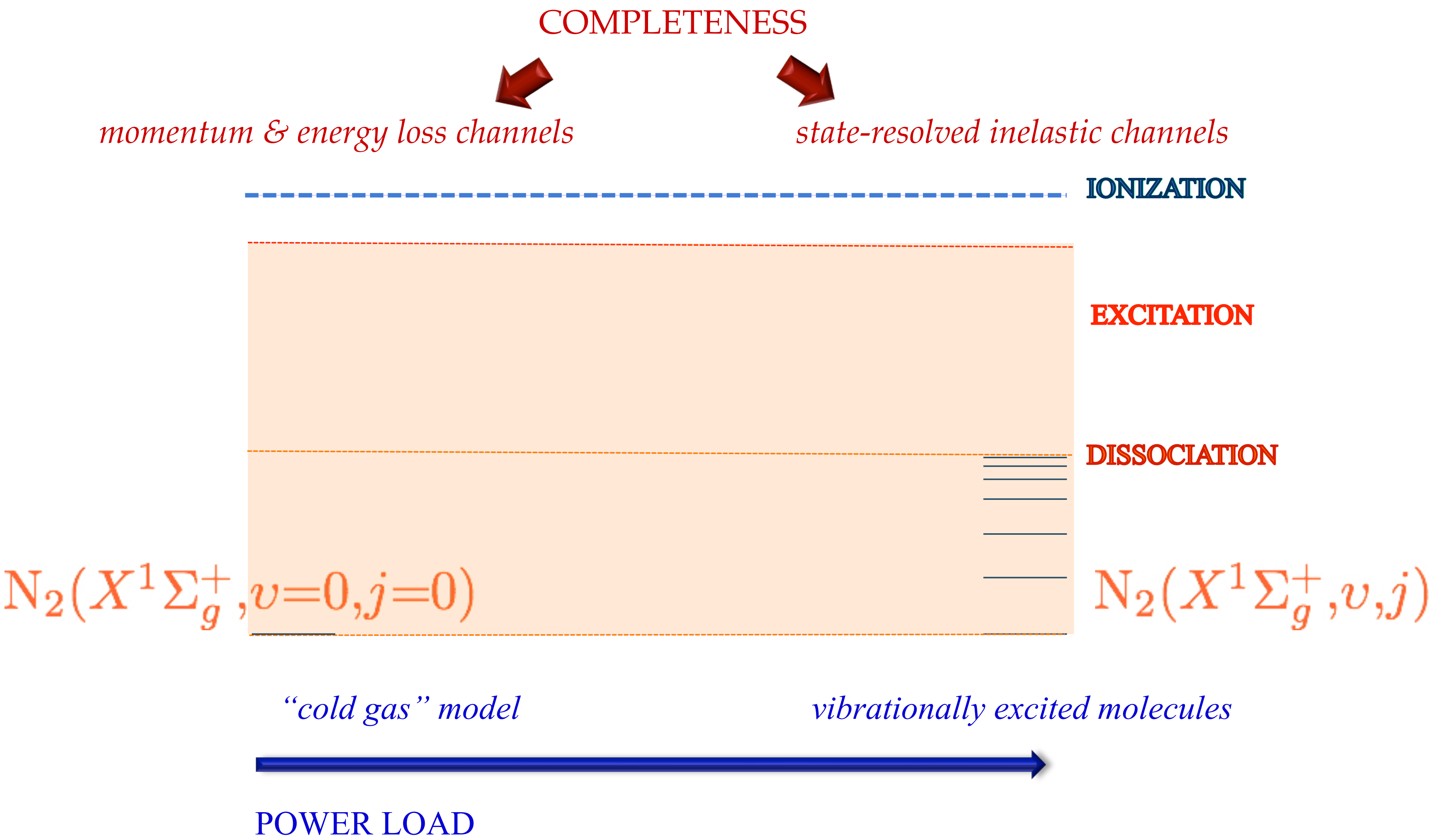
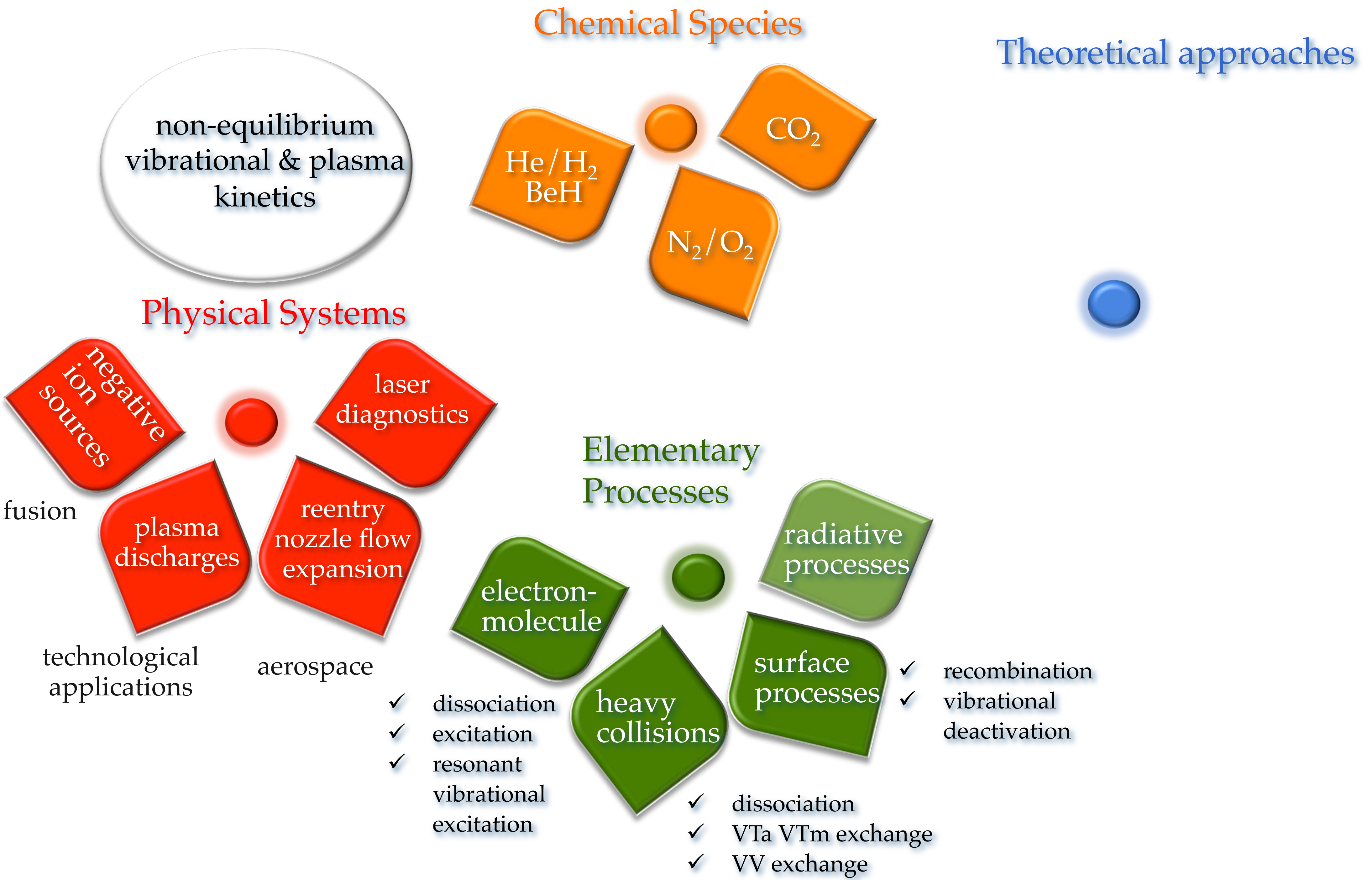
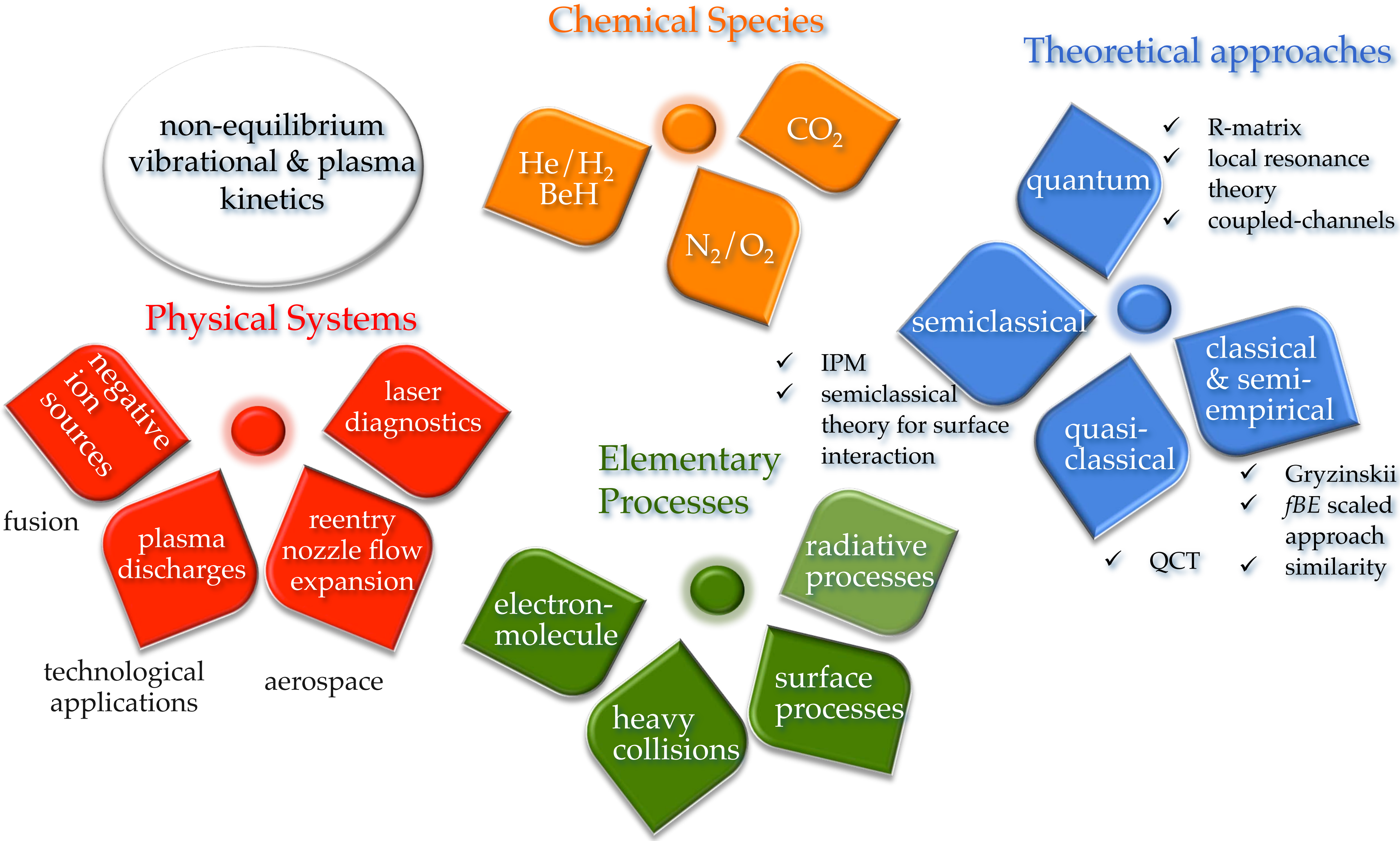
The state-of-the-art description of vibrational-electronic excitations

A. Laricchiuta

CNR IMIP Bari (Italy)


COMPLETENESS
momentum & energy loss channels
state-resolved inelastic channels
IONIZATION
EXCITATION
DISSOCIATION
$N_2(X^1\Sigma_g^+, v=0, j=0)$
$N_2(X^1\Sigma_g^+, v, j)$
"cold gas" model
vibrationally excited molecules
POWER LOAD


Chemical Species
Theoretical approaches
non-equilibrium vibrational & plasma kinetics
He/H_2
BeH
CO_2
N_2/O_2
Physical Systems
negative ion sources
laser diagnostics
fusion
plasma discharges
reentry nozzle flow expansion
technological applications
aerospace
Elementary Processes
radiative processes
electron-molecule
heavy collisions
surface processes
✓ recombination
✓ vibrational deactivation
✓ dissociation
✓ excitation
✓ resonant vibrational excitation
✓ dissociation
✓ VTa VTm exchange
✓ VV exchange



A. LARICCHIUTA *The state-of-the-art description of vibrational-electronic excitations*
MASTER CLASS 2014 Physikzentrum Bad Honnef (Germany), October 10th, 2014

ELEMENTARY PROCESS DATA

F Esposito, I Armenise, G Capitta, M Capitelli, **O–O_2 state-to-state vibrational relaxation and dissociation rates based on quasiclassical calculations**, Chemical Physics 351 (2008) 91-98

Panesi, M., Jaffe, R.L., Schwenke, D.W., Magin, T.E., **Rovibrational internal energy transfer and dissociation of $N_2(^1\Sigma_g^+)$-$N(^4S_u)$ system in hypersonic flows**, J. Chem. Phys. 138 (2013) 044312

Kim, J.G., Kwon, O.J., Park, C., **Non-equilibrium rotation-vibration transitions and chemical reactions in H +H_2 and He+H_2**, AIP Conf Proc 1084 (2009) 813-818, RGD26

A Kurnosov, M Cacciatore, A Laganà, F Pirani, M Bartolomei, E Garcia, **The effect of the intermolecular potential formulation on the state-selected energy exchange rate coefficients in N_2–N_2 collisions**, J. comp. chem. 35 (2014), 722-736

A Lombardi, A Laganà, F Pirani, M Bartolomei, **Carbon dioxide dynamics in earth and planetary atmospheres: vibrational energy transfer in CO_2+ CO_2 collisions**, Virt&l-Comm 1 (2012), pp. 16-17

Cacciatore, M. , Rutigliano, M., **The semiclassical and quantum-classical approaches to elementary surface processes: Dissociative chemisorption and atom recombination on surfaces**, Physica Scripta 78 (2008) 058115

Capitelli, M., Laricchiuta, A., Celiberto, R., Kosarim, A.V., Smirnov, B.M., **Electron-molecule collision cross-sections for air kinetics**, AIP Conf. Proc. 762 (2005) 914-919, (RGD24)

V Laporta, R Celiberto, J Tennyson, **Resonant vibrational-excitation cross sections and rate constants for low-energy electron scattering by molecular oxygen**, Plasma Sources Science and Technology 22 (2013), 025001

DATABASEs

LXCAT DATABASE

http://fr.lxcat.net/home/

ALADDIN IAEA DATABASE

https://www-amdis.iaea.org/ALADDIN/

PHYS4ENTRY DATABASE

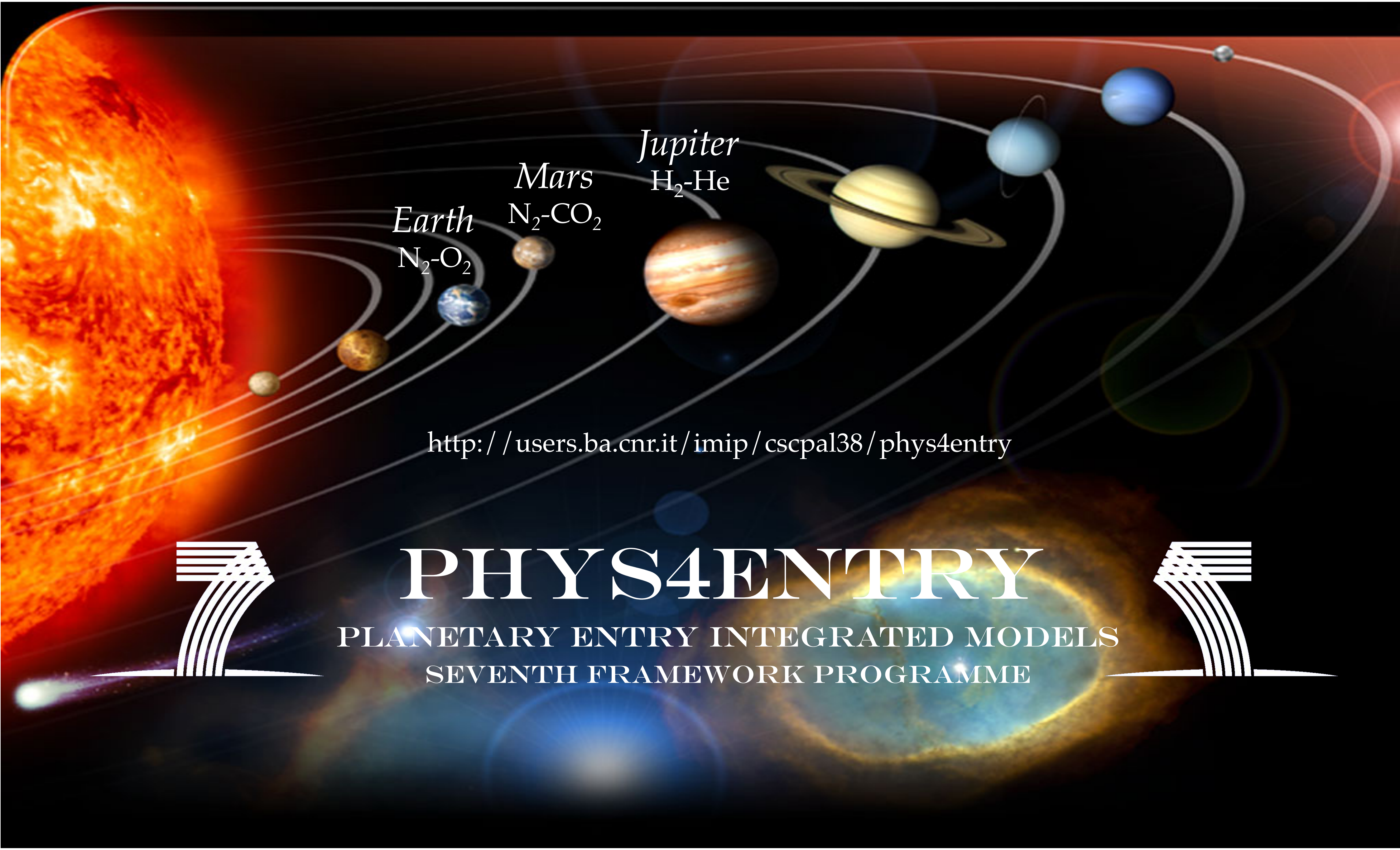
http://users.ba.cnr.it/imip/cscpal38/phys4entry/database.html

STELLAR DATABASE

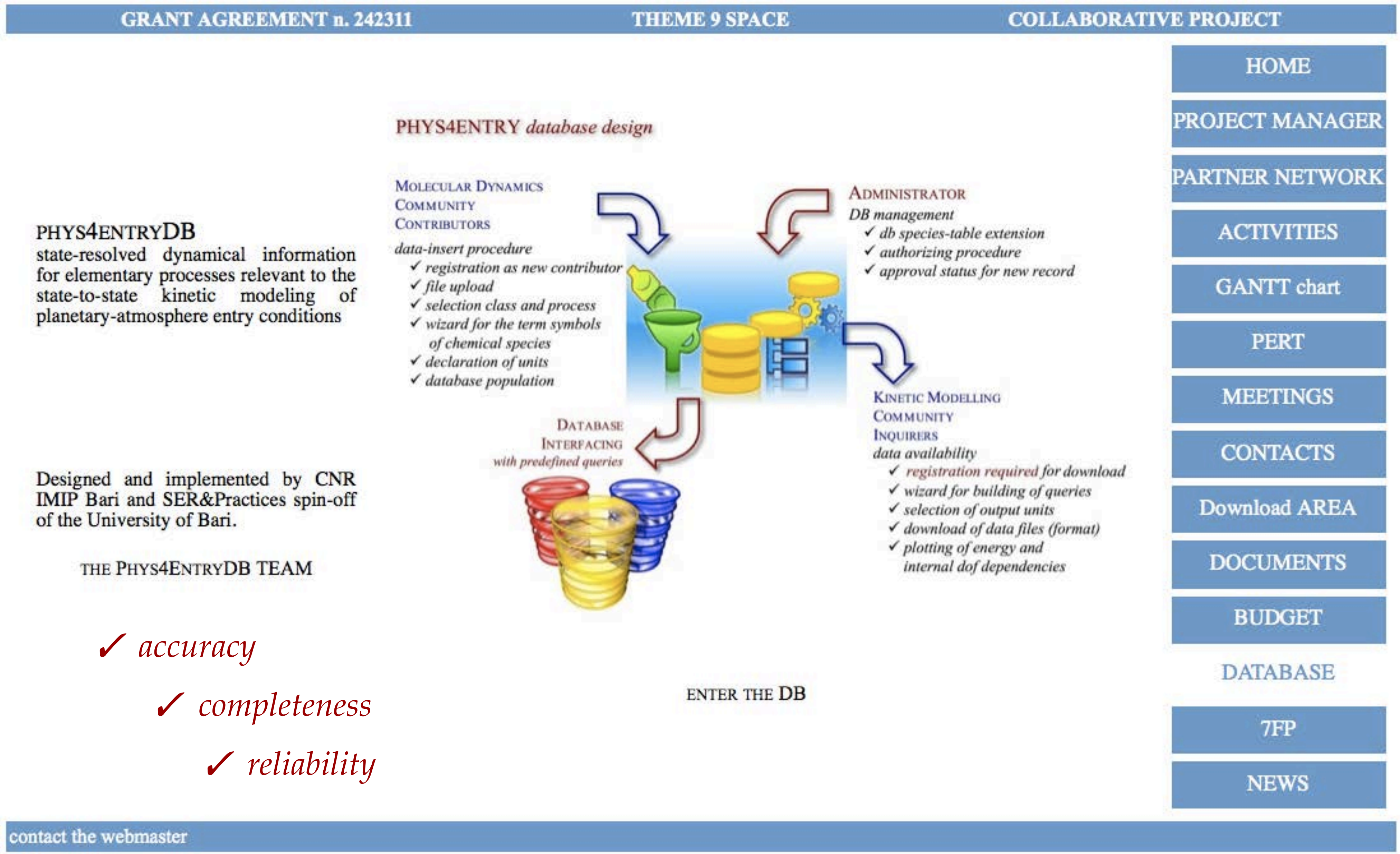
http://esther.ist.utl.pt/pages/stellar.html

POTLIB DATABASE

http://comp.chem.umn.edu/potlib


Earth
N_2-O_2
Mars
N_2-CO_2
Jupiter
H_2-He
http://users.ba.cnr.it/imip/cscpal38/phys4entry
PHYS4ENTRY
PLANETARY ENTRY INTEGRATED MODELS
SEVENTH FRAMEWORK PROGRAMME

The Phys4EntryDB

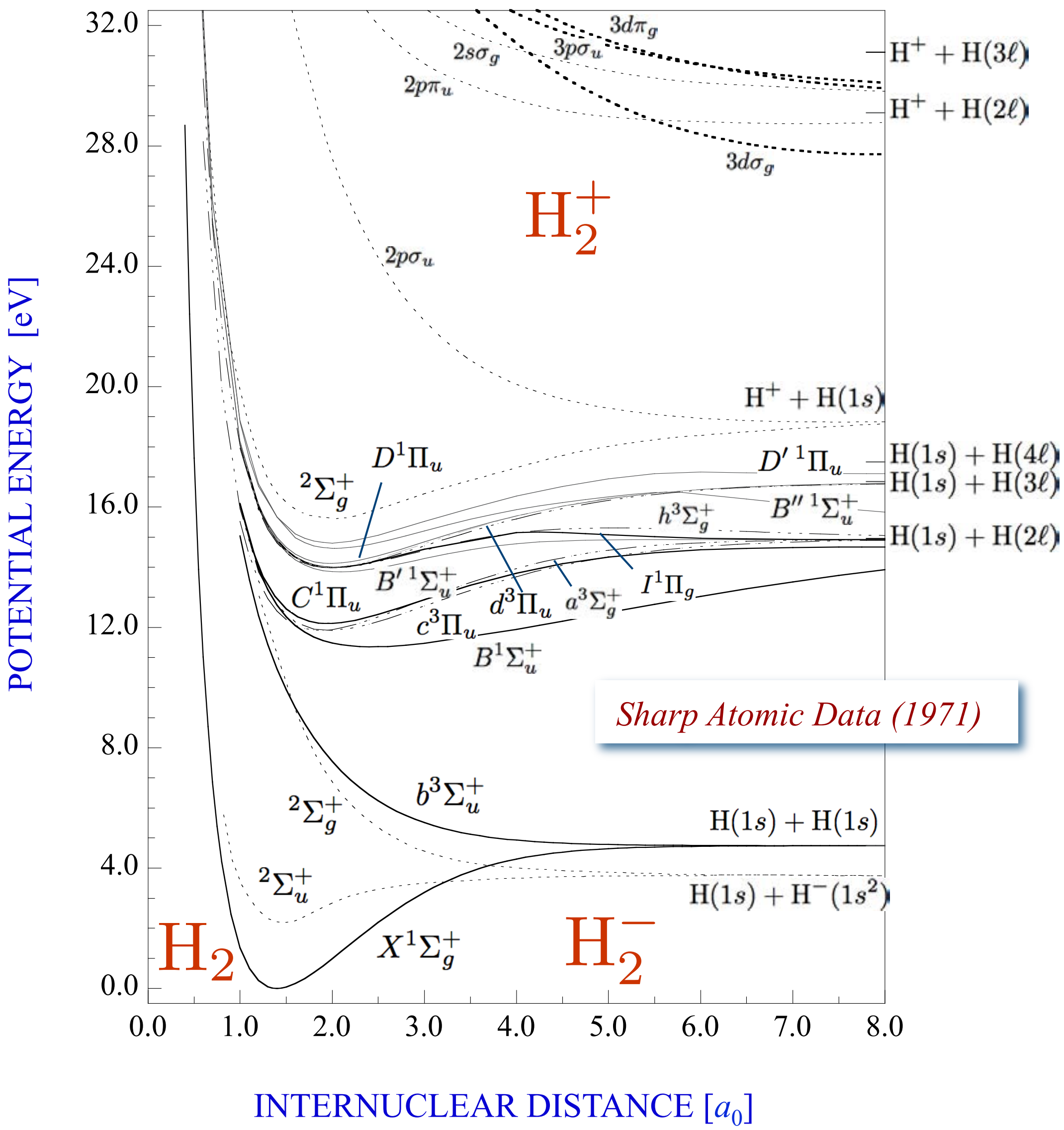


✓ *accuracy*

✓ *completeness*

✓ *reliability*

ELECTRON IMPACT INDUCED PROCESSES: THE DATA SET FOR H_2



Sharp Atomic Data (1971)

RESONANT PROCESSES

$$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2^- \rightarrow H^-(^1S) + H(n)$$

$$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2^- \rightarrow H_2(X^1\Sigma_g^+, v_f) + e$$

Celiberto et al, Chemical Physics (2012)
Celiberto et al, Physical Review A (2013)
Horáček et al, Physical Review A (2004) and (2006)

non-RESONANT VIBRONIC EXCITATION

$$e + H_2(X^1\Sigma_g^+, v_i) \rightarrow e + H_2^\star \rightarrow e + H(^2S) + H(n \leq 4)$$

Celiberto et al., AtomicData&NuclearDataTables (2001)

Laricchiuta et al., Physical Review A (2004)

