Resonant electron-molecular cation collisions in the edge plasmas of fusion devices: new state-to-state cross sections and rate coefficients

J. Zsolt Mezei

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Introduction: Elementary processes

Dissociative recombination

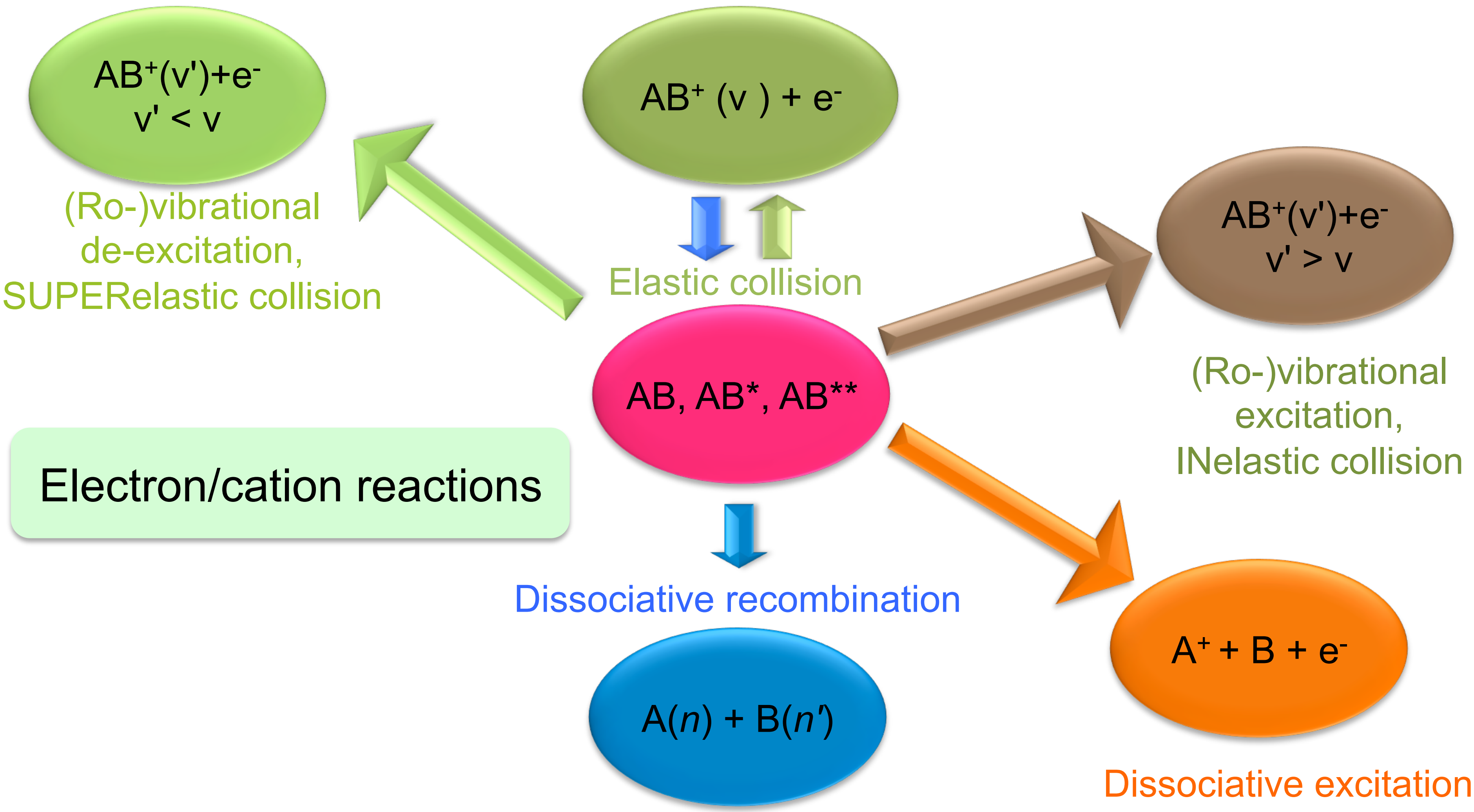
Introduction: Elementary processes

Vibrational excitation

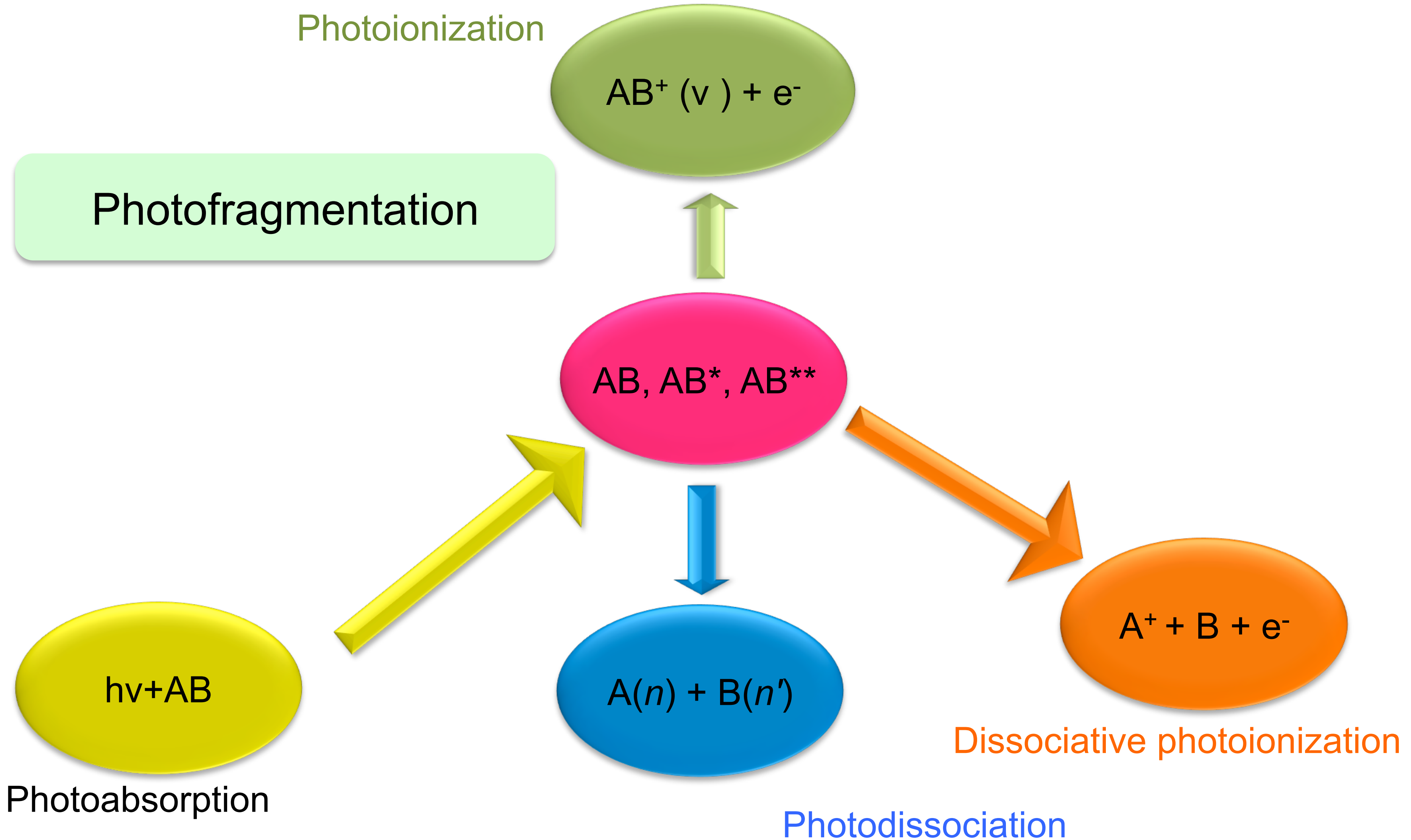
Introduction: Elementary processes

Dissociative excitation

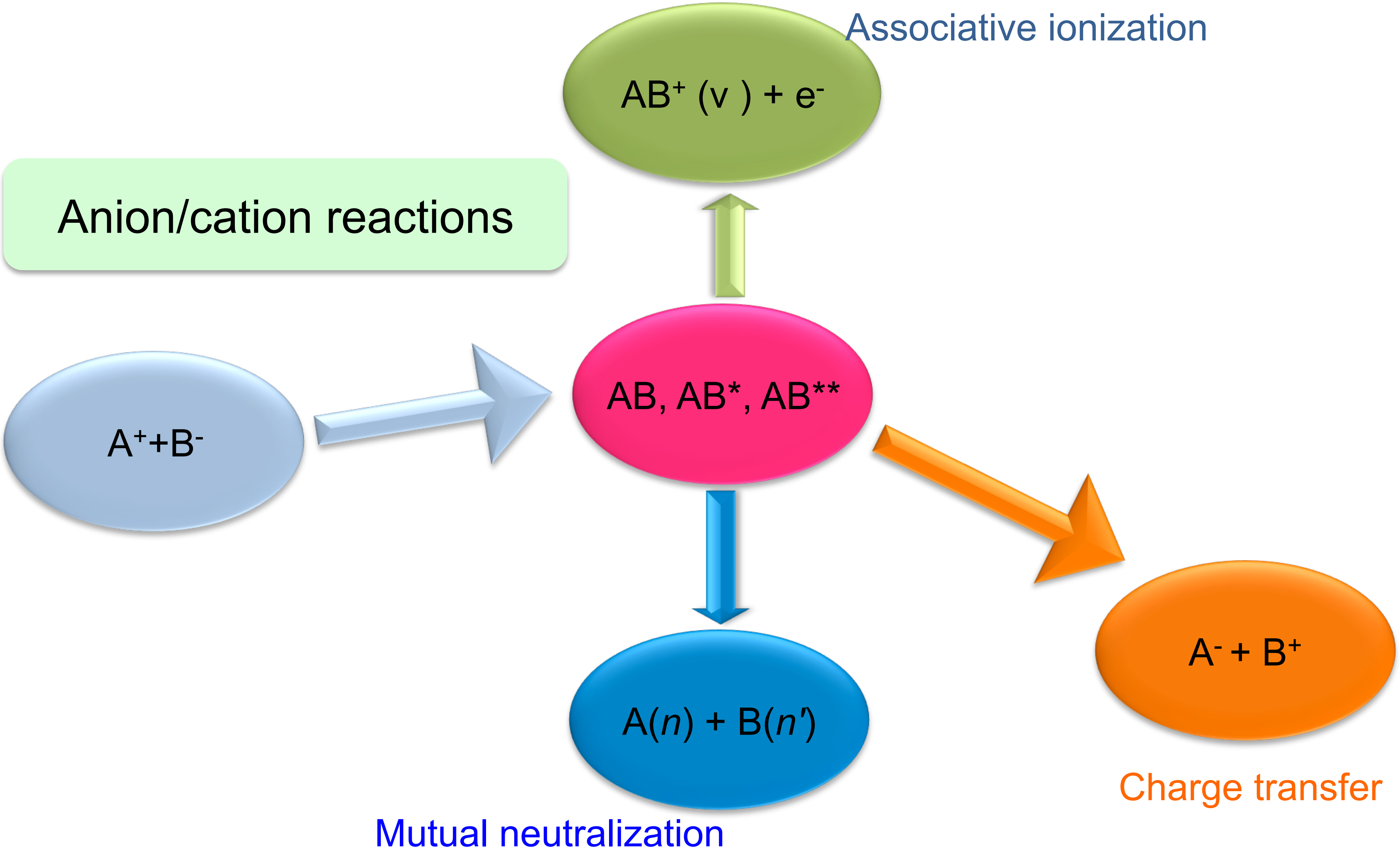
