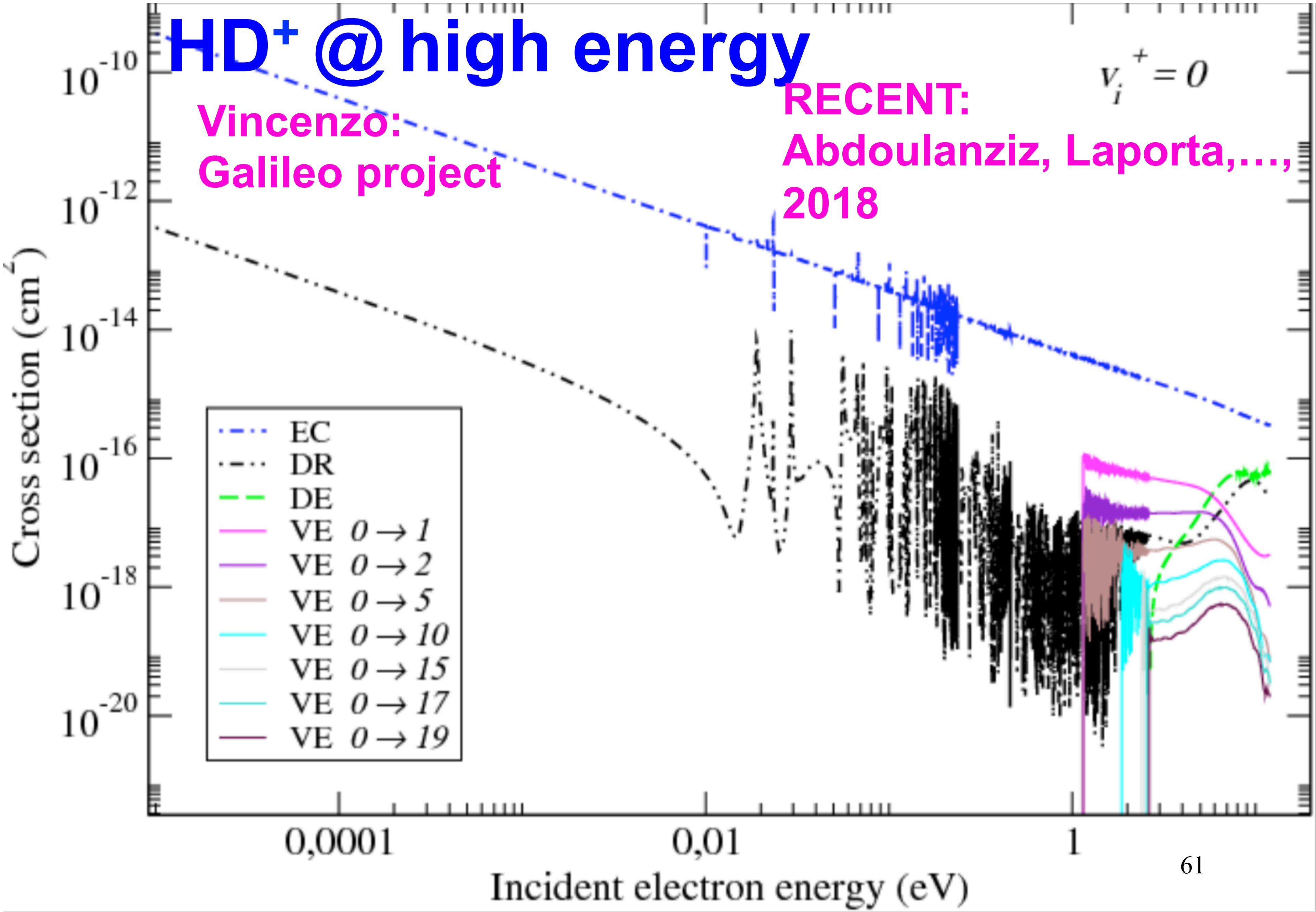
The competition between dissociative recombination, vibrational excitation, and dissociative excitation of H_2^+ molecular cations in electron-impact collisions is discussed within the formalism of the Multichannel Quantum Defect Theory...