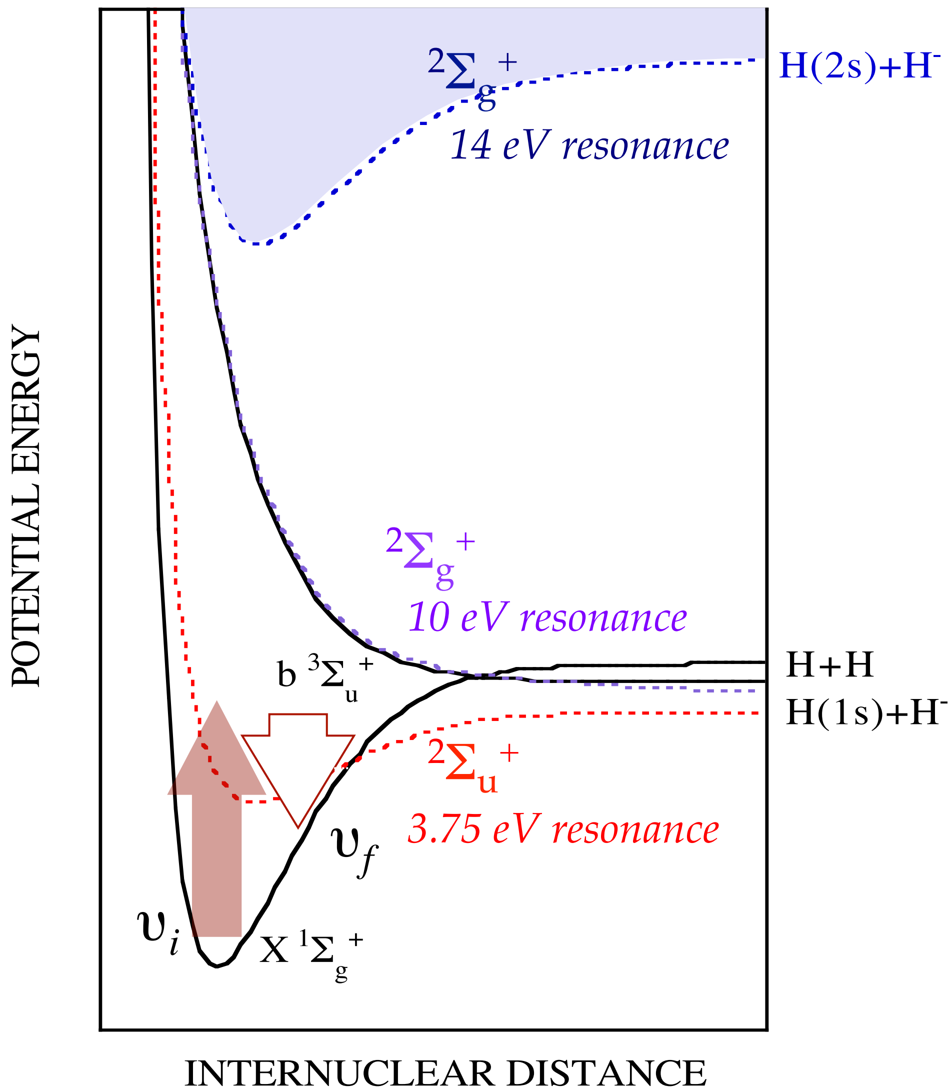
Liu et al J Phys B 45 (2012) 015201

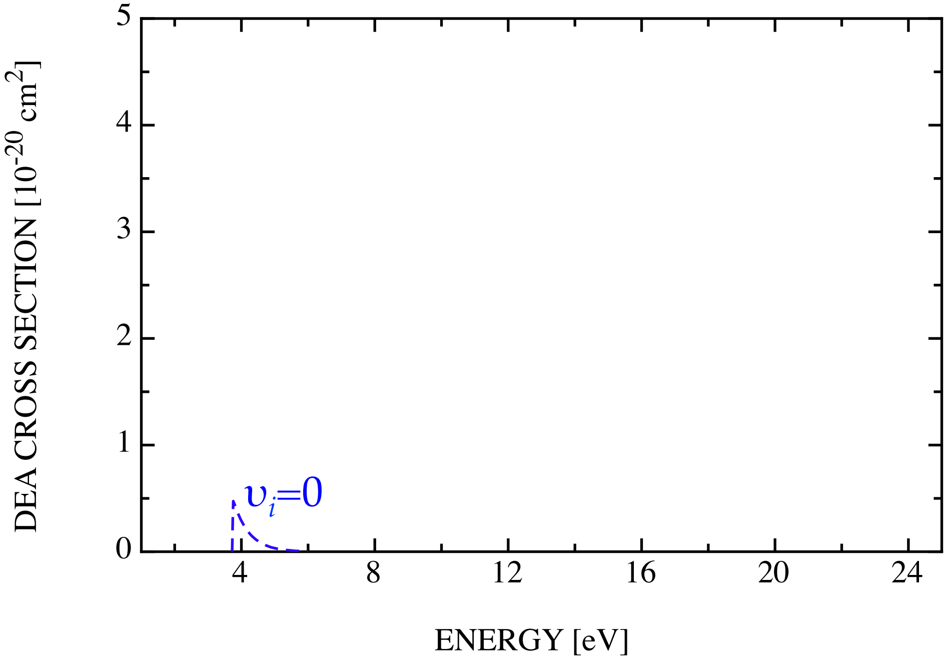
DISSOCIATIVE & non-DISSOCIATIVE IONIZATION

$$e + H_2(X^1\Sigma_g^+, v_i) \longrightarrow 2e + H_2^+ \rightarrow 2e + H + H^+$$

Wünderlich Chemical Physics 390 (2011) 75–82

H_2 Dissociative Attachment

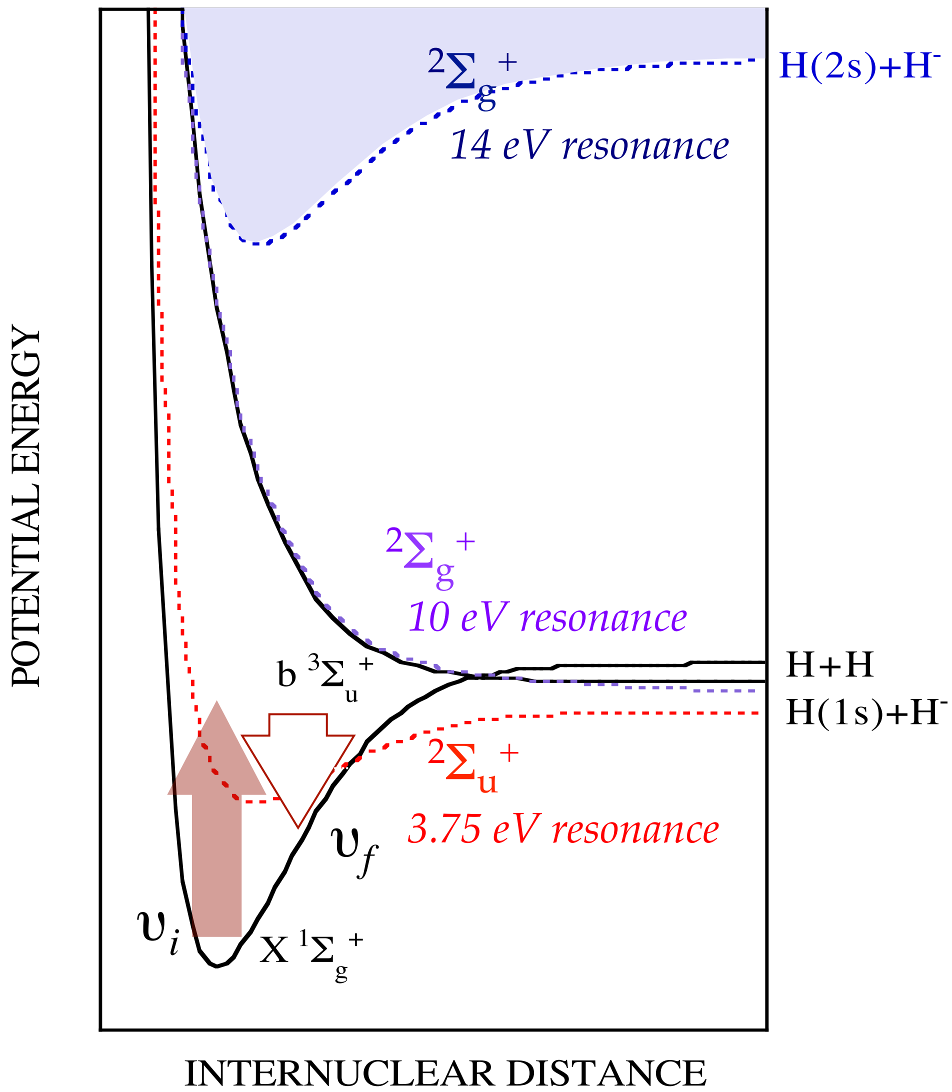


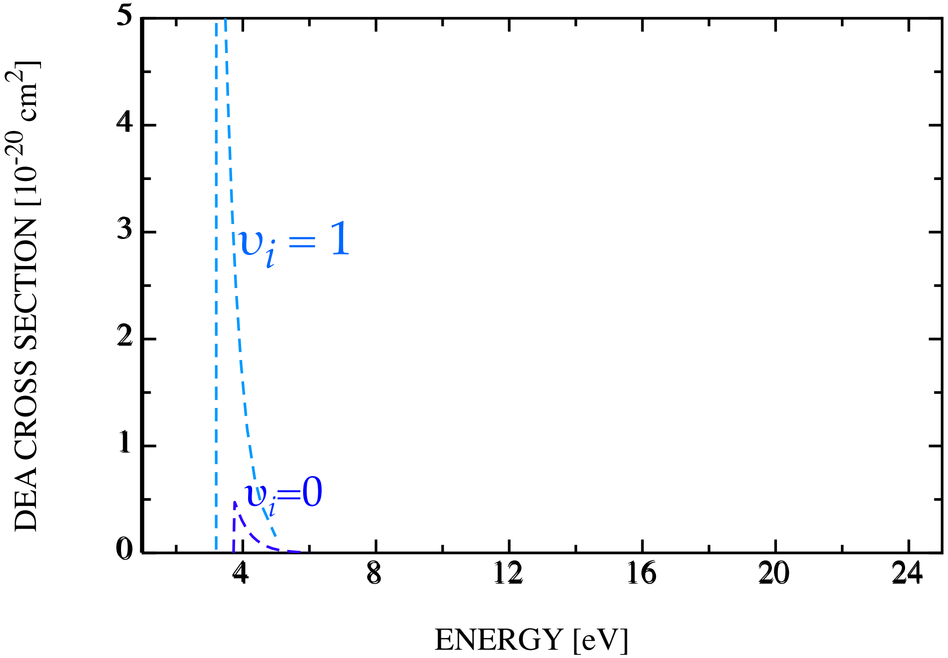


Horáček et al, Physical Review A (2004)

3.75 eV resonance

H_2 Dissociative Attachment

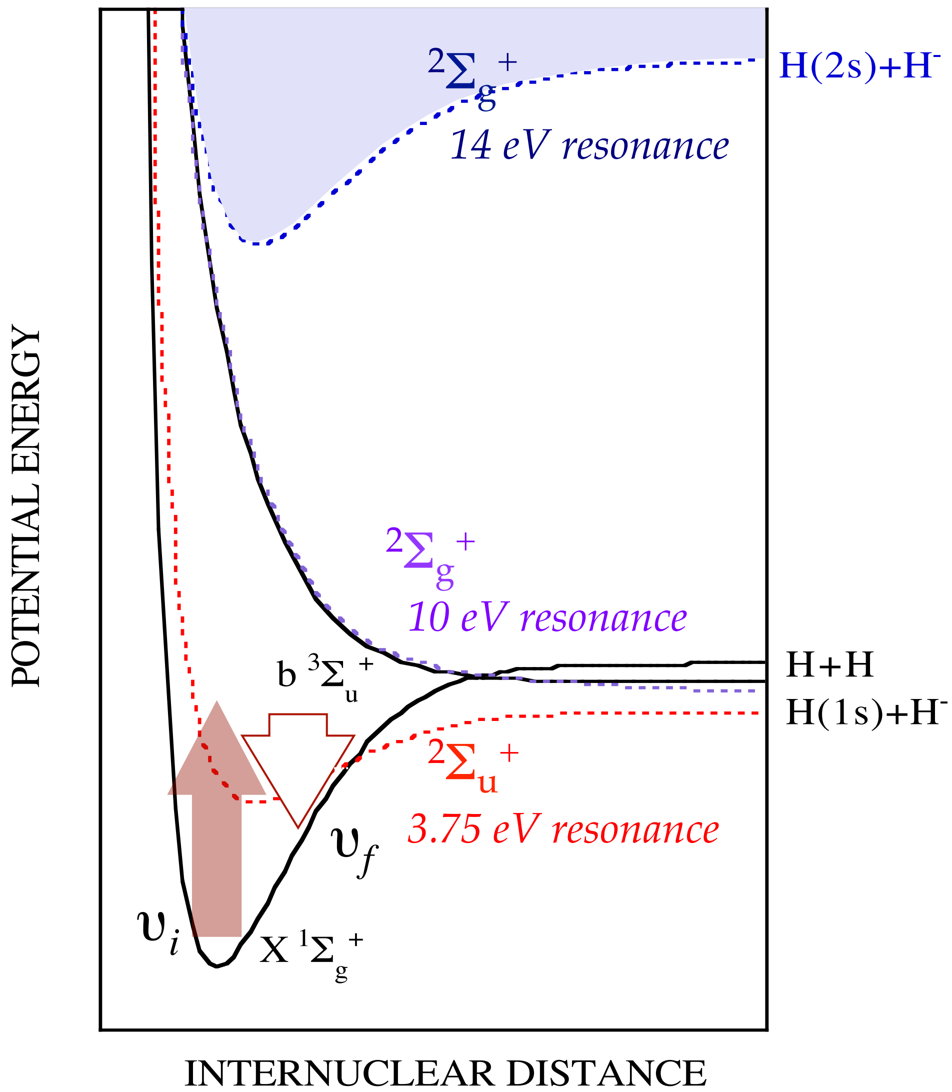


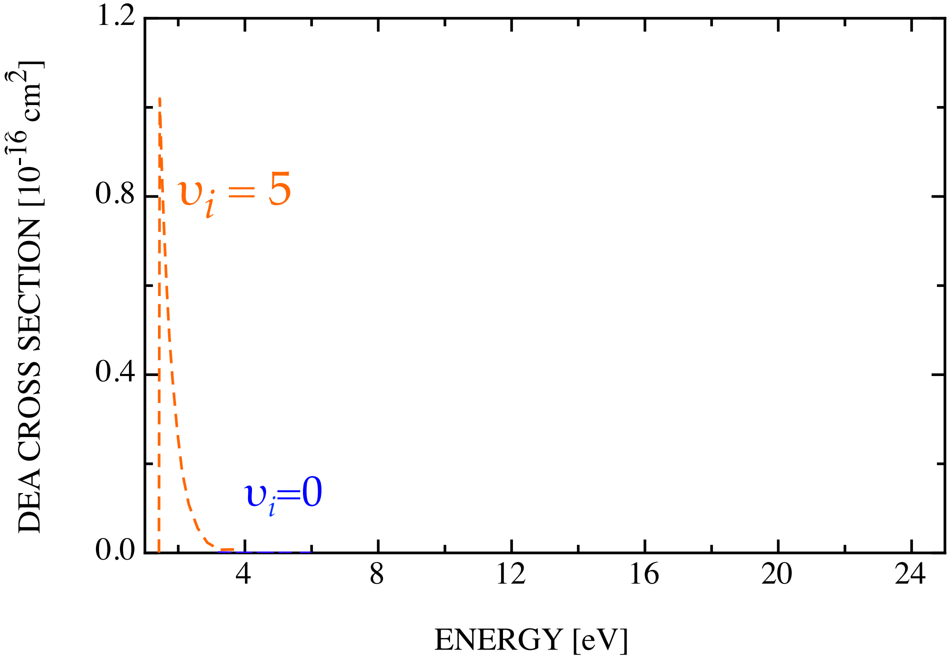


Horáček et al, Physical Review A (2004)

3.75 eV resonance

H_2 Dissociative Attachment





Horaček et al, Physical Review A (2004)

3.75 eV resonance

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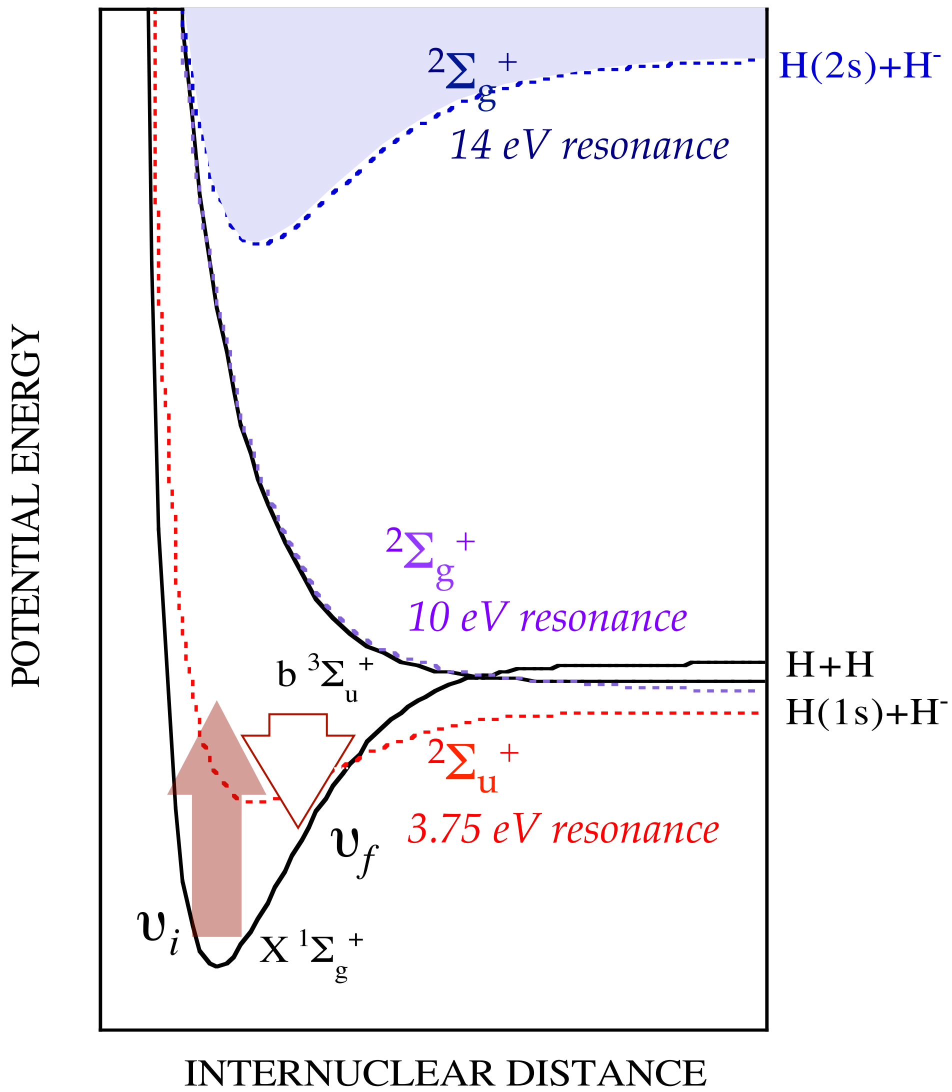
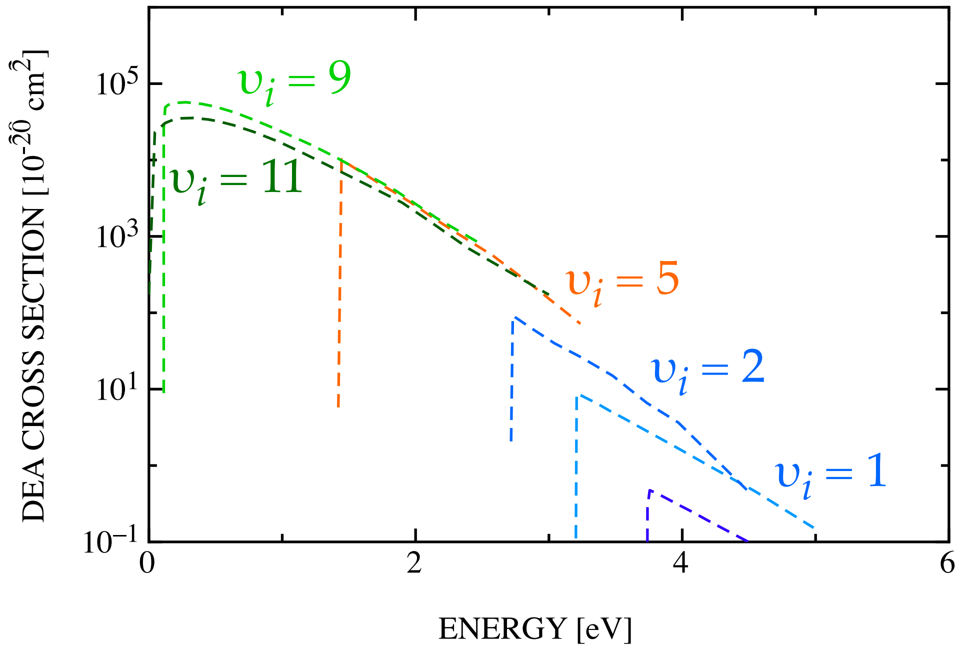
H_2 Dissociative Attachment





Horačék et al, Physical Review A (2004)

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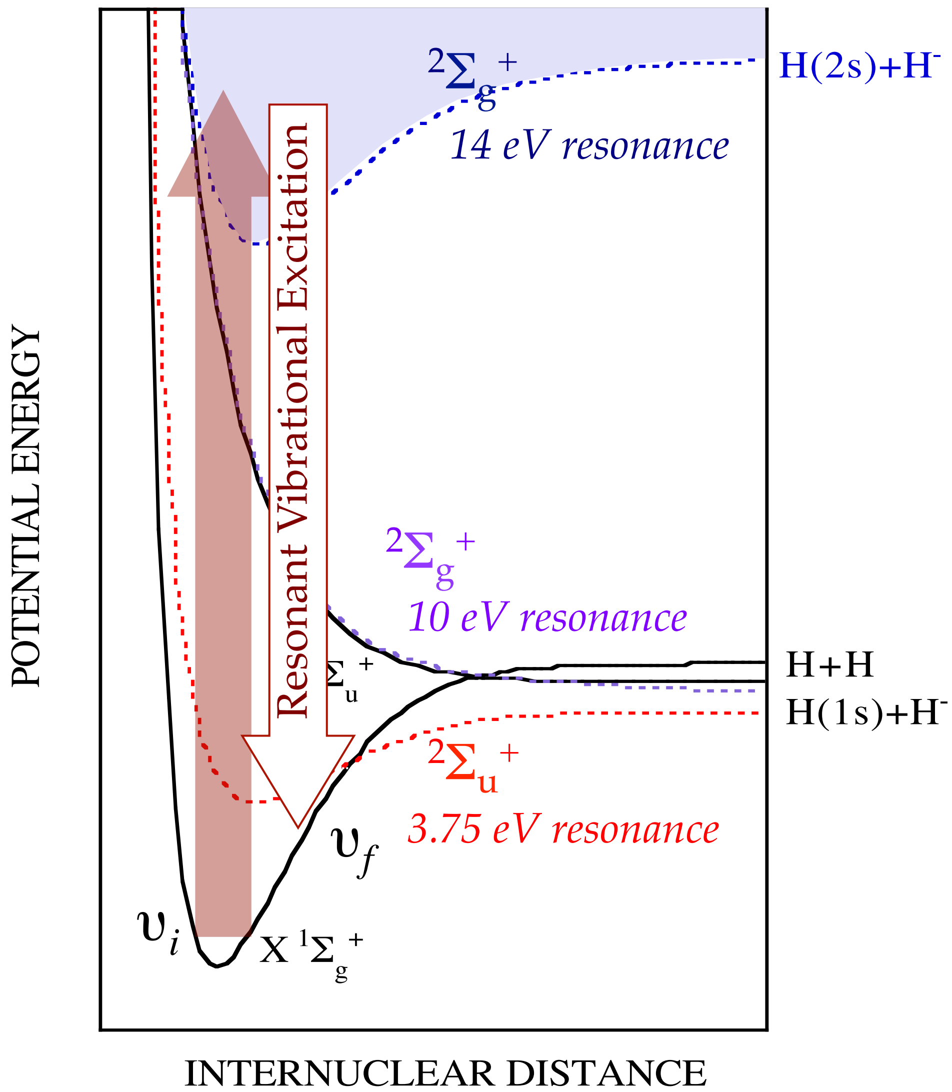
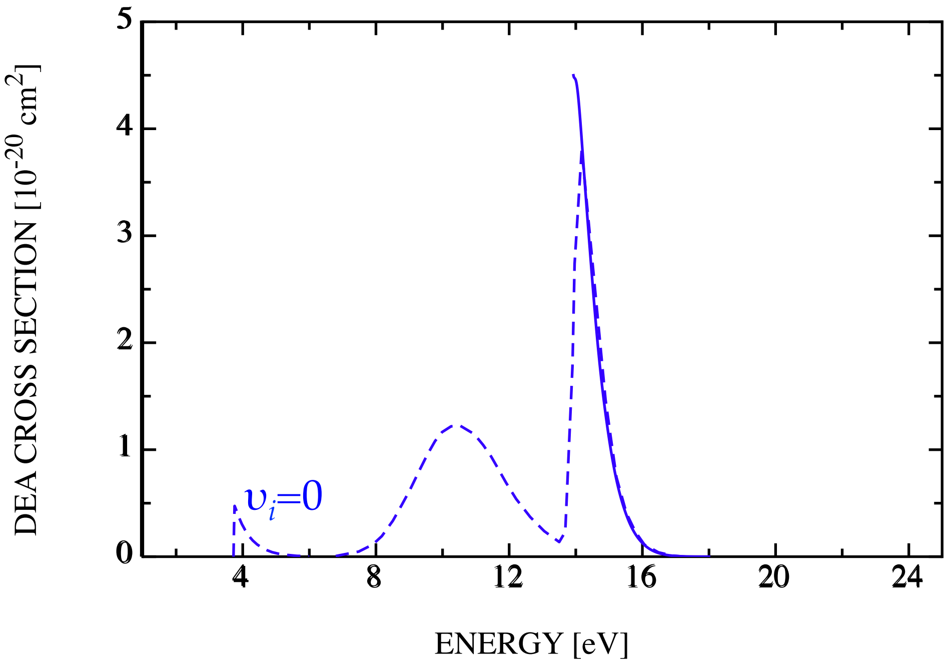
H_2 Dissociative Attachment

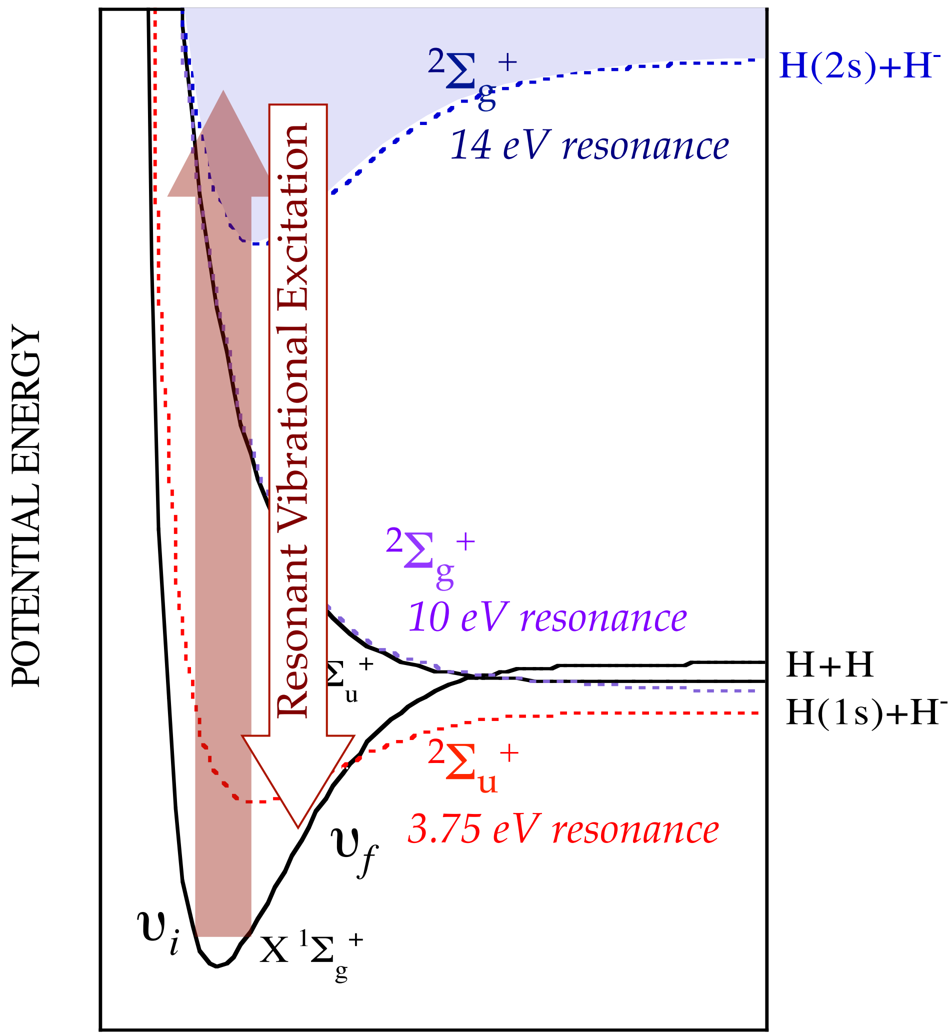


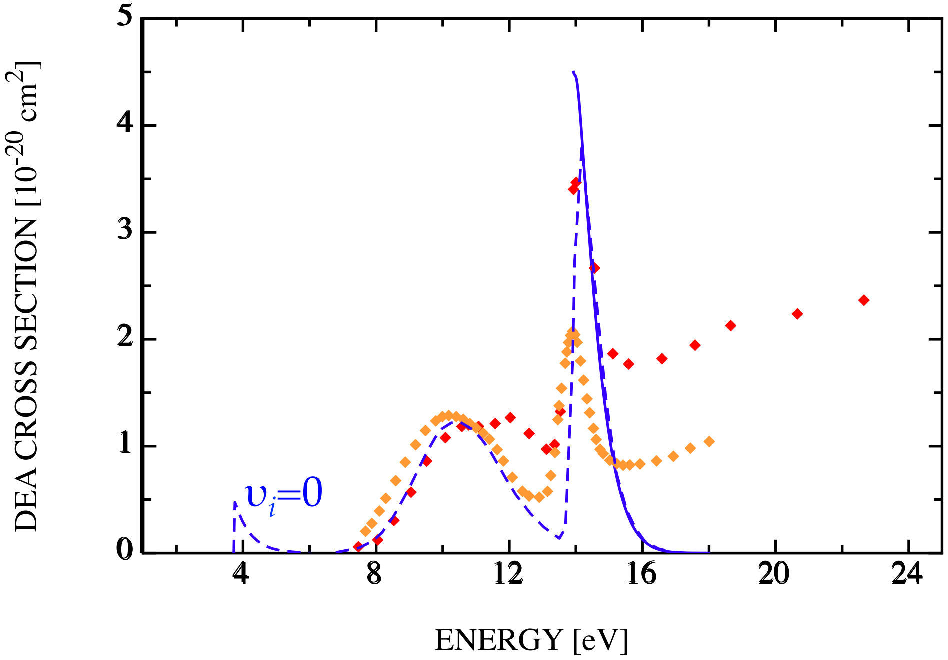


Horáček et al, Physical Review A (2004)