Introduction: Elementary processes



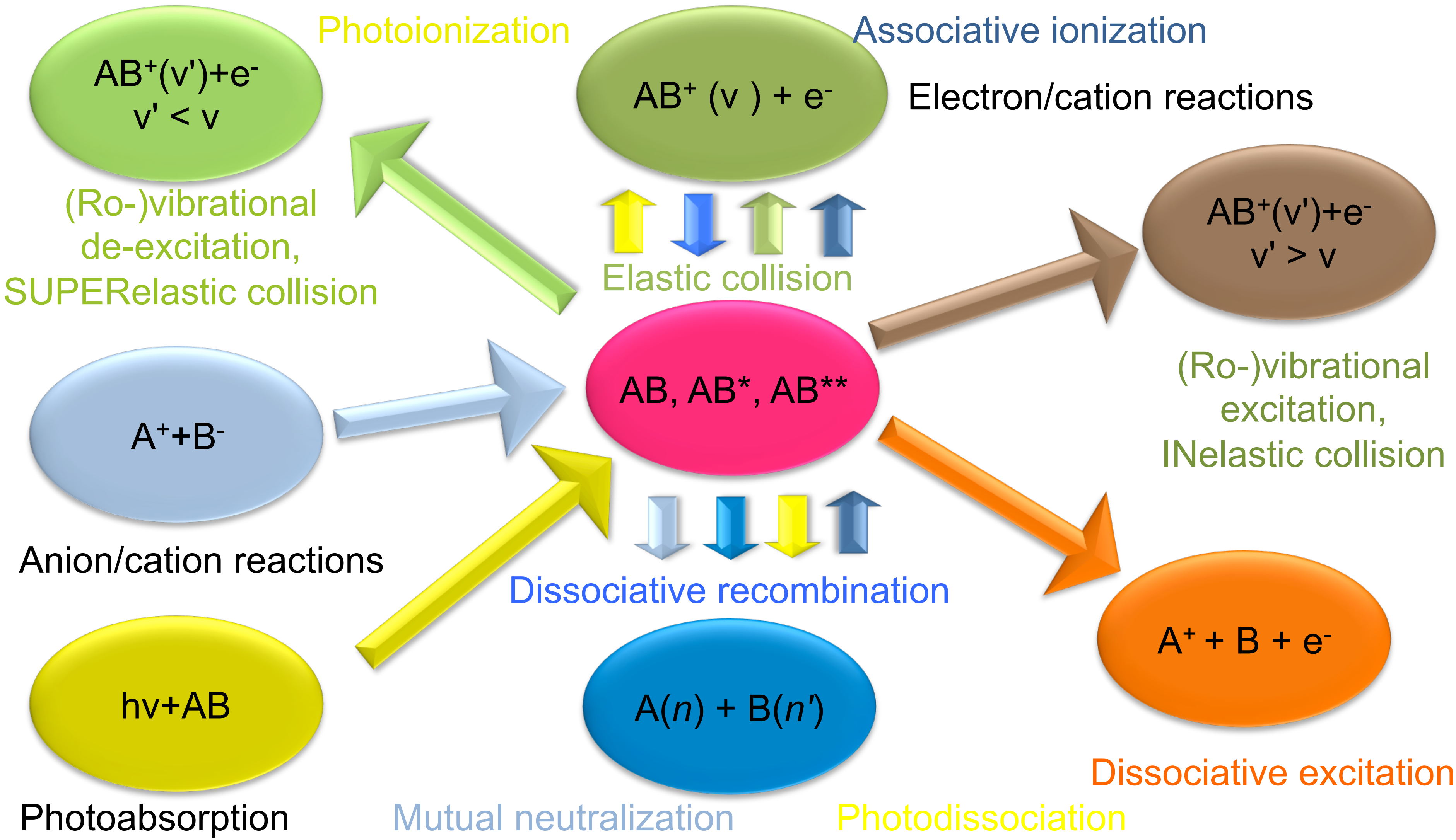
Introduction: Elementary processes



Introduction: Elementary processes



Introduction: Elementary processes

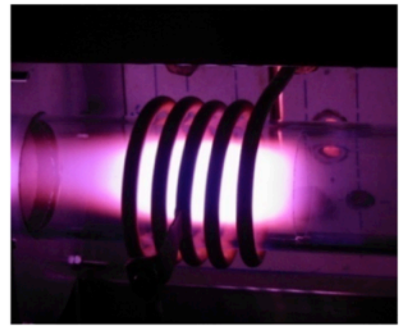


Introduction: Cold ionized media

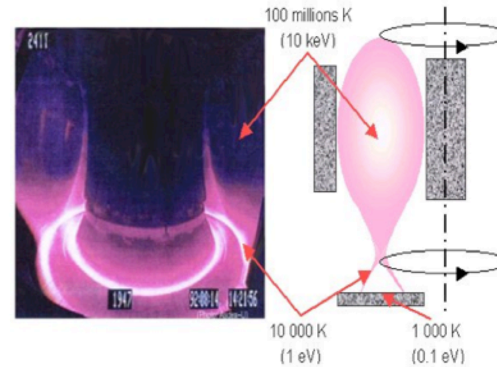
Interstellar molecular clouds

Planetary atmospheres

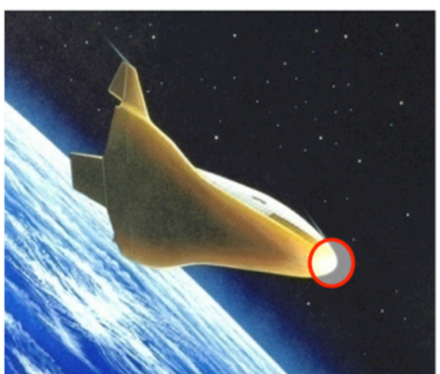
Cold laboratory plasmas



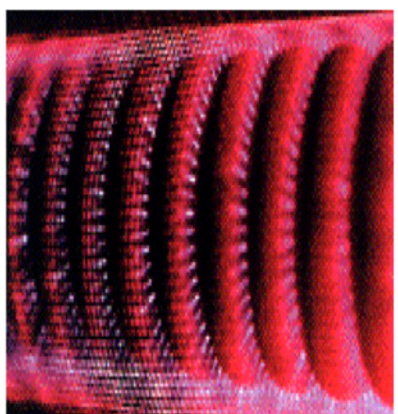
At the wall of the fusion devices (ITER) project



