Electronic and photonic reactive collisions in edge fusion plasma: Application to H_2, BeH, CH and N_2 systems

$$AB^+(v_i^+) + e^- \longrightarrow A + B$$

$$AB^+(v_i^+) + e^- \longrightarrow AB^+(v_f^+) + e^-$$

$$AB^+(v_i^+) + e^- \longrightarrow A + B^+ + e^-$$

$$AB(v_i) + h\nu \longrightarrow A + B^+ + e^-, A + B$$

J. Zs. MEZEI & I. F. SCHNEIDER

Université du Havre, LOMC-UMR-6294,
Université Paris-Sud, LAC-UPR-3321

2014/09/29: ADAS @ Warszawa

Electronic and photonic reactive collisions in edge fusion plasma: Application to H_2, BeH, CH and N_2 systems

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Université du Havre, LOMC-UMR-6294,
Université Paris-Sud, LAC-UPR-3321

Results of … and collaboration with: Ch. Jungen, O. Dulieu, J. Robert (Orsay), F. O. Waffeu Tamo, D. Backodissa, (Le Havre), O. Motapon (Douala), S. Niyonzima (Bujumbura) ,K. Chakrabarti (Kolkatta), N. Pop, S. Ilie (Timisoara), A. Wolf (Heidelberg), J. Tennyson, D. Little (London),…

Electron/Molecular cation collisions studied with stepwise-MQDT approach

2014/09/29: ADAS @ Warszawa

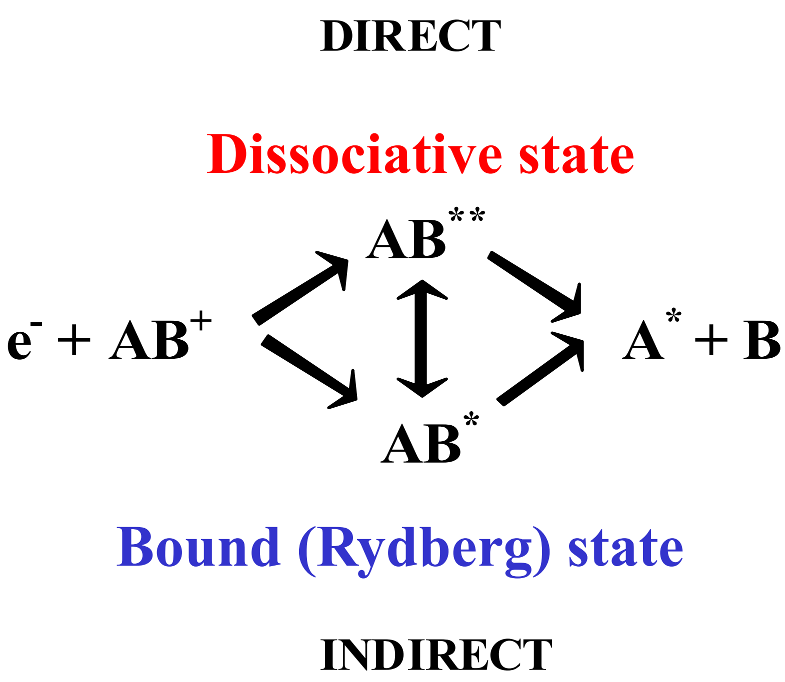
Electron/molecular cation reactive collisions

Main THEORETICAL approach: MQDT

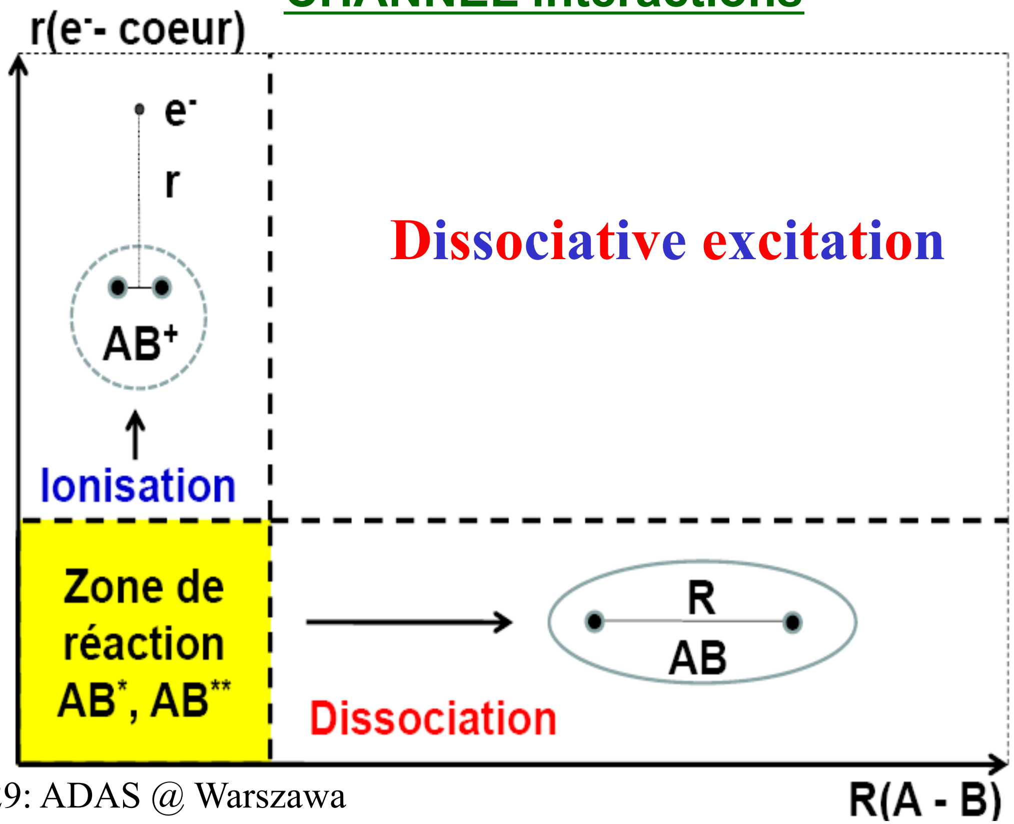
Multichannel Quantum Defect Theory

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

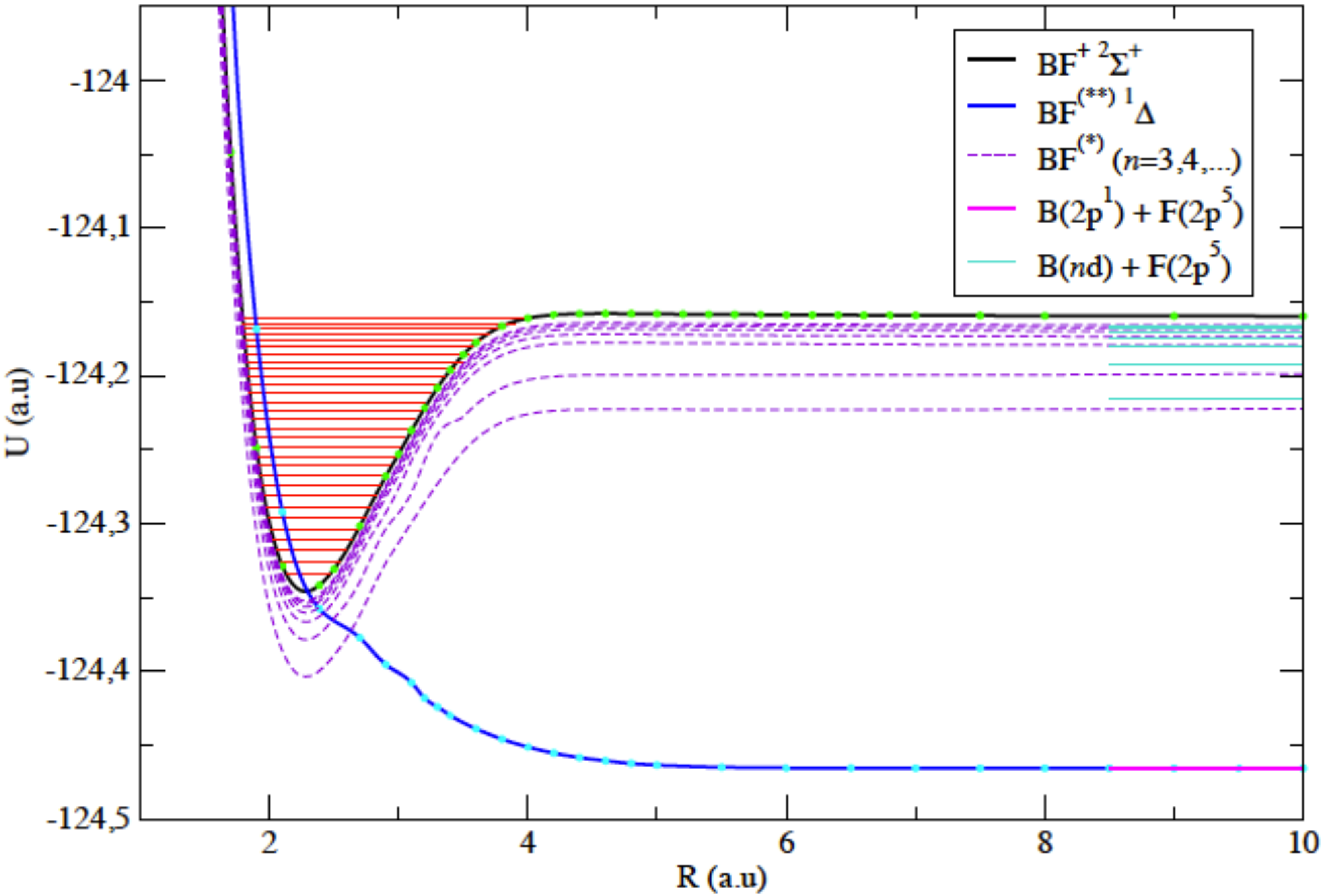
Quantum Interferences



CHANNEL interactions



Example: $BF^{+} + e^{-}$



-124
-124,1
-124,2
-124,3
-124,4
-124,5
U (a.u)
2
4
6
8
10
R (a.u)
BF+ 2Σ+
BF(**) 1Δ
BF(*) (n=3,4,...)
B(2p1) + F(2p5)
B(nd) + F(2p5)

The 18th ADAS Workshop
28-30 September 2014
Regent Warsaw Hotel, Poland

Monday 29th September

14:00 – 15:30 Session 3: Fundamental data (I)

Nigel Badnell	*Dielectronic recombination of W^{18+}: Theory vs. Storage ring measurements*
Matthew Bluteau	*Relativistic R-matrix and Breit-Pauli distorted wave calculations of the electron impact excitation of W^{44+}*
Duck-Hee Kwon	*Electron-impact ionization of complex atoms and ions*
Kanti Aggarwal	*Energy levels, radiative rates and lifetimes for Br-like ions with $Z \geq 38$*

H_2^+ (or isotopomers) + e^-

Atomic Data and Nuclear Data Tables **77,** 161–213 (2001)
doi:10.1006/adnd.2000.0850, available online at http://www.idealibrary.com on IDEAL®

CROSS SECTION DATA FOR ELECTRON-IMPACT INELASTIC PROCESSES OF VIBRATIONALLY EXCITED MOLECULES OF HYDROGEN AND ITS ISOTOPES

R. CELIBERTO

Politecnico di Bari, Italy and Centro di Studio per la Chimica dei Plasmi del C.N.R., Bari, Italy

R. K. JANEV

National Institute for Fusion Science, Toki, Japan, and Macedonian Academy of Sciences and Arts, Skopje, Macedoni

A. LARICCHIUTA

Dipartimento di Chimica, Università di Bari, Italy

M. CAPITELLI

Centro di Studio per la Chimica dei Plasmi del C.N.R., Bari, Italy and Dipartimento di Chimica, Università di Bari, Ital

and

J. M. WADEHRA and D. E. ATEMS

Department of Physics and Astronomy, Wayne State University, Detroit, Michigan 48202

2014/09/29: ADAS @ Warszawa

H_2^+ (or isotopomers) + e^-

LOW energy

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

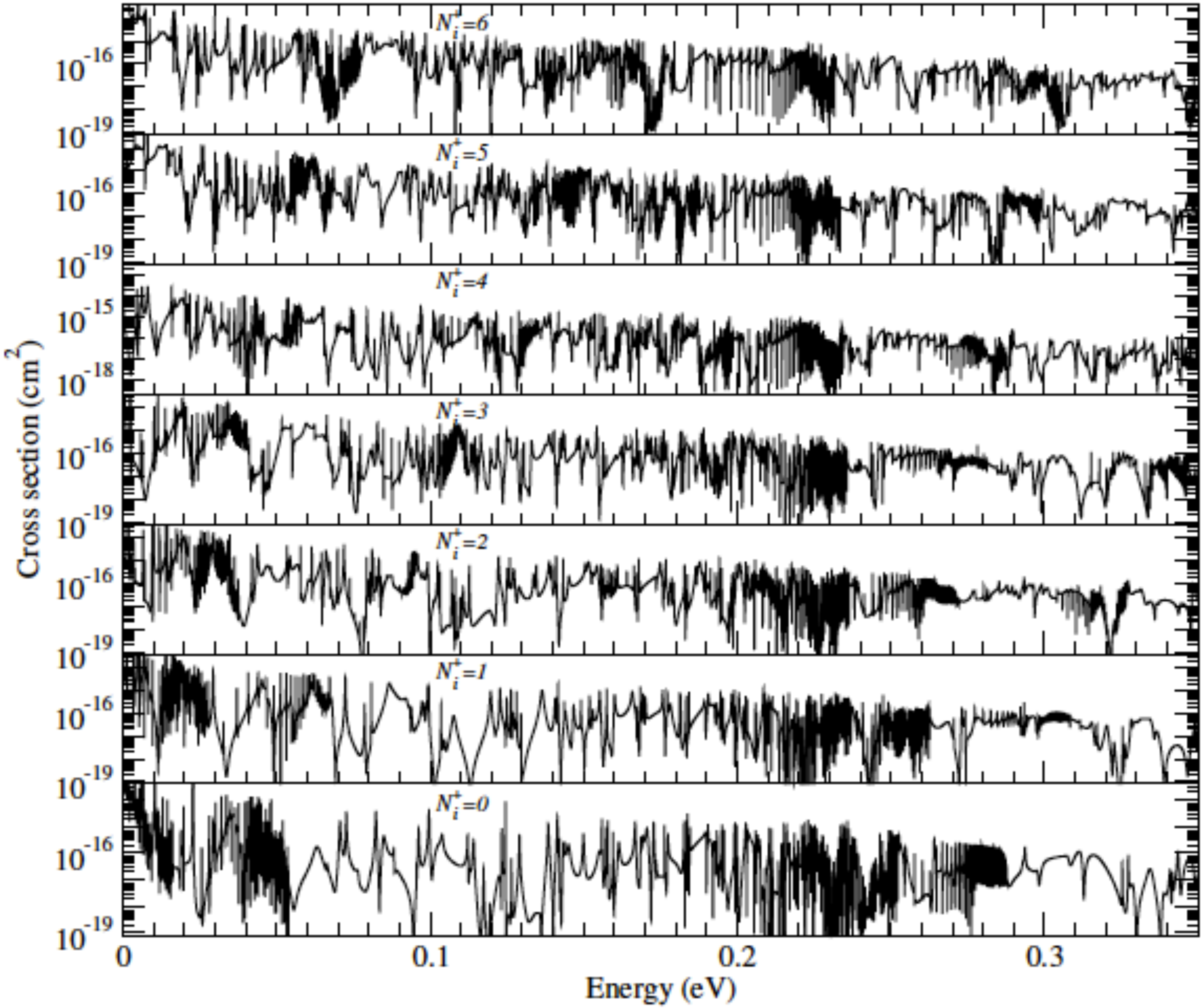


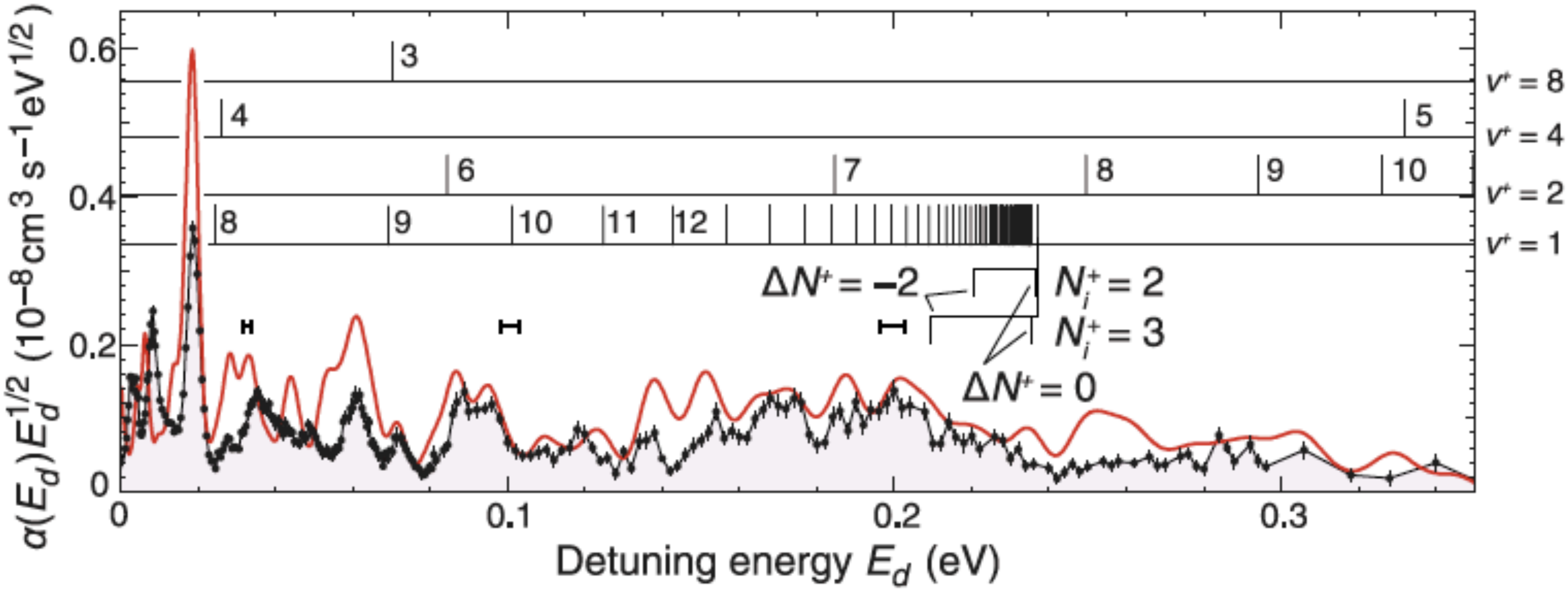
Figure 3. DR cross sections of HD^+ initially in one of its lowest rotational level N_i^+ (vibrational ground state).