Perspectives

HD^+ @ high energy

Vincenzo:
Galileo project

RECENT:
Abdoulanziz, Laporta,…,
2018



HD^+ @ LOW energy

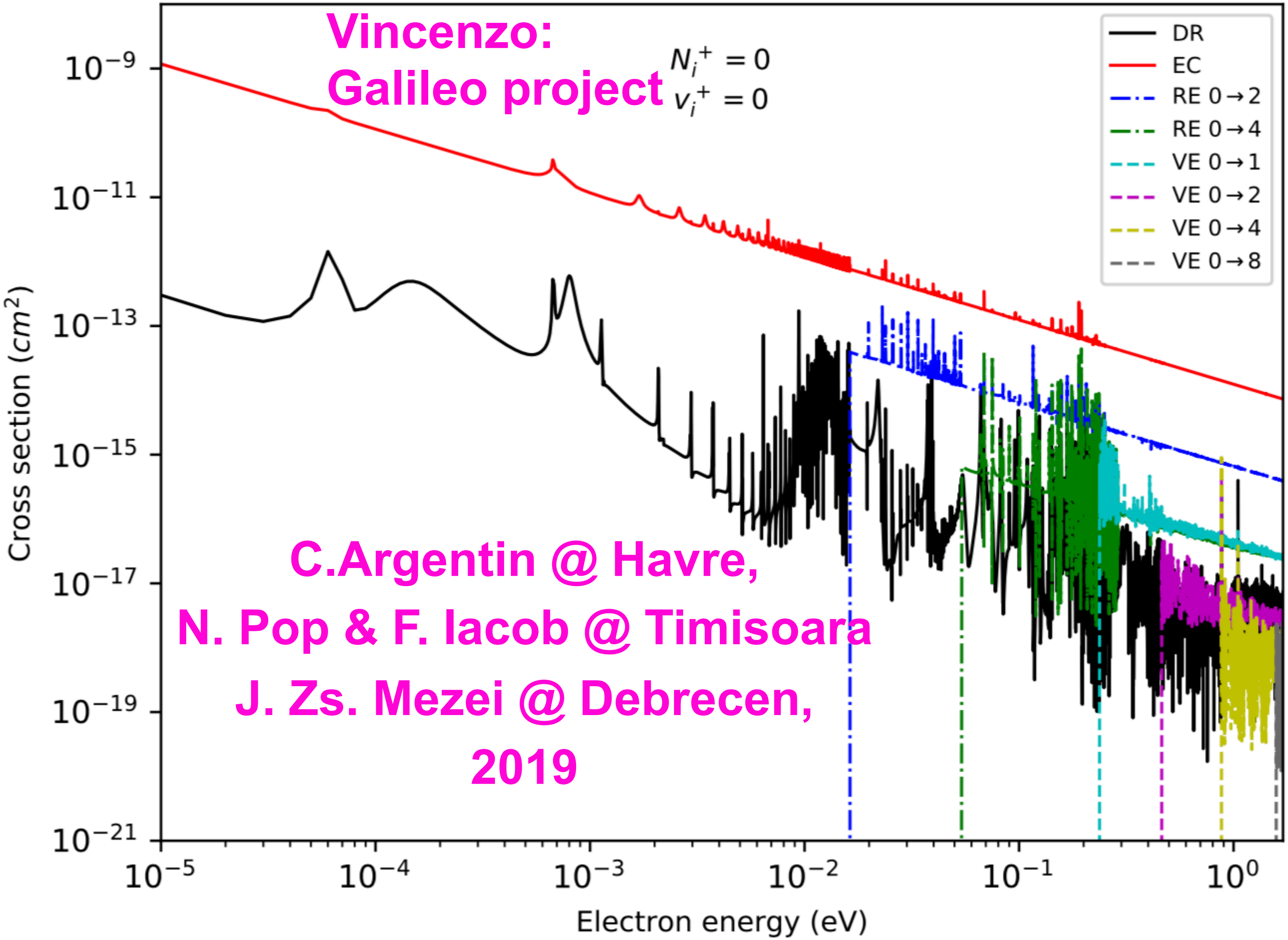
F. Iacob & N. Pop

Energy levels of HD+ rescaled to the lowest
* The energy in (cm-1) is measured against the ion dissociation limit
** The energy in (eV) is measured against the fundamental level (N+ = 0, v+ = 0)