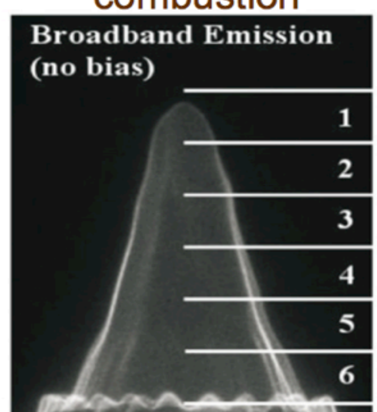
Hypersonic entry of spacecrafts



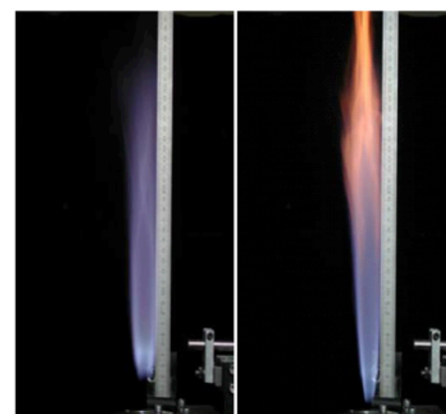
Plasma-assisted depollution



Electric-field-assisted combustion



Plasma-assisted-combustion



Theoretical approach: Reactive collisions

$$e^- + \mathrm{AB}^+(v_i^+, N_i^+) \rightarrow \mathrm{AB}^*, \mathrm{AB}^{**} \rightarrow \begin{cases} \mathrm{AB}^+(v_f^+, N_f^+) + e^- & \text{EC,IC,SEC} \\ [\mathrm{A} + \mathrm{B}]_{(\epsilon)} & \text{DR} \\ \mathrm{A}^+ + \mathrm{B} + e^- & \text{DE} \end{cases}$$