PHYSICAL REVIEW A **84**, 022710 (2011)

Assignment of resonances in dissociative recombination of HD⁺ ions: High-resolution measurements compared with accurate computations

F. O. Waffeu Tamo,[1,2,3] H. Buhr,[4,5] O. Motapon,[6] S. Altevogt,[4] V. M. Andrianarijaona,[4,*] M. Grieser,[4] L. Lammich,[4,†] M. Lestinsky,[4,‡] M. Motsch,[4,§] I. Nevo,[5] S. Novotny,[4] D. A. Orlov,[4] H. B. Pedersen,[4,†] D. Schwalm,[4,5] F. Sprenger,[4] X. Urbain,[7] U. Weigel,[4] A. Wolf,[4,‖] and I. F. Schneider[1,¶]

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



HOW was Dissociative Recombination cross section MEASURED ?

The 18th ADAS Workshop
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Monday 29th September

14:00 – 15:30 Session 3: Fundamental data (I)

Nigel Badnell	*Dielectronic recombination of W^{18+}: Theory vs. Storage ring measurements*
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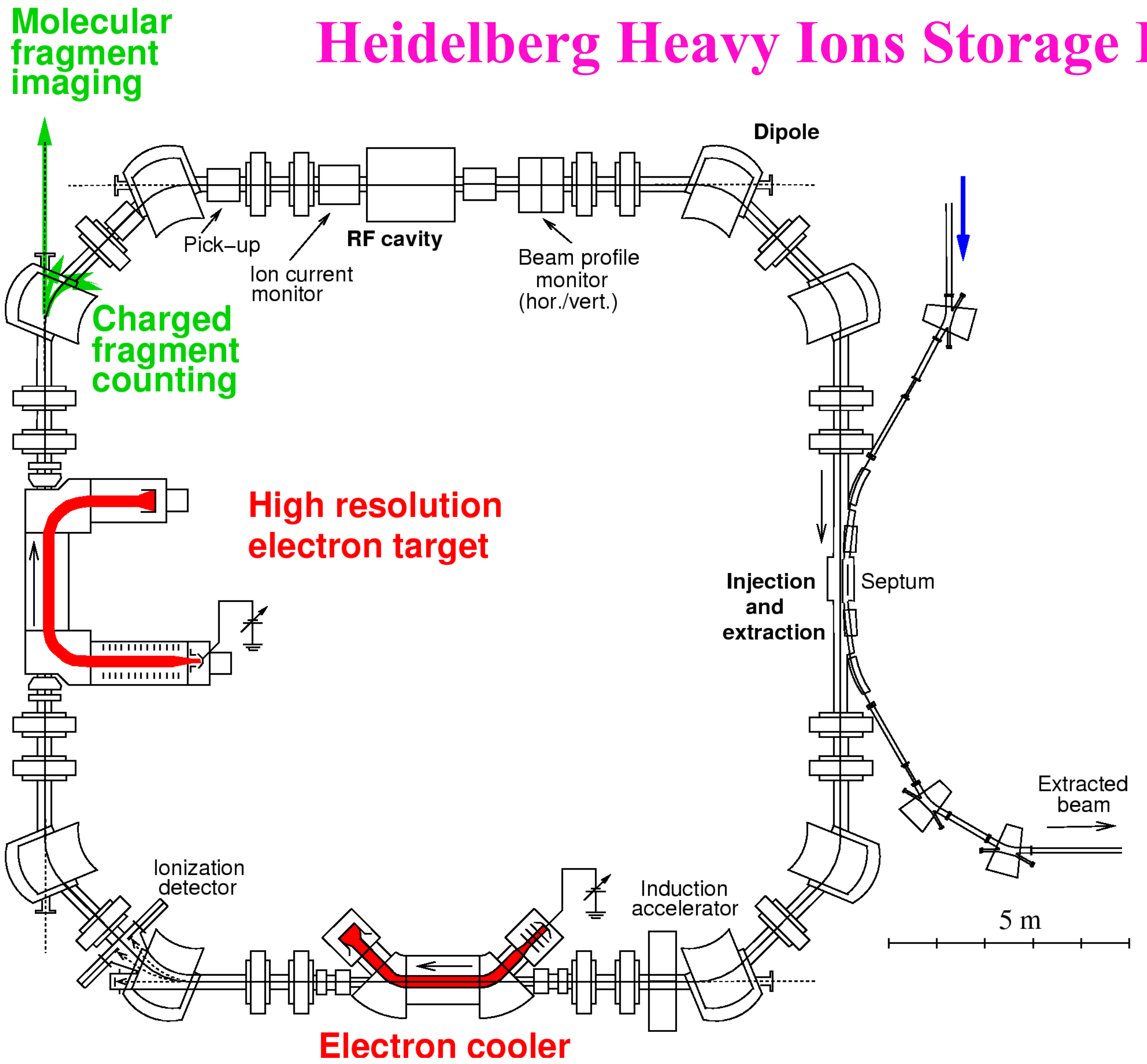
Kanti Aggarwal	*Energy levels, radiative rates and lifetimes for Br-like ions with $Z \geq 38$*

Heidelberg Heavy Ions Storage Ring



Electronic and photonic reactive collisions in edge fusion plasma and interstellar space: Application to H_2 and BeH systems

J. Zs. Mezei[1,2,3], S. Niyonzima[1,4], D. Backodissa[1], N. Pop[5], F. O. Waffeu Tamo[1], K. Chakrabarti[6], O. Motapon[7], A. Wolf[8], J. Robert[2], O. Dulieu[2], Å. Larson[9], A. E. Orel[10], A. Bultel[11] and I. F. Schneider[1,*]

In press @ J. Phys.Conference Series 2014 (IOP)
Report after IAEA-CRP "Light Elements…"

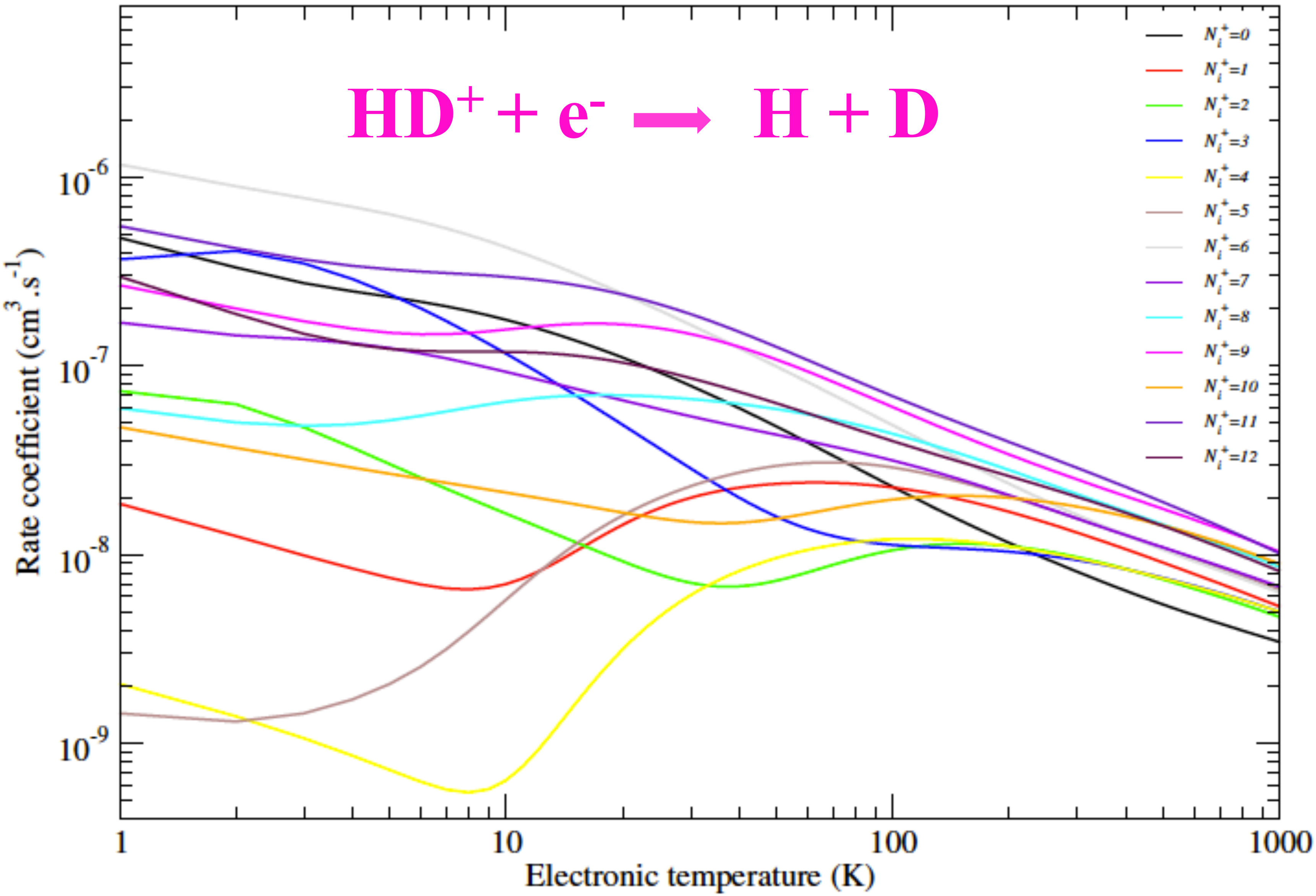


Figure 5. DR rate coefficients of HD^+ initially in one of its lowest rotational level N_i^+ (vibrational ground state).

$$k^{DR}_{(HD^+),N_i^+}(T_e) = A_{N_i^+}\, T_e^{\alpha_{N_i^+}} \exp\left[-\sum_{j=1}^{7} \frac{B_{N_i^+}(j)}{j\, T_e^j}\right],$$

$$k^{DR}_{(HD^+),N_i^+}(T_e) = A_{N_i^+}\, T_e^{\alpha_{N_i^+}} \exp\left[-\sum_{j=1}^{7} \frac{B_{N_i^+}(j)}{j\, T_e^j}\right],$$

Table A4. List of the parameters used in Eq.(A.3) for the DR rate coefficients of HD^+, Fig. 5.

N_i^+	$A_{N_i^+}$	$\alpha_{N_i^+}$	$B_{N_i^+}(1)$	$B_{N_i^+}(2)$	$B_{N_i^+}(3)$	$B_{N_i^+}(4)$	$B_{N_i^+}(5)$	$B_{N_i^+}(6)$	$B_{N_i^+}(7)$
0	0.222071374×10^{-5}	-0.932864010×10^{0}	0.739191072×10^{2}	-0.154789113×10^{5}	0.103315553×10^{7}	-0.316311988×10^{8}	0.493047262×10^{9}	$-0.380248534\times10^{10}$	0.115087036×10^{11}
1	0.128851757×10^{-4}	-0.110718597×10^{1}	0.171547468×10^{3}	-0.133254014×10^{5}	0.636973066×10^{6}	-0.162724883×10^{8}	0.225760856×10^{9}	$-0.161473237\times10^{10}$	0.465576516×10^{10}
2	0.114310768×10^{-4}	-0.109891626×10^{1}	0.228874916×10^{3}	-0.626220862×10^{4}	-0.292604786×10^{6}	0.162301810×10^{8}	-0.292959848×10^{9}	0.235215411×10^{10}	$-0.713445323\times10^{10}$
3	0.210694935×10^{-4}	-0.115741172×10^{1}	0.387330067×10^{3}	-0.458061947×10^{5}	0.215862337×10^{7}	-0.524142418×10^{8}	0.692418139×10^{9}	$-0.472234646\times10^{10}$	0.130101406×10^{11}
4	0.104194981×10^{-4}	-0.107653008×10^{1}	0.259272046×10^{3}	-0.225402550×10^{5}	0.113744859×10^{7}	-0.302083722×10^{8}	0.434933765×10^{9}	$-0.321416426\times10^{10}$	0.951009824×10^{10}
5	0.134920614×10^{-4}	-0.109088522×10^{1}	0.147709496×10^{3}	-0.107365043×10^{5}	0.588051475×10^{6}	-0.175373466×10^{8}	0.276671733×10^{9}	$-0.217615510\times10^{10}$	0.671291314×10^{10}
6	0.874218683×10^{-5}	-0.104397770×10^{1}	0.847564491×10^{2}	-0.147034346×10^{5}	0.931407905×10^{6}	-0.280229117×10^{8}	0.434010714×10^{9}	$-0.333951526\times10^{10}$	0.101015040×10^{11}
7	0.130857676×10^{-4}	-0.107990536×10^{1}	0.164277599×10^{3}	-0.169491618×10^{5}	0.867333556×10^{6}	-0.237117821×10^{8}	0.350008362×10^{9}	$-0.262310582\times10^{10}$	0.781247654×10^{10}
8	0.206886625×10^{-4}	-0.111130085×10^{1}	0.161516618×10^{3}	-0.169829856×10^{5}	0.933477114×10^{6}	-0.266848249×10^{8}	0.404489322×10^{9}	$-0.308099132\times10^{10}$	0.927053336×10^{10}
9	0.323544041×10^{-4}	-0.114880459×10^{1}	0.190230296×10^{3}	-0.277588793×10^{5}	0.167583946×10^{7}	-0.488514291×10^{8}	0.739258454×10^{9}	$-0.559128198\times10^{10}$	0.166941689×10^{11}
10	0.474515481×10^{-4}	-0.120225797×10^{1}	0.320379237×10^{3}	-0.242842906×10^{5}	0.891353217×10^{6}	-0.189565820×10^{8}	0.237461583×10^{9}	$-0.161098316\times10^{10}$	0.452761220×10^{10}
11	0.439397909×10^{-4}	-0.119221433×10^{1}	0.177276579×10^{3}	-0.239180085×10^{5}	0.135806621×10^{7}	-0.381412189×10^{8}	0.563259564×10^{9}	$-0.418763908\times10^{10}$	0.123461437×10^{11}
12	0.246800711×10^{-4}	-0.113548321×10^{1}	0.210755163×10^{3}	-0.267666526×10^{5}	0.148126308×10^{7}	-0.412669275×10^{8}	0.608552008×10^{9}	$-0.452848138\times10^{10}$	0.133722848×10^{11}

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]

PHYSICAL REVIEW A 90, 012706 (2014)

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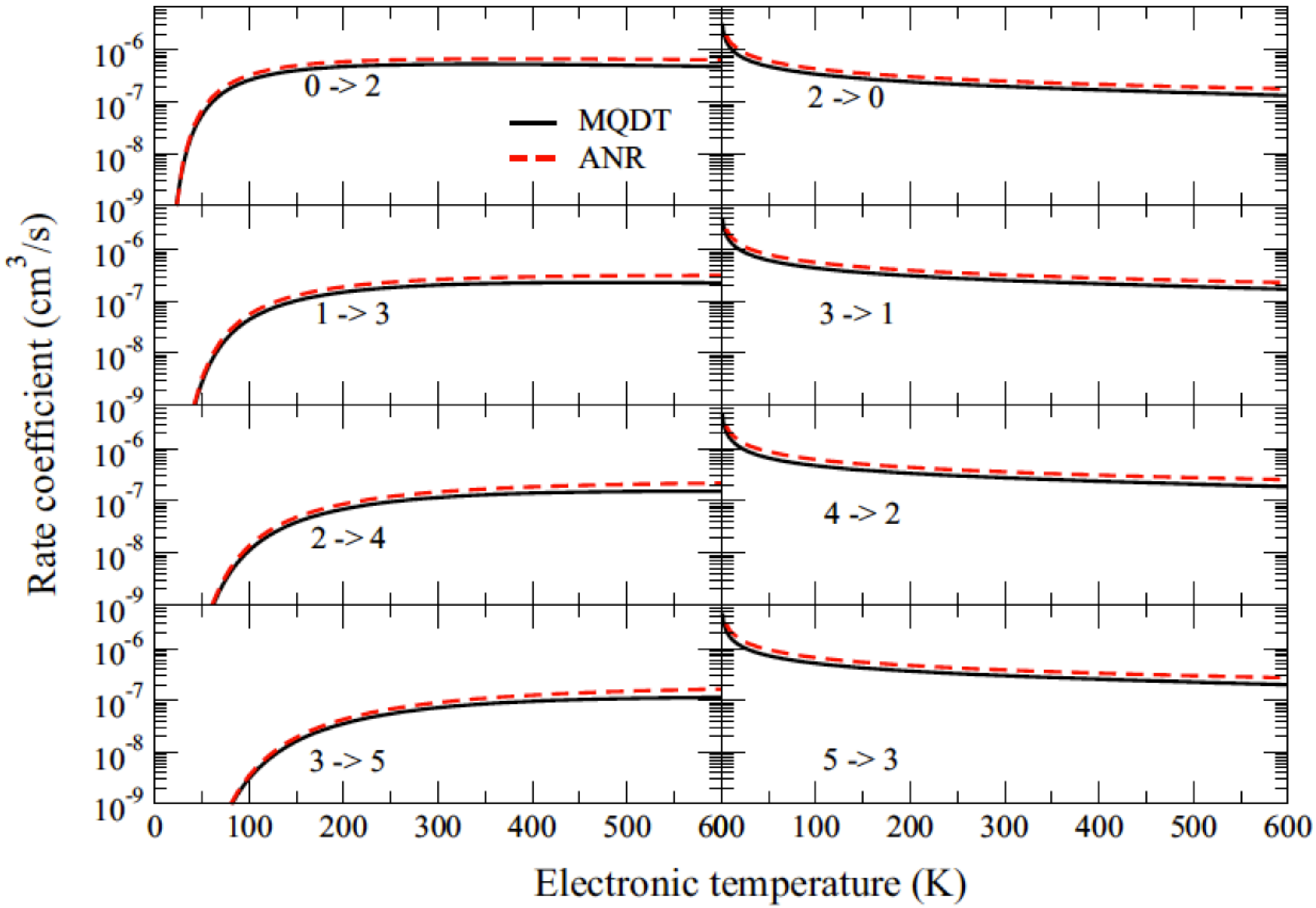
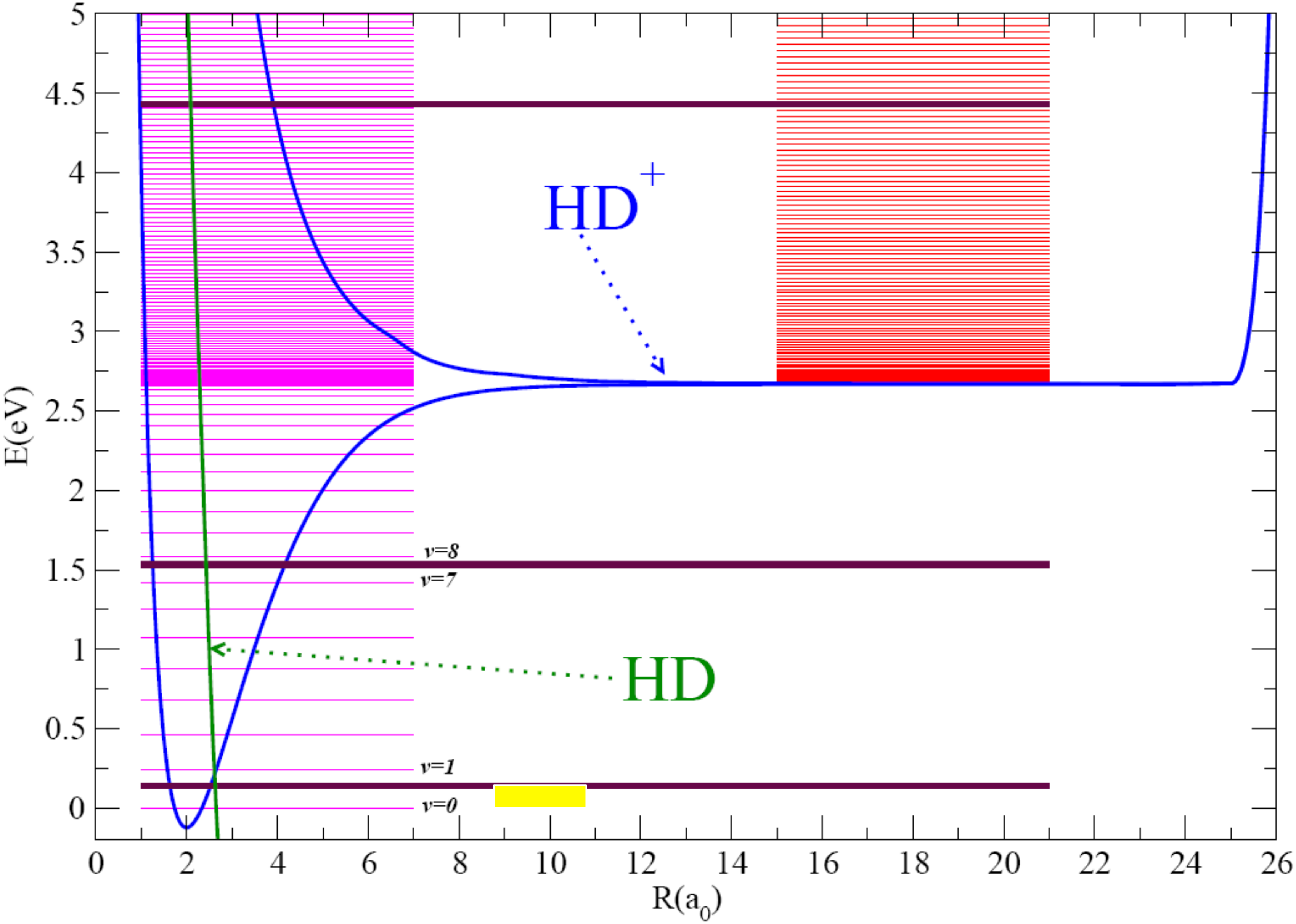