Celiberto et al, Chemical Physics (2012)

H_2 Dissociative Attachment



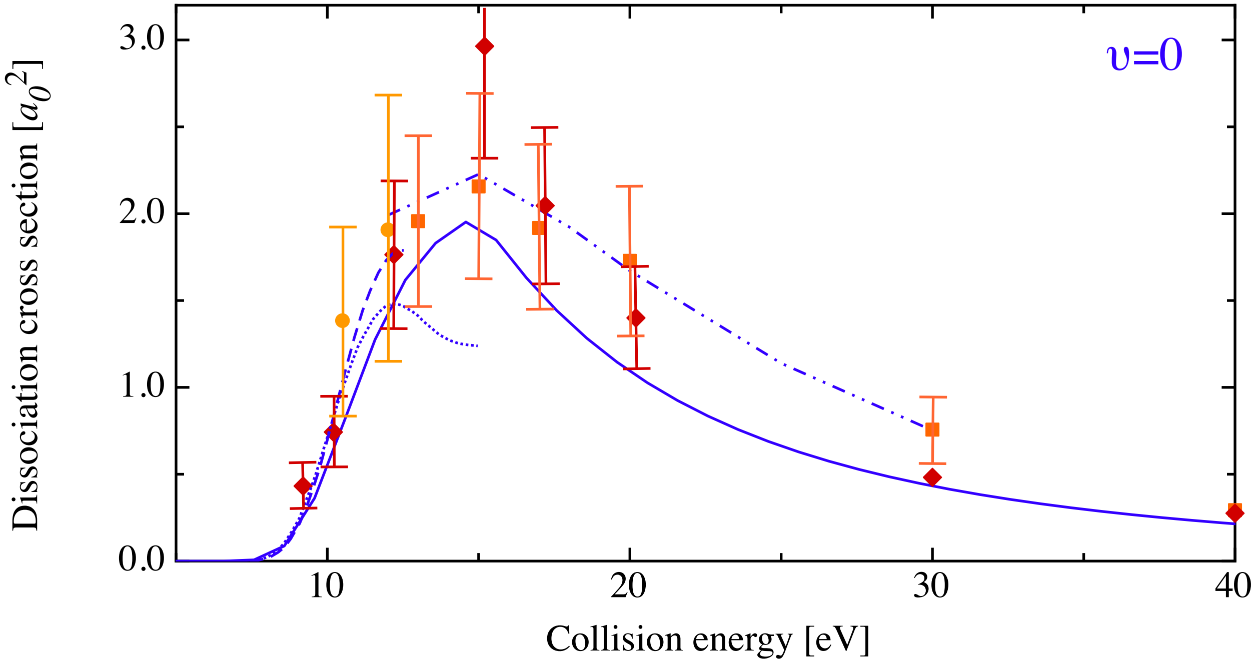


Horáček et al, Physical Review A (2004)

Celiberto et al, Chemical Physics (2012)

G. J. Schulz, Phys. Rev. 113 (1959) 816
D. Rapp et al, Phys. Rev. Lett. 14 (1965) 533

H_2 Direct Dissociation trough *b* state



Khakoo & Segura, J Phys B (1994)
Khakoo et al., Phys Rev A (1987)

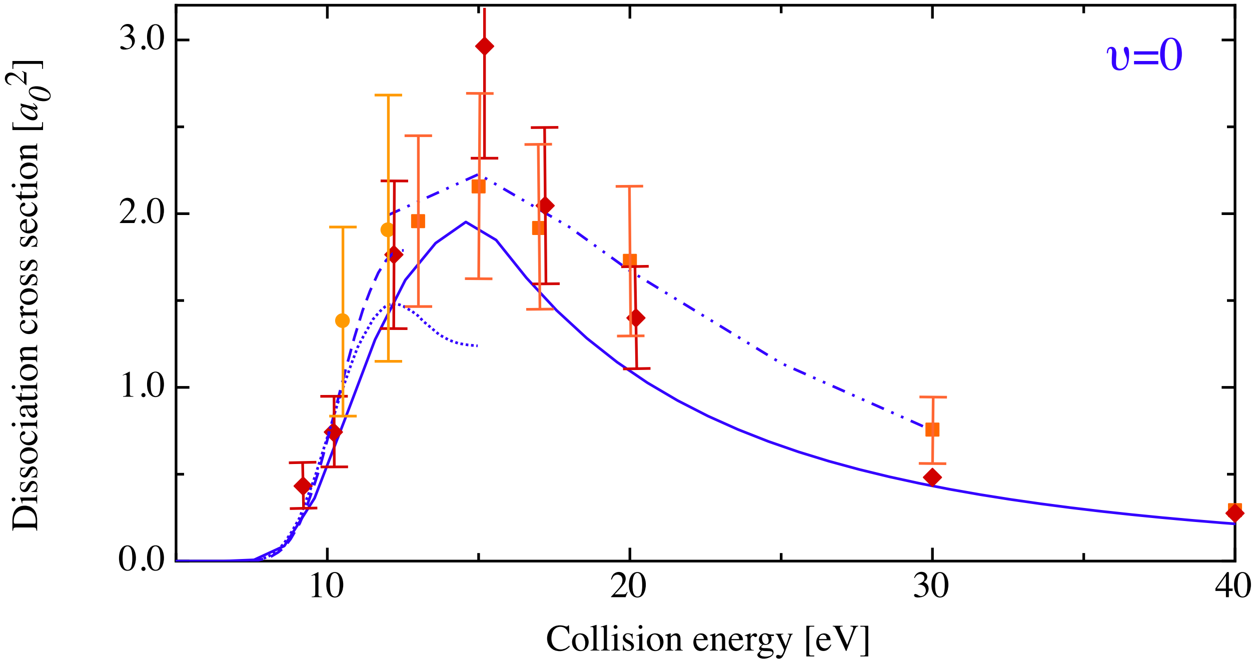
H. Nishimura, J. Phys. Soc. Jpn. 55 (1986) 3031

R-matrix
Stibbe & Tennyson,
The Astrophysical Journal (1999)
Trevisan&Tennyson,
Plasma Phys & Controlled Fusion (2002)

Gryzinskii approach
Celiberto et al.,
AtomicData&NuclearDataTables (2001)

Complex Khon method
Rescigno & Schneider, J Phys B (1988)

H_2 Direct Dissociation trough *b* state



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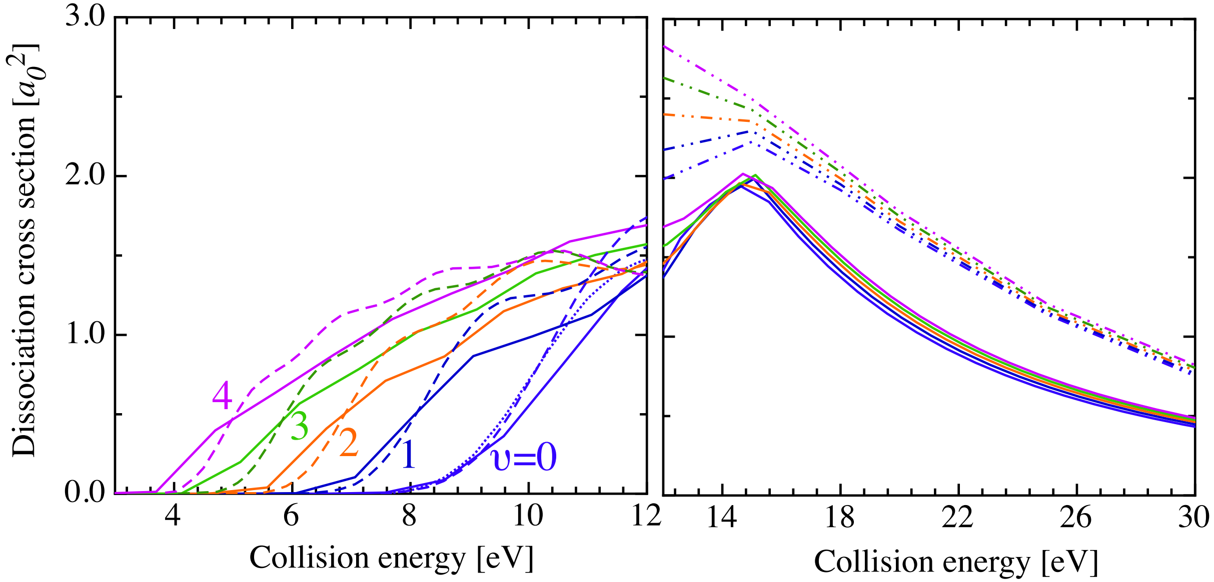

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Trevisan&Tennyson,
Plasma Phys & Controlled Fusion (2002)

Gryzinskii approach
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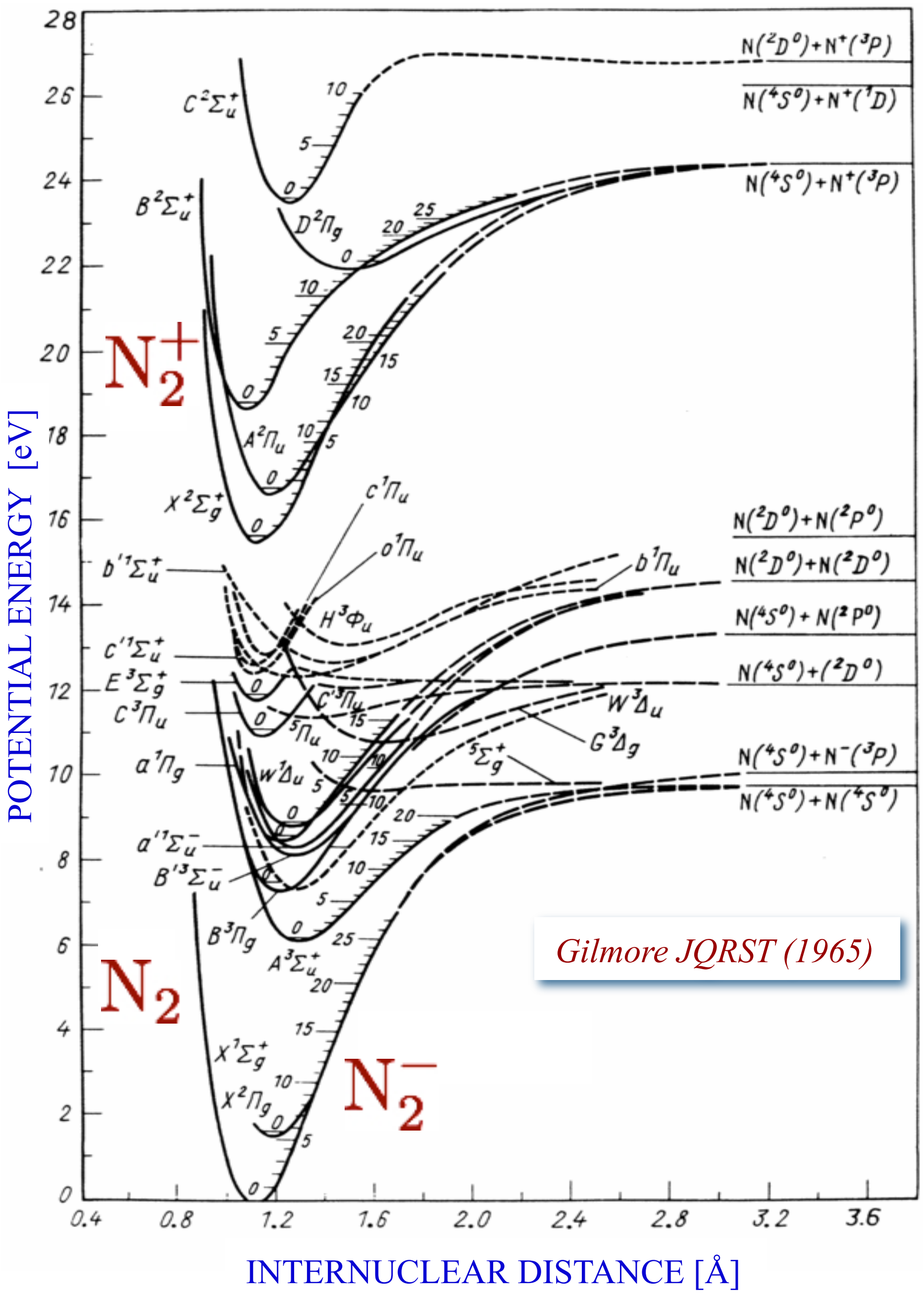
ELECTRON IMPACT INDUCED PROCESSES: THE DATA SET FOR N_2



RESONANT VIBRATIONAL EXCITATION

$$N_2(X^1\Sigma_g^+, v_i, j_i) + e \rightarrow N_2(X^1\Sigma_g^+, v_f, j_f) + e$$

Laporta et al PlasmaSourcesScience&Tech (2012)

VIBRONIC EXCITATION

$$N_2(^1\Sigma_g^+, v_i, j_i = 0) + e \rightarrow N_2^\star(triplets) + 2e$$

$$N_2(^1\Sigma_g^+, v_i, j_i = 0) + e \rightarrow N_2^\star(singlets) + 2e$$
$$\rightarrow N(^4S) + N(^2D)$$

Capitelli&Celiberto in
"Novel Aspects of Electron-Molecule Collisions"
Ed KH Becker (1998)

NON-DISSOCIATIVE IONIZATION

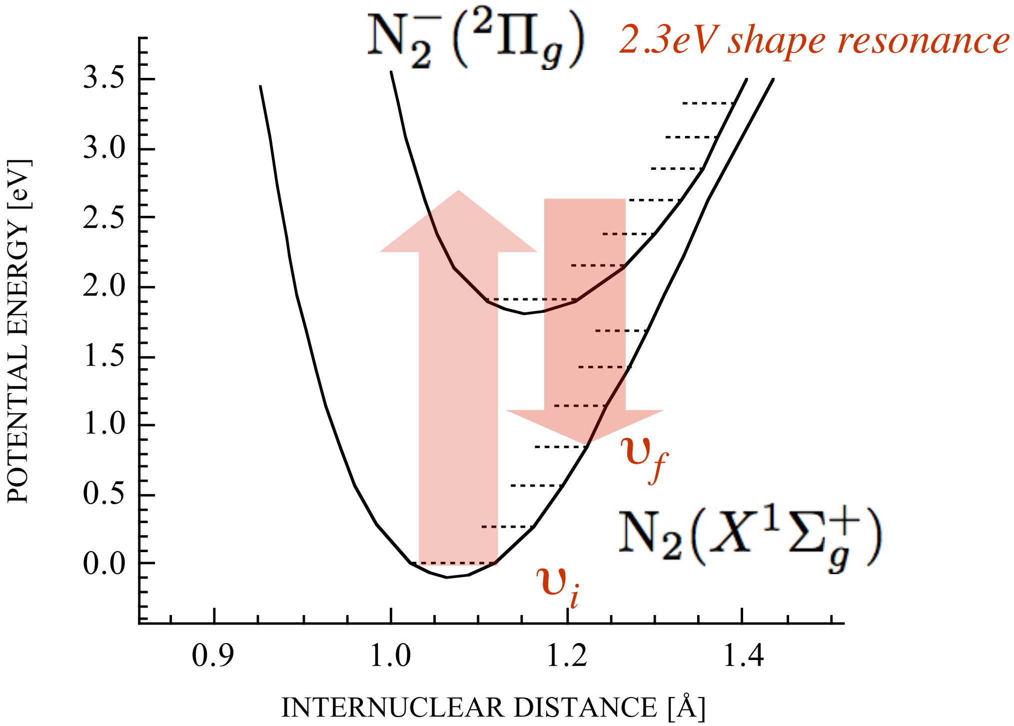
$$N_2(^1\Sigma_g^+, v_i, j_i = 0) + e \rightarrow N_2^+(^2\Sigma_g^+) + 2e$$

Kosarim et al ChemPhysLett (2005)
Laricchiuta et al. AIAA paper 2006-2898 (2006)

Electron-Impact induced Vibrational Pumping

resonant vibrational excitation (eV *processes*)

$$N_2(^1\Sigma_g^+, \upsilon_i) + e \rightarrow N_2^-(^2\Pi_g) \rightarrow N_2(^1\Sigma_g^+, \upsilon_f) + e$$



V. Laporta, R. Celiberto, J.M. Wadehra, Plasma Sources Sci. Technol. 21 (2012) 055018

M. Capitelli et al., Plasma Chemistry & Plasma Proc. 32 (2012) 427

OLD DATASET

collection of theoretical and experimental cross sections

$\upsilon_i = 0 \rightarrow \upsilon_f = 1-17$
M.Allan, J.Phys.B (1985)

$\upsilon_i = 0 \rightarrow \upsilon_f = 18-19$
L.A.Morgan, J.Phys.B (1986)

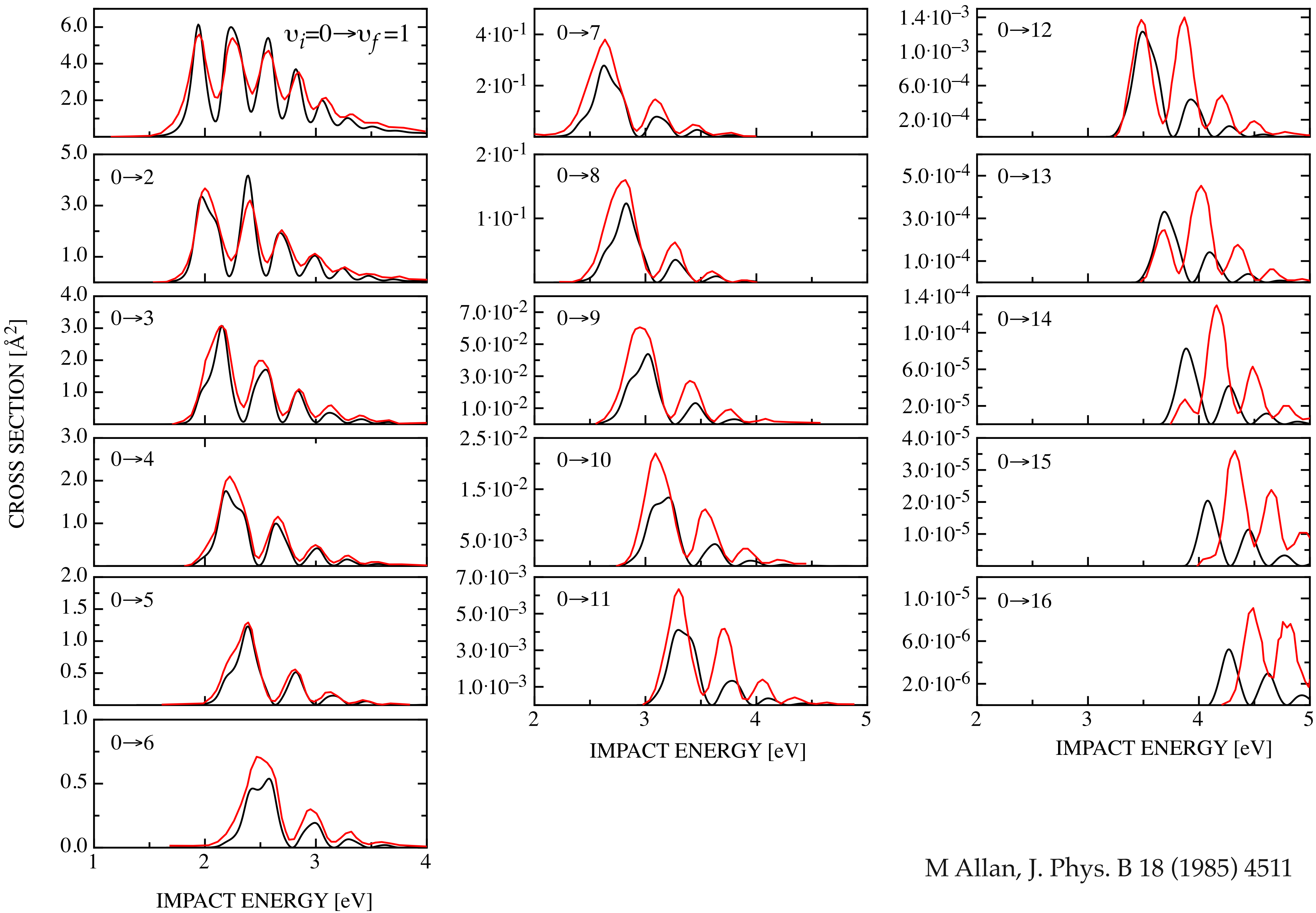
$\upsilon_i = 1-7 \rightarrow \upsilon_f = \upsilon_i + 1-8$
N. Chandra & A.Temkin, NASA-TN (1976)

⇩

NEW DATASET

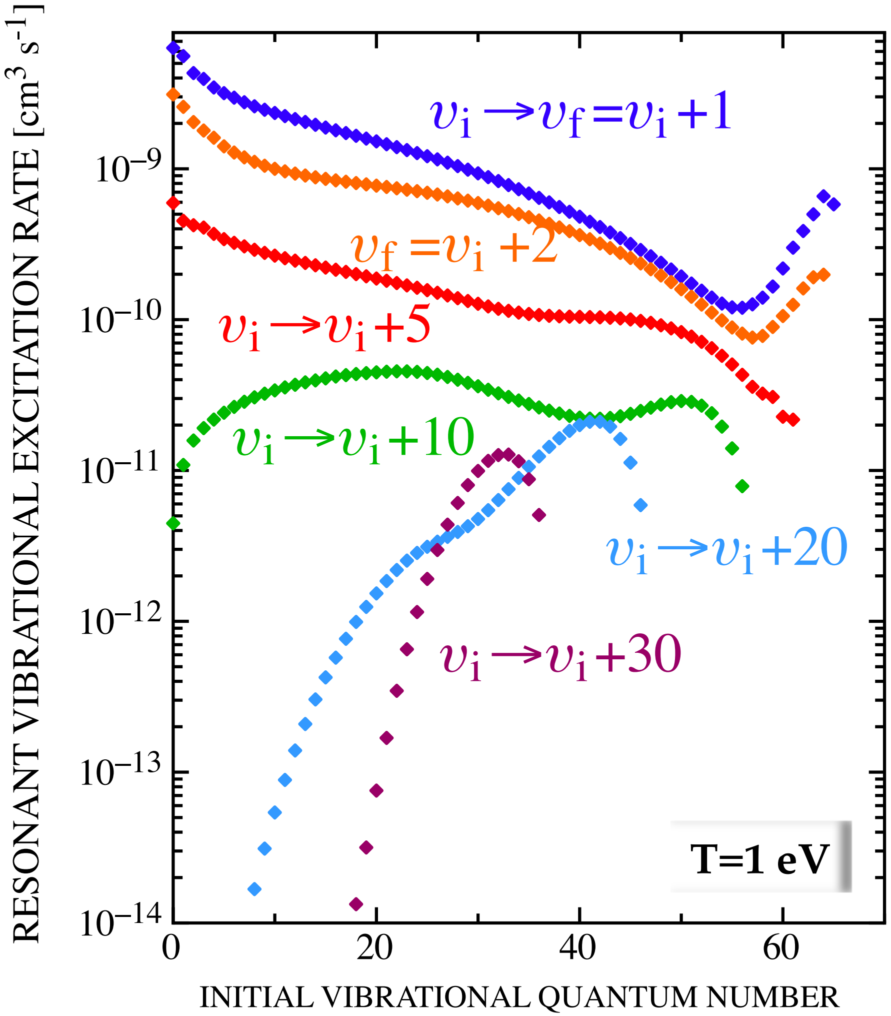
local theory of resonance
complete set of cross sections for transitions among all the levels in the vibrational ladder

Electron-Impact induced Vibrational Pumping



M Allan, J. Phys. B 18 (1985) 4511

Electron-Impact induced Vibrational Pumping



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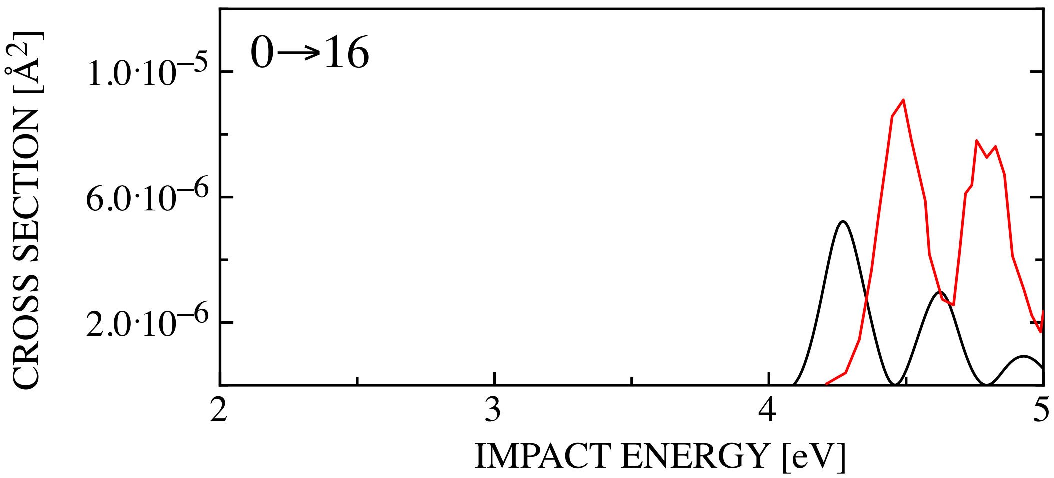
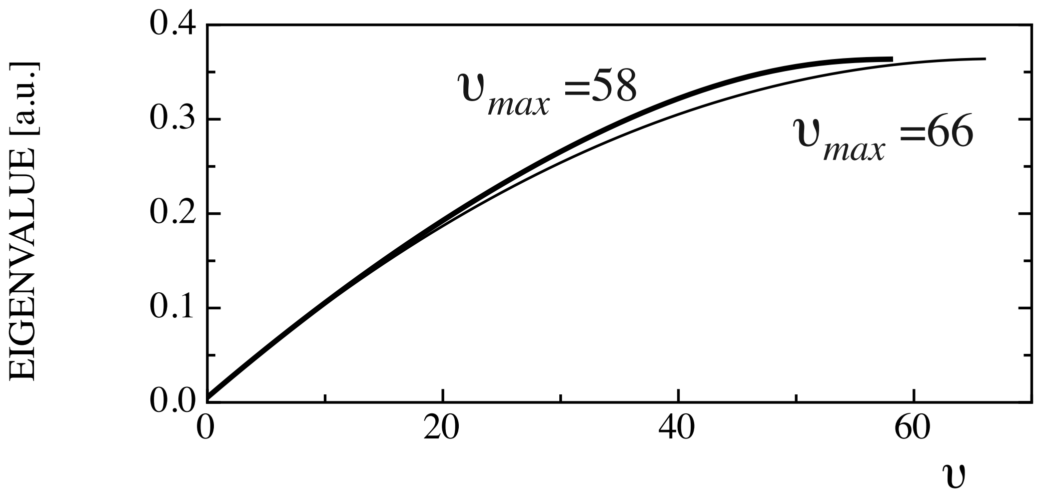
Electron-Impact induced Vibrational Pumping