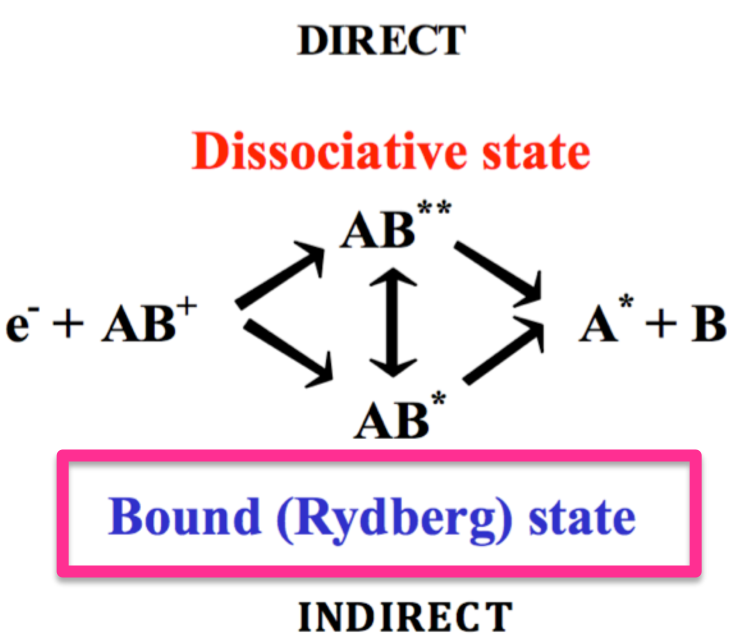
Poster of J. Zs. Mezei *et al*

Theoretical approach: MQDT

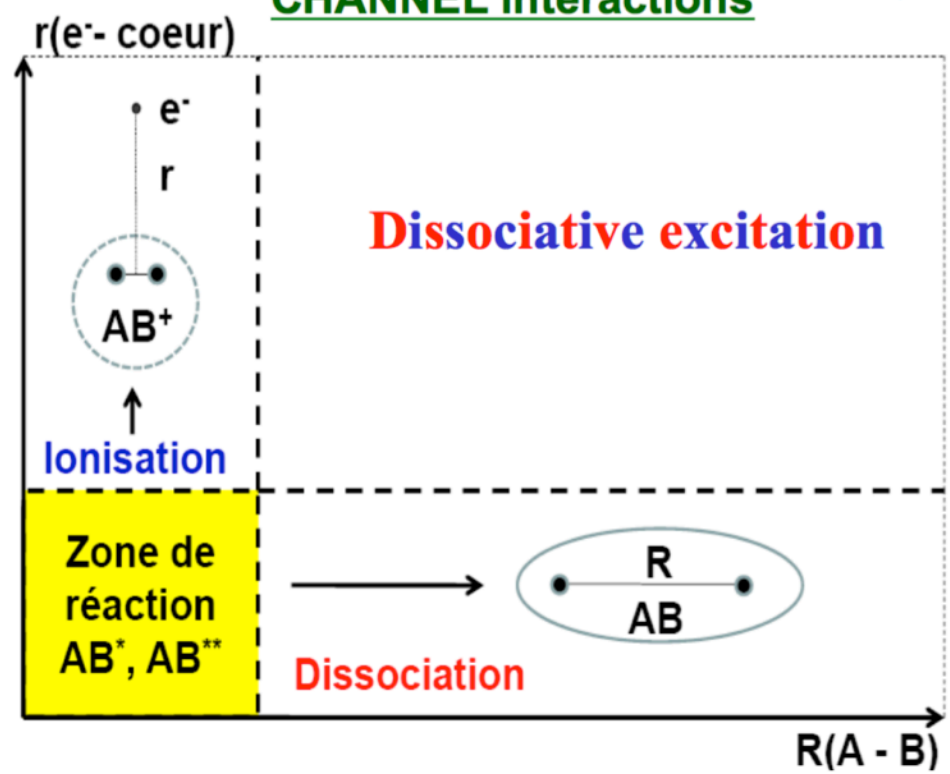
Multichannel Quantum Defect Theory

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

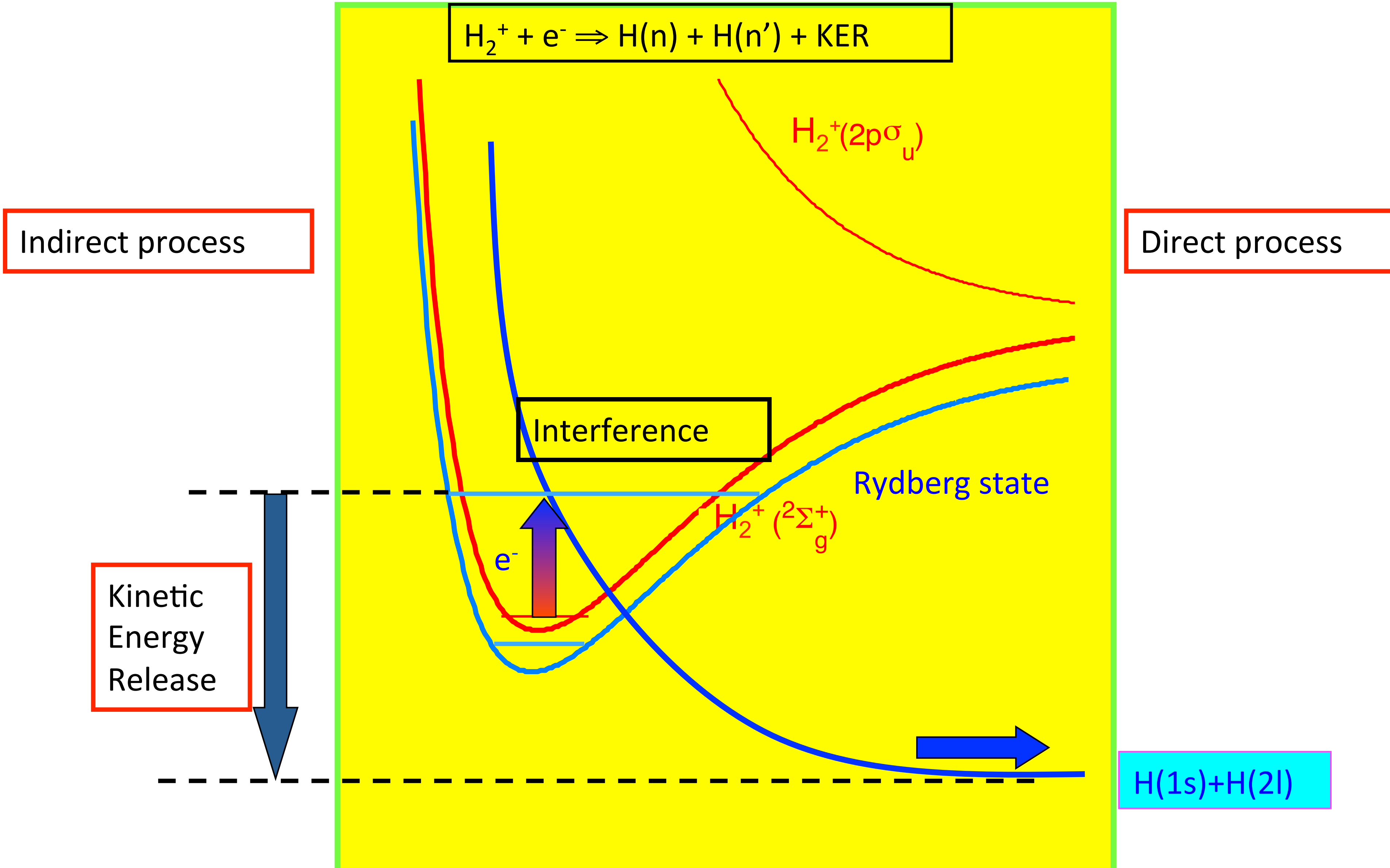
Quantum Interferences



CHANNEL interactions

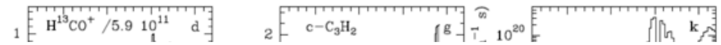


MQDT: DR mechanisms



Case study: SH+

K. M. Menten et al: Submillimeter absorption from SH+, a new widespread interstellar radical, 13CH+ and HCl, A&A 525, A77 (2011)



THE JOURNAL OF CHEMICAL PHYSICS **146**, 204109 (2017)

Discovery: Benz *et al* (2010)

A theoretical study of the dissociative recombination of SH^+ with electrons through the $^2\Pi$ states of SH

D. O. Kashinski,[1,a)] D. Talbi,[2,b)] A. P. Hickman,[3,c)] O. E. Di Nallo,[1] F. Colboc,[4,d)] K. Chakrabarti,[5] I. F. Schneider,[4,e)] and J. Zs. Mezei[4,6,7]

[1]*Department of Physics and Nuclear Engineering, United States Military Academy, West Point, New York 10996, USA*
[2]*Laboratoire Univers et Particules de Montpellier, Université de Montpellier, CNRS, Place Eugène Bataillon, 34095 Montpellier, France*
[3]*Department of Physics, Lehigh University, 16 Memorial Drive East, Bethlehem, Pennsylvania 18015, USA*
[4]*Laboratoire Ondes et Milieux Complexes, UMR 6294, Université Le Havre, 25, Rue Philippe Lebon, BP 540, F-76058 Le Havre, France*
[5]*Department of Mathematics, Scottish Church College, 1 and 3 Urquhart Square, Calcutta 700 006, India*