H_2^+ (or isotopomers) + e^-

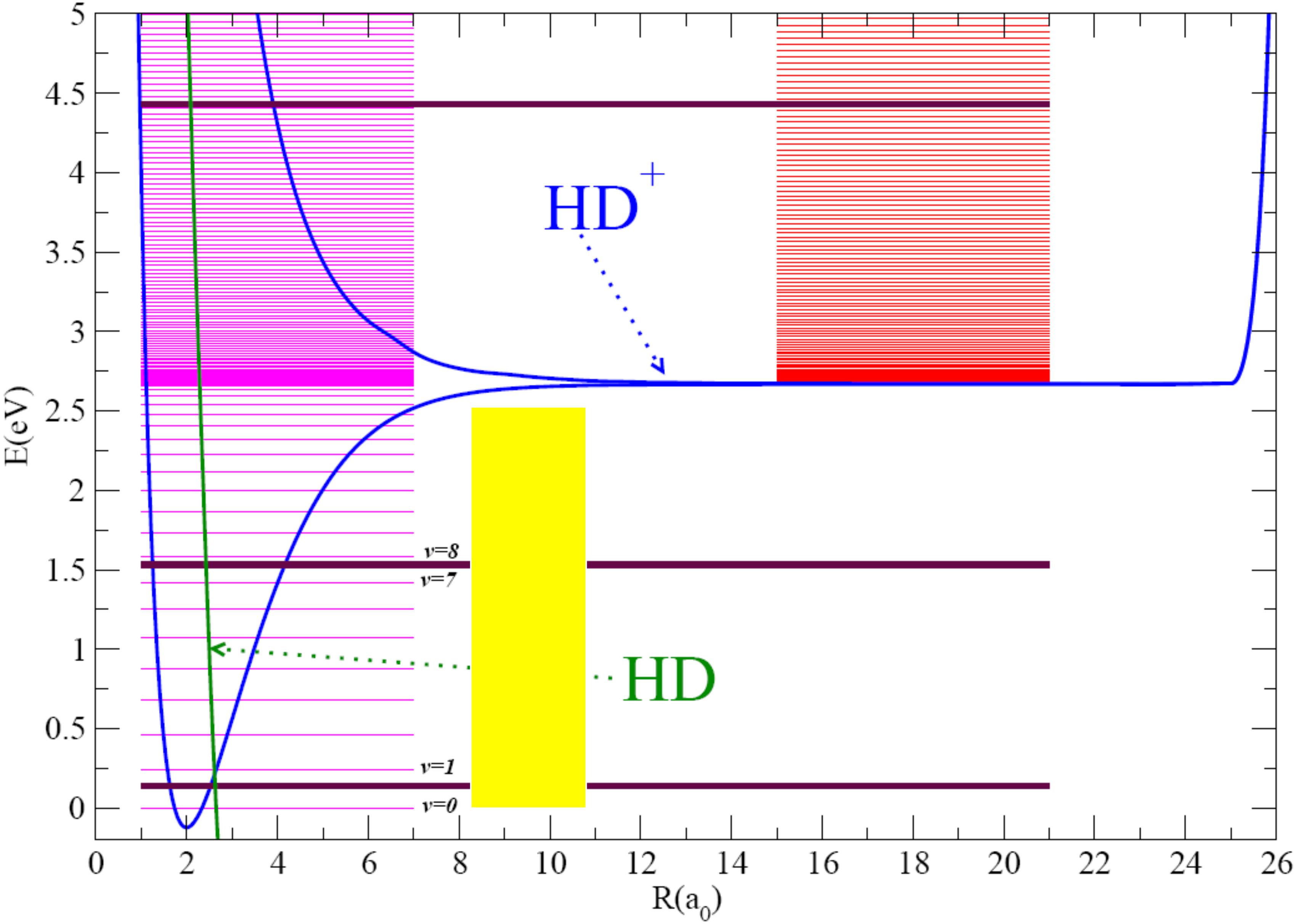
HIGH energy

HIGH energy: the role of DISSOCIATIVE EXCITATION

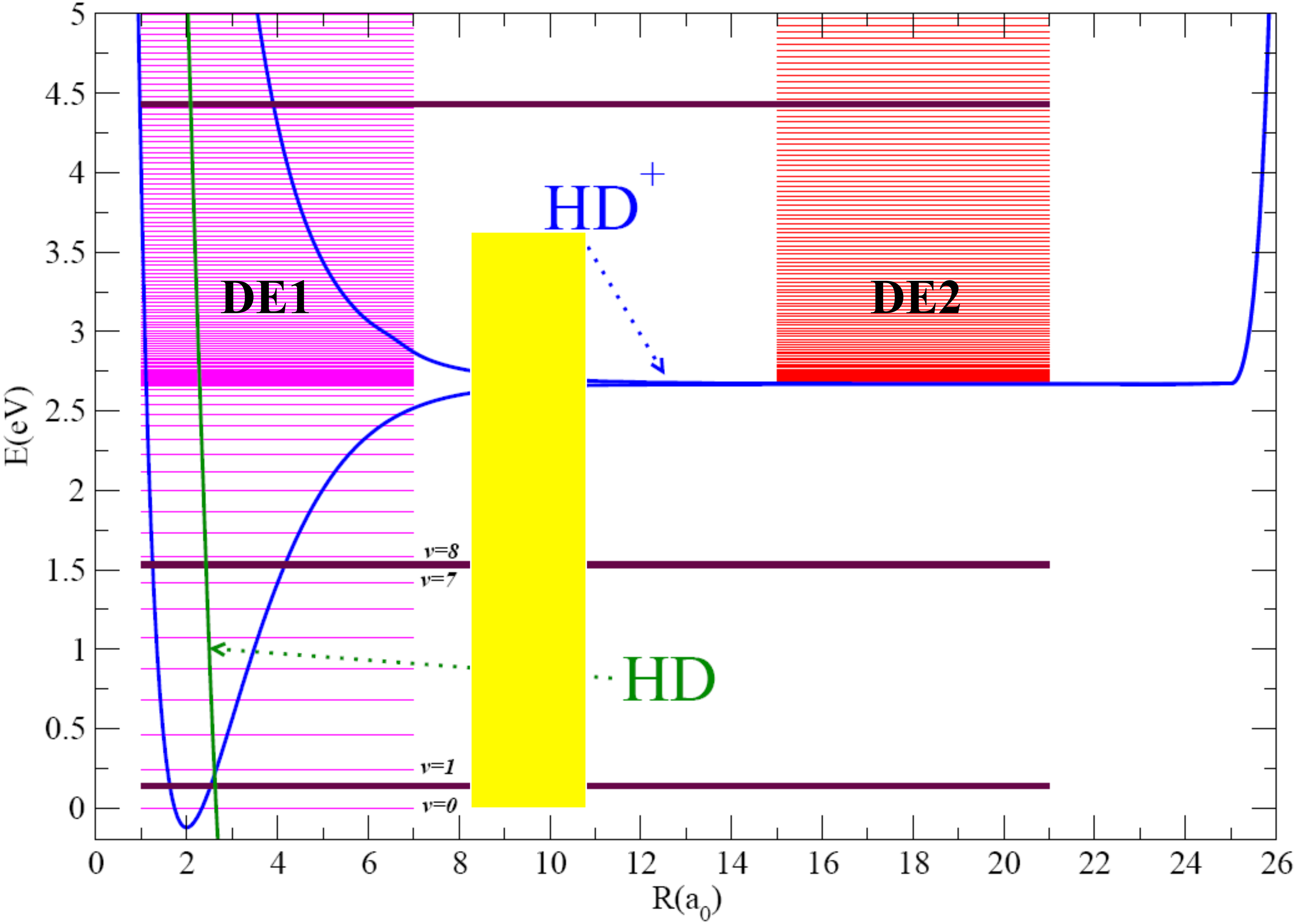
2014/09/29: ADAS @ Warszawa



E(eV)
R(a$_0$)
HD$^+$
HD
v=8
v=7
v=1
v=0



HD+
HD
v=8
v=7
v=1
v=0
E(eV)
R(a0)



HD+
DE1
DE2
HD
v=8
v=7
v=1
v=0
E(eV)
R(a_0)

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

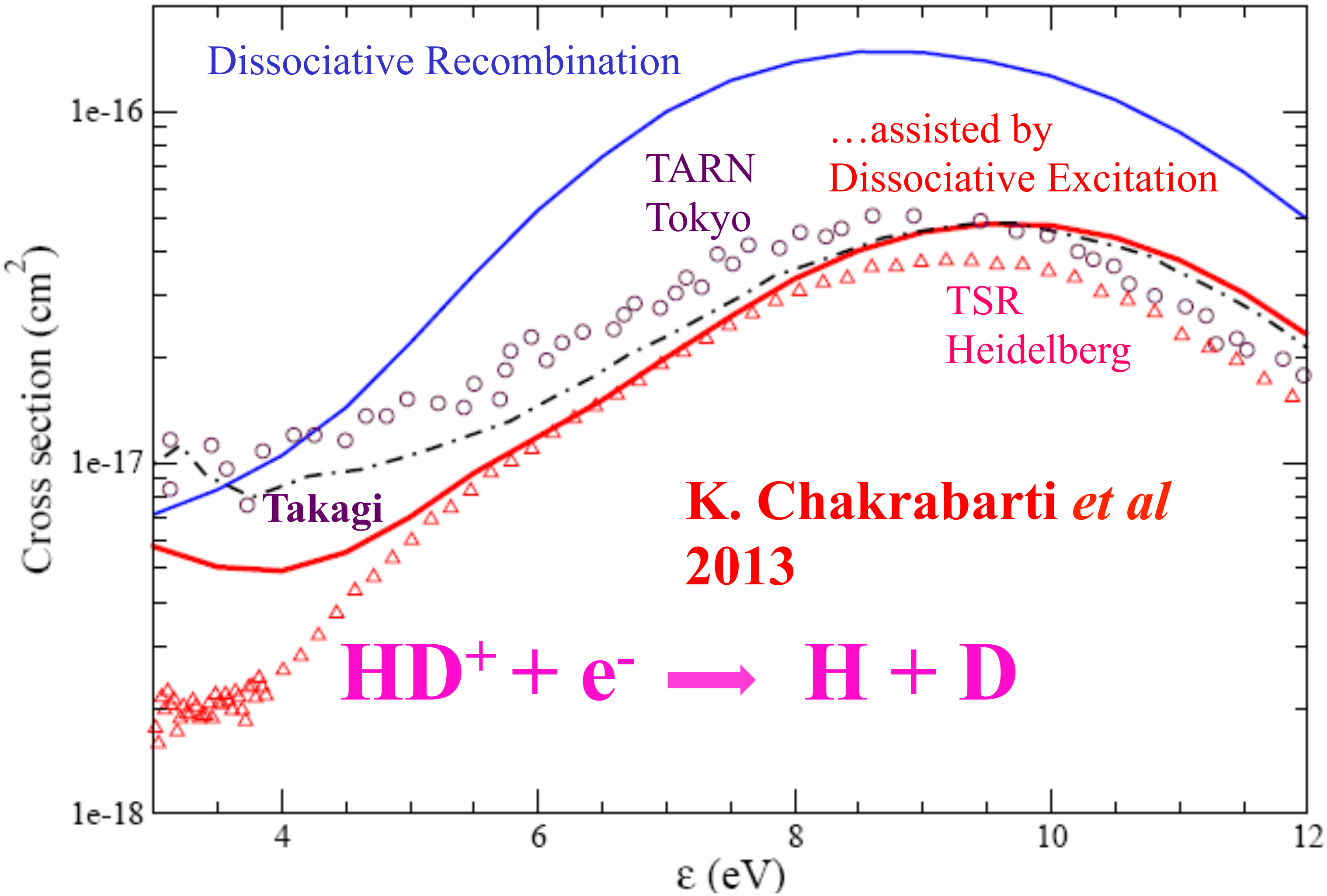
Dissociative recombination of electrons with diatomic molecular cations above dissociation threshold: Application to H_2^+ and HD^+

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]

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]



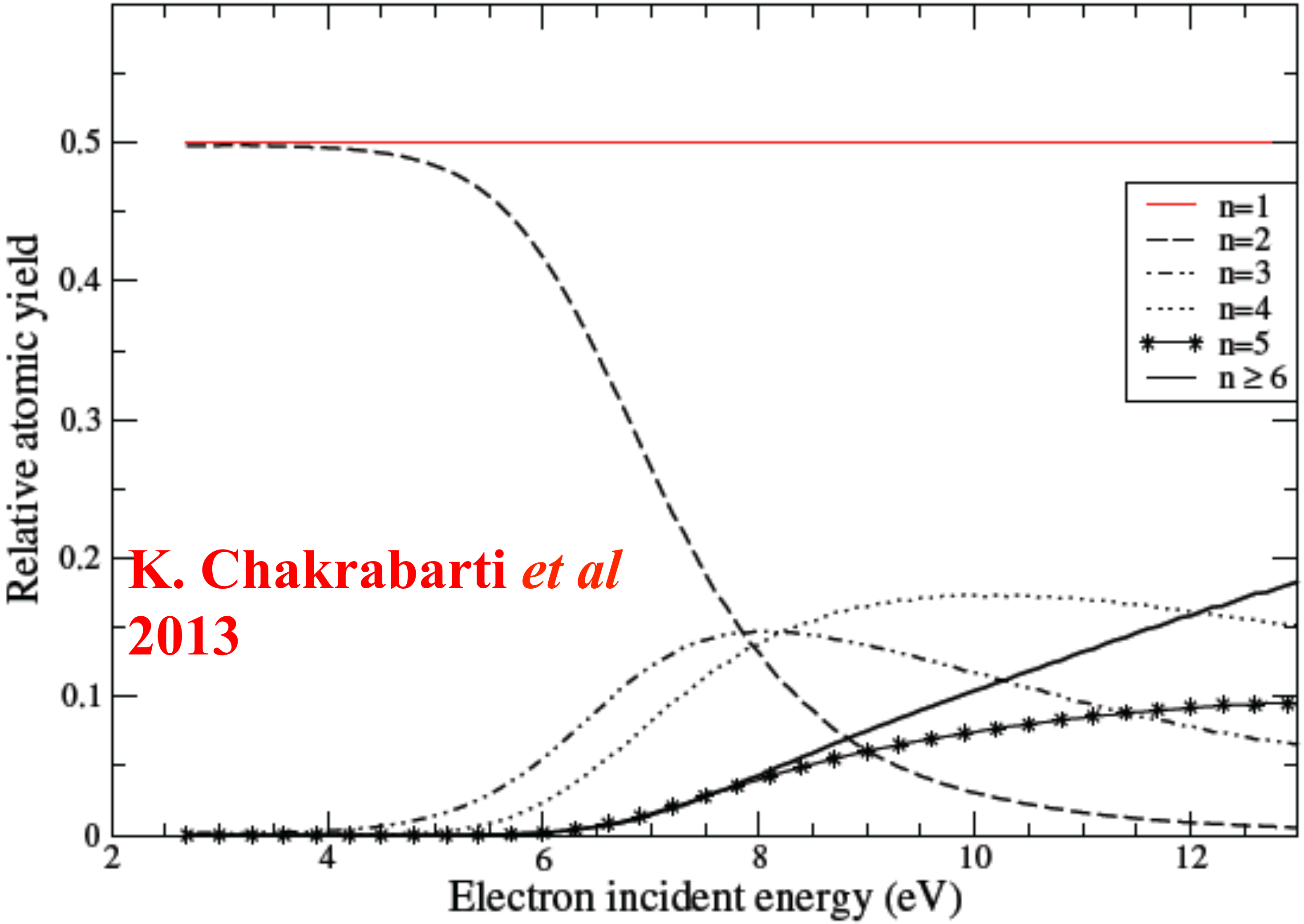


FIG. 7: (Colour online) Dissociative recombination of ground state HD^+ ion, relative atomic H(n) or D(n) final states yields.