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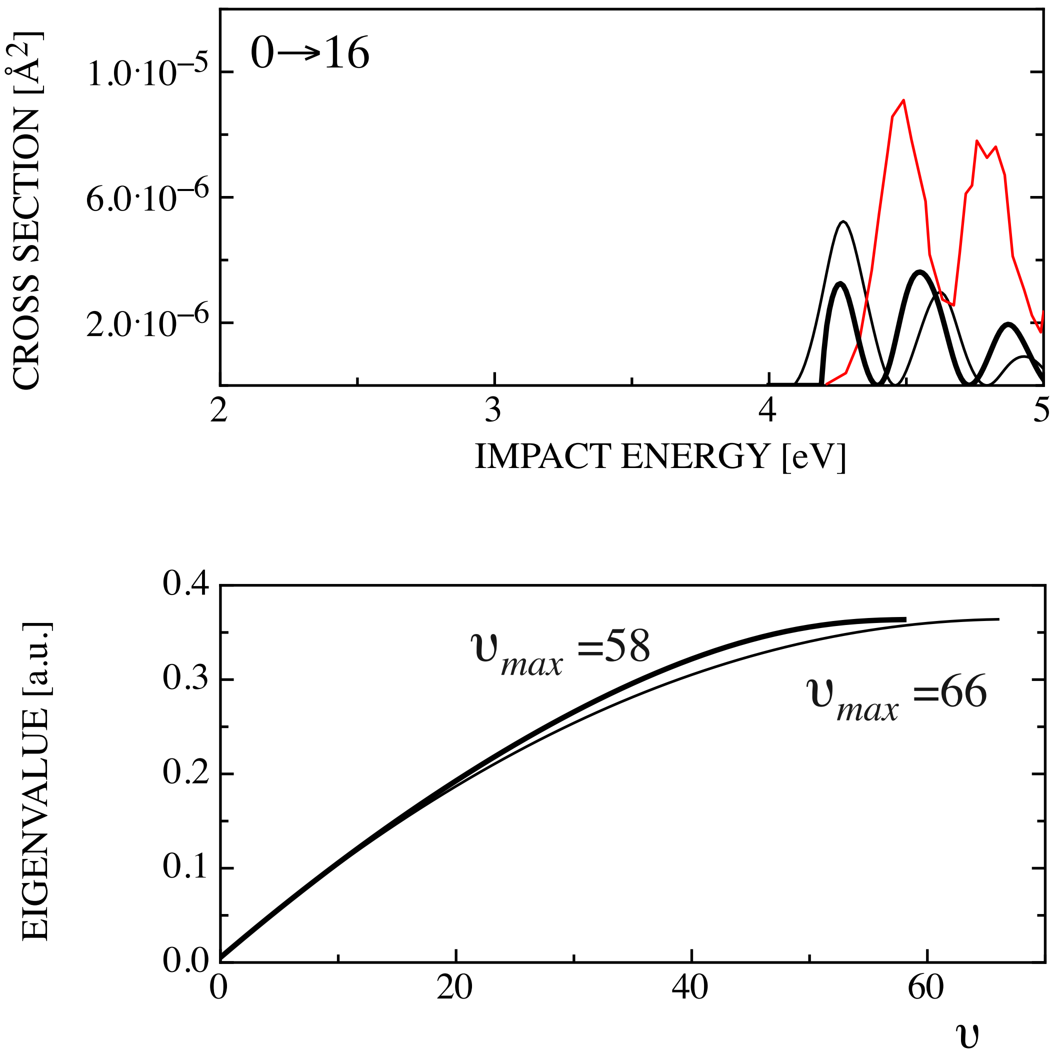
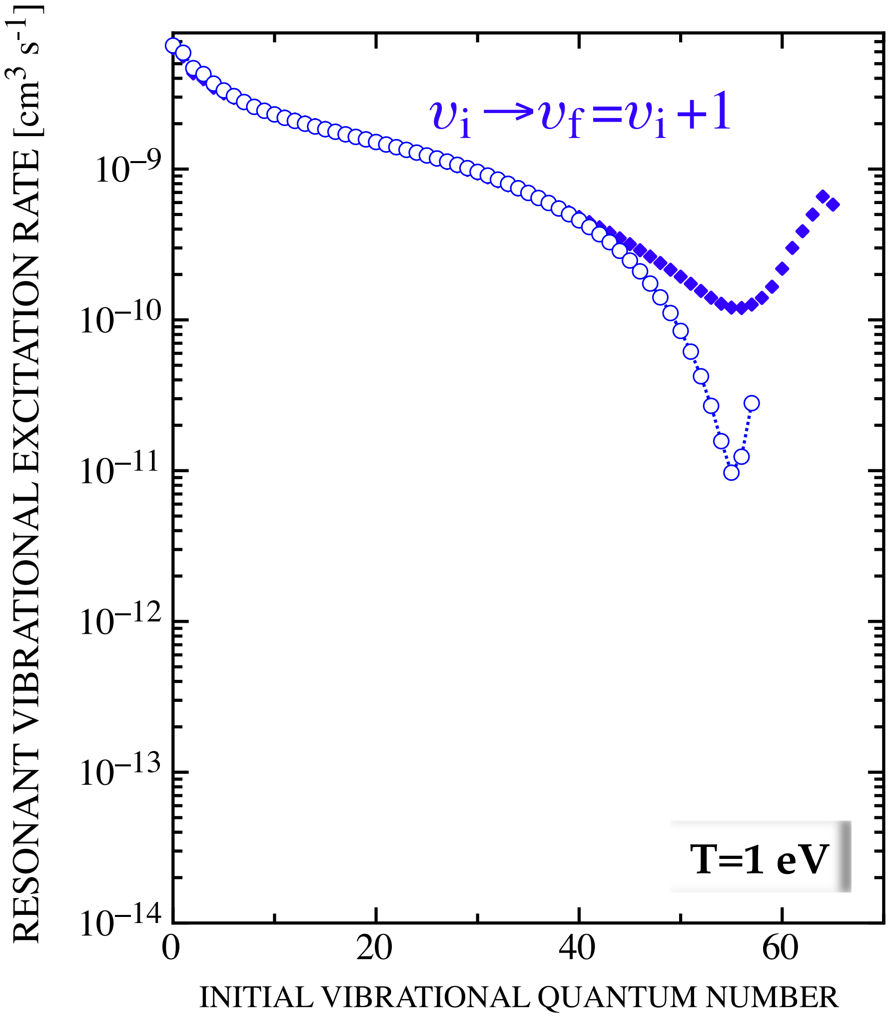
Electron-Impact induced Vibrational Pumping



Laporta et al. Plasma Sources Sci. Technol. (2014)

Electron-Impact induced Vibrational Pumping



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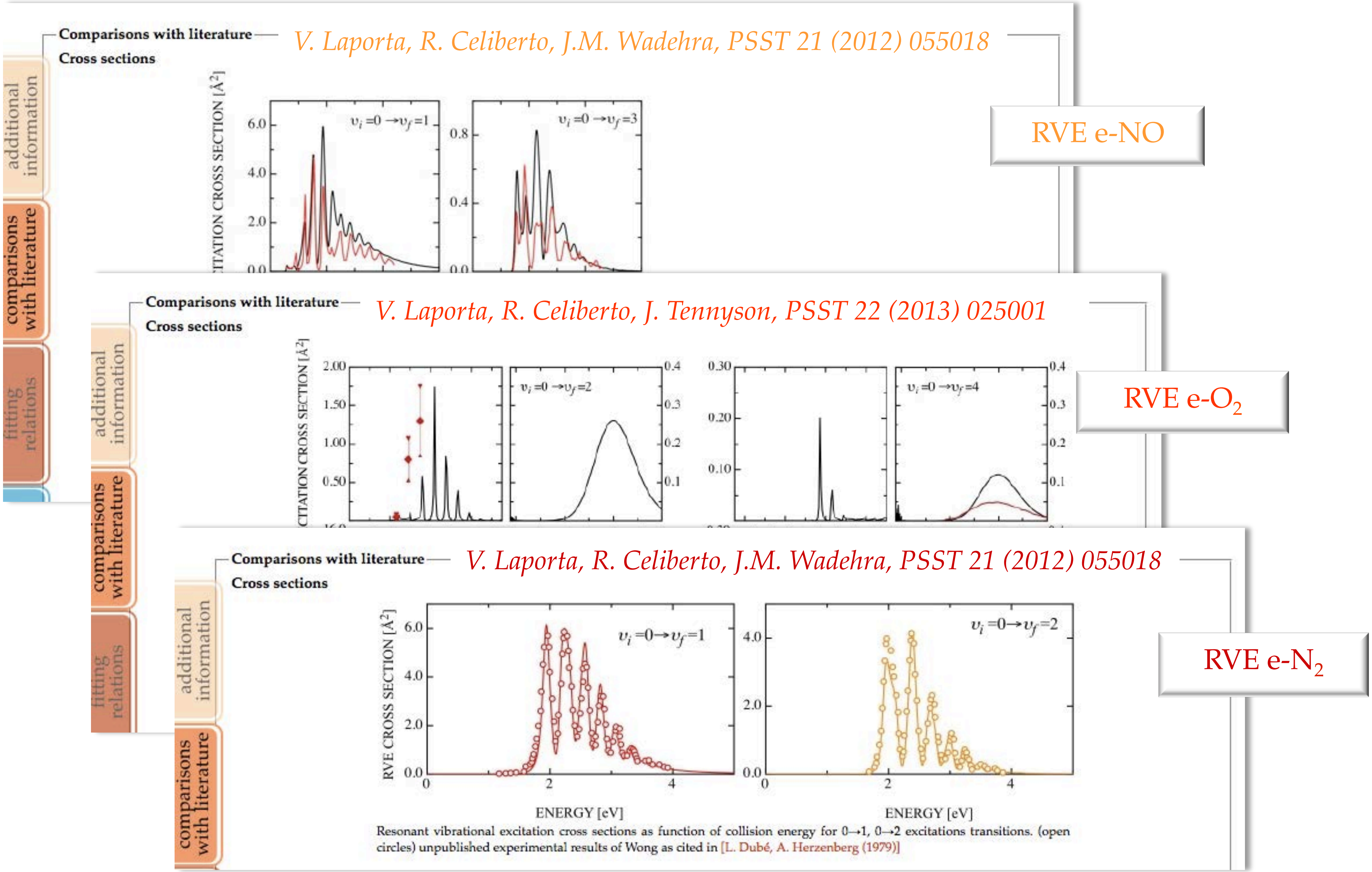
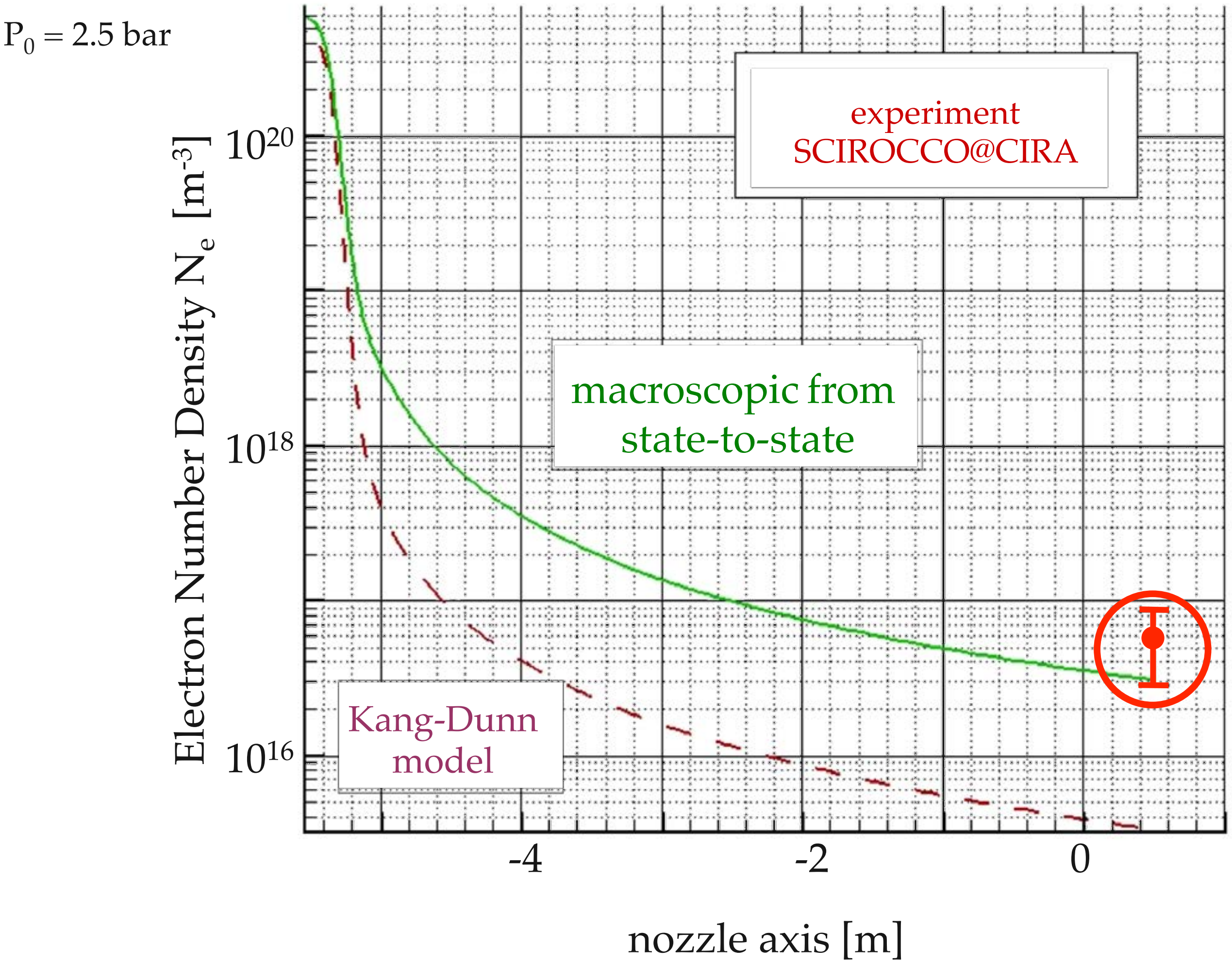
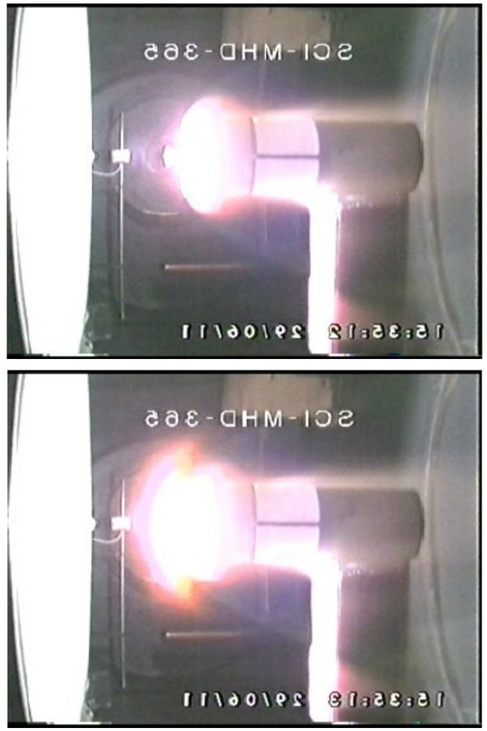
The Phys4EntryDB : Resonant Vibrational Excitation



Experimental / theoretical investigation of MHD interaction in Air

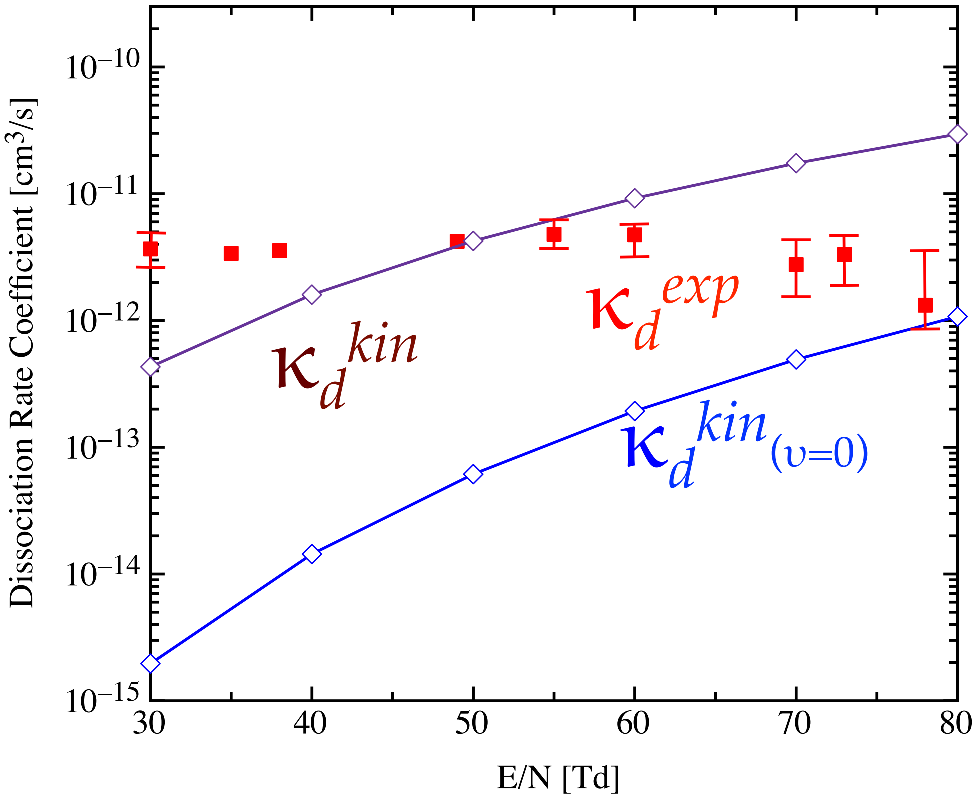


A. Schettino & D. D'Ambrosio,
The Open Plasma Physics Journal 7 (Special Issue) (2014)



A. Cristofolini et al.,
AIAA paper 2012-3179 (2012)

N_2 continuous discharge: dissociation rate coefficient at stationary state



$T = 1000$ K
$p = 5.6$ torr
SS at 0.1*s*

κ_d^{exp}

experimental global dissociation rate

L. S. Polak et al. in Proceedings 12th ICPIG 1975

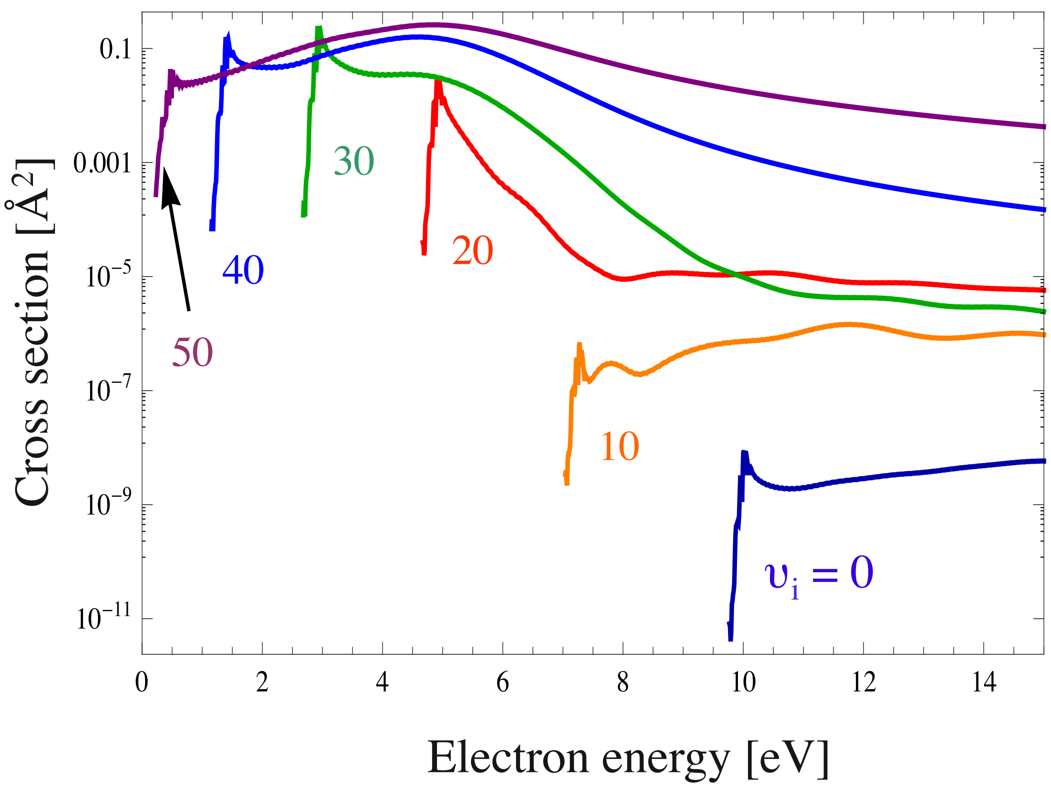
$$\kappa_d^{kin} = \sum_{\upsilon=0}^{\upsilon_{max}} k_d(\upsilon) \frac{N_\upsilon}{N_{tot}}$$

$$e + N_2(X, v) \rightarrow e + N(^4S) + N(^4S)$$

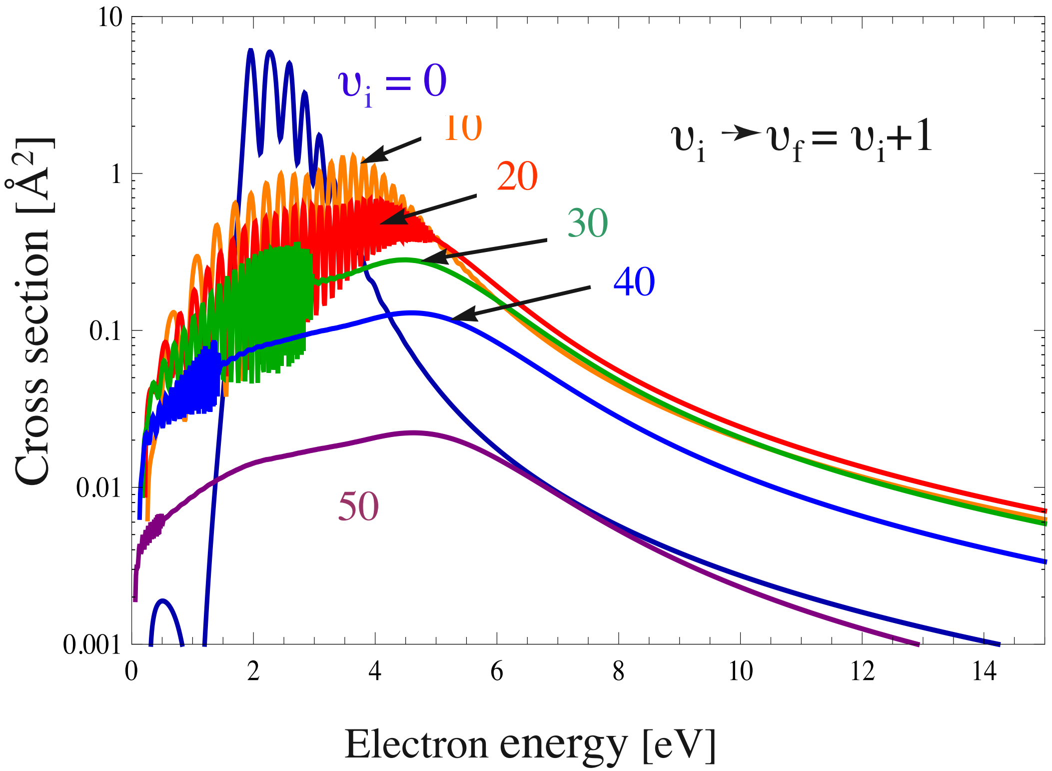
direct dissociation (predissociation)

resonant dissociation *vs* mono-quantum excitation in e-N_2 collisions

$$e + N_2(X, v) \rightarrow N_2^- \rightarrow e + N(^4S) + N(^4S)$$

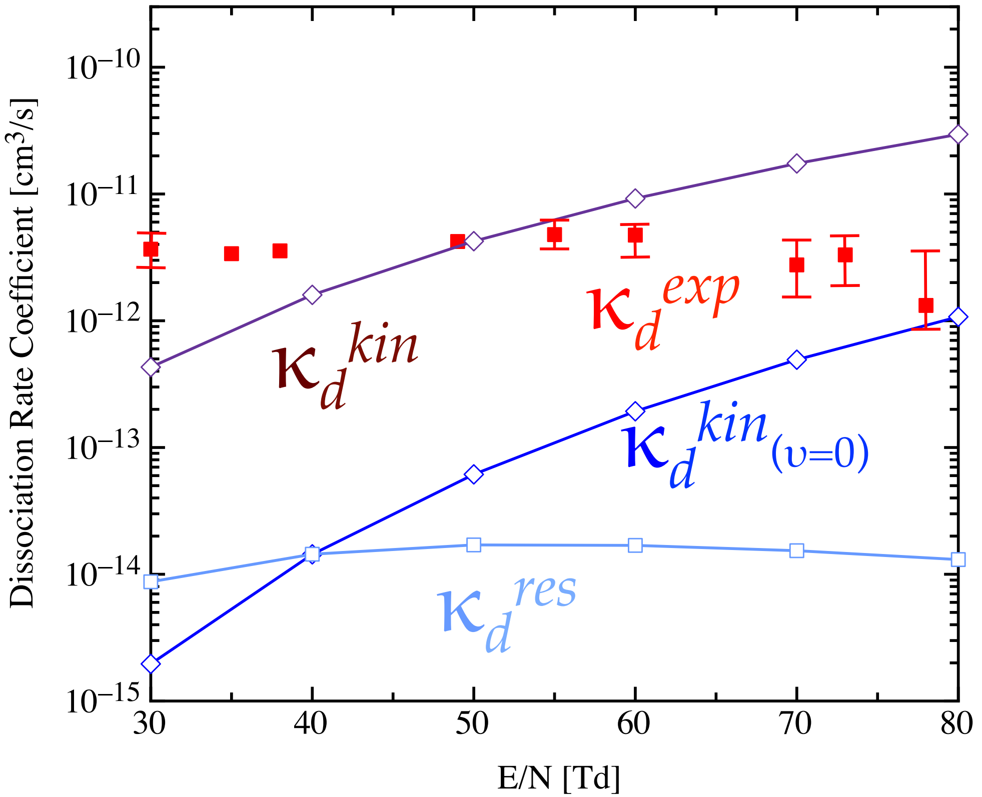


$$e + N_2(v_i) \rightarrow N_2^- \rightarrow e + N_2(v_i + 1)$$



Laporta et al. Plasma Sources Sci. Technol. (2014)