[6]*Laboratoire Aimé Cotton UMR 9188 CNRS, University Paris-Sud/ENS Cachan, Bâtiment 505, Campus d'Orsay, 91405 Orsay Cedex, France*
[7]*Laboratoire des Sciences des Procédés et des Matériaux, UPR 3407, Université Paris 13, 99 Avenue Jean-Baptiste Clément, F-93430 Villetaneuse, France*

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A quantitative theoretical study of the dissociative recombination of SH^+ with electrons has been carried out. Multireference, configuration interaction calculations were used to determine accurate potential energy curves for SH^+ and SH. The block diagonalization method was used to disentangle strongly interacting SH valence and Rydberg states and to construct a diabatic Hamiltonian whose diagonal matrix elements provide the diabatic potential energy curves. The off-diagonal elements are related to the electronic valence-Rydberg couplings. Cross sections and rate coefficients for the dissociative recombination reaction were calculated with a stepwise version of the multichannel quantum defect theory, using the molecular data provided by the block diagonalization method. The calculated rates are compared with the most recent measurements performed on the ion Test Storage Ring (TSR) in Heidelberg, Germany. *Published by AIP Publishing.* [http://dx.doi.org/10.1063/1.4983690]

[1] LERMA, CNRS UMR 8112, École Normale Supérieure & Observatoire de Paris, Paris, France
[2] Institut d'Astrophysique Spatiale, CNRS UMR 8617, Université Paris-Sud, Orsay, France