The 18th ADAS Workshop
28-30 September 2014
Regent Warsaw Hotel, Poland

Monday 29th September

09:10 – 10:30 Session 1: Reports from Laboratories

Andrzej Fludra	*EUV spectroscopy of the solar atmosphere from the SPICE spectrometer on the Solar Orbiter mission*
Andy Meigs	*Electron temperature from high-n Balmer series at JET: A question of spectra? Or more?*
Stuart Loch	*Recent progress on SXBs for complex species and light species excited state ionization calculations for GCR data*
Amy Shumack	*High-resolution X-Ray diagnostic upgrade for ITER-like wall experiments at JET*

The 18th ADAS Workshop
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However, Kurt Behringer sais

MAR doesn't matter…☹

Monday 29th September

09:10 – 10:30 Session 1: Reports from Laboratories

Andrzej Fludra	*EUV spectroscopy of the solar atmosph… from the SPICE spectrometer on the Solar Orbiter mission*
Andy Meigs	*Electron temperature from high-n Balmer series at JET: A question of spectra? Or more?*
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$BeH^{+} + e^{-}$

IOP PUBLISHING PLASMA PHYSICS AND CONTROLLED FUSION
Plasma Phys. Control. Fusion 54 (2012) 035012 (11pp) doi:10.1088/0741-3335/54/3/035012

State-to-state electron impact cross sections for BeH^+ molecular ions in ITER-like fusion edge plasmas with Be walls

R Celiberto[1,2], R K Janev[3,4] and D Reiter[4]

[1] Department of Water Engineering and Chemistry, Polytechnic of Bari, 70125 Bari, Italy
[2] Institute of Inorganic Methodologies and Plasmas, CNR, 70125 Bari, Italy
[3] Macedonian Academy of Sciences and Arts, PO Box 428, 1000 Skopje, Macedonia
[4] Institute of Energy and Climate Research - Plasma Physics, Forschungszentrum Jülich GmbH Association EURATOM-FZJ, Partner in Trilateral Euregio Cluster, 52425 Jülich, Germany

The 18th ADAS Workshop
28-30 September 2014
Regent Warsaw Hotel, Poland

Tuesday 30th September

09:00 – 10:30 Session 5: Spectroscopy

Kurt Behringer	*Modelling of Lyman and Fulcher Band Spectra – Vibrational and Rotational Population*
Dmitry Borodin	*Interpretation of the Be and BeD spectroscopy in the recent plasma-wall interaction experiments*
Matthew Carr	*CXRS diagnostics on MAST*
Yang Yang	*Spectroscopic results of W^{11+}-W^{15+}in EUV region, observed in the SH-HtscEBIT (Shanghai High-Temperature-Super-Conduct Electron Beam Ion Trap), and relative calculations*
Stuart Loch	*Discrepancies in Fe XVII line ratios*

PHYSICAL REVIEW A **87**, 022713 (2013)

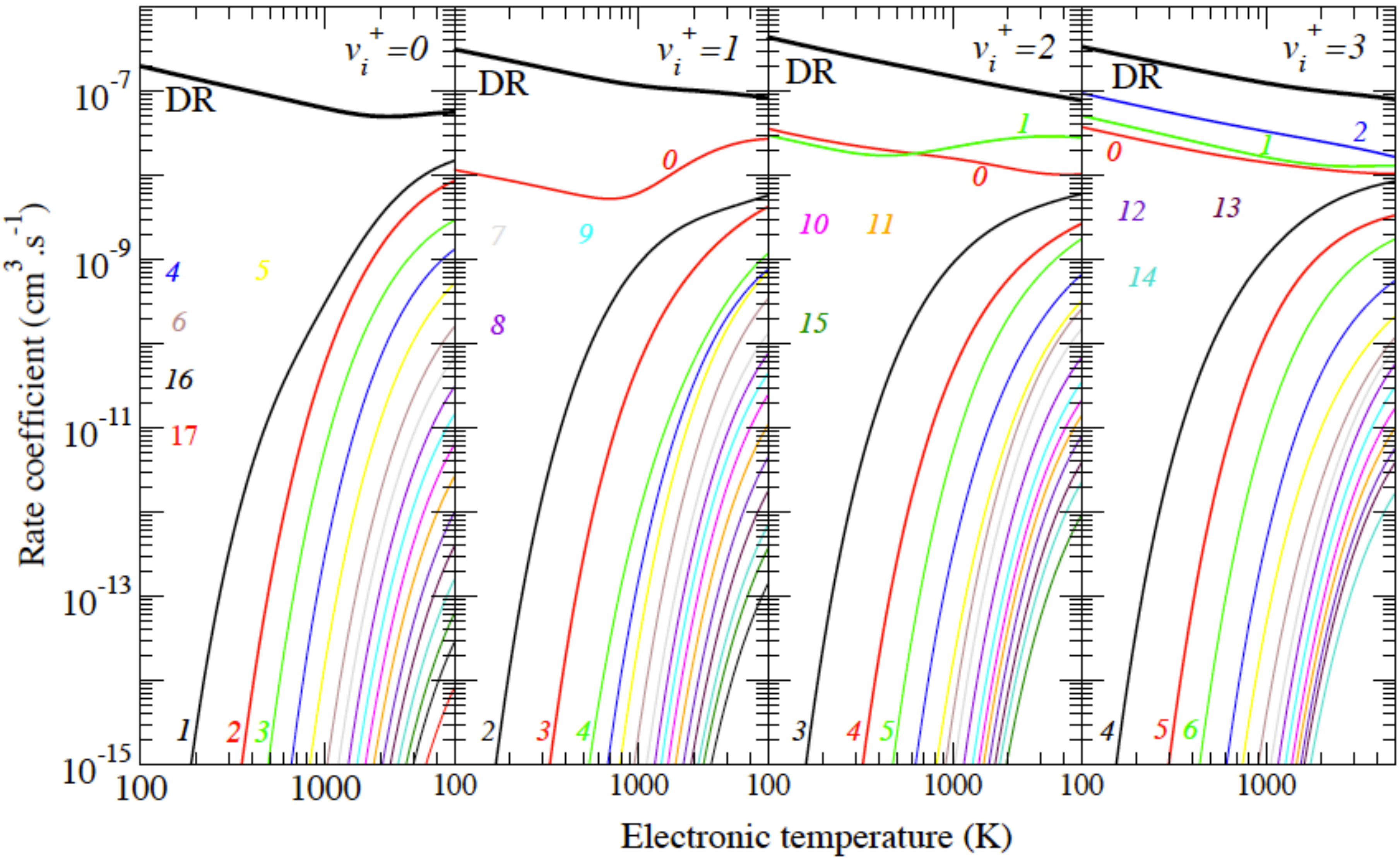
Multichannel-quantum-defect-theory treatment of reactive collisions between electrons and BeH^+

S. Niyonzima,[1,2] F. Lique,[1] K. Chakrabarti,[3] Å. Larson,[4] A. E. Orel,[5] and I. F. Schneider[1,*]

PHYSICAL REVIEW A **87**, 022713 (2013)

Multichannel-quantum-defect-theory treatment of reactive collisions between electrons and BeH^+

S. Niyonzima,[1,2] F. Lique,[1] K. Chakrabarti,[3] Å. Larson,[4] A. E. Orel,[5] and I. F. Schneider[1,*]



Electronic and photonic reactive collisions in edge fusion plasma and interstellar space: Application to H_2 and BeH systems

J. Zs. Mezei[1,2,3], S. Niyonzima[1,4], D. Backodissa[1], N. Pop[5], F. O. Waffeu Tamo[1], K. Chakrabarti[6], O. Motapon[7], A. Wolf[8], J. Robert[2], O. Dulieu[2], Å. Larson[9], A. E. Orel[10], A. Bultel[11] and I. F. Schneider[1,*]

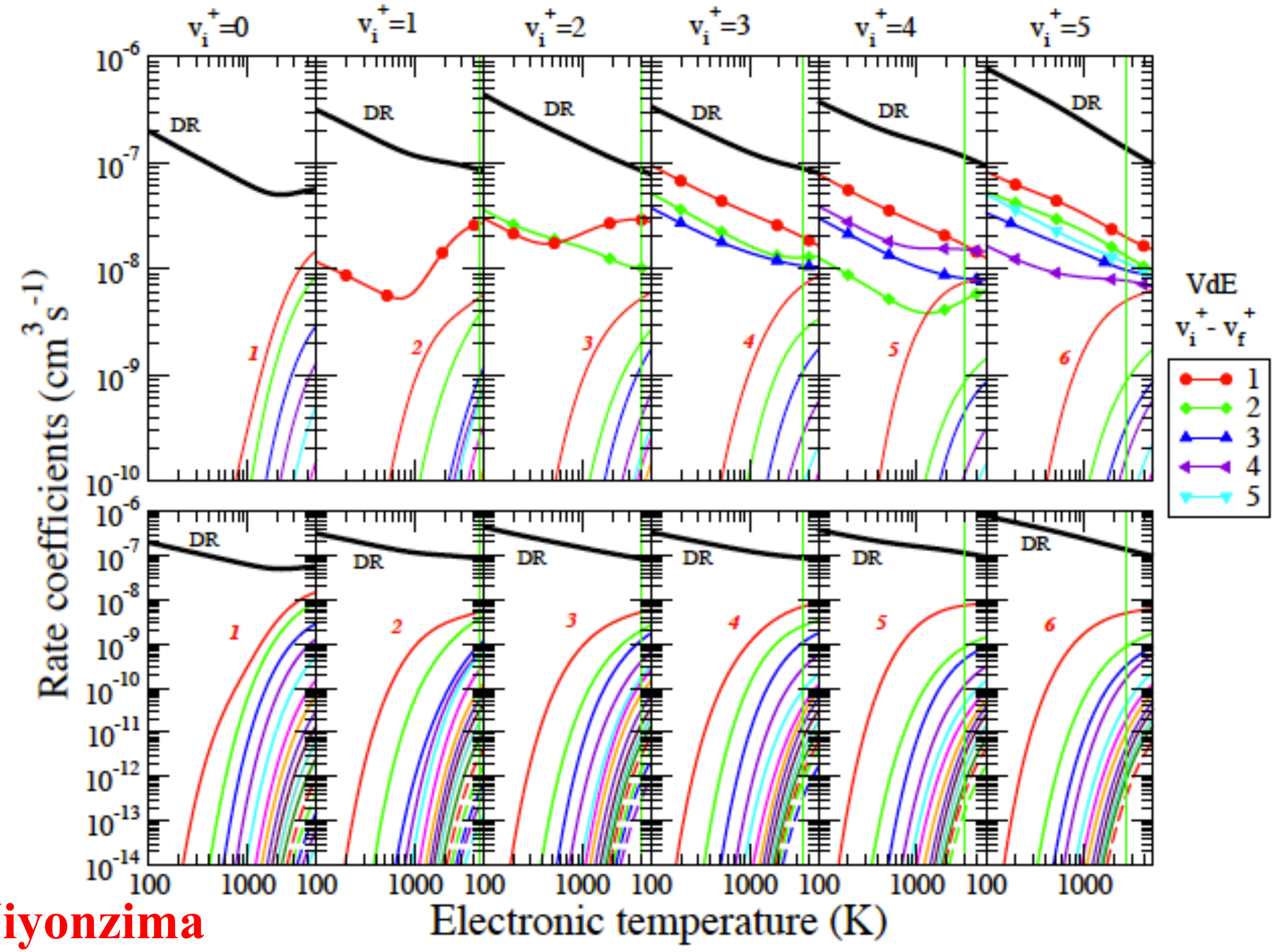
In press @ J. Phys.Conference Series 2014 (IOP)
Report after IAEA-CRP "Light Elements…"

$$k^{DR}_{(BeH^+),v_i^+}(T_e) = A_{v_i^+}\, T_e^{\alpha_{v_i^+}} \exp\left[-\sum_{j=1}^{7} \frac{B_{v_i^+}(j)}{j\, T_e^j}\right],$$

$$k^{VE}_{(BeH^+),v_i^+\to v_f^+}(T_e) = A_{v_i^+\to v_f^+}\, T_e^{\alpha_{v_i^+\to v_f^+}} \exp\left[-\sum_{j=1}^{7} \frac{B_{v_i^+\to v_f^+}(j)}{j\, T_e^j}\right]$$

Table A5. Parameters used in Eq. (A.4) for the DR rate coefficients of BeH^+ displayed in Fig. 8.

v_i^+	$A_{v_i^+}$	$\alpha_{v_i^+}$	$B_{v_i^+}(1)$	$B_{v_i^+}(2)$	$B_{v_i^+}(3)$	$B_{v_i^+}(4)$	$B_{v_i^+}(5)$	$B_{v_i^+}(6)$	$B_{v_i^+}(7)$
0	0.253513120×10^{-9}	0.592469479	-0.190649410×10^{4}	0.123315004×10^{7}	-0.388342503×10^{9}	0.647265585×10^{11}	$-0.566722264\times10^{13}$	0.232068987×10^{15}	$-0.295078806\times10^{16}$
1	0.314462330×10^{-5}	-0.407538250	0.958577714×10^{3}	-0.135957934×10^{7}	0.725436198×10^{9}	$-0.192640935\times10^{12}$	0.271812541×10^{14}	$-0.194765942\times10^{16}$	0.557221814×10^{17}
2	0.114678715×10^{-5}	-0.322376187	-0.265630394×10^{3}	0.219601686×10^{6}	-0.916549130×10^{8}	0.207255861×10^{11}	$-0.259613563\times10^{13}$	0.169396874×10^{15}	$-0.449074035\times10^{16}$
3	0.849641548×10^{-6}	-0.275140774	0.171673351×10^{3}	-0.451956583×10^{6}	0.285096525×10^{9}	$-0.827403486\times10^{11}$	0.123588751×10^{14}	$-0.921680323\times10^{15}$	0.271612346×10^{17}



S. Niyonzima *et al* 2014

Figure 5. *DR and state-to-state VE and VdE global rate coefficients of* BeH^+ *in its ground electronic state (*v_i^+ *standing for the vibrational quantum number of the target ion) in the upper panels. In all panels, curves of same color show VE global rate coefficients in relation with the same* $\Delta v = v_f^+ - v_i^+$ *in the transition while only the lowest final vibrational quantum number of* BeH^+ *is indicated in each panel.*

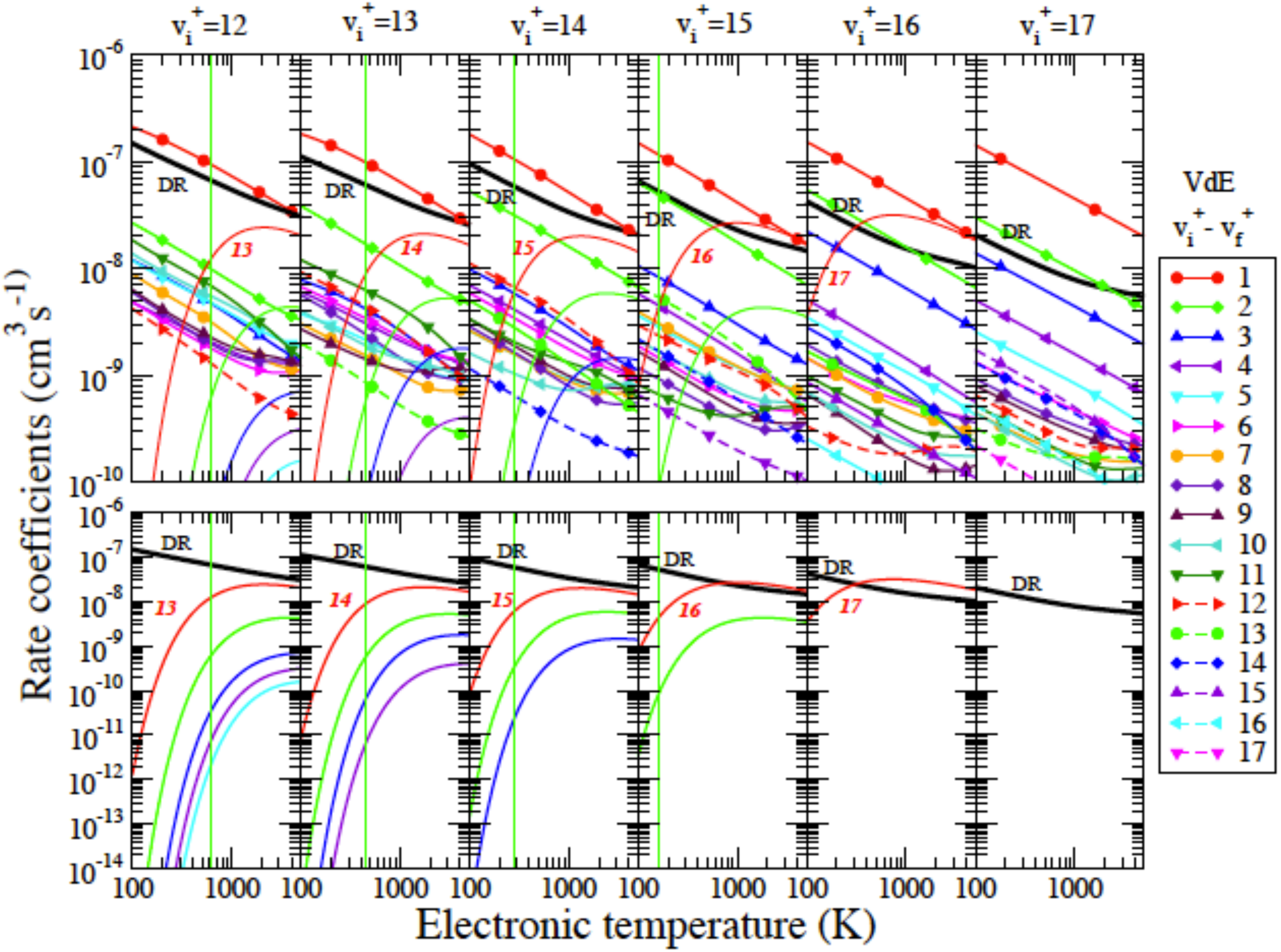
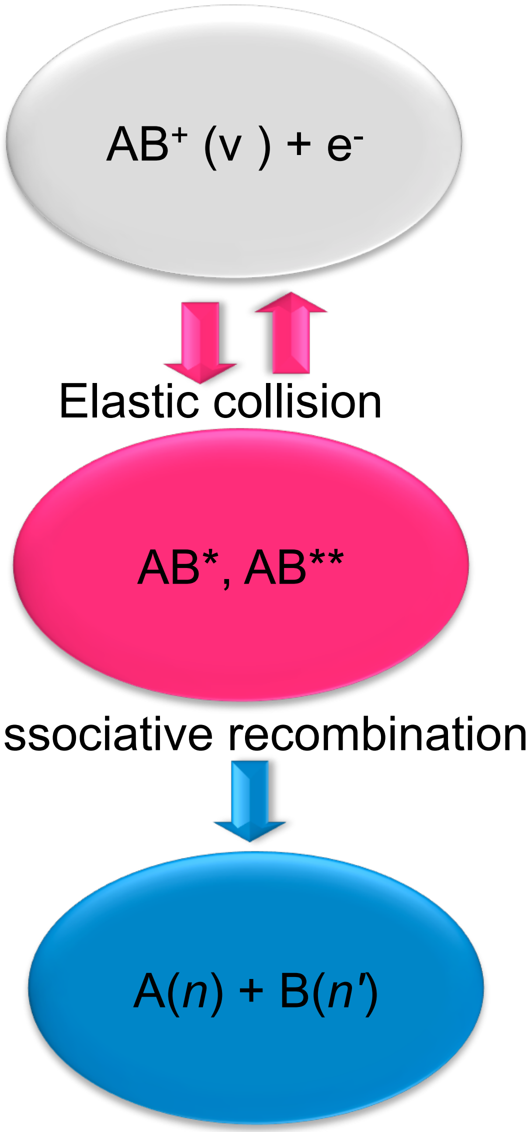


Figure 7. *DR and state-to-state VE and VdE global rate coefficients of* BeH^+ *in its ground electronic state* (v_i^+ *standing for the vibrational quantum number of the target ion) in the upper panels. In all panels, curves of same color show VE global rate coefficients in relation with the same* $\Delta v = v_f^+ - v_i^+$ *in the transition while only the lowest final vibrational quantum number of* BeH^+ *is indicated in each panel.*