N_2 continuous discharge: dissociation rate coefficient at stationary state



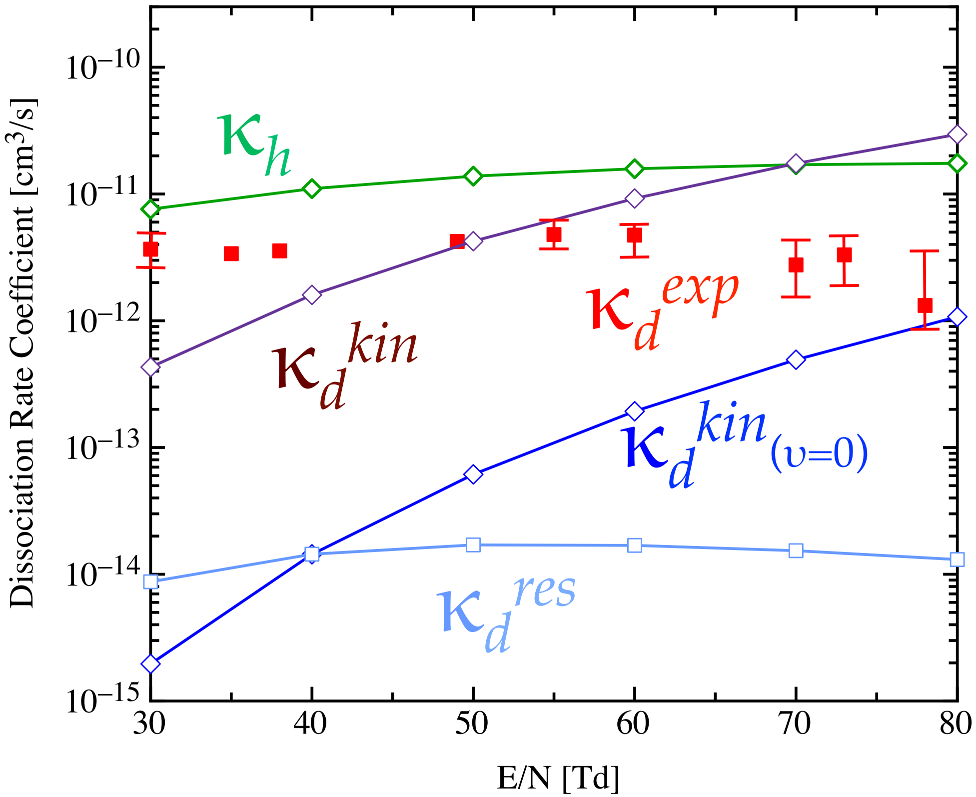
κ_d^{res}

$$e + N_2(v_i) \rightarrow N_2^- \rightarrow e + N(^4S) + N(^4S)$$

resonant dissociation

M. Capitelli et al. Chemical Physics (2014)

N_2 continuous discharge: dissociation rate coefficient at stationary state



κ_h

heavy collisions involving electronically and vibrationally excited molecules

$$N_2(X,v)+N_2(X,v) \rightarrow N_2(X)+2N(^4S)$$
$$10 < v < 25$$

$$N_2(X,v)+N_2(A^3\Sigma) \rightarrow N_2(B^3\Pi,v')+N_2(X)$$
$$\rightarrow N_2(X)+2N$$
$$14 \le v \le 19 \qquad v' \ge 13$$

V. Guerra, E. Galiaskarov, J. Loureiro, Chem. Phys. Lett. 371 (2003) 576

M. Capitelli et al. Chemical Physics (2014)

Simplified Theoretical Approaches

✓ *Gryzinskii approach*

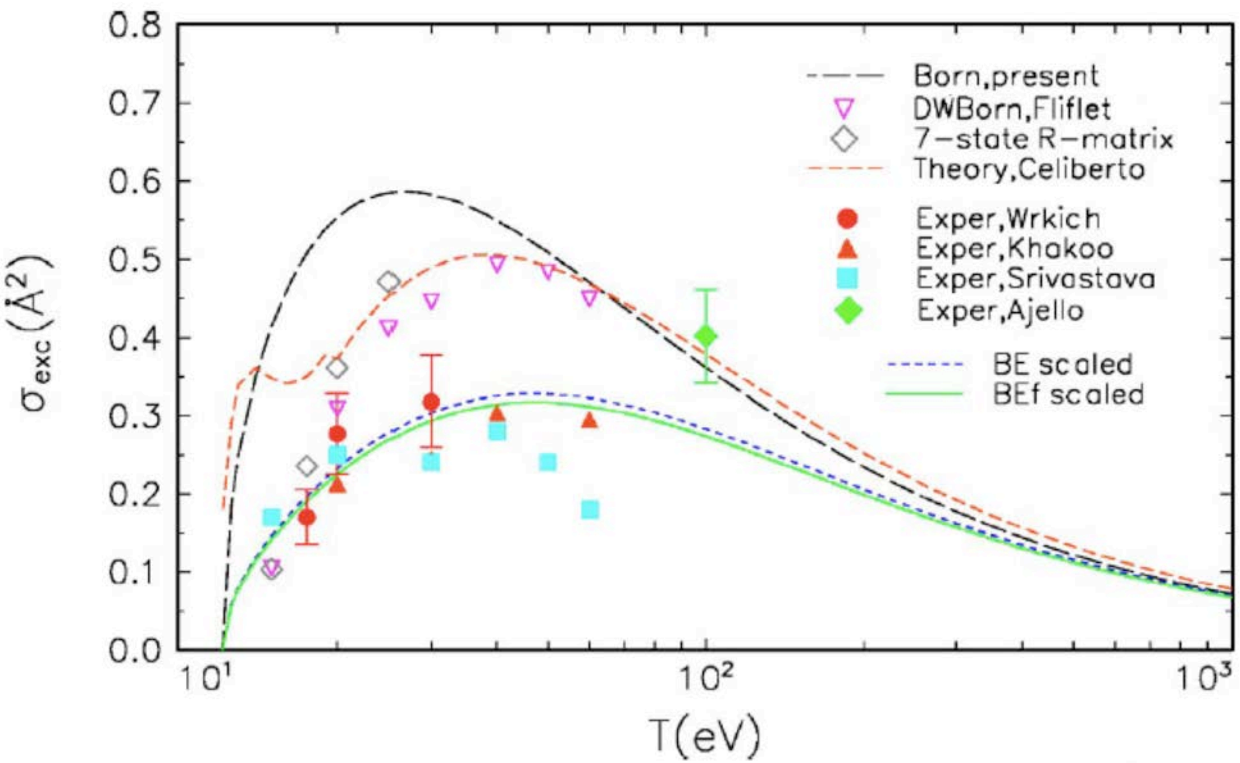
✓ *Bef-scaled approach*

✓ *Similarity approach*

Simplified Theoretical Approaches

- ✓ *Gryzinskii approach*
- ✓ *Bef-scaled approach*
- ✓ *Similarity approach*

$$e + H_2\,(X^1\Sigma_g{}^+, \upsilon'') \rightarrow e + H_2\,(B^1\Sigma u^+)$$

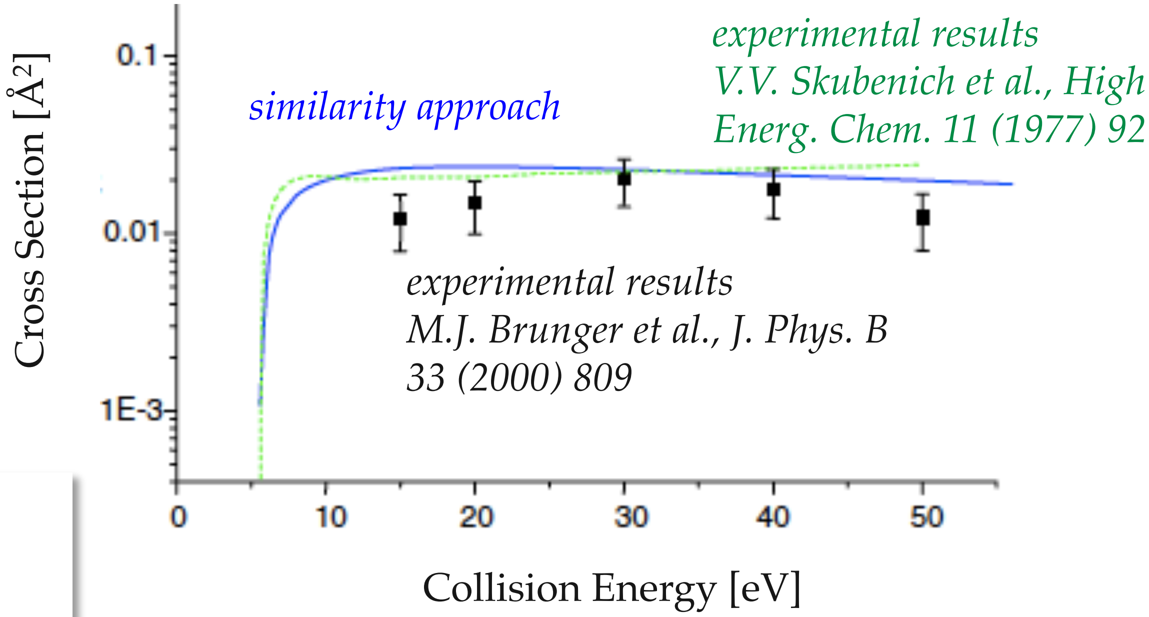


Y.K. Kim, J. Chem. Phys. 126 (2007) 064305

Simplified Theoretical Approaches

- ✓ *Gryzinskii approach*
- ✓ *Bef-scaled approach*
- ✓ *Similarity approach*

$$e+NO\,(X^2\Pi) \rightarrow e+NO\,(A\,^2\Sigma^+)$$



S. Adamson, Chem.Phys. Letters 436 (2007) 308
A.V. Eletskii & B.M. Smirnov, Zh. Eksp. Teor. Fiz. 84 (1983) 1639

N_2 e-impact induced allowed excitation

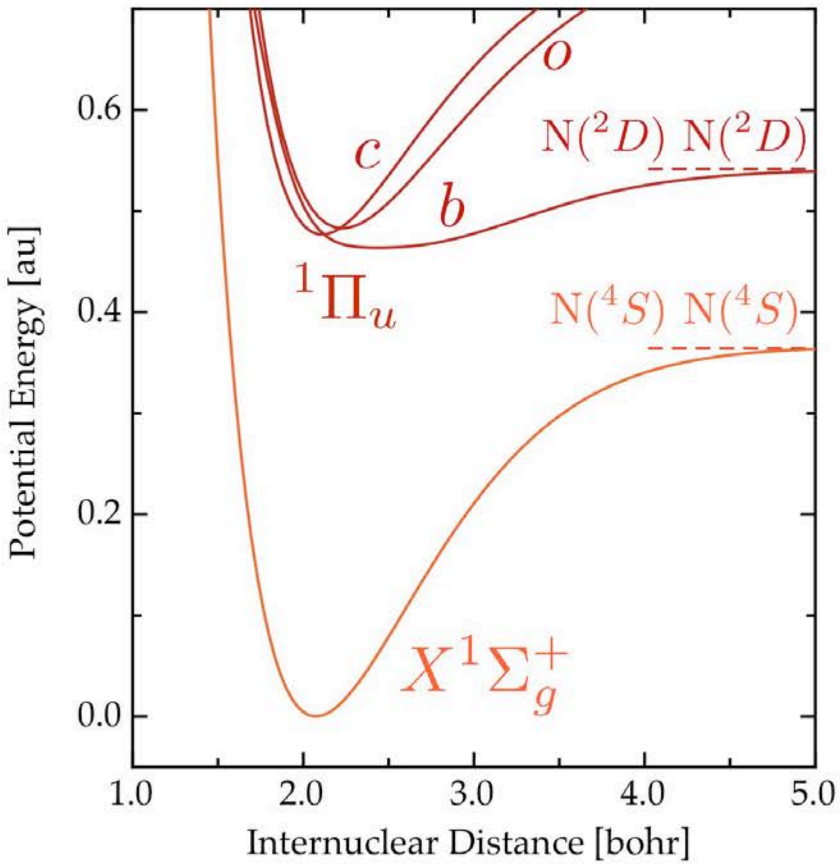
$$a^1\Pi_g \rightarrow a'^1\Sigma_u^-, a^1\Pi_g \rightarrow w^1\Delta_u, A^3\Sigma_u^+ \rightarrow B^3\Pi_g,$$

$$B^3\Pi_g \rightarrow C^3\Pi_u, B^3\Pi_g \rightarrow W^3\Delta_u, \text{and } B^3\Pi_g \rightarrow B'^3\Sigma_u^-,$$

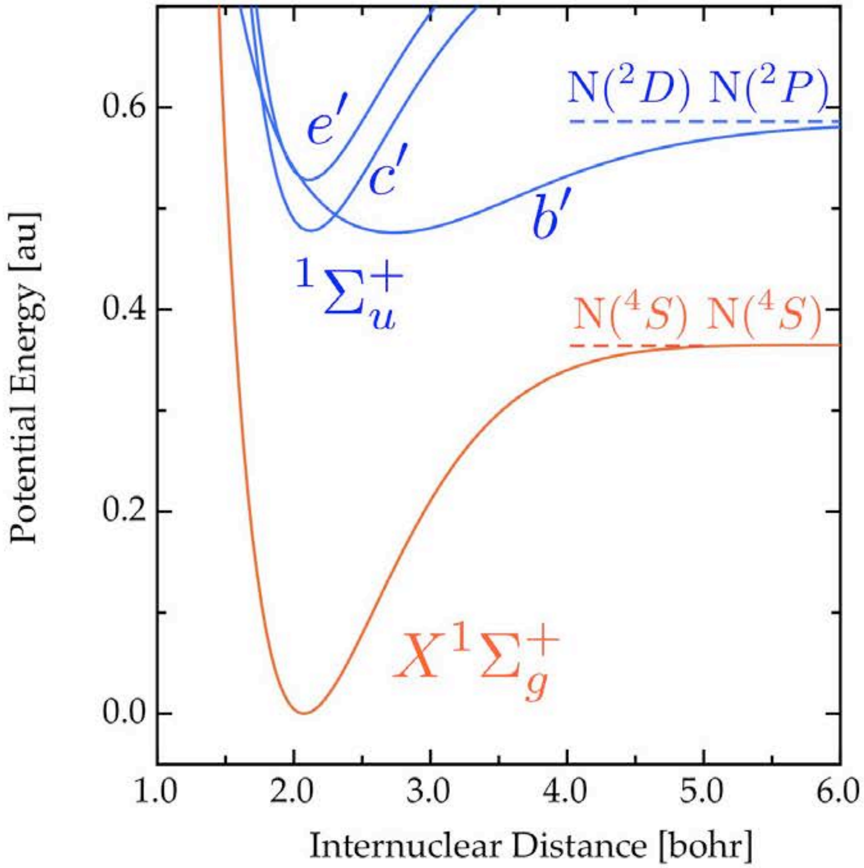
Xin&Ding, Plasma Science and Tech. 16 (2014) 104

Electron-Impact Vibronic Excitation of Singlet Terms in N_2 Spectrum

$$e + N_2(X^1\Sigma_g^+, v'') \rightarrow e + N_2^\star\left(\begin{matrix} b \\ c \\ o \end{matrix}\ {}^1\Pi_u, v'\right)$$



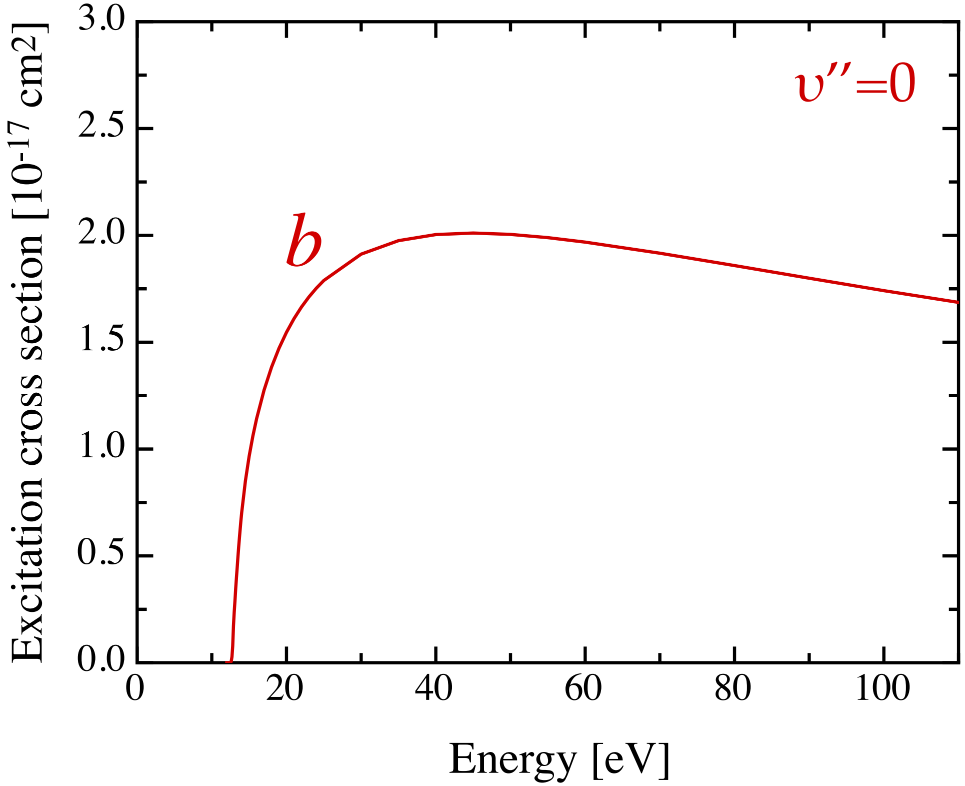
$$e + N_2(X^1\Sigma_g^+, v'') \rightarrow e + N_2^\star\left(\begin{matrix} b' \\ c' \\ e' \end{matrix}\ {}^1\Sigma_u^+, v'\right)$$

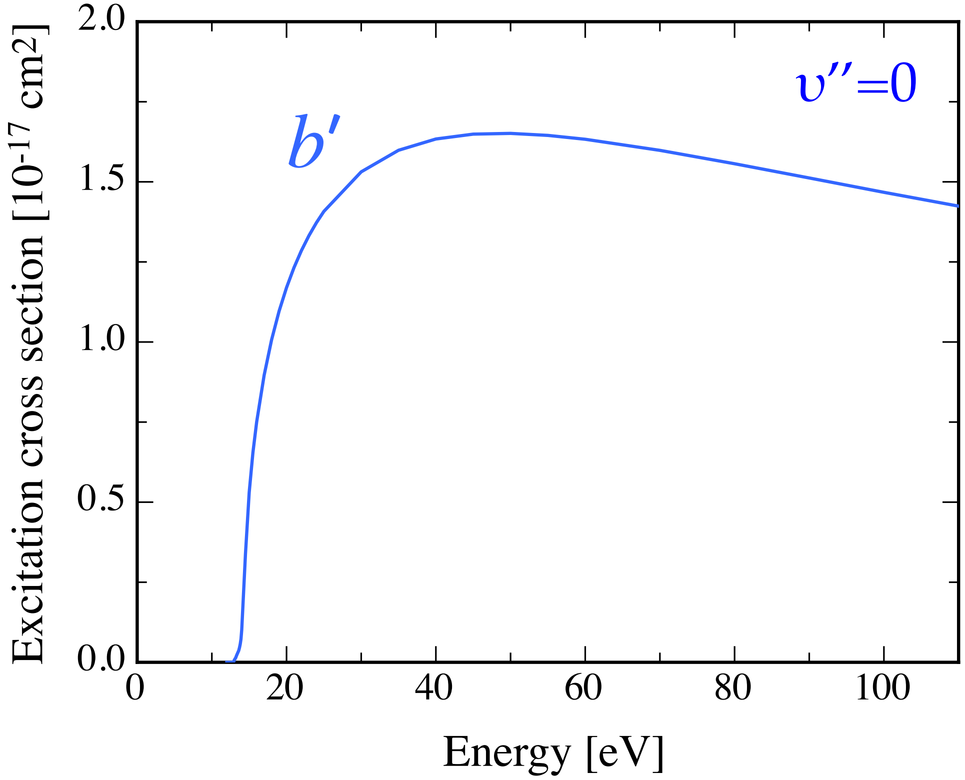


- ✓ *perturbed vibrational progression*
- ✓ *responsible of emission in VUV region*
- ✓ *efficiently predissociated*

D. Spelsberg & W. Meyer, J.Chem.Phys 115 (2001) 6438
Z. Fan et al., Molecular Physics (2014)

Vibronic Excitation Cross Sections: comparison with experiments



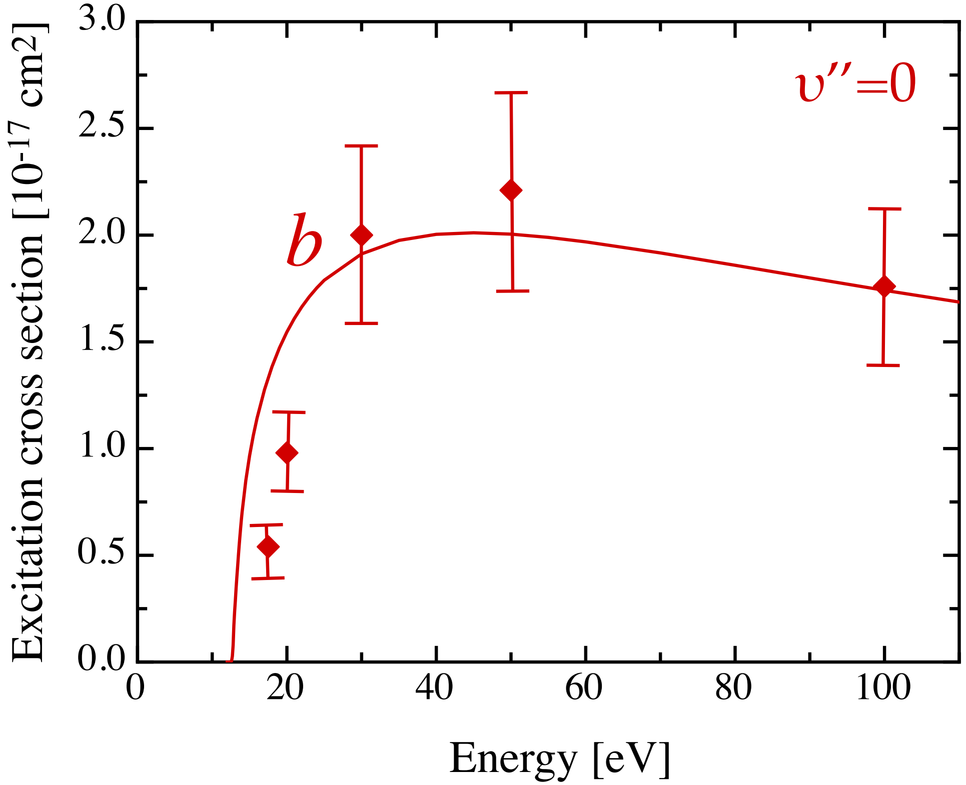


excitation from theoretical state-to-state cross sections

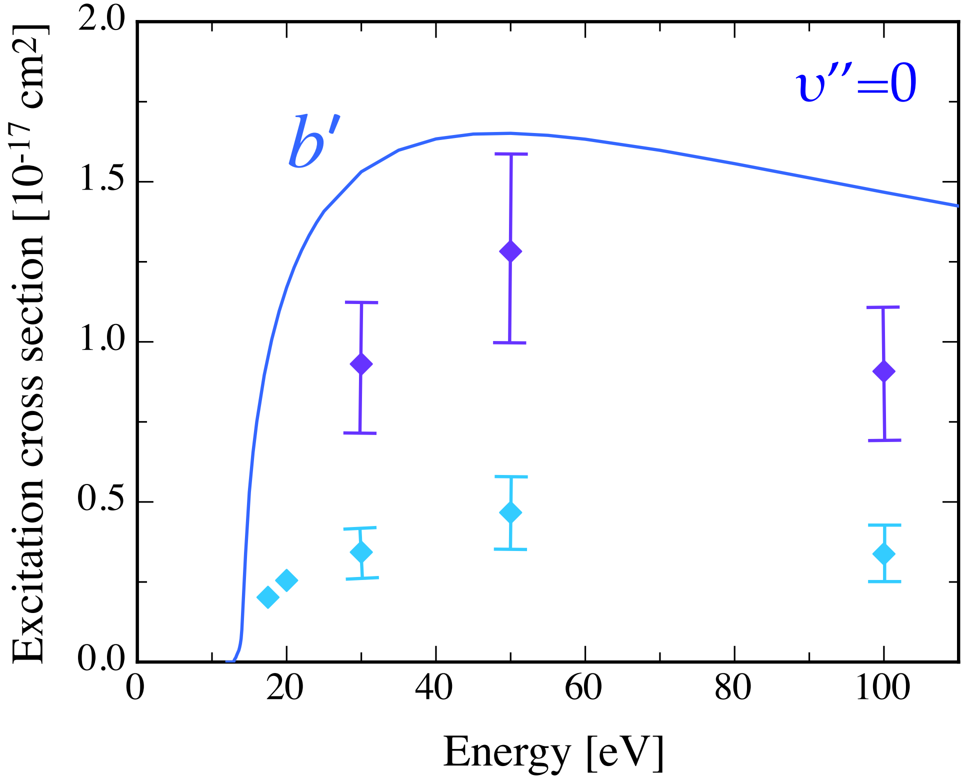
$$\sigma^{b}_{v''=0}(E) = \sum_{v'} \sigma_{v'v''}(E) P_{v'}(b)$$ *state character*

R. Celiberto et al., The Open Plasma Physics Journal 7 (Special Issue) (2014)

Vibronic Excitation Cross Sections: comparison with experiments



spectral range [12.00-13.82 eV]
vibrational analysis b[v′ 0-14] c[v′ 0-3] o[v′ 0-3]

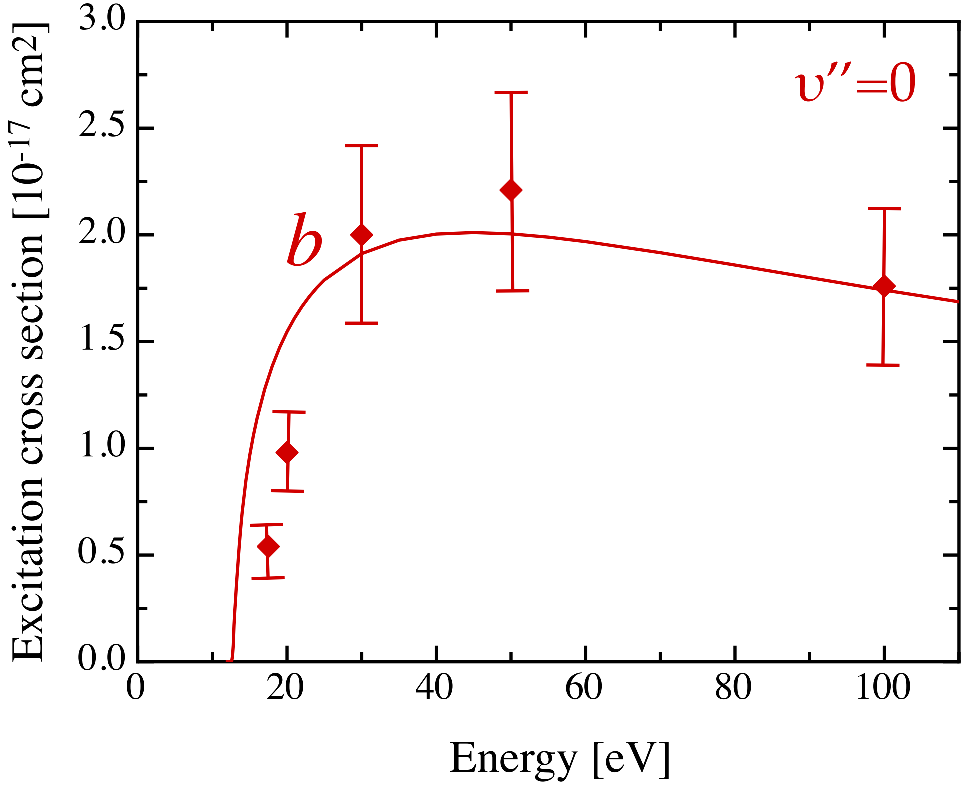


vibrational analysis b′[v′ 0-10] c′[v′ 0-3]
or
b′[v′ 0-16] c′[v′ 0-5]