Received 28 January 2014 / Accepted 19 July 2014

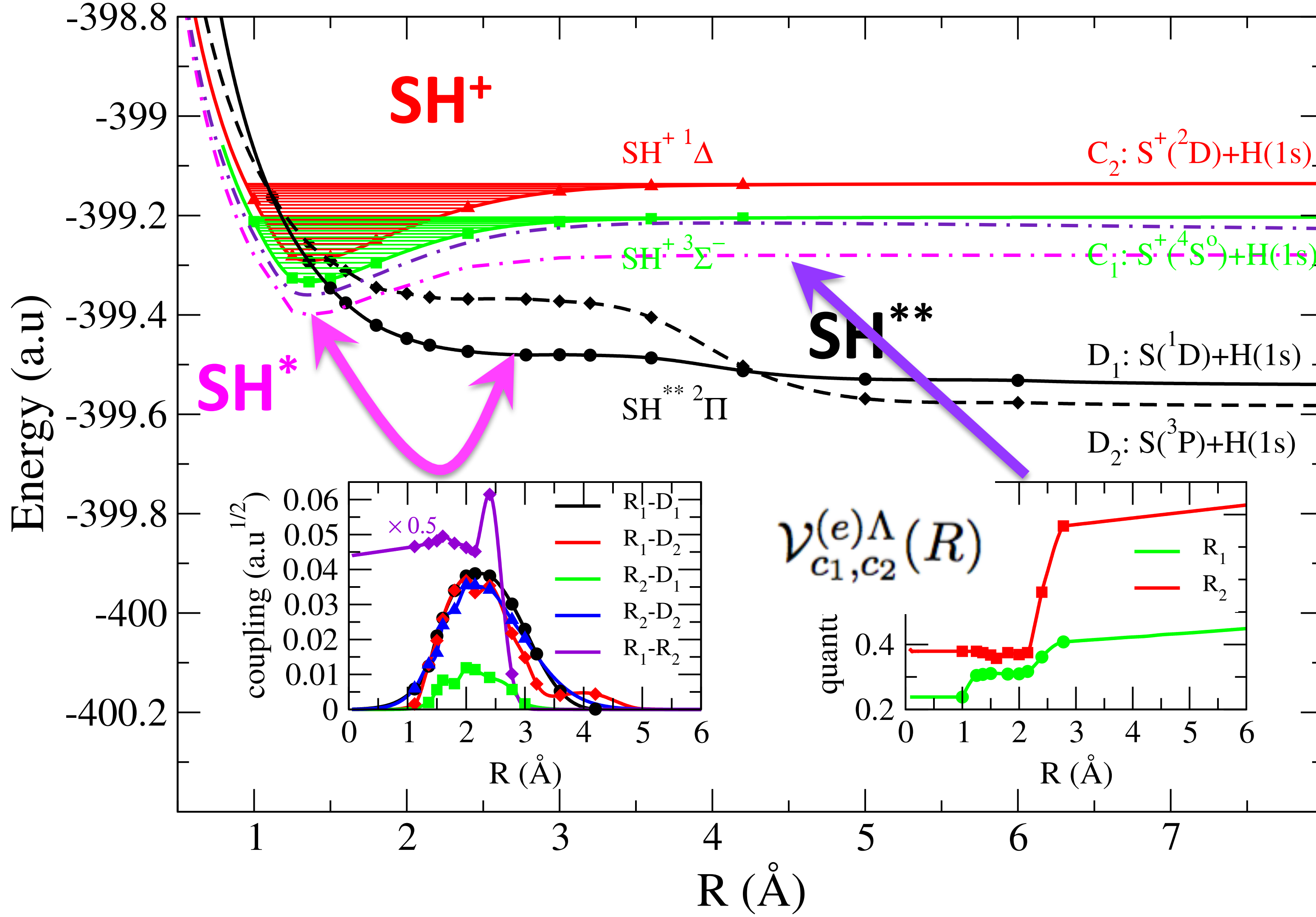
Formation and destruction routes

$S^+ + H_2 \rightarrow SH^+ + H$ (-0.86 eV)

Abstract

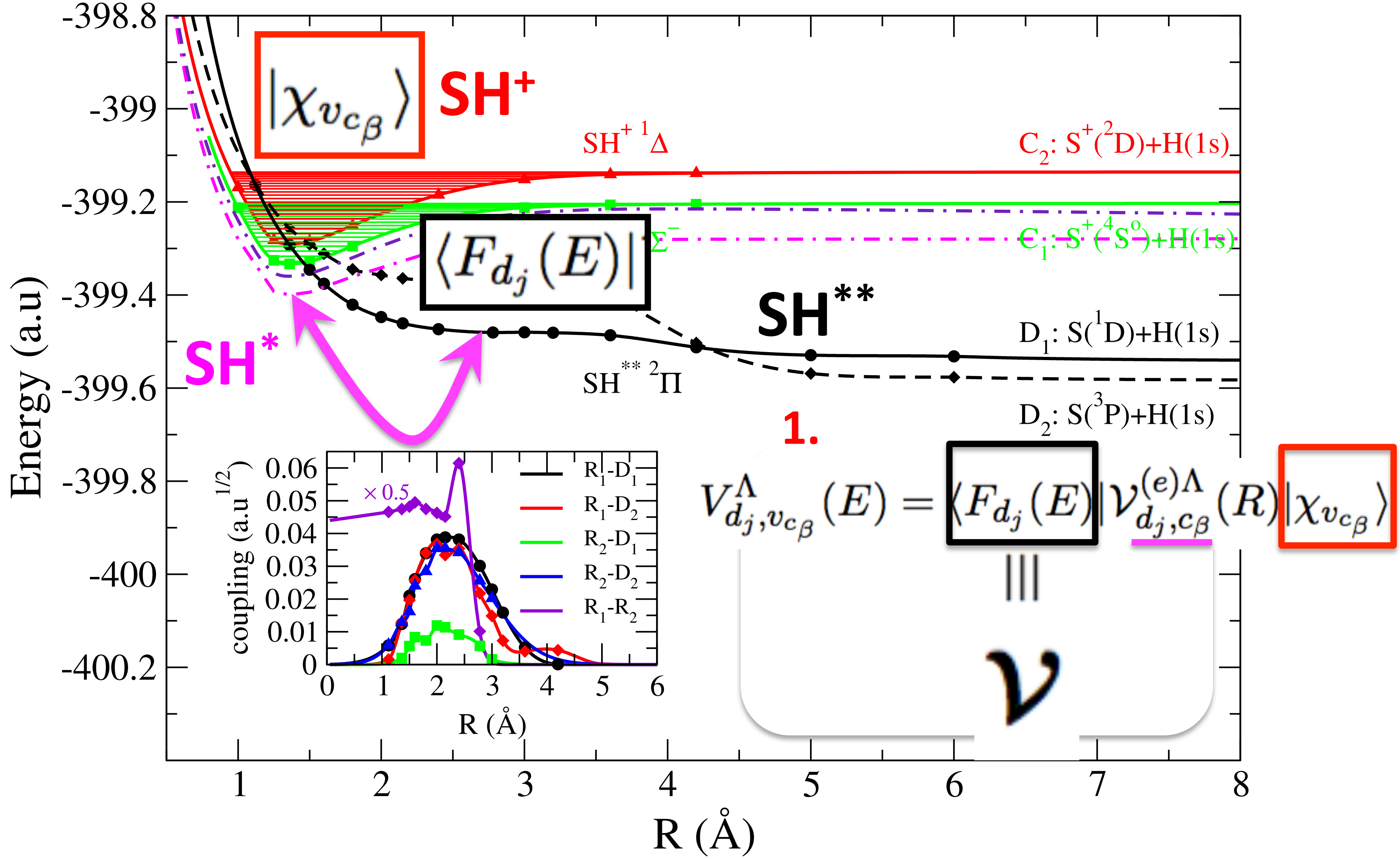
Context. Tens of light hydrides and small molecules have now been detected over several hundreds sightlines sampling the diffuse interstellar medium (ISM) in both the Solar neighbourhood and the inner Galactic disk.
Aims. These new data confirm the limitations of the traditional chemical pathways driven by the UV photons and the cosmic rays (CR) and the need for additional energy sources, such as turbulent dissipation, to open highly endoenergetic formation routes. The goal of the present paper is to further investigate the link between specific species and the properties of the turbulent cascade in particular its space-time intermittency.
Methods. We have analysed ten different atomic and molecular species in the framework of the updated model of turbulent dissipation regions (TDR). We study the influence on the abundances of these species of parameters specific to chemistry (density, UV field, and CR ionisation rate) and those linked to turbulence (the average turbulent dissipation rate, the dissipation timescale, and the ion-neutral velocity drift in the regions of dissipation).
Results. The most sensitive tracers of turbulent dissipation are the abundances of CH^+ and SH^+, and the column densities of the $J = 3, 4, 5$ rotational levels of H_2. The abundances of CO, HCO^+, and the intensity of the 158 μm [CII] emission line are significantly