Partial conclusion:…

Electron/molecular cation reactive collisions

Rich dynamics, many continua, unified treatment



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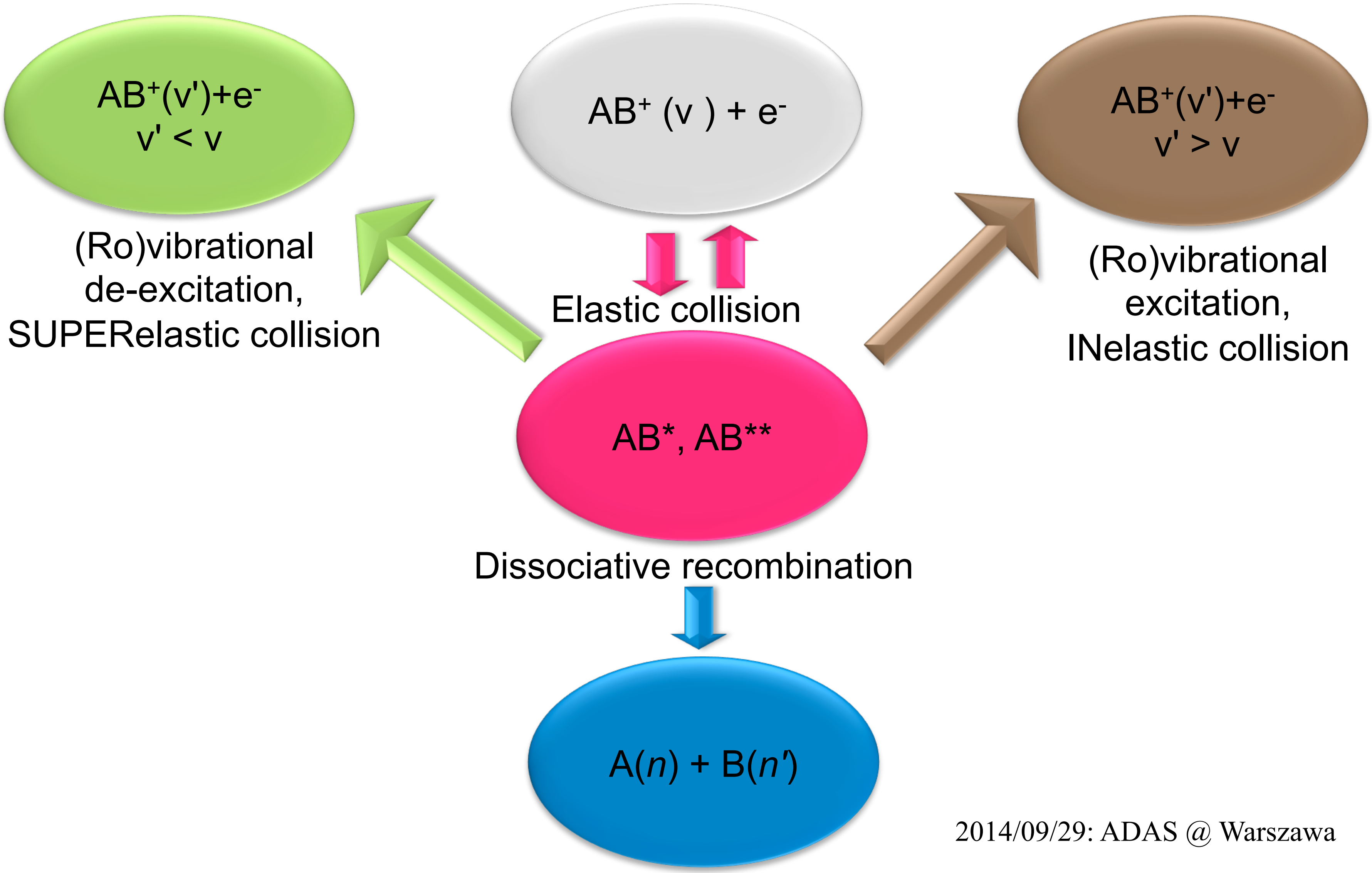

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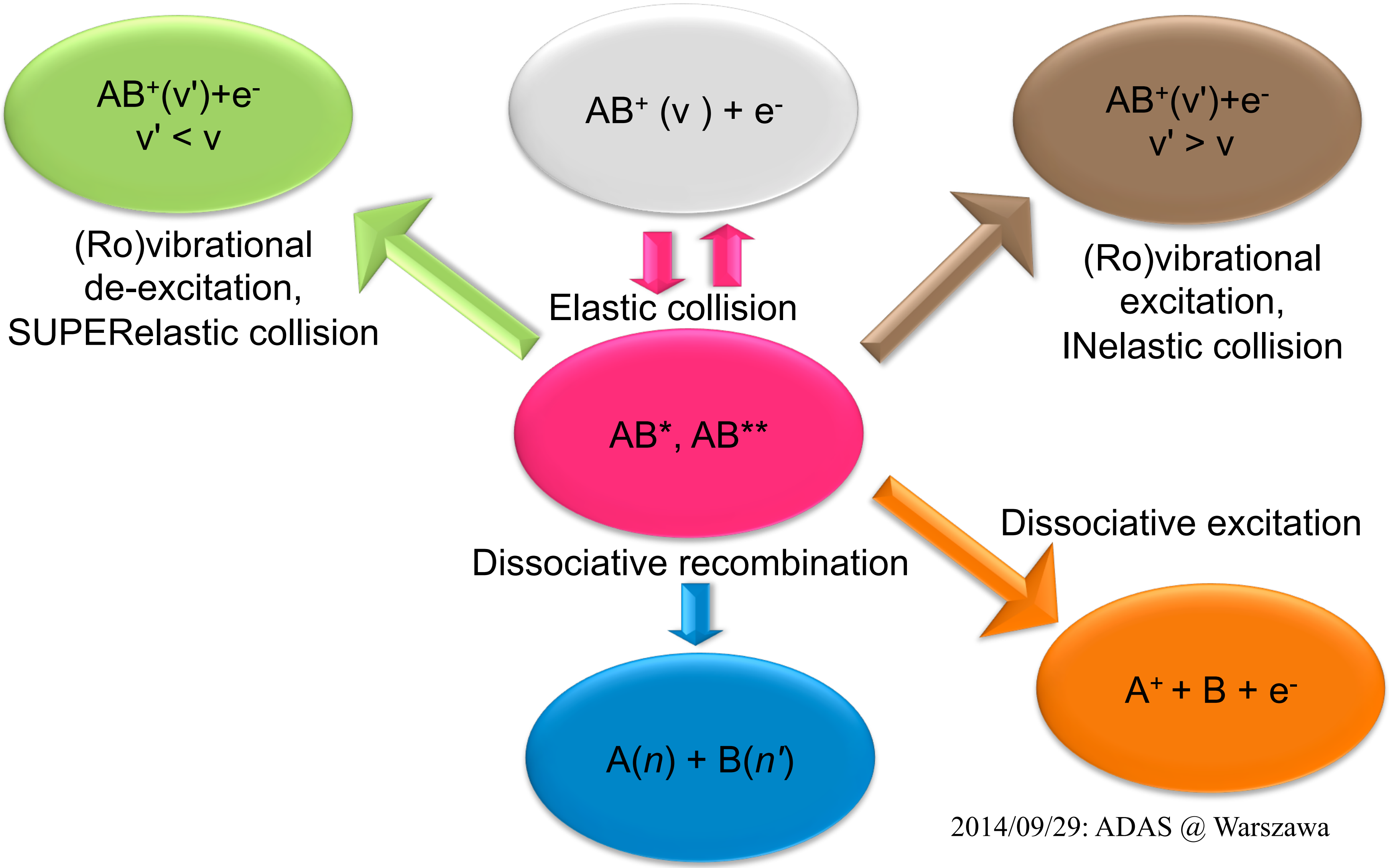

…and OPENING to OTHER processes:…

The SAME

Rydberg resonances

(related to CLOSED channels !)

have a HUGE role in the

PHOTOABSORPTION (PHOTOIONIZATION and PHOTODISSOCIAION)

of H_2

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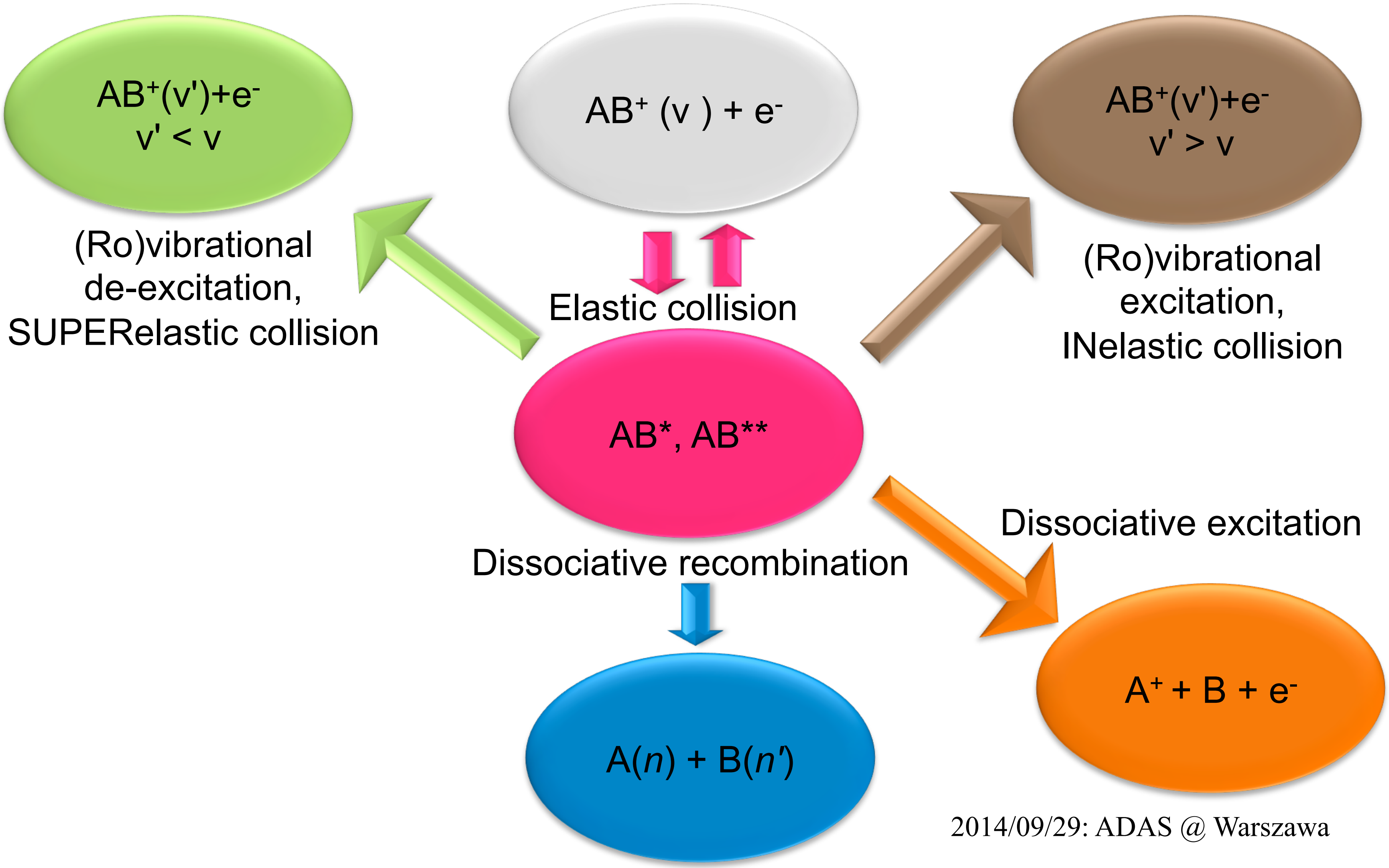
IAEA-CRP “H & He containing systems…”

Electron/molecular cation reactive collisions

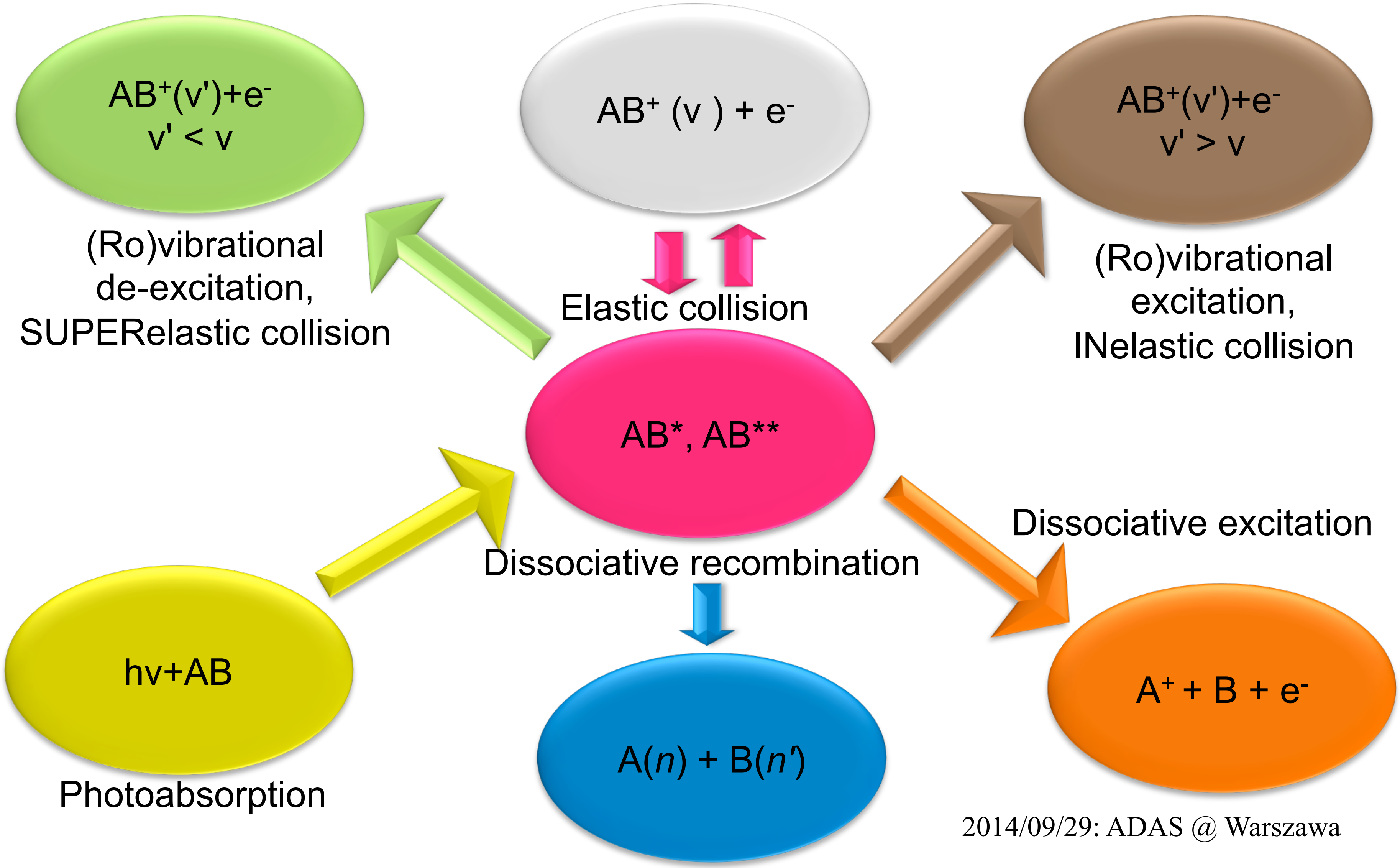
Rich dynamics, many continua, unified treatment



Electron/molecular cation reactive collisions

AND photoabsorption by neutral molecules

Rich dynamics, many continua, unified treatment



The 18th ADAS Workshop
28-30 September 2014
Regent Warsaw Hotel, Poland

Tuesday 30th September

09:00 – 10:30 Session 5: Spectroscopy

Kurt Behringer	*Modelling of Lyman and Fulcher Band Spectra – Vibrational and Rotational Population*
Dmitry Borodin	*Interpretation of the Be and BeD spectroscopy in the recent plasma-wall interaction experiments*
Matthew Carr	*CXRS diagnostics on MAST*
Yang Yang	*Spectroscopic results of W^{11+}-W^{15+}in EUV region, observed in the SH-HtscEBIT (Shanghai High-Temperature-Super-Conduct Electron Beam Ion Trap), and relative calculations*
Stuart Loch	*Discrepancies in Fe XVII line ratios*

Use of the GLOBAL version of the MQDT (Ch. Jungen)

Use of the GLOBAL version of the MQDT (Ch. Jungen)

PHYSICAL REVIEW A **85**, 043411 (2012)

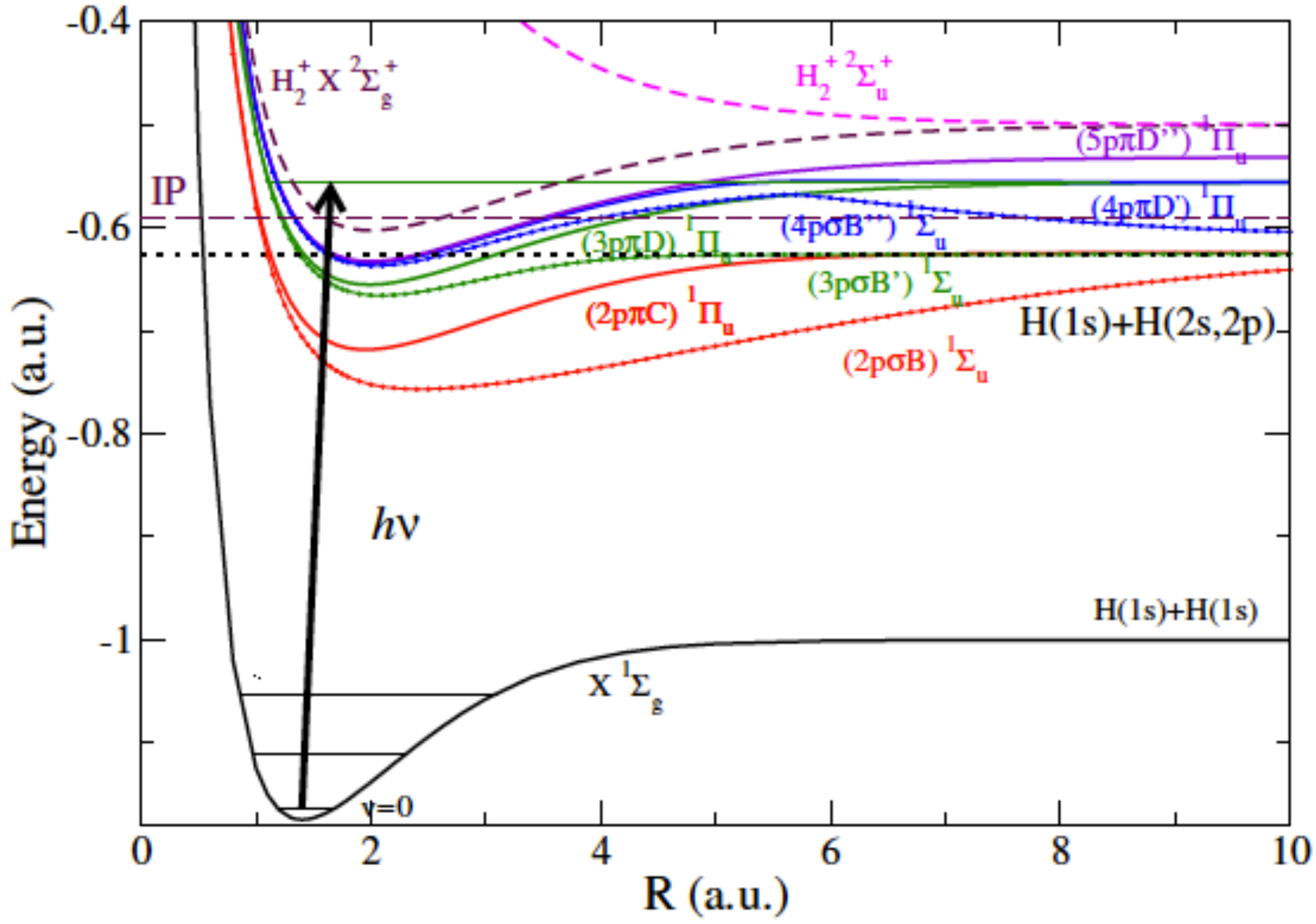
Resonances in photoionization: Cross sections for vibrationally excited H_2