M.A. Khakoo et al., Phys.Rev.A 77 (2008) 012704

C.P. Malone et al., Phys.Rev.A 85 (2012) 062704

Vibronic Excitation Cross Sections: comparison with experiments



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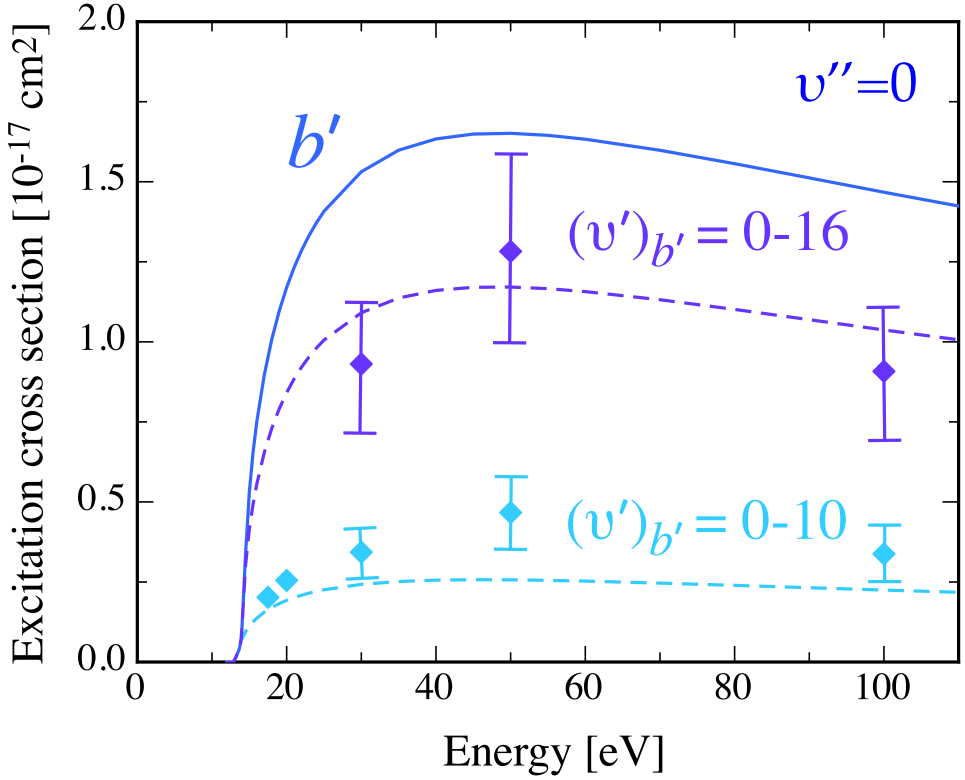

vibrational analysis b′[v′ 0-10] c′[v′ 0-3]
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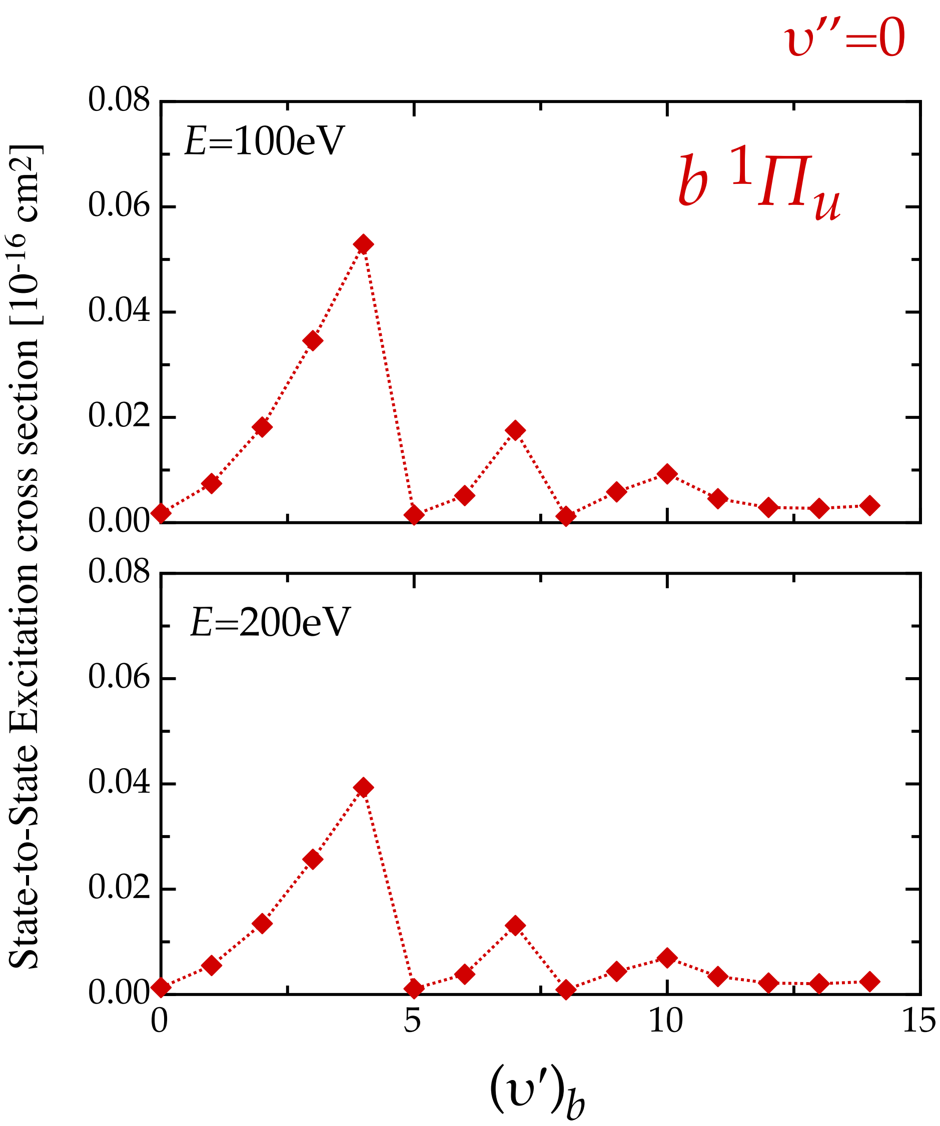
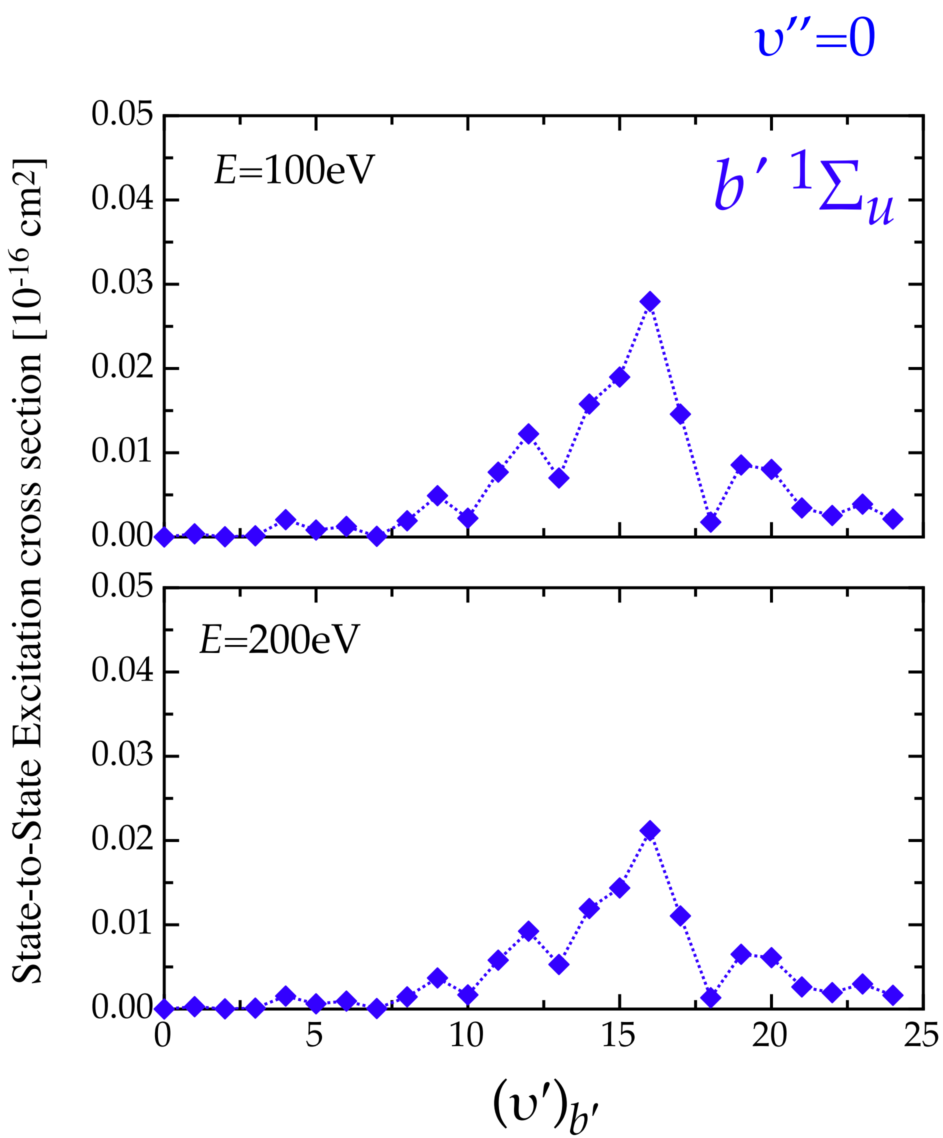
M.A. Khakoo et al., Phys.Rev.A 77 (2008) 012704
C.P. Malone et al., Phys.Rev.A 85 (2012) 062704

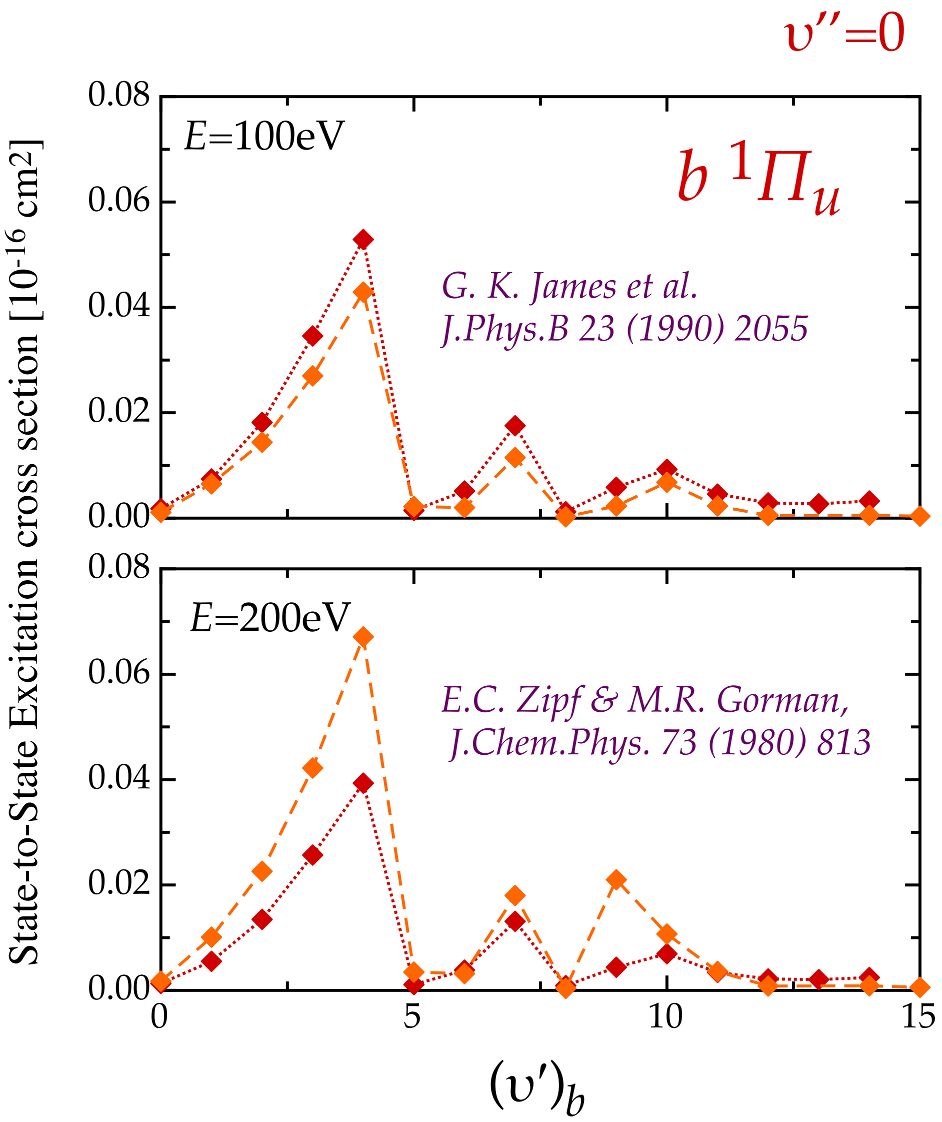
State-to-State Vibronic Excitation Cross Sections: comparison with experiments

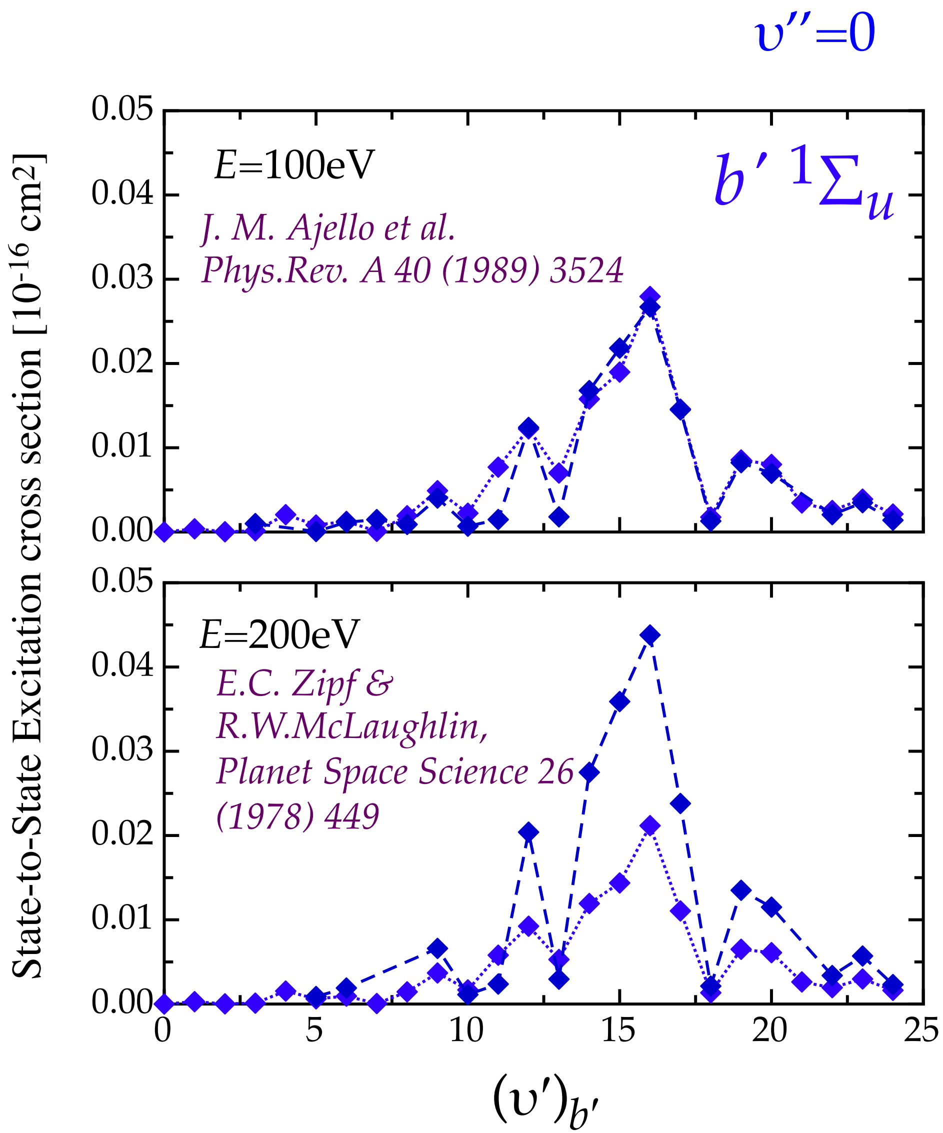




A. Laricchiuta *The state-of-the-art description of vibrational-electronic excitations*
Master Class 2014 Physikzentrum Bad Honnef (Germany), October 10th, 2014

State-to-State Vibronic Excitation Cross Sections: comparison with experiments





N-N_2 collisional-induced processes

PROCESSES

$$N + N_2(v_i) \rightarrow N + N + N$$ collisional-induced dissociation

$$N_2(v_i) + N \rightarrow N_2(v_f) + N$$ vibration-translation energy transfer

CANCULATION FEATURES

Theoretical approach	*QCT* method [Blais&Truhlar (1976)] [M. Pattengill "Rotational excitation III: Classical trajectory methods, in: Atom-molecule Collision Theory; a Guide for the Experimentalist" (1979) Plenum Press, NewYork and London]	translational energy range [0.001-10 eV] stratified sampling trajectory density per eV and per Angstrom of impact parameter: 96000 up to 0.5 eV 24000 up to 3.0 eV 6000 up to 10 eV
Potential energy surface of N_3	LEPS PES [Laganà et al (1987)] and [Laganà & Garcia (1994)]	

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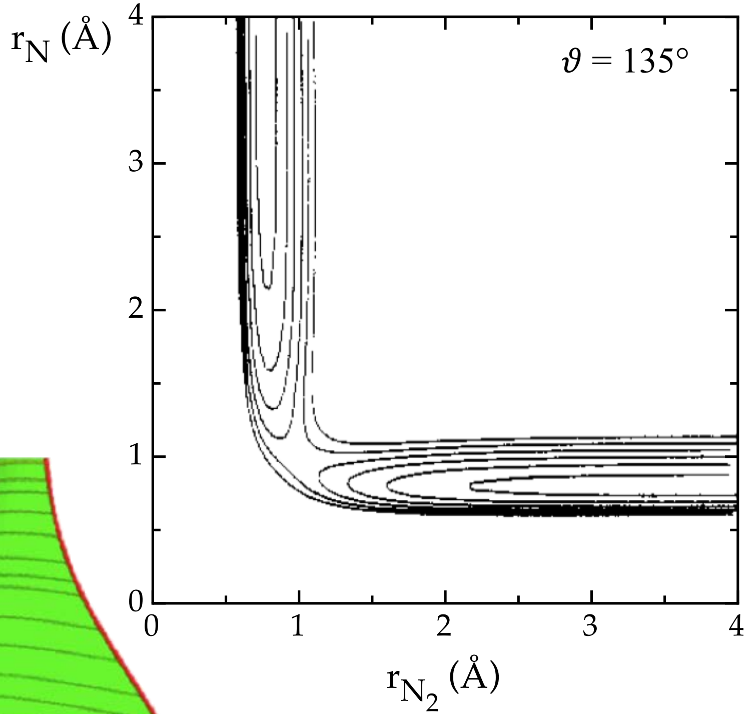
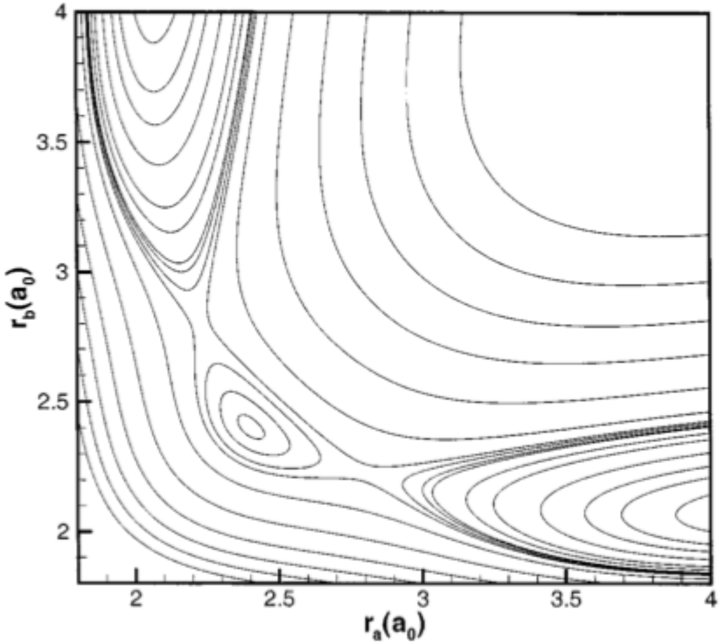
F. Esposito, M. Capitelli, C. Gorse, Chemical Physics 257 (2000) 193–202

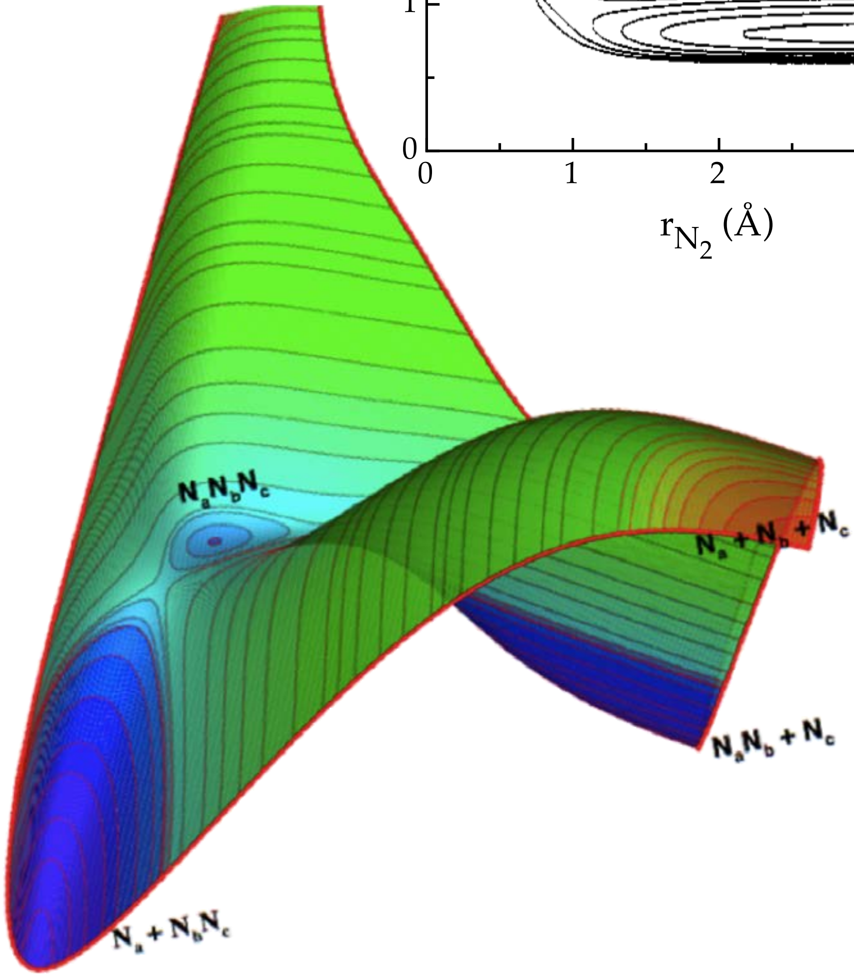
F. Esposito et al., Chem Physics (2006)

F. Esposito & M. Capitelli, Chem Phys Lett (2006)



LEPS
A. Laganà, E. Garcia, L. Ciccarelli,
J. Phys. Chem. 91 (1987) 312-314



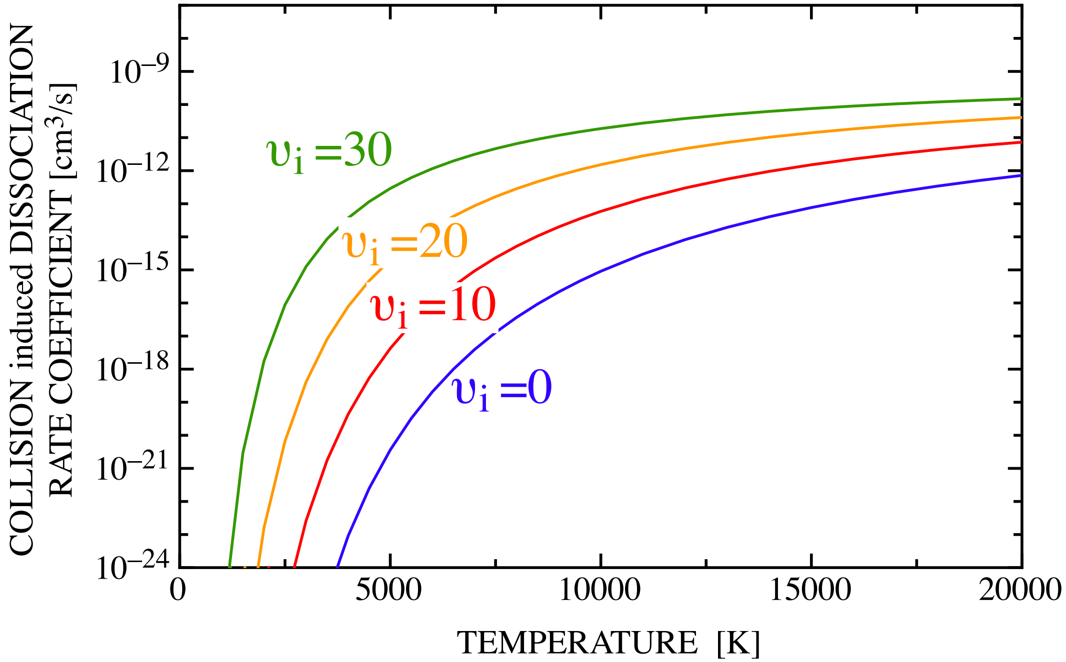


ab-initio
D. Wang, W.M. Huo, C.E. Dateo, D.W. Schwenke, J.R. Stallcop,
J. Chem. Phys. 120 (2004) 6041

P.J.S.B.Caridade, B.R.L. Galvao, A.J.C. Varandas
J. Phys. Chem. A 114 (2010) 6063–6070