MQDT: molecular data



GAMESS + Block diagonalization method (Kashinki, Hickman, Talbi)

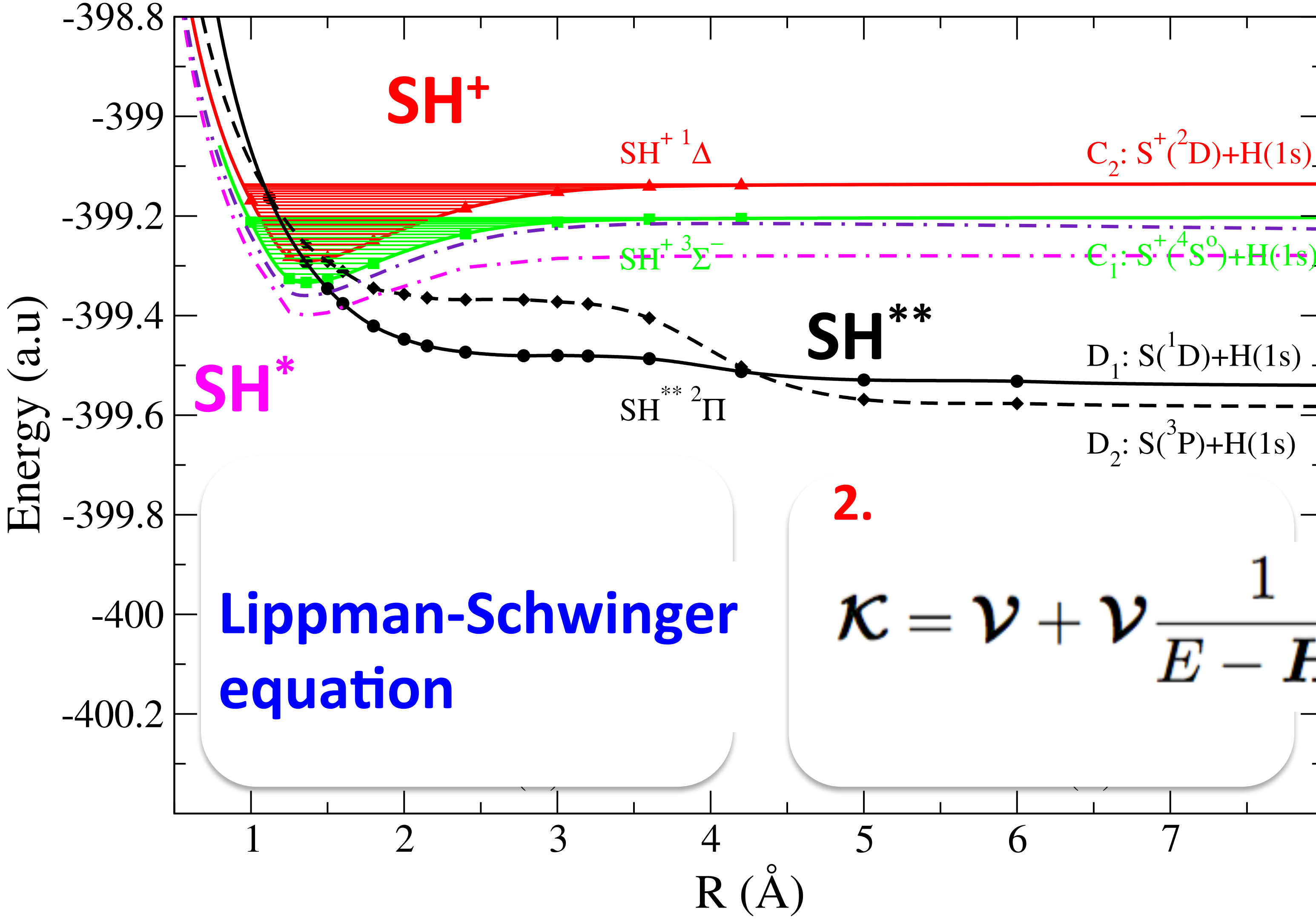
MQDT: The formalism



$$V^{\Lambda}_{d_j,v_{c_\beta}}(E) = \langle F_{d_j}(E)|\mathcal{V}^{(e)\Lambda}_{d_j,c_\beta}(R)|\chi_{v_{c_\beta}}\rangle$$