J. Zs. Mezei,[1,2,*] I. F. Schneider,[1,†] E. Roueff,[3] and Ch. Jungen[2,‡]

2014/09/29: ADAS @ Warszawa

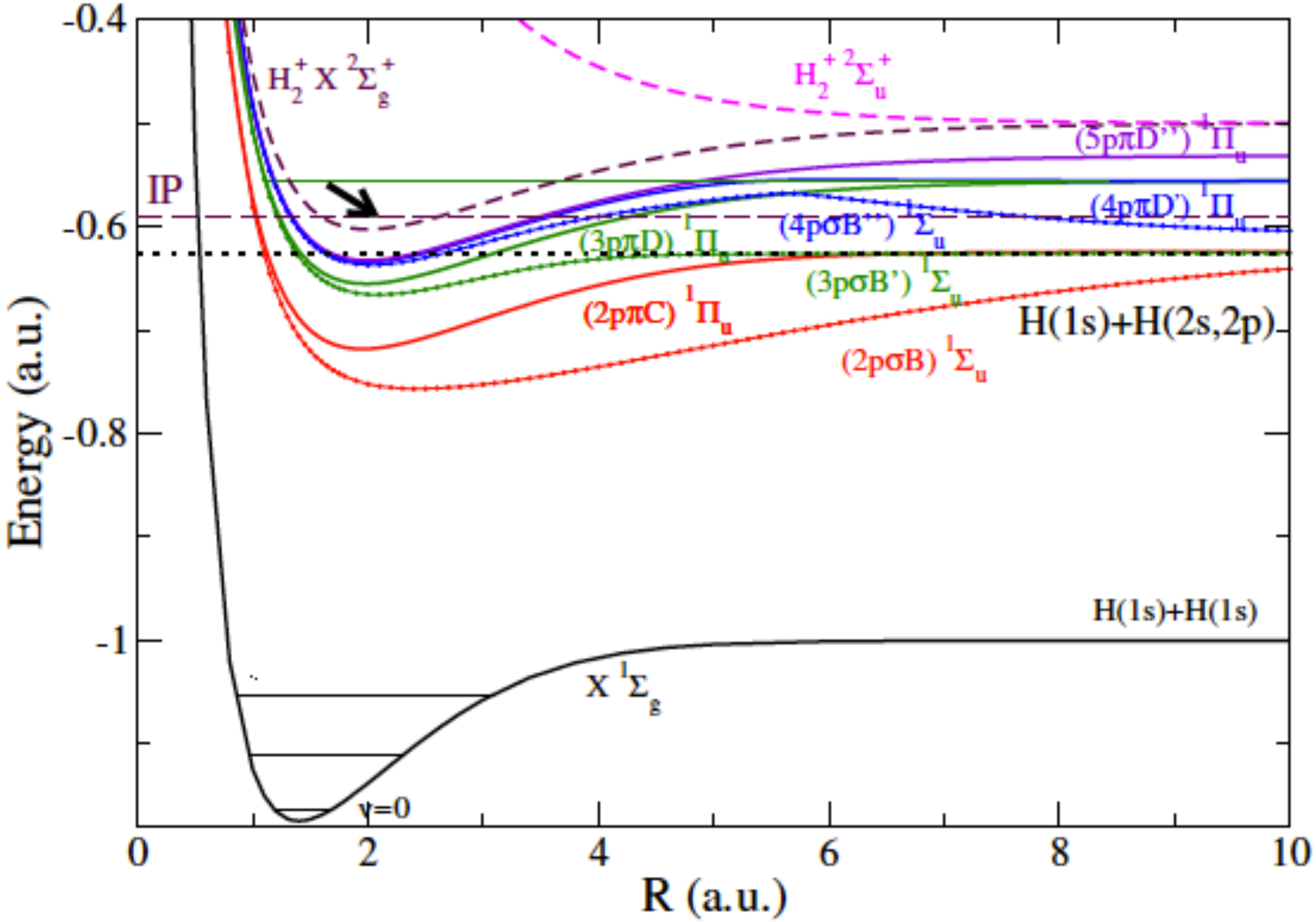
Photoinduced processes

$$H_2(v'', N'') + h\nu \to H_2^{(*)}$$



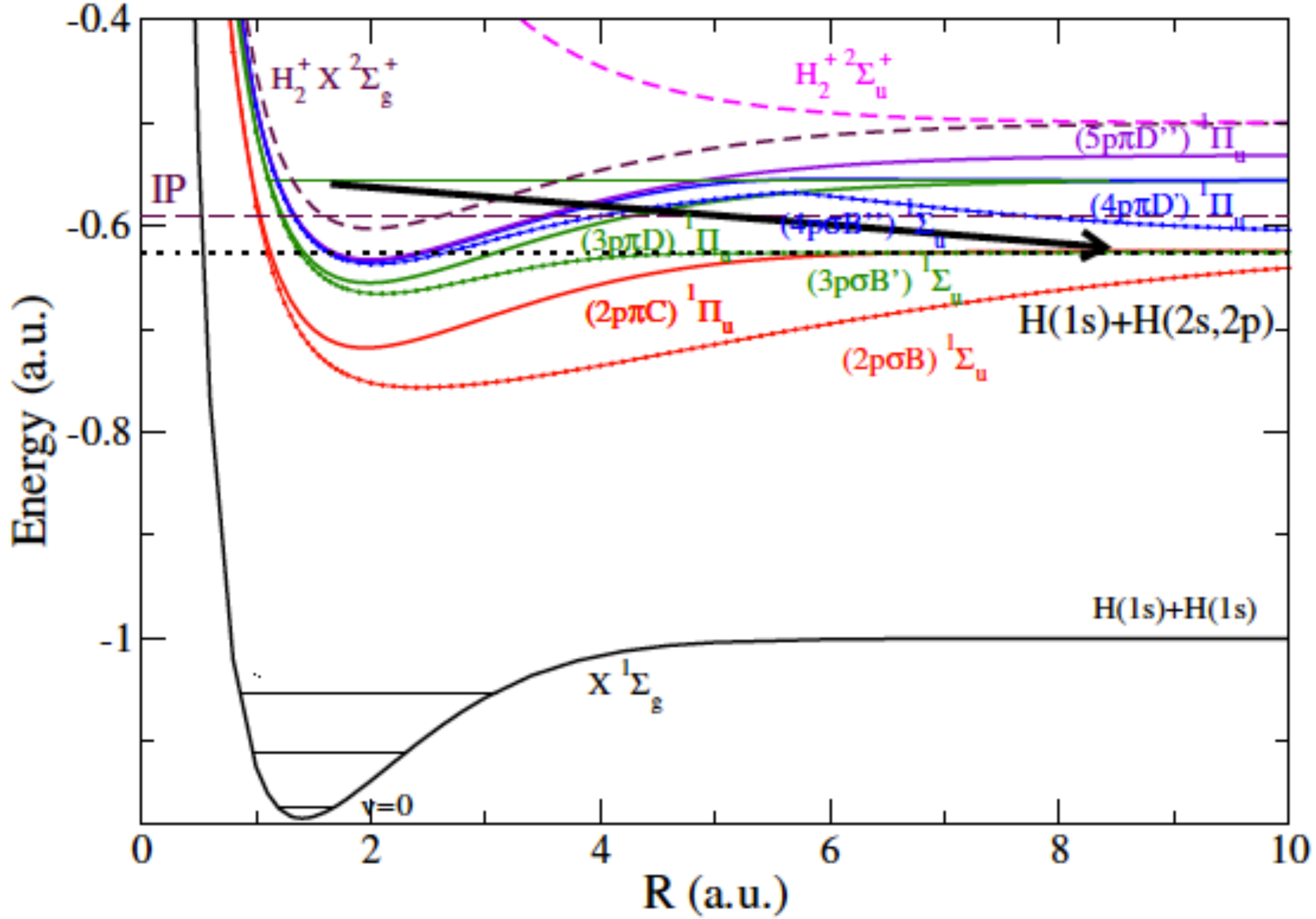
Photoinduced processes

$$H_2(v'', N'') + h\nu \rightarrow H_2^{(*)}(v', N') \rightarrow H_2(v^+, N^+) + e^-$$



Photoinduced processes

$$H_2(v'', N'') + h\nu \to H_2^{(*)}(v', N') \to H(n) + H(m)$$



Photoinduced processes

$$H_2(v'', N'') + h\nu \rightarrow H_2^{(*)}(v', N') \rightarrow H_2(v''_f, N''_f) + h\nu$$

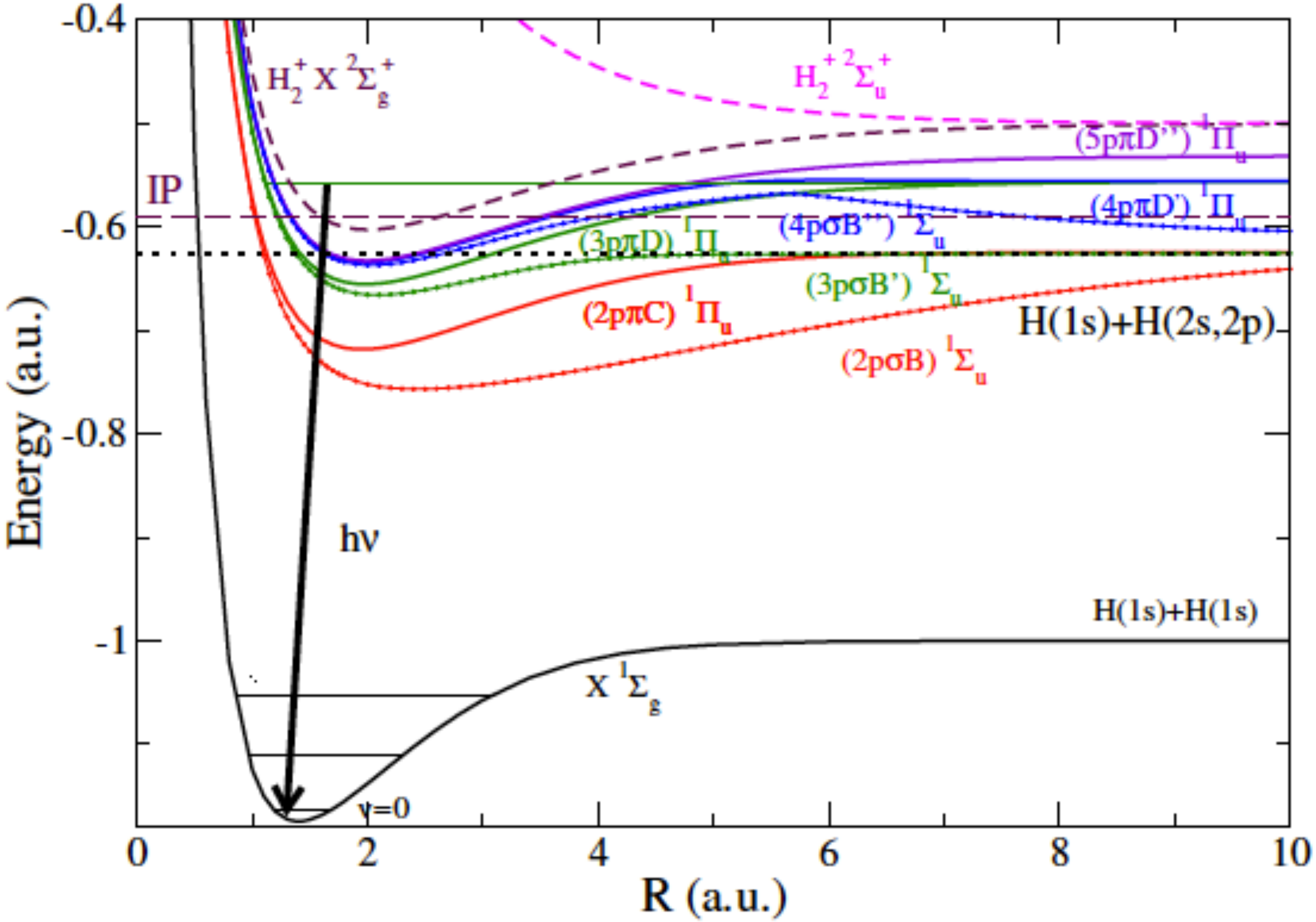
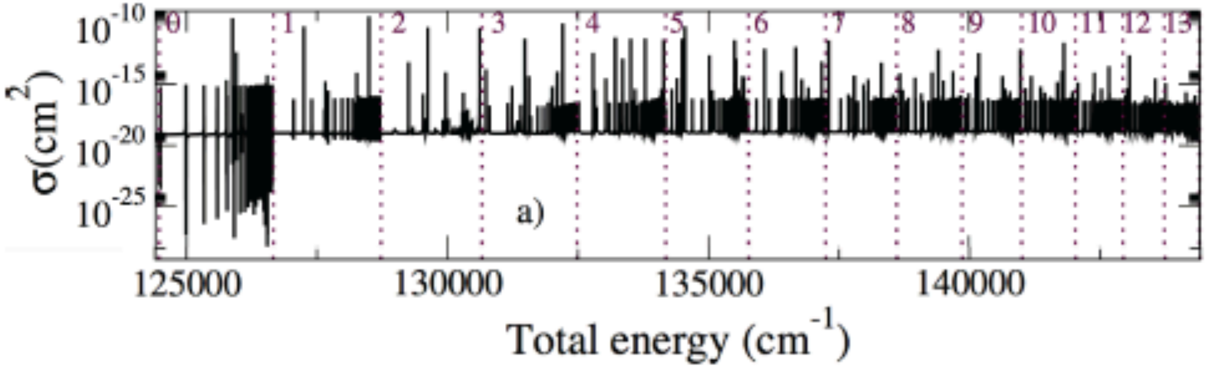


TABLE I. Properties of the peaks characterized as resonances connected to vibrational levels of the different electronic states lying above the ionization limit for $Q(1)$ transitions of H_2. The notation (n,v') refers to the principal and vibrational quantum numbers of the upper state, e.g., $(3,7) = 3p\pi\, D(v' = 7)$. ν_n/c and $\nu(\text{obs})/c$ are the calculated and observed transition frequencies in cm^{-1}, and $[\nu_n - \nu(\text{obs})]/c$ is their difference (where available). The corresponding energies, E_n, of the upper state levels above $v'' = 0, N'' = 0$ are obtained by adding 4273.7371 cm^{-1} [36]. Γ are the calculated autoionization widths, A is the spontaneous emission probability, and $\Delta A/A$ the relative difference of the present calculation and the earlier calculations of Abgrall *et al.* [8]. A/A_{approx} is the ratio of the Einstein coefficients calculated with Eqs. (11) and (16), respectively. Horizontal gaps are indicative of the positions of the vibrational ionization thresholds $v^+, N^+ = 1$. *Threshold* stands for the closest higher vibrational level of the ion. The *relative contribution* is defined by Eq. (17).

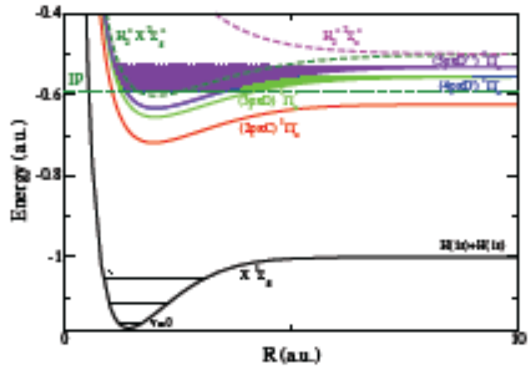
								Ionization		Absorption	
Upper state (n,v')	ν_n/c (cm^{-1})	$[\nu_n - \nu(\text{obs})]/c$ (cm^{-1})	Γ (10^{-4} cm^{-1})	A (10^6 s^{-1})	$\Delta A/A$	A/A_{approx}	Threshold (v^+)	Relative contrib.	Total vs backgr.	Relative contrib.	Total vs backgr.
(5,2)	120 227.40		131.0	0.25		0.95		0.01		0.01	
(6,2)	121 490.07		668.8	2.48		0.86		0.13		0.05	
(3,7)	121 603.97	0.55	0.05	27.36	0.11	0.96	1	$<10^{-2}$	5.9	0.59	15.1
(4,4)	121 678.08	−0.22	1.0	0.94		0.98		0.01		0.02	
(5,3)	122 163.19		58.1	0.13		0.97		0.01		$<10^{-2}$	
(3,8)	122 974.34	−0.29	0.2	24.17	0.08	0.97		$<10^{-2}$		0.32	
(4,5)	123 387.07	−0.03	0.5	6.52		0.97		$<10^{-3}$		$<10^{-2}$	
(6,3)	123 437.68		349.8	0.22		0.97	2	0.03	1.9	$<10^{-2}$	15.9
(5,4)	123 988.41		47.7	1.26		0.97		0.13		0.02	
(3,9)	124 222.40	−0.44	0.02	20.44	0.08	0.97		0.01		0.56	
(4,6)	124 983.98		75.2	9.96		0.97		0.50		0.24	
(6,4)	125 256.71		1399.6	0.74		0.97		0.05		0.02	
(3,10)	125 347.34	−0.36	0.04	16.20	0.06	0.97	3	$<10^{-3}$	4.2	0.19	9.5
(5,5)	125 695.41		141.0	3.32		0.97		0.19		0.09	
(3,11)	126 344.18	0.09	0.2	14.89	0.2	0.97		$<10^{-2}$		0.35	

Photoionization - Q(1) results

$$X^1\Sigma_g^+(v''=1, J=1) + h\nu \rightarrow (n^1\Pi_u^-) \rightarrow H_2^+(v^+, J^+=1) + e^-$$



a) ionization profile



Mezei, Schneider, Roueff and Jungen: Phys. Rev. A **85**, 043411 (2012).