Crt. No.	J	v+	* energy(cm-1)	** energy (eV)	cm-1 to eV
1	0	0	-21515.56	0.00E+00	0.000123985
2	1	0	-21471.7	5.44E-03	
3	2	0	-21384.27	1.63E-02	
4	3	0	-21253.75	3.25E-02	
5	4	0	-21080.96	5.39E-02	
6	5	0	-20866.86	8.04E-02	
7	6	0	-20612.67	1.12E-01	
8	7	0	-20319.79	1.48E-01	
9	8	0	-19989.82	1.89E-01	
10	9	0	-19624.47	2.34E-01	
11	0	1	-19602.72	2.37E-01	
12	1	1	-19560.89	2.42E-01	
13	2	1	-19477.44	2.53E-01	
14	3	1	-19352.9	2.68E-01	
15	10	0	-19225.58	2.84E-01	
16	4	1	-19188.01	2.89E-01	
17	5	1	-18983.74	3.14E-01	
18	11	0	-18795.07	3.37E-01	
19	6	1	-18741.23	3.44E-01	
20	7	1	-18461.87	3.79E-01	
21	12	0	-18334.99	3.94E-01	
22	8	1	-18147.15	4.18E-01	
23	13	0	-17847.37	4.55E-01	
24	9	1	-17798.76	4.61E-01	
25	0	2	-17786.24	4.62E-01	
26	1	2	-17746.31	4.67E-01	
27	2	2	-17666.78	4.77E-01	
28	3	2	-17548.03	4.92E-01	