$$\equiv \mathcal{V}$$

MQDT: The formalism

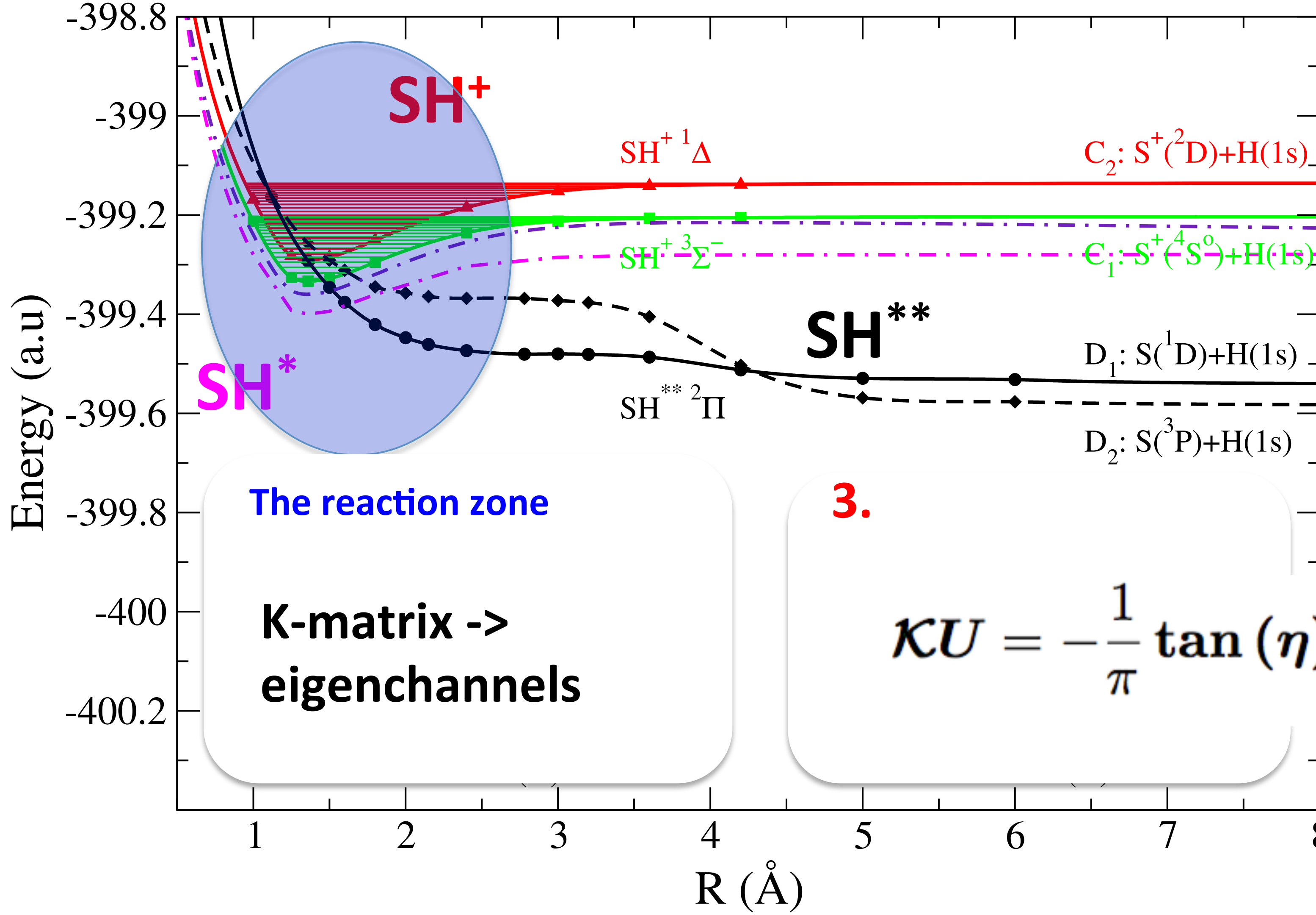


Lippman-Schwinger equation

2.

$$\mathcal{K} = \mathcal{V} + \mathcal{V}\frac{1}{E - \boldsymbol{H_0}}\mathcal{V},$$

MQDT: The formalism



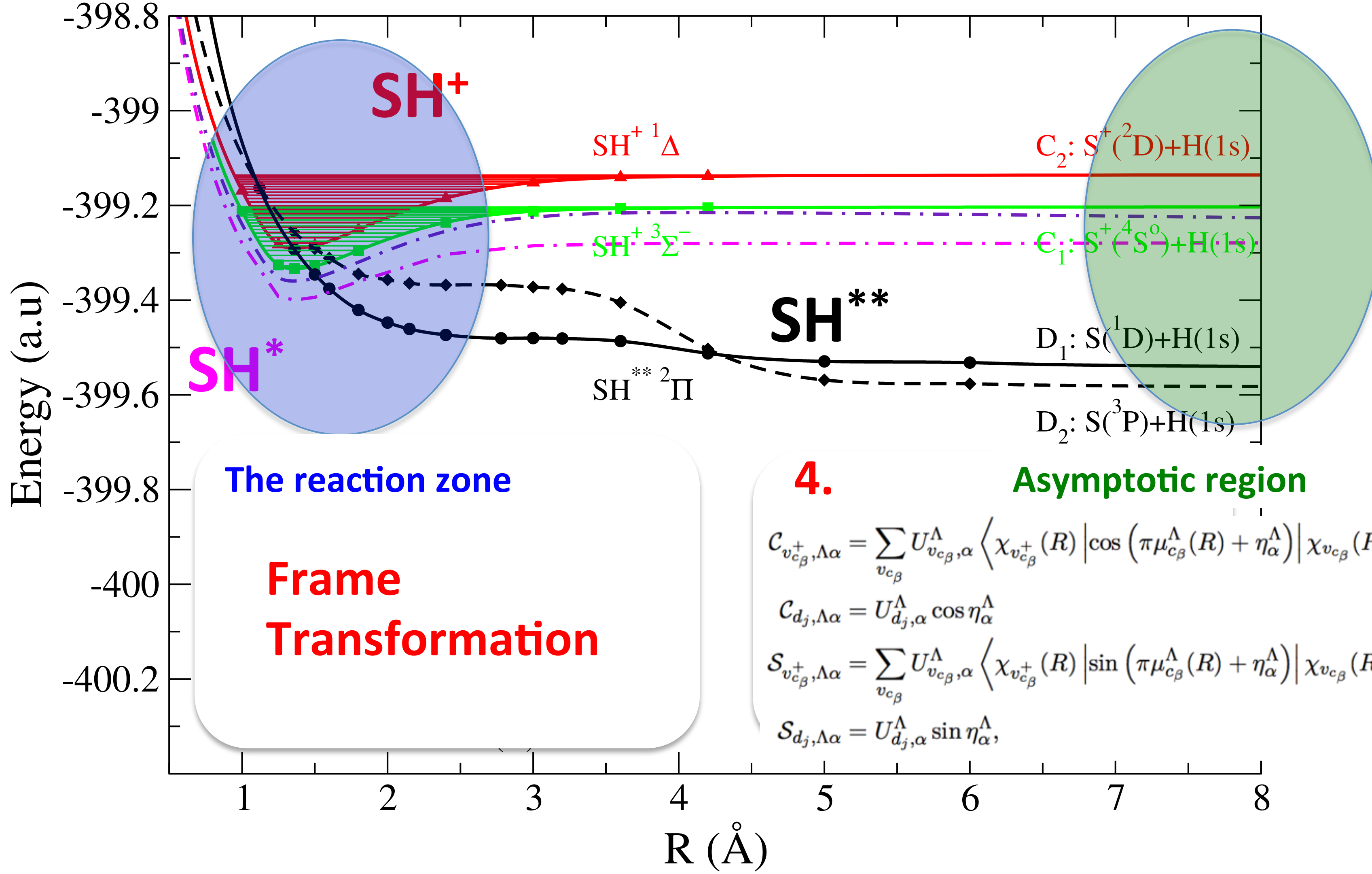
The reaction zone

K-matrix -> eigenchannels

3.

$$\mathcal{K}U = -\frac{1