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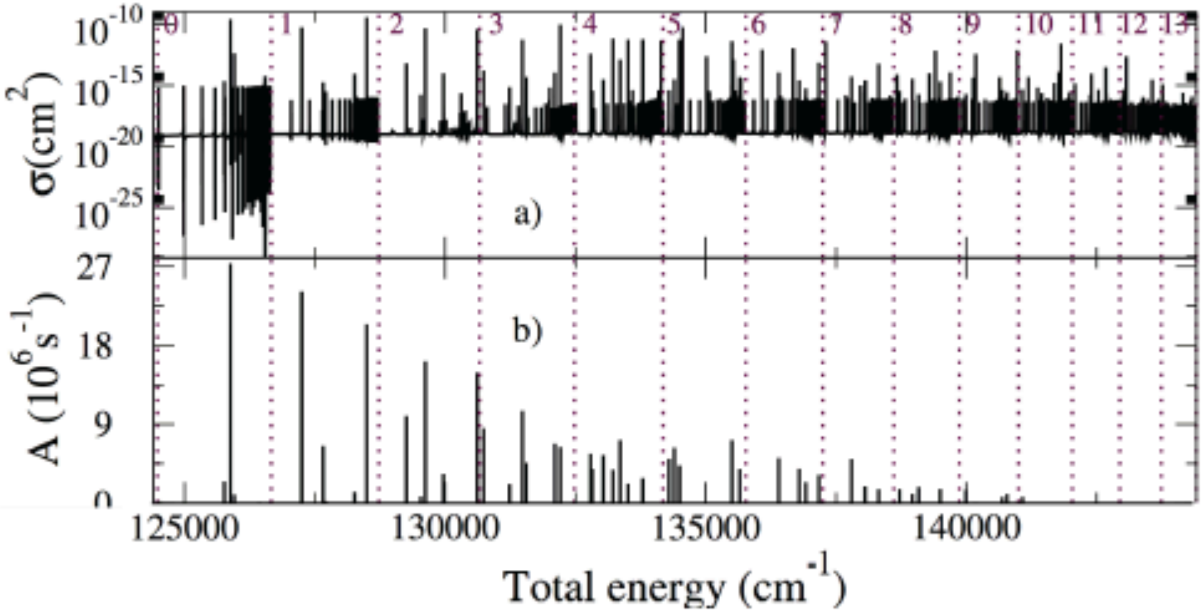
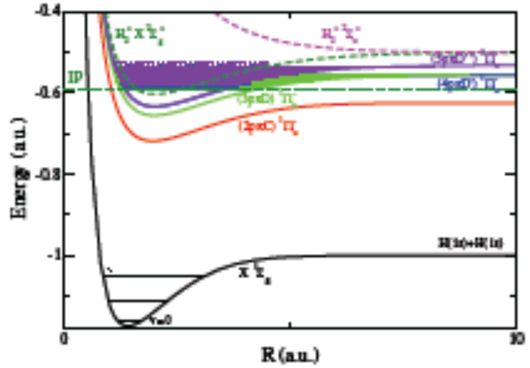


a) ionization profile

b) most intense lines



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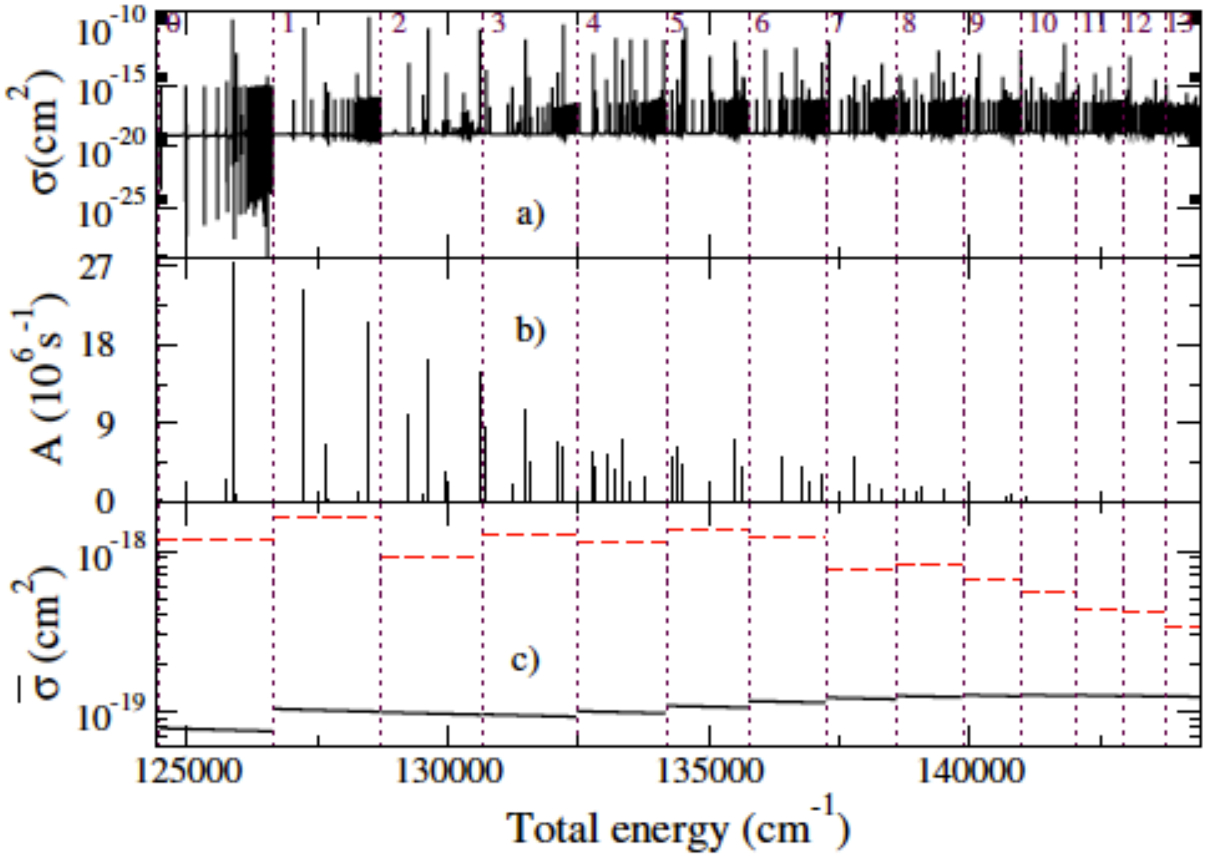

a) ionization profile

b) most intense lines

c) averaged cross section

Autoionization: very important !!

Mezei, Schneider, Roueff and Jungen: Phys. Rev. A **85**, 043411 (2012).

THE JOURNAL OF CHEMICAL PHYSICS **141**, 064305 (2014)

Resonances in photoabsorption: Predissociation line shapes in the $3p\pi\, D\, ^1\Pi_u^+ \leftarrow X\, ^1\Sigma_g^+$ system in H_2

J. Zs. Mezei,[1,2,a)] I. F. Schneider,[2] M. Glass-Maujean,[3] and Ch. Jungen[1,4,b)]

THE JOURNAL OF CHEMICAL PHYSICS **141**, 064305 (2014)

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J. Zs. Mezei,[1,2,a)] I. F. Schneider,[2] M. Glass-Maujean,[3] and Ch. Jungen[1,4,b)]

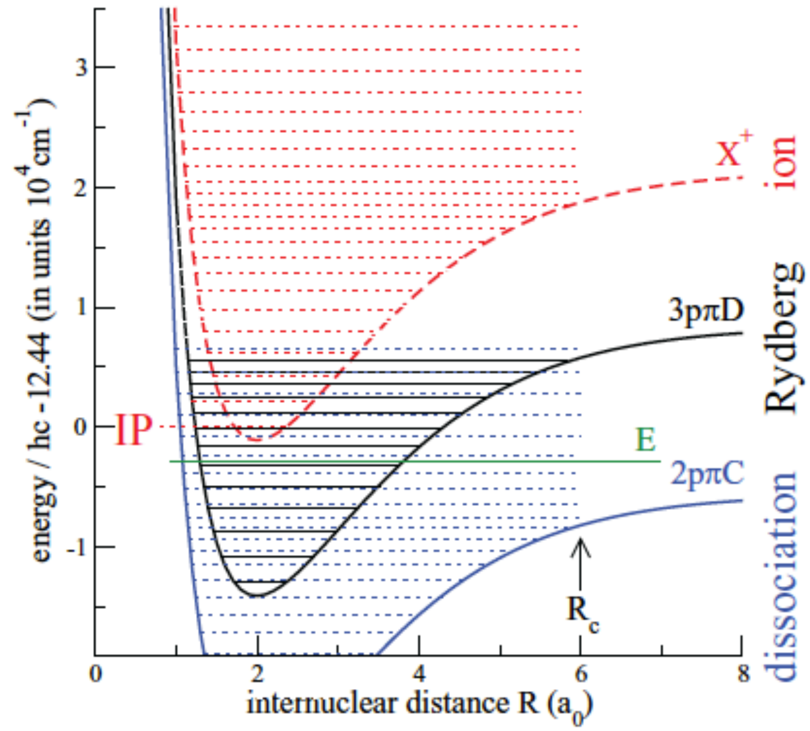


FIG. 1. Molecular (solid lines) and ion (dashed line) potential energy curves with vibronic levels (black horizonal solid lines and blue horizontal dotted lines), and vibrational ionization thresholds (red horizontal dotted lines), illustrating the discretization of the dissociation continuum through application of a fixed boundary condition at $R = R_c$. E (green horizontal solid line) is the total energy under consideration. Rydberg levels with $n > 3$ are not shown for clarity.

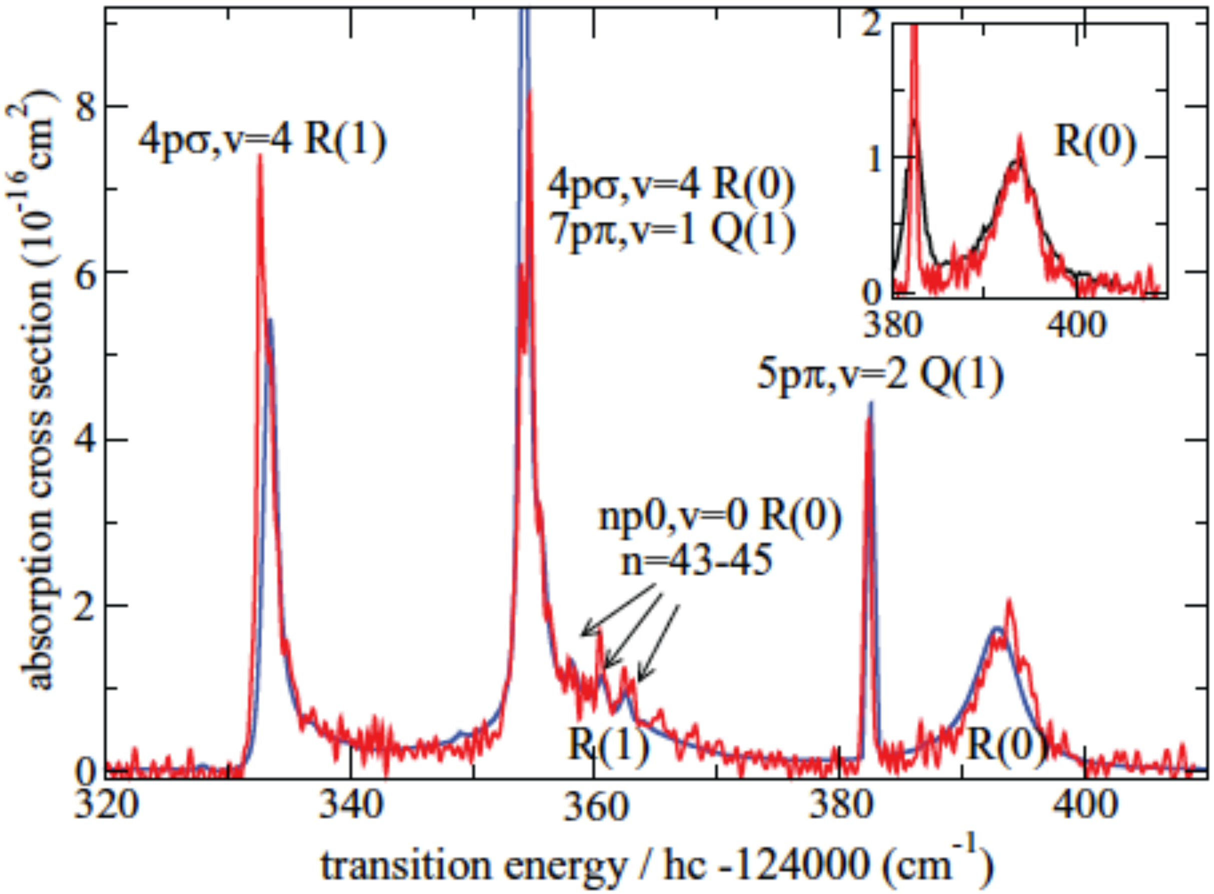


FIG. 3. Absorption cross section profile near the $3p\pi D\ ^1\Pi_u^+, v = 6 \leftarrow X\ ^1\Sigma_g^+, v'' = 0\ R(0)$ and $R(1)$ transitions. The red lines are the spectral recordings of Dickenson *et al.*[10] taken at SOLEIL. The inset shows how the approximate calibration of these data with respect to the absolute measurements made at BESSY,[9] represented by the black curve in the inset, is made using the $R(0)$ transition (cf. the text). The blue lines represent the present first-principles calculations.

PERSPECTIVES

1) **Diatomics:**

H_2^+, CO^+, CH^+, N_2^+, BeH^+, SH^+, BF^+, …

FeO^+, AlO^+, …

2) **Polyatomics: H_3^+, HCO^+, HCN^+, CO_2^+…**

3) **Heavy/Heavy collisions (J. Zs. Mezei !):**

Associative Ionization, Ion Pair Production, etc.

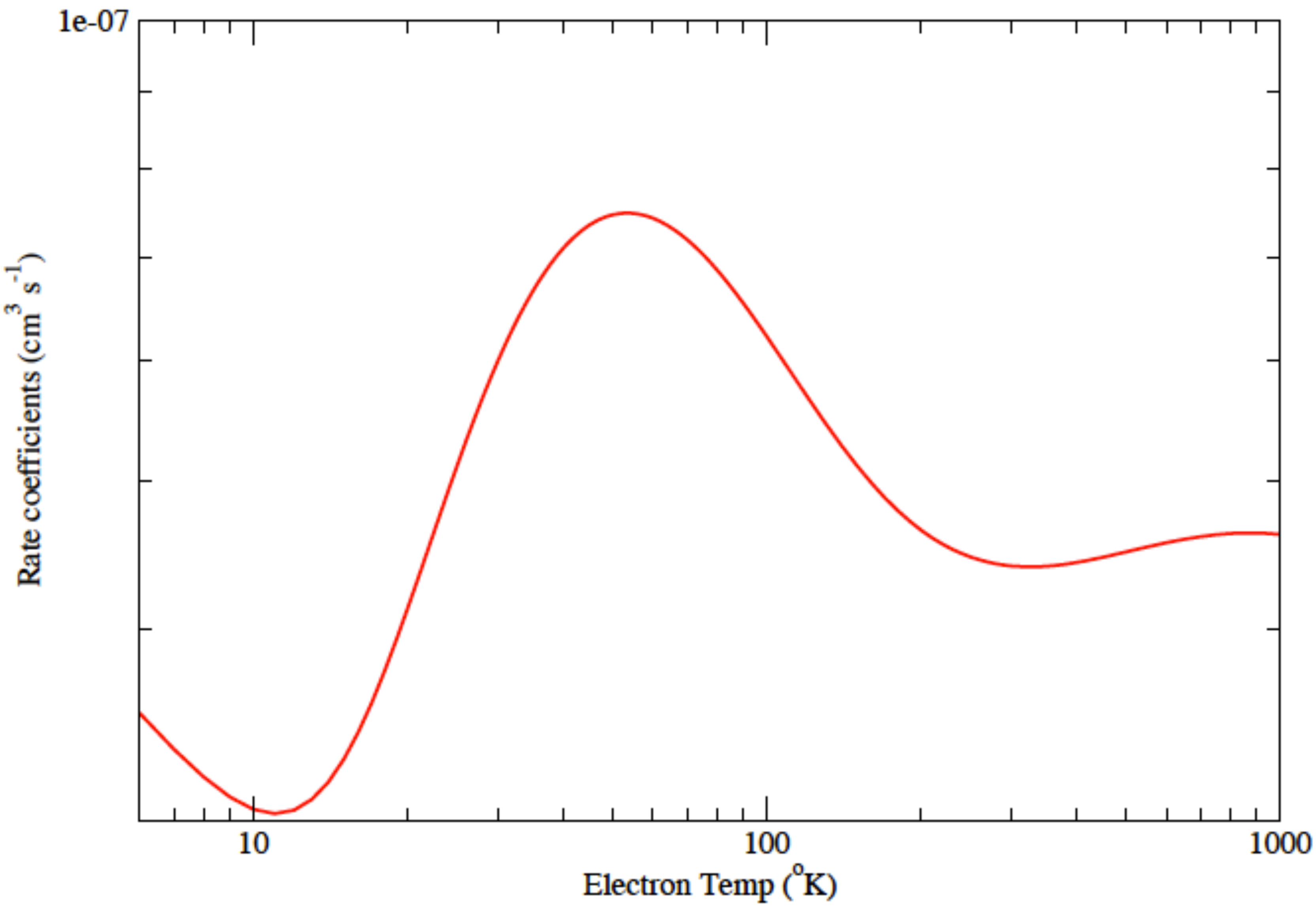
Catalytic mechanism of divertor plasma recombination provided by hydrocarbon impurities