N-N_2 collisional-induced dissociation

$$N+N_2(v_i) \rightarrow N+N+N$$



F. Esposito & M. Capitelli, Chem Phys Lett (2006)
F. Esposito et al., Chem Physics (2006)

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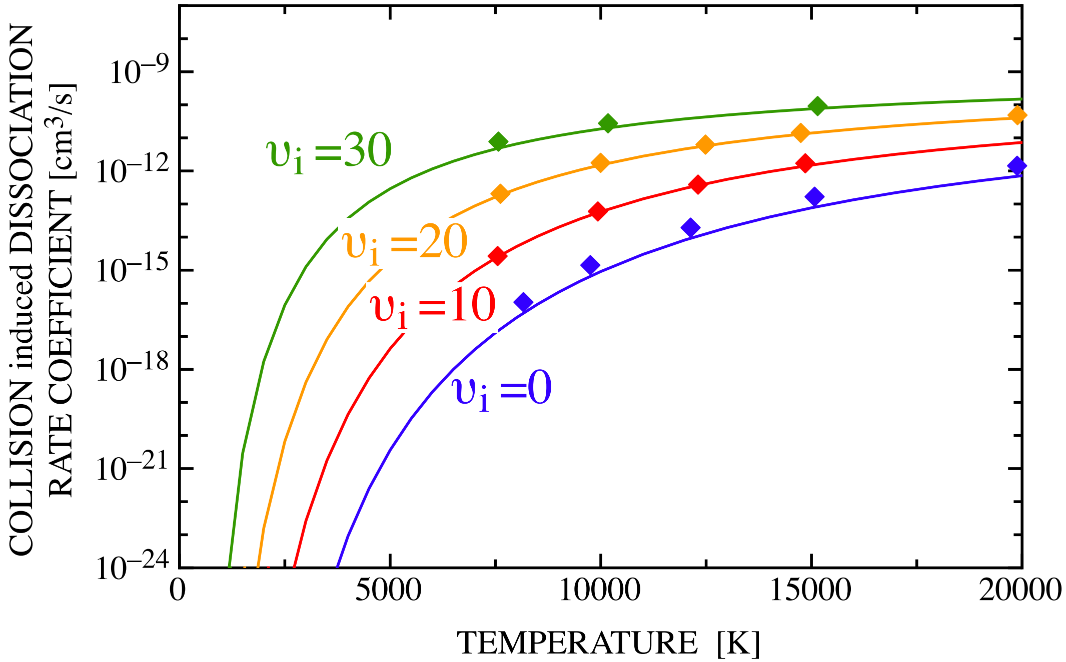
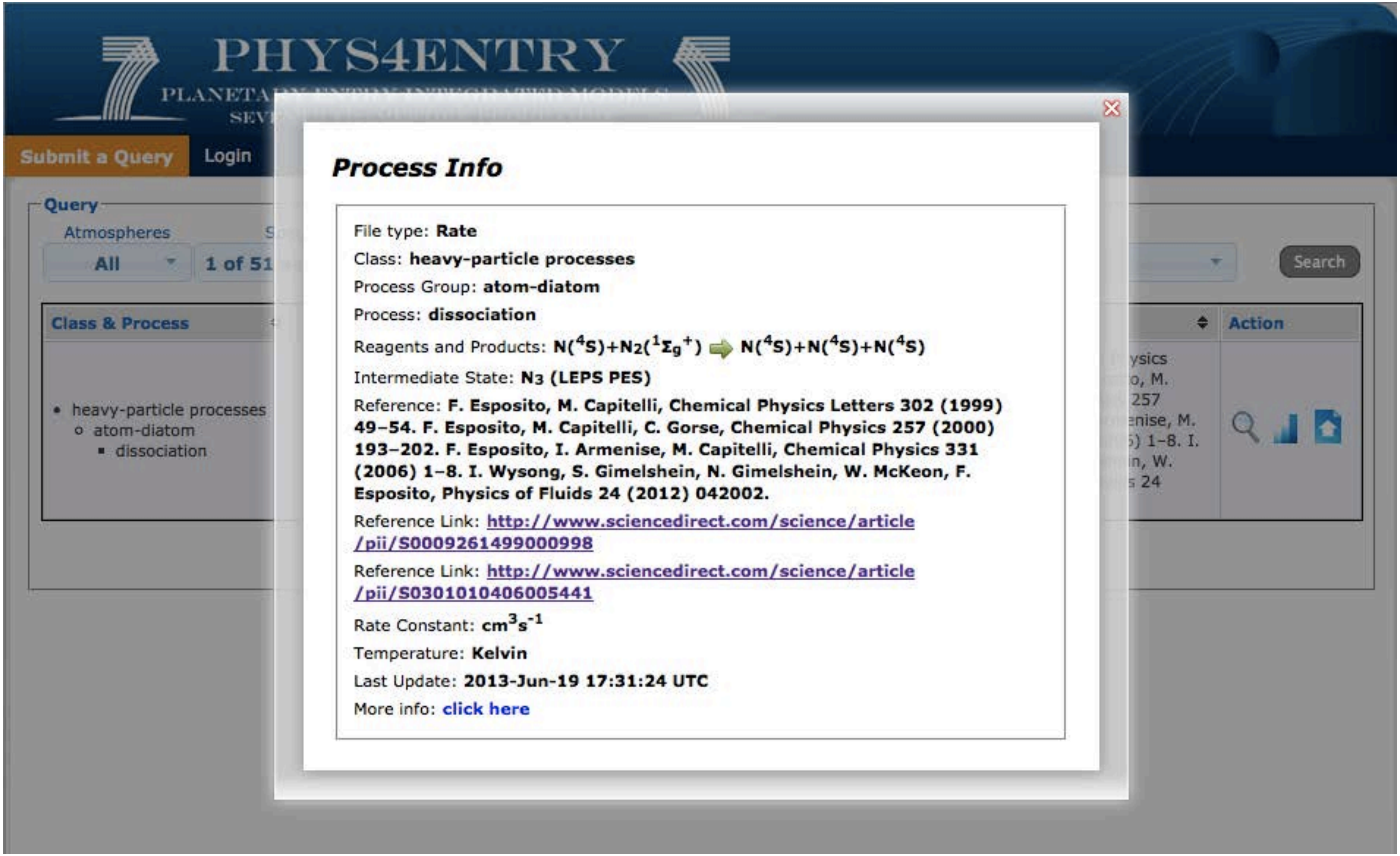


R.L. Jaffe, D.W. Schwenke, and G. Chaban,
AIAA Paper 2010-4517 (2010)
Munafò et al, Eur. Phys. J. D (2012)

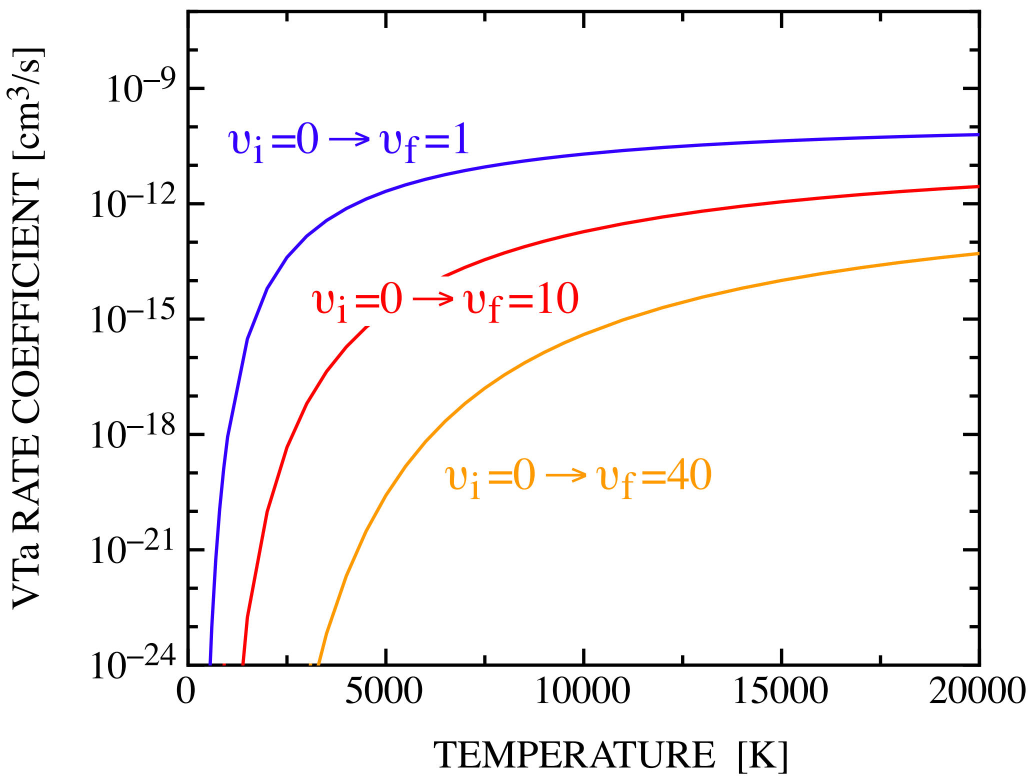
F. Esposito & M. Capitelli, Chem Phys Lett (2006)
F. Esposito et al., Chem Physics (2006)

N-N_2 collisional-induced dissociation: global dissociation rate coefficient

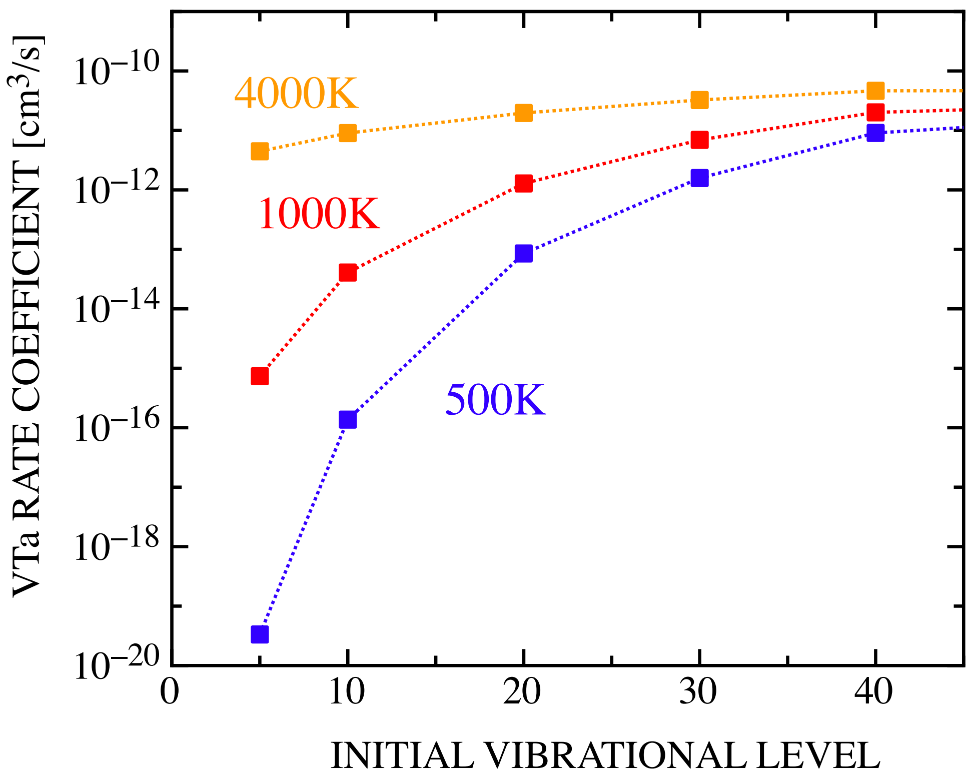


VT energy transfer processes in N-N_2 collisions

$$v_i = 0 \rightarrow v_f$$



$$v_i \rightarrow v_f = v_i - 1$$



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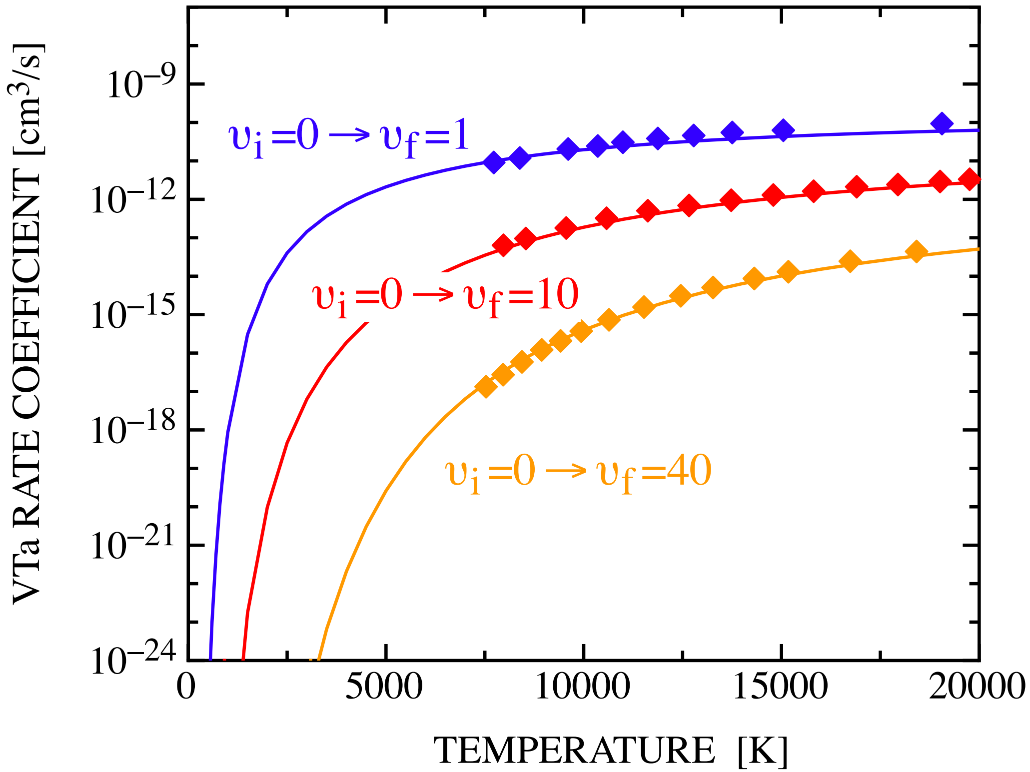

R.L. Jaffe, D.W. Schwenke, and G. Chaban,
AIAA Paper 2010-4517 (2010)
Munafò et al, Eur. Phys. J. D (2012)

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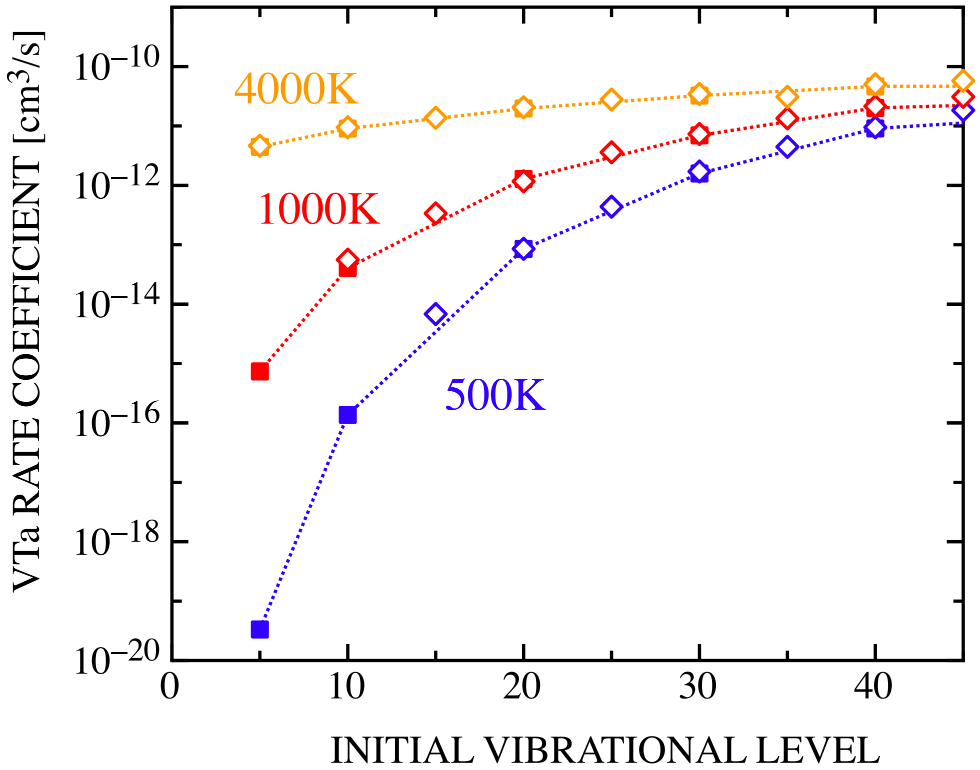
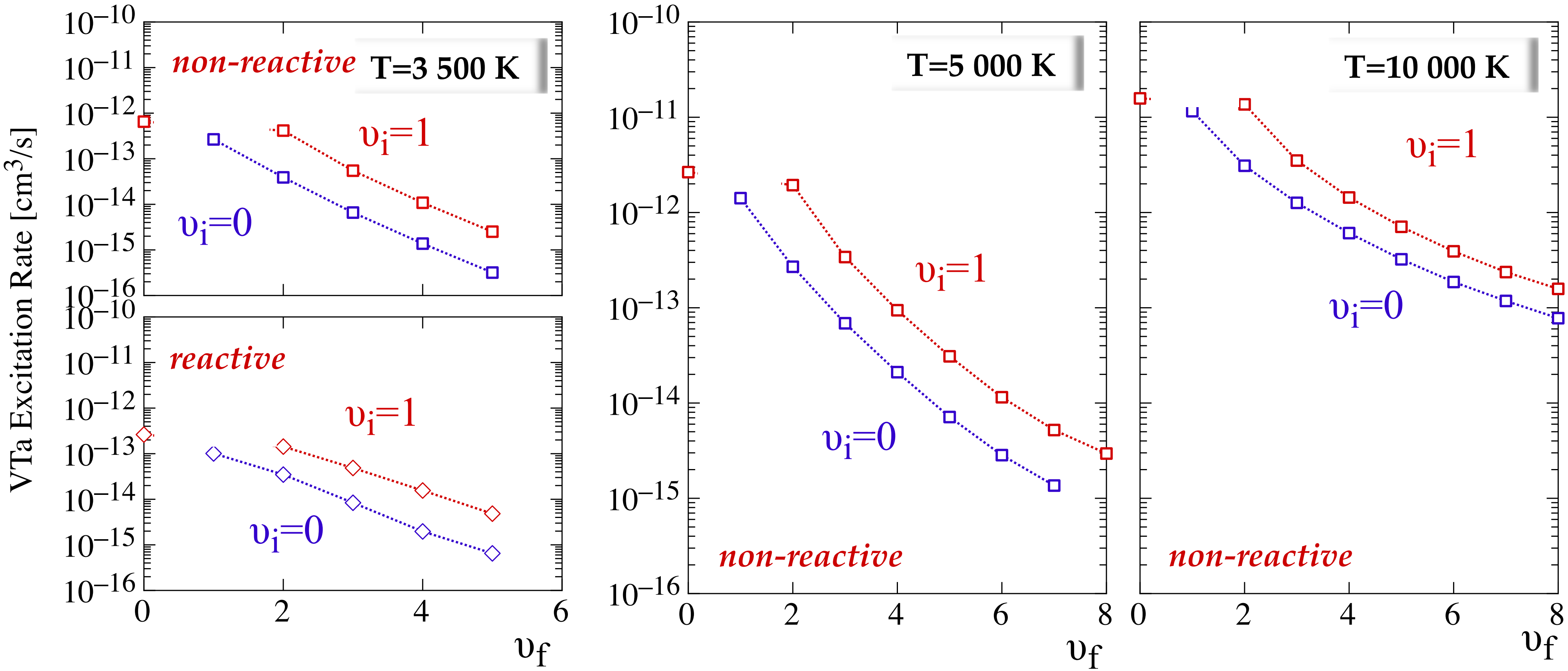


A. Laganà , G. Ochoa De Aspuru, E. Garcia,
Temperature dependence of quasiclassical and quantum rate coefficients for N + N_2
Dip Chimica, Università di Perugia, Italy (1996)

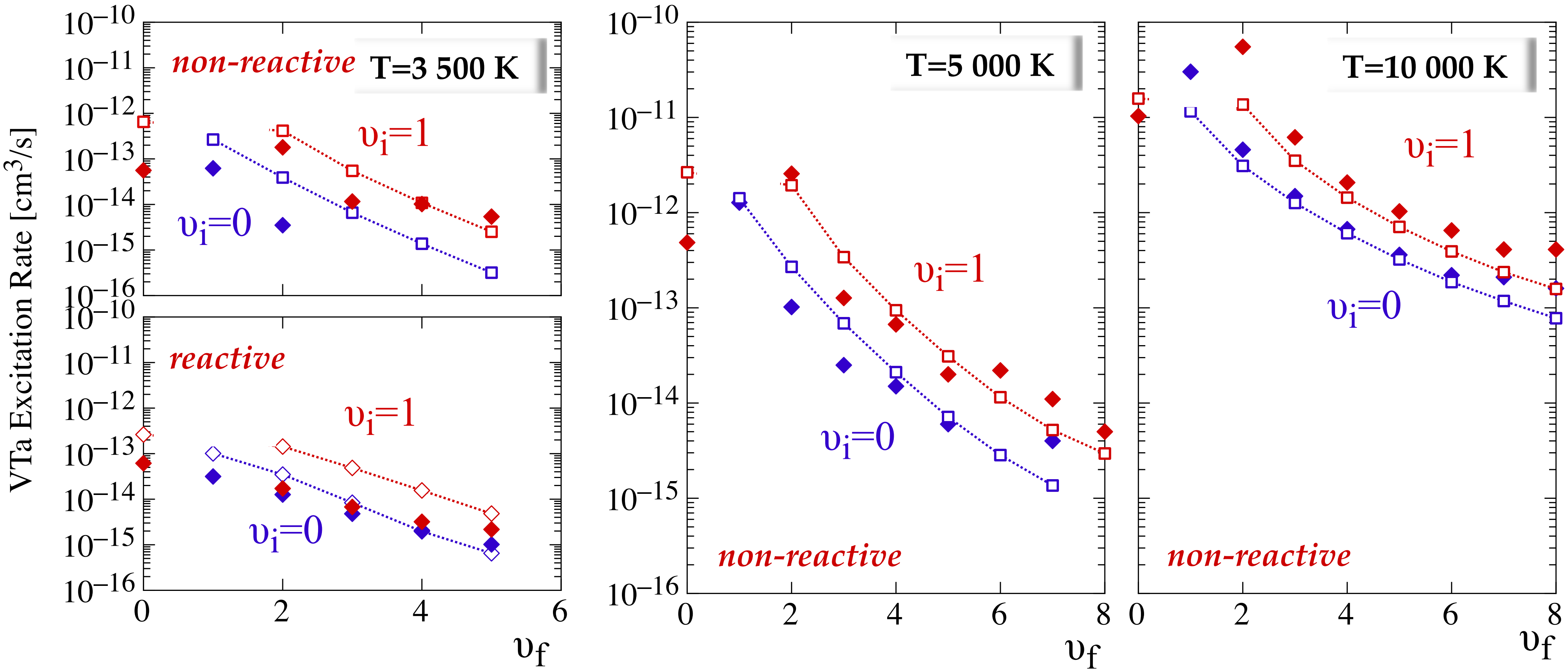
VT energy transfer processes in N-N_2 collisions

$$N_2(\upsilon_i)+N \rightarrow N_2(\upsilon_f)+N$$



VT energy transfer processes in N-N_2 collisions

$$N_2(v_i)+N \rightarrow N_2(v_f)+N$$

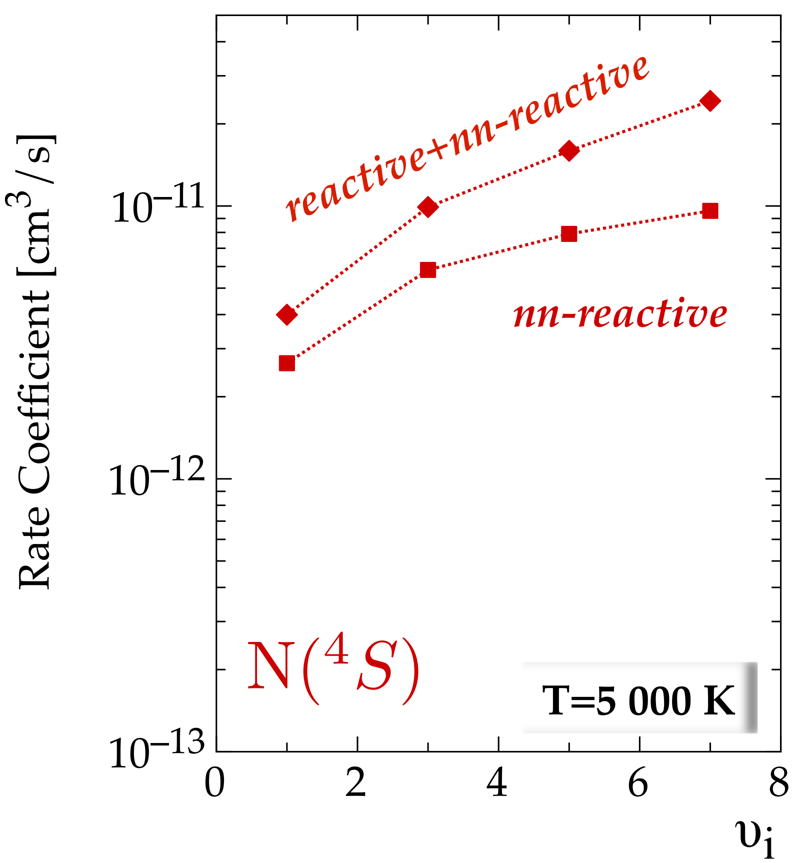


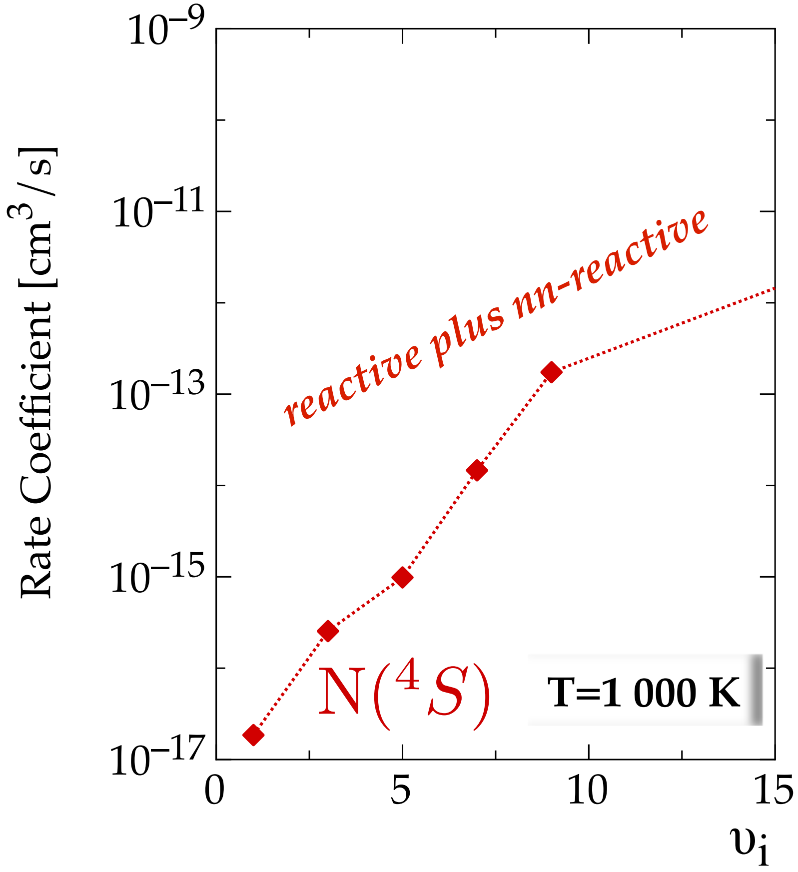
P.J.S.B.Caridade, B.R.L. Galvao, A.J.C. Varandas
J. Phys. Chem. A 114 (2010) 6063–6070