Vincenzo:
Galileo project

HD^+ @ LOW energy



Need of NEW molecular structure data

? Jonathan

? M. Telmini, Ch. Jungen, Zsolt
PhD @ Tunis & Le Havre, 2019-…

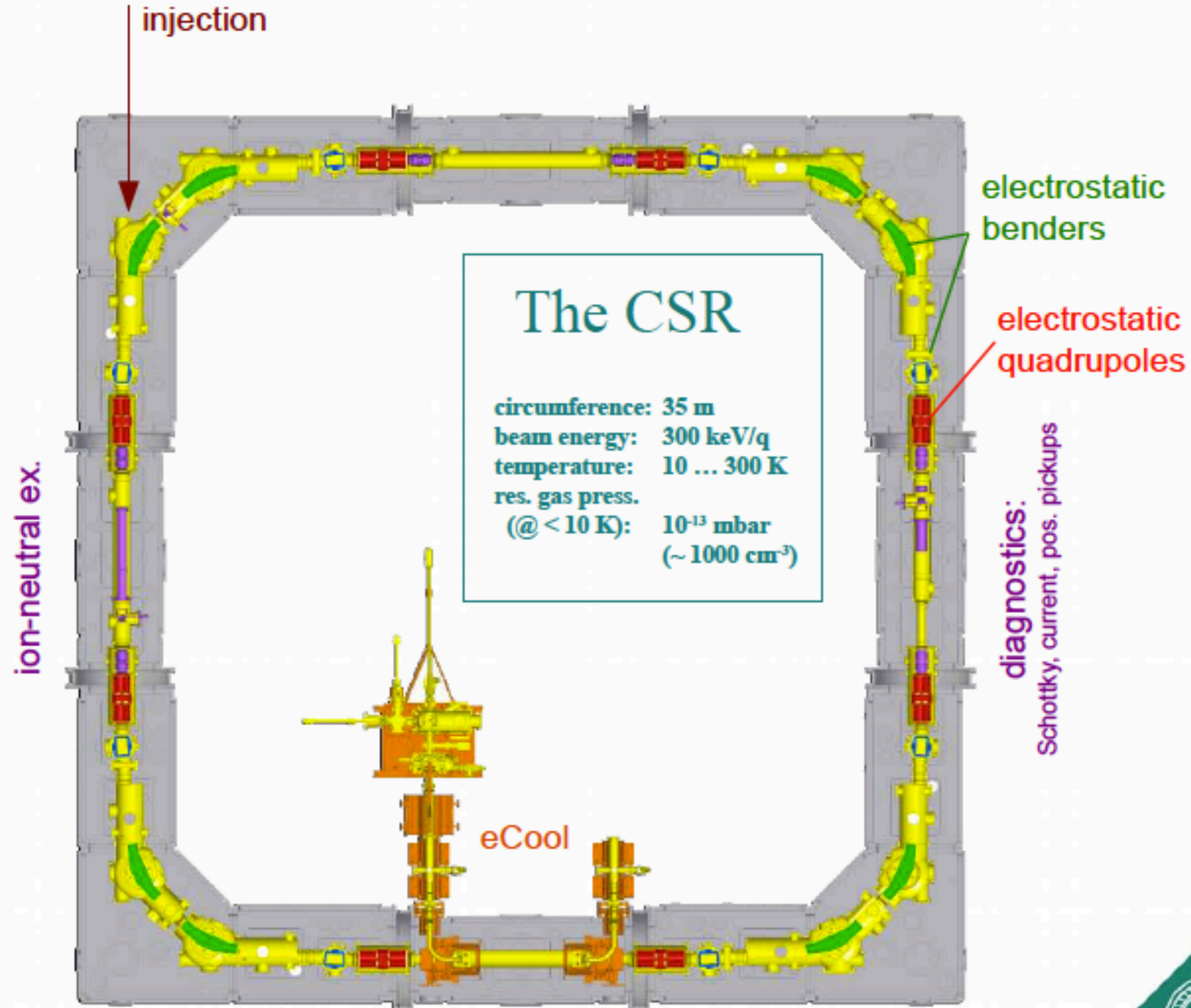
Branching Ratios

NOT very precise with MQDT

And …

the “experimental “

FUTURE



The CSR

circumference:	35 m
beam energy:	300 keV/q
temperature:	10 … 300 K
res. gas press.	
(@ < 10 K):	10^{-13} mbar
	(~ 1000 cm^{-3})

SUPPORT, CONTRATS

esa space for europe

European Space Agency

Fundamental Issues in the Aerothemodynamics of Planetary Atmosphere Re-entry

ESA General Study Programme

University of Perugia

University of Siena

Bergische Universitat Wuppertal

University of Coimbra

University of LeHavre

Istituto Superior Técnico

Université Libre de Bruxelles

Polytechnic Marseille

St Petersburg State Polytechnic University

CNR Institute of Inorganic Methodologies & Plasmas

IAEA

International Atomic Energy Agency

Atoms For Peace

ADAS

Atomic Data and Analysis Structure

SUPORT

AGENCE NATIONALE DE LA RECHERCHE
ANR

PROGRAMME BLANC
Acronyme SUMOSTAI
EDITION 2009

SUperexcited MOlecular STates of Astrophysical Importance : dissociative recombination and spectroscopy

REGION HAUTE NORMANDIE

INSTITUT
Energie
Fluides
Environnement
iefe

FR FCM
Fédération de Recherche
Fusion par Confinement Magnétique - ITER

Project 2009-2010: Reactive Collisions in the Fusion Plasma Edge

Financement

PicoLIBS (2014-2018)

EMoPlaf (2017-2019)

RIN-VIRIDIS-CO2 (2018-2019)

PCMI/INSU (2018-2020)


1 16:30


Thank you for
your attention !