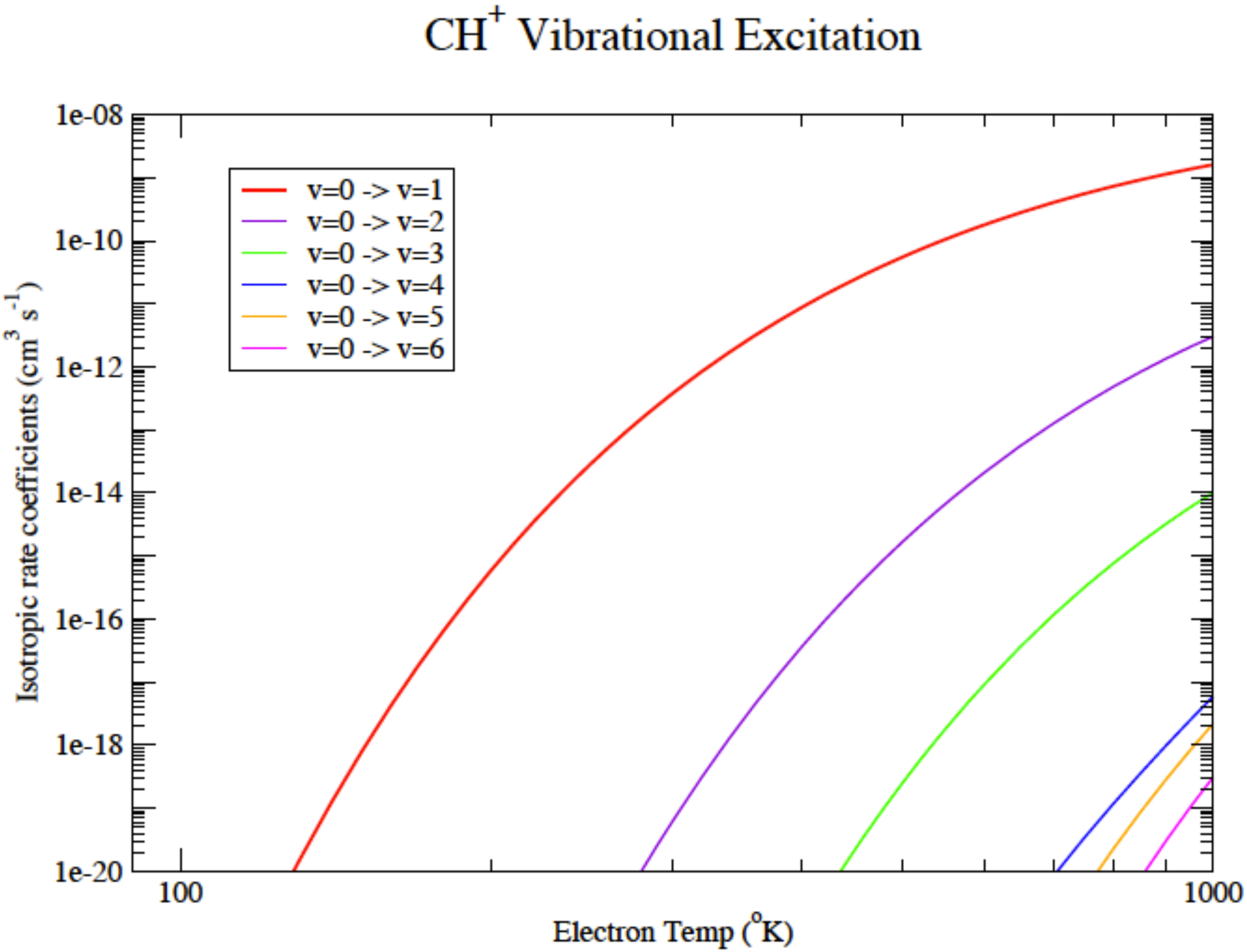
R. K. Janev, T. Kato, and J. G. Wang

Citation: Physics of Plasmas (1994-present) **7**, 4364 (2000); doi: 10.1063/1.1316082
View online: http://dx.doi.org/10.1063/1.1316082
View Table of Contents: http://scitation.aip.org/content/aip/journal/pop/7/11?ver=pdfcov
Published by the AIP Publishing

$CH^{+} + e^{-}$

CH^+ v_i^+=0 Dissociative Recombination




CH+ Vibrational Excitation
v=0 -> v=1
v=0 -> v=2
v=0 -> v=3
v=0 -> v=4
v=0 -> v=5
v=0 -> v=6
1e-08
1e-10
1e-12
1e-14
1e-16
1e-18
1e-20
Isotropic rate coefficients (cm3 s-1)
100
1000
Electron Temp (oK)

$$N_2^+ + e^-$$

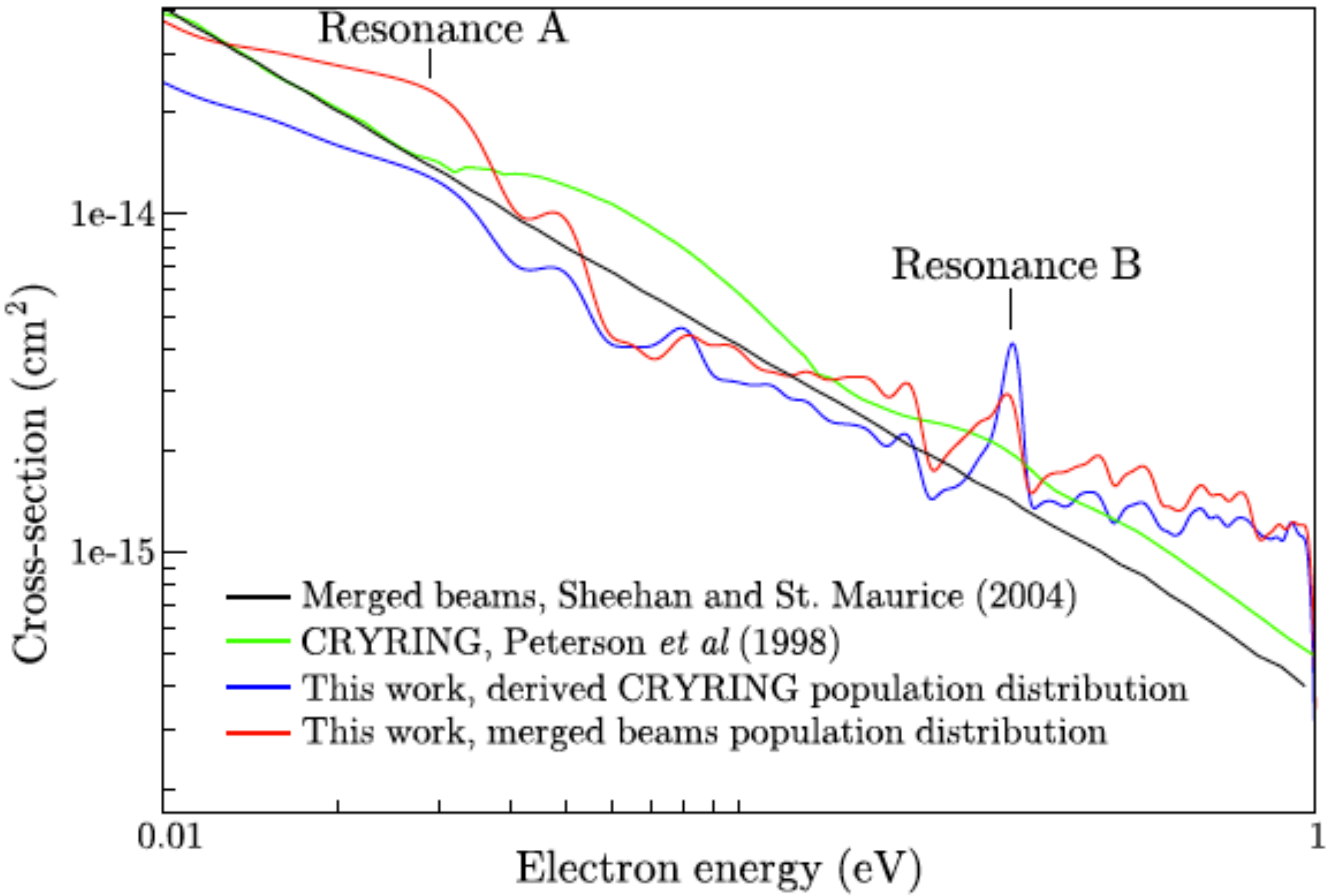


FIG. 14: Comparison of our computed N_2^+ DR effective cross sections with those measured using CRYRING [7] and by Sheehan and St. Maurice [8].

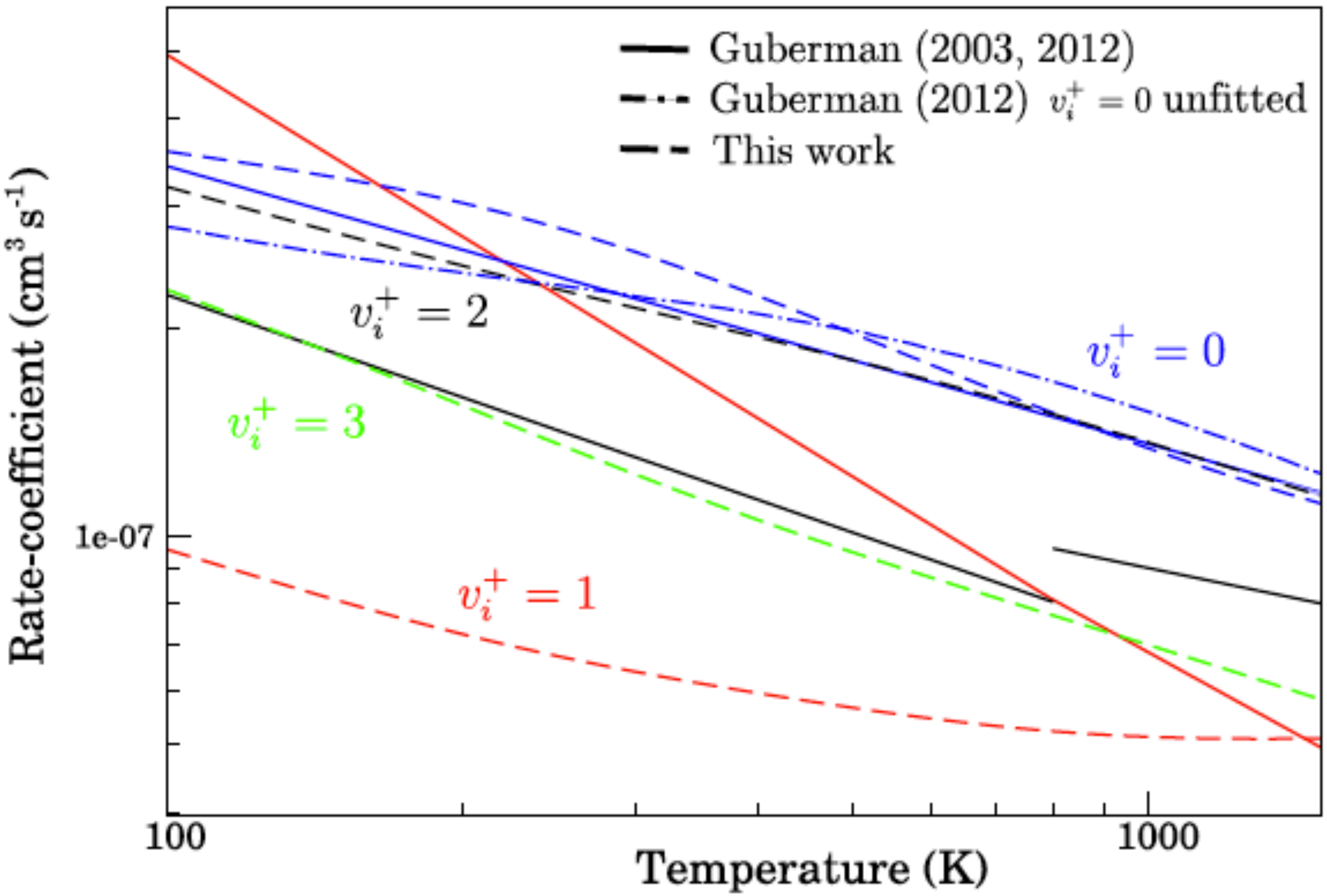
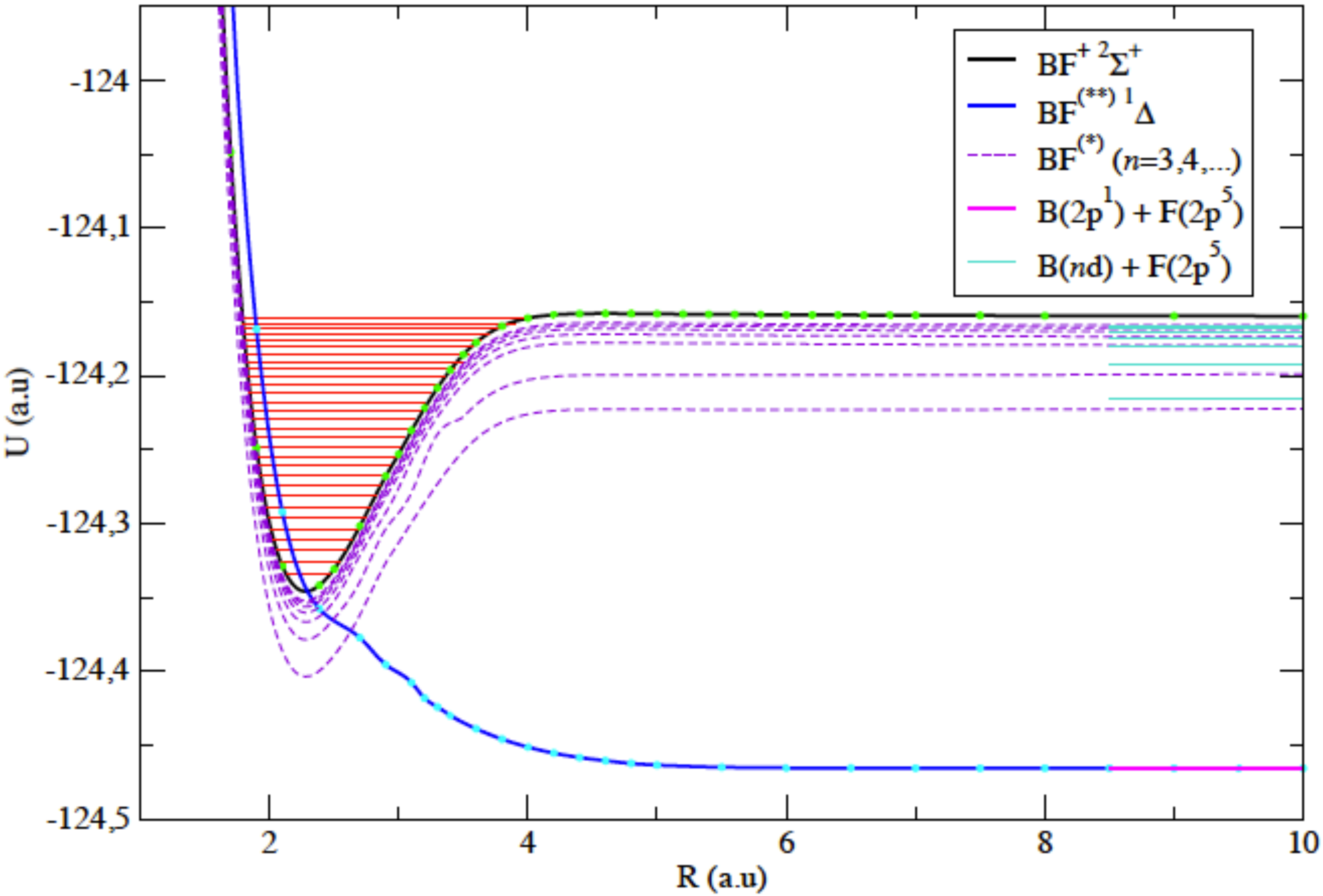


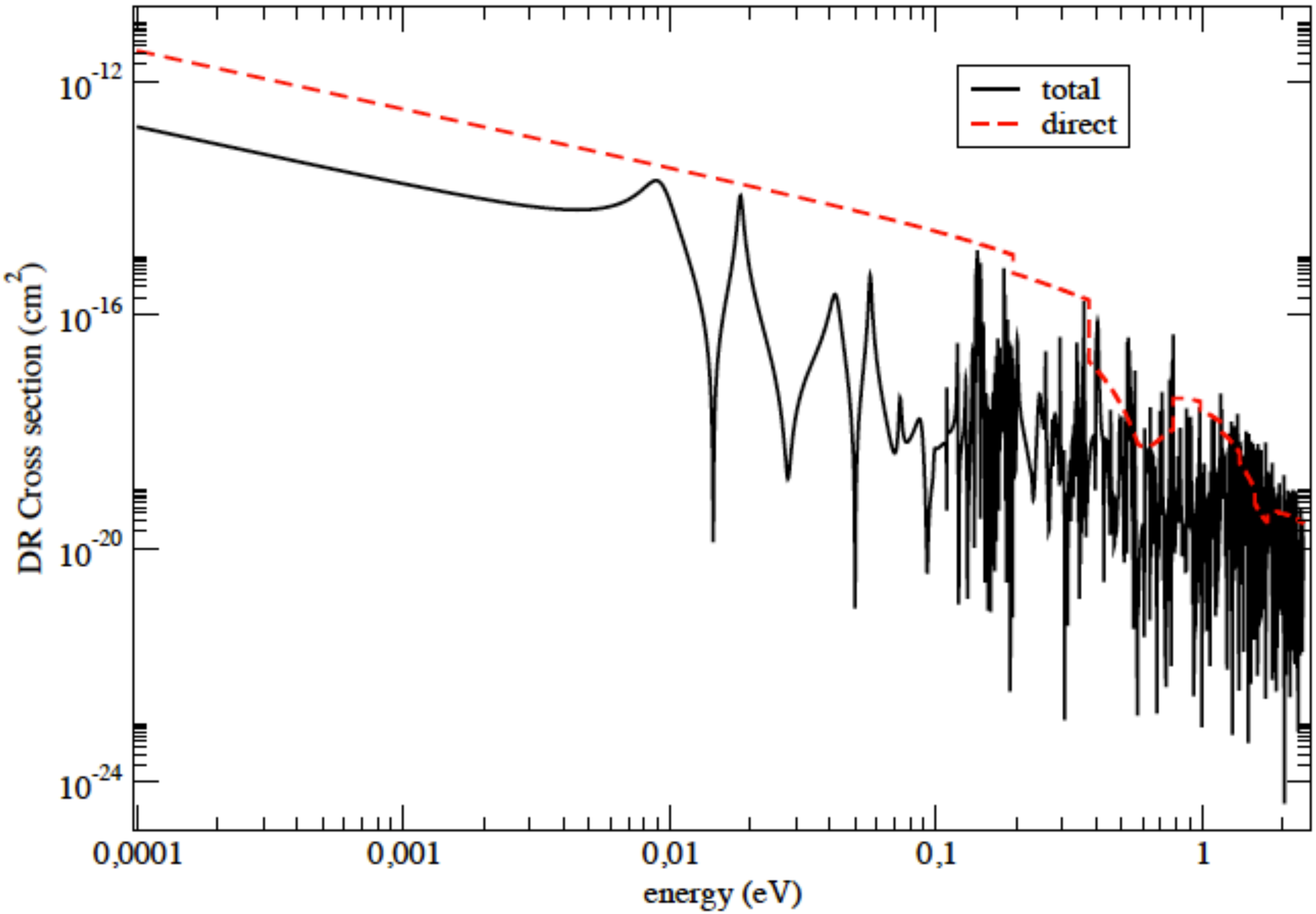
FIG. 17: Comparison with Guberman's [15, 17] isotropic N_2^+ DR rate coefficients. Guberman's fitted and unfitted values for $v_i^+ = 0$ are displayed for comparison.

$BF^{+} + e^{-}$

Example: $BF^+ + e^-$



BF+ 2Σ+
BF(**) 1Δ
BF(*) (n=3,4,...)
B(2p1) + F(2p5)
B(nd) + F(2p5)
-124
-124,1
-124,2
-124,3
-124,4
-124,5
U (a.u)
2
4
6
8
10
R (a.u)



total
direct
DR Cross section (cm^2)
10^{-12}
10^{-16}
10^{-20}
10^{-24}
0,0001
0,001
0,01
0,1
1
energy (eV)

http://www.paris-dr2013.com/

LOCAL ORGANIZING COMMITTEE

by Anna da Costa (28/11/2012)

- I. F. Schneider (Le Havre University),
- O. Dulieu (Paris-Sud University),
- J. Robert (Paris-Sud University)
- and A. da Costa (Triangle de la Physique)

You can contact the local organizing committee, if you have any question: ✉local-committee@paris-dr2013.com

Proceedings

to appear in EPJ/WoC

THANKS

four your attention !