VT energy transfer processes in N-N_2 collisions

$$N_2(v_i)+N \rightarrow N_2(v_f)+N \text{ with } v_f < v_i$$

$$k^{VT}(v_i) = \sum_{0}^{v_f=v_i-1} k^{VT}(v_i, v_f)$$





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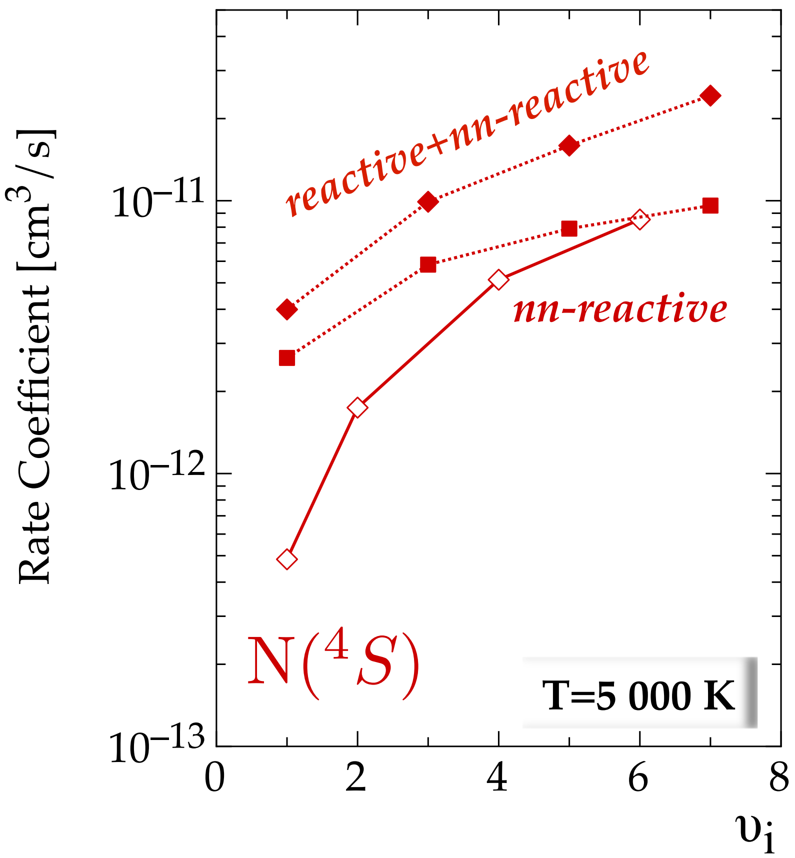
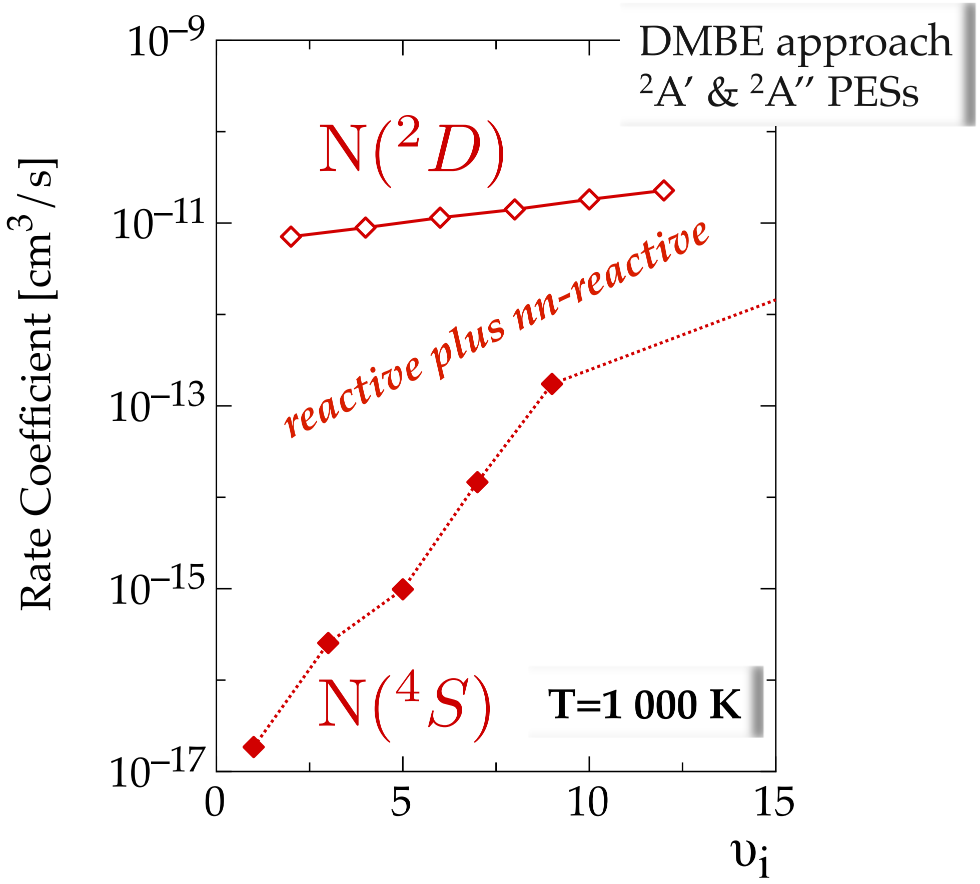
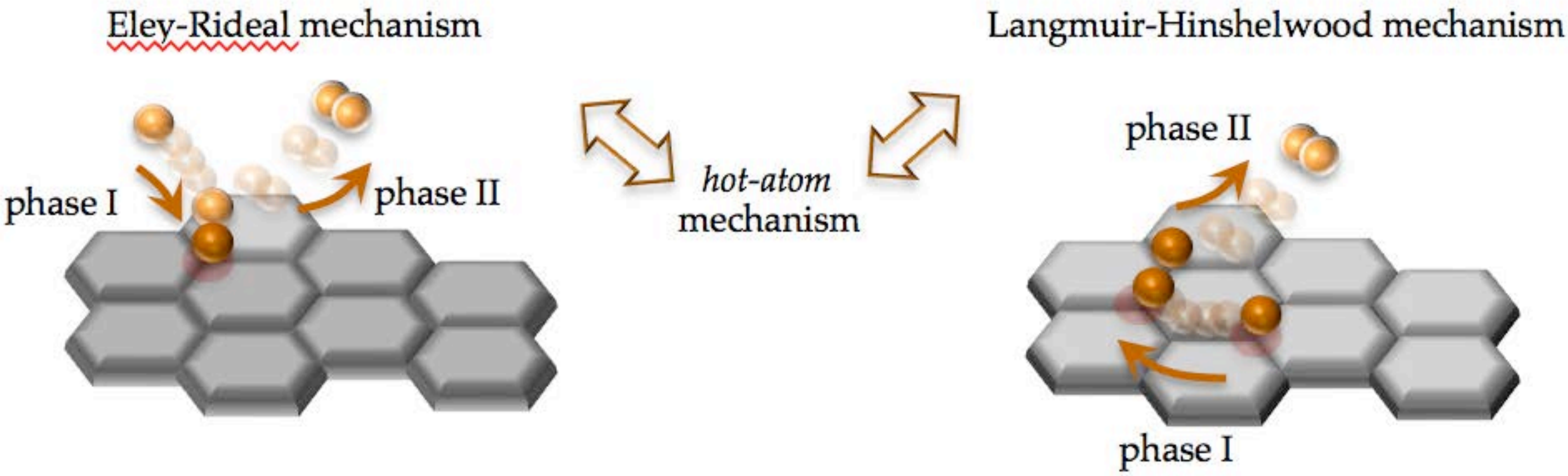




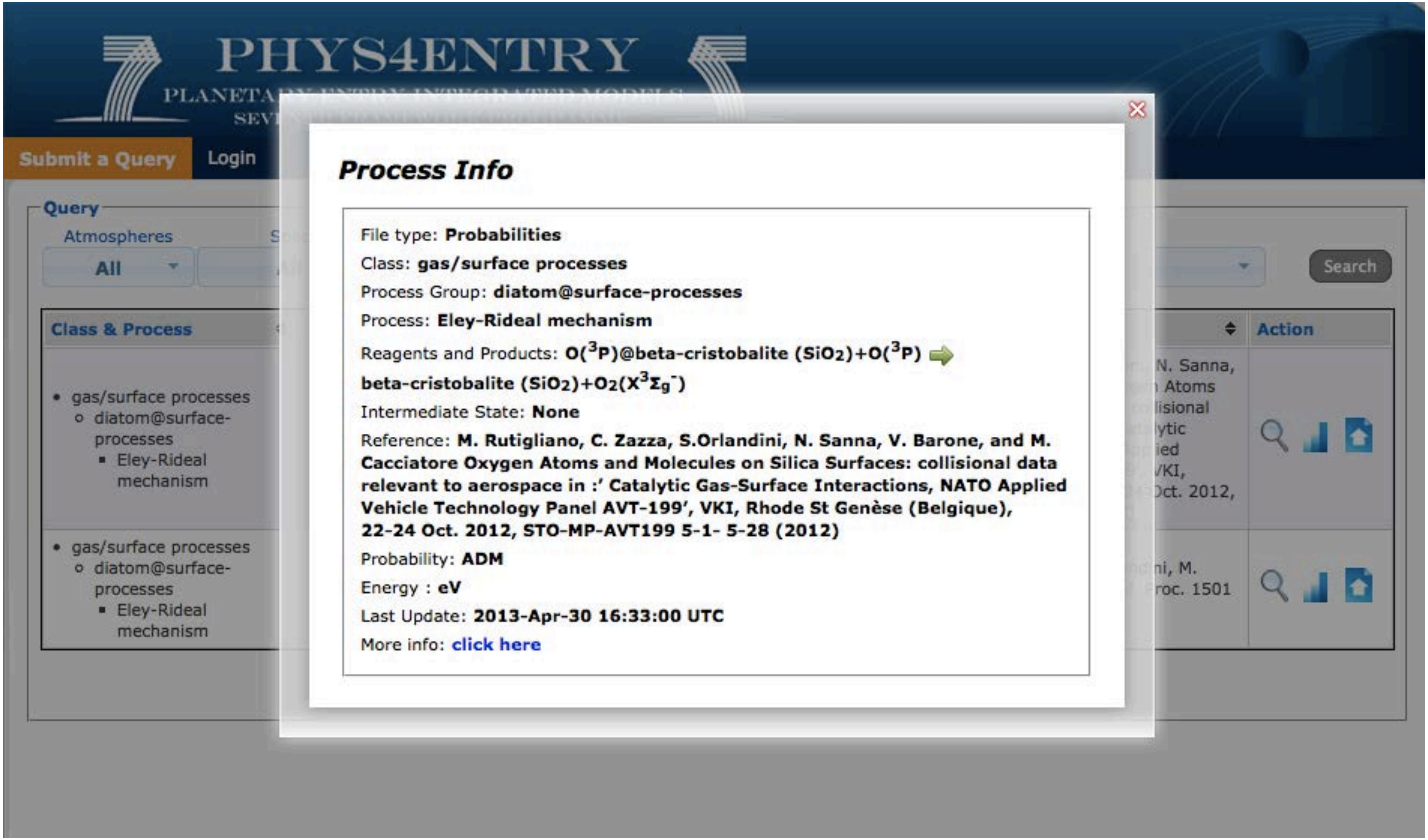
P.J.S.B.Caridade, B.R.L. Galvao, A.J.C. Varandas
J. Phys. Chem. A 114 (2010) 6063–6070

B.R.L. Galvão, A.J.C. Varandas, J.P. Braga, J.C. Belchior
Chemical Physics Letters 577 (2013) 27–31

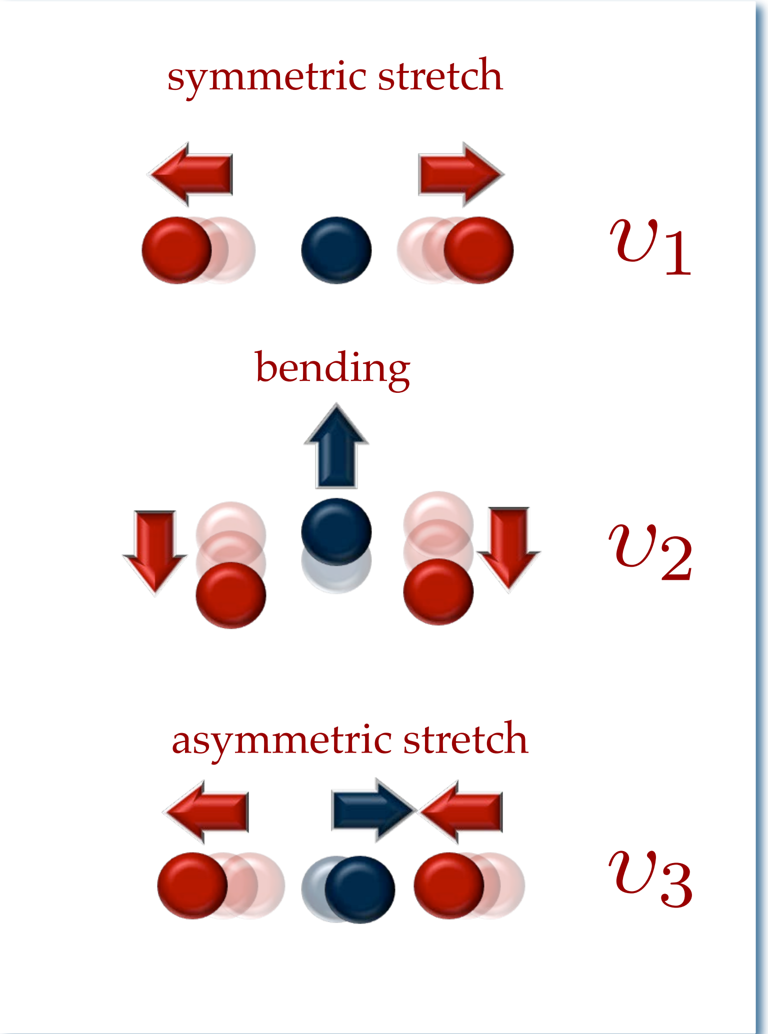
heterogeneous recombination at surface



heterogeneous recombination at surface



CO_2 vibrational kinetics

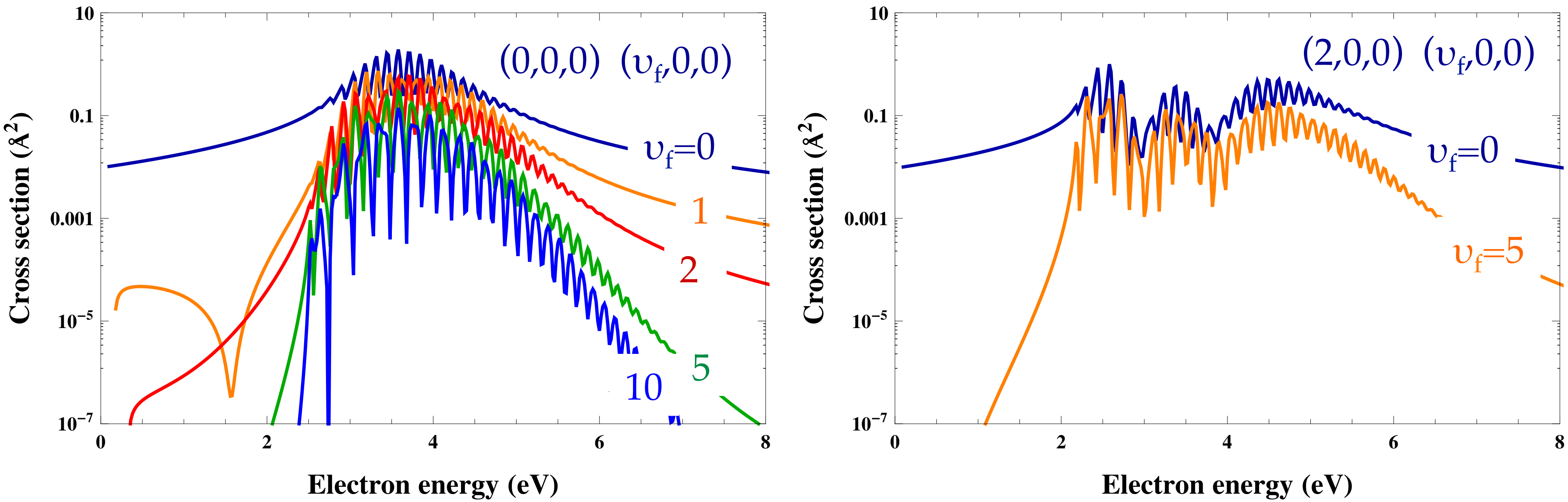


Armenise & Kustova,
Chemical Physics (2013) and (2014)

Tomáš Kozák and Annemie Bogaerts,
Plasma Sources Science &Technology (2014)

Resonant vibrational excitation in e-CO_2 collisions

$$e^- + CO_2(X^1\Sigma_g^+, \upsilon_i) \rightarrow CO_2^-(^2\Pi_u) \rightarrow e^- + CO_2(^1\Sigma_g^+, \upsilon_f)$$



R. Celiberto, V. Laporta, A. Laricchiuta, J. Tennyson and J.M. Wadehra, The Open Plasma Physics Journal, 2014, 7, (Suppl 1: M2) 33-47

energy transfer processes in CO_2-CO_2 collisions

PROCESSES

$$\mathrm{CO_2}(^1\Sigma,v_1^i,v_2^i,v_3^i)+\mathrm{CO_2}(^1\Sigma,w_1^i,w_2^i,w_3^i)\rightarrow \mathrm{CO_2}(^1\Sigma,v_1^f,v_2^f,v_3^f)+\mathrm{CO_2}(^1\Sigma,w_1^f,w_2^f,w_3^f)$$

CANCULATION FEATURES

Theoretical approach	*QCT* method [Blais&Truhlar (1976)] [M. Pattengill "Rotational excitation III: Classical trajectory methods, in: Atom-molecule Collision Theory; a Guide for the Experimentalist" (1979) Plenum Press, NewYork and London]
Potential energy surface	intra-molecule potential [JS. Carter and N. Murrel, Croat. Chem. Acta 57 (1984) 355] inter-molecule potential [Bartolomei et al (1976)]
Rotational levels	a Boltzmann distribution is assumed for rotational levels at the translational temperature

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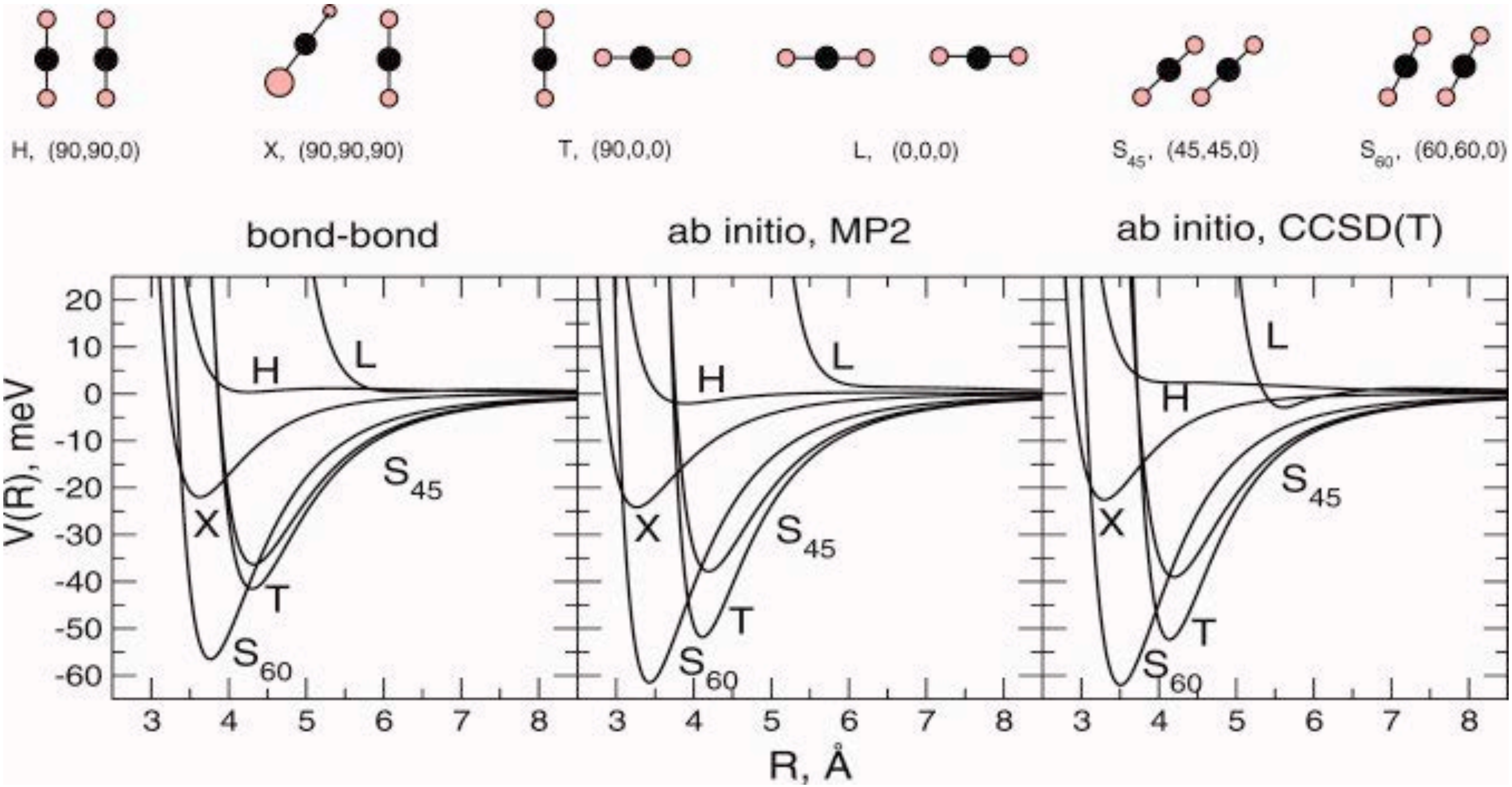
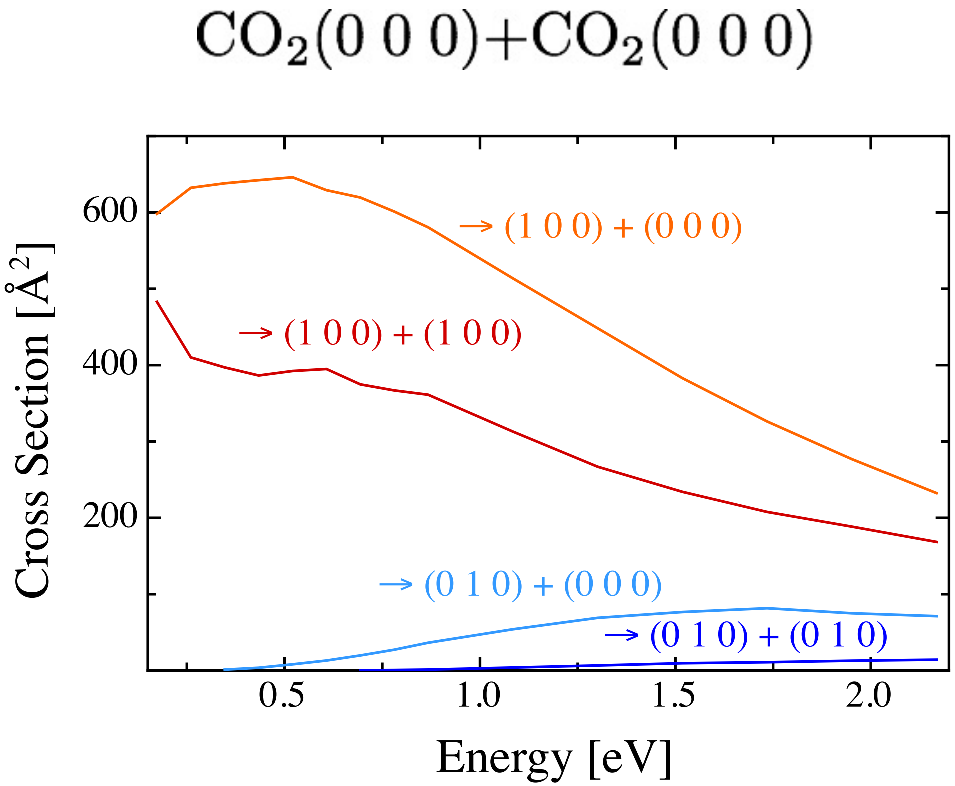
in: Murgante, B., Gervasi, O., Misra, S., Nedjah, N., Rocha, A.M.A.C., Taniar, D., Apduhan, B.O. (eds.) ICCSA 2012, Part I. LNCS, vol. 7333, pp. 387–400. Springer, Heidelberg (2012)

energy transfer processes in CO_2-CO_2 collisions



rigid-monomers ➡ stretched&bent monomers

energy transfer processes in CO_2-CO_2 collisions



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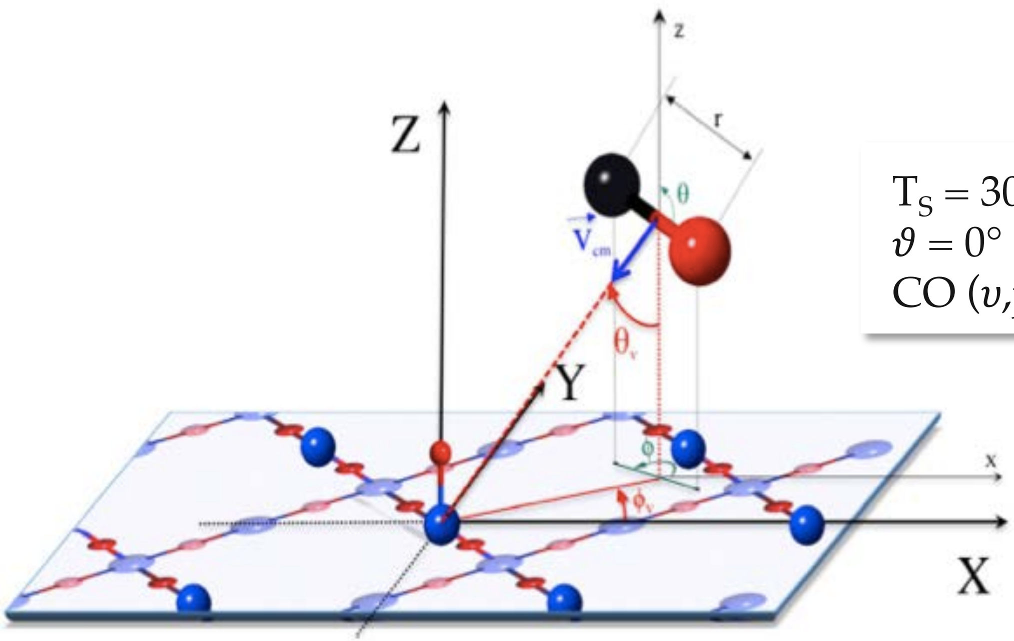
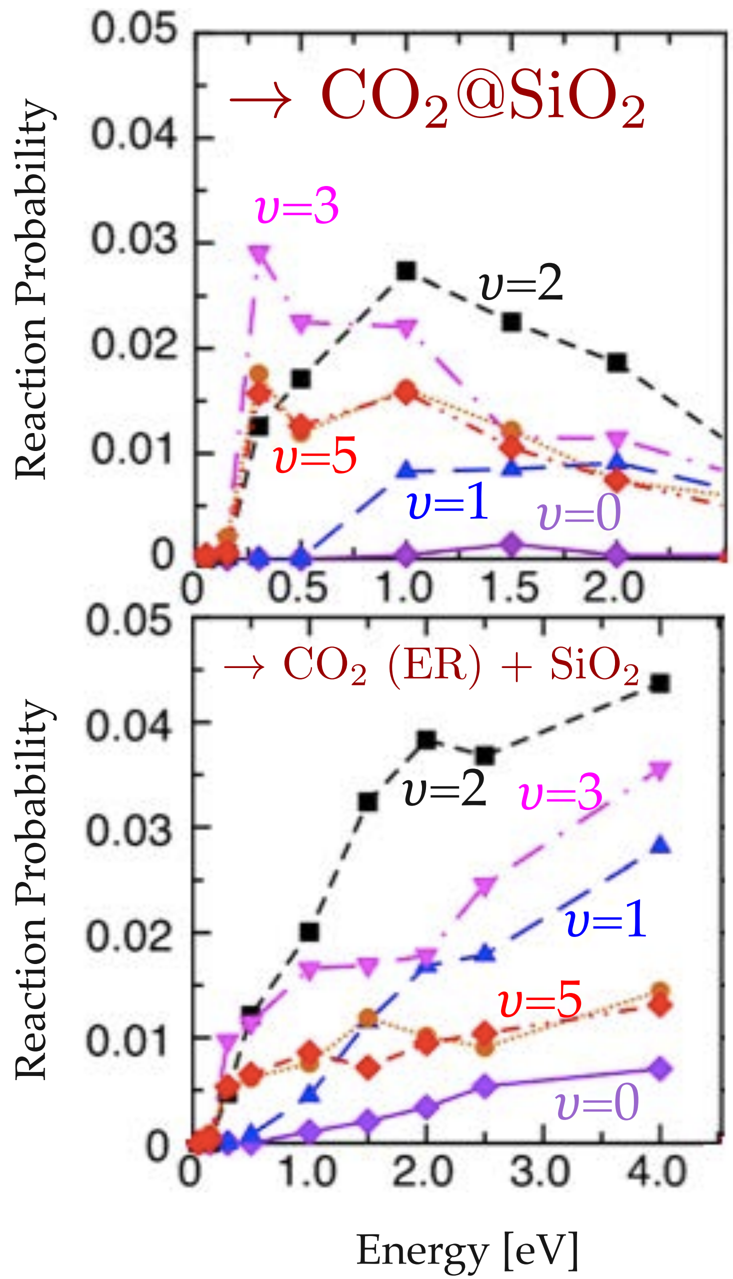
MASTER CLASS 2014 Physikzentrum Bad Honnef (Germany), October 10th, 2014

$$\mathrm{CO}(X^1\Sigma^+, v, j) + \mathrm{O@SiO_2}$$



T_S = 300K
ϑ = 0°
CO (v,j=0)



REFLECTED CO

$$\rightarrow \mathrm{CO}(X^1\Sigma^+, v') + \mathrm{O@SiO_2}$$

Pablo Gamallo, Hèctor Prats and Ramón Sayós
Journal of Molecular Modeling 20 (2014) 2160

A clear research imperative in the next decade will therefore be to increase our knowledge of the chemical and physical interactions in such plasmas of electrons, ions and radicals with neutral species

N. Mason "The 2012 Plasma Roadmap" J. Phys. D: Appl. Phys. 45 (2012) 253001
citing the report of the Washington: National Research Council (1996)
Database Needs for Modeling and Simulation of Plasma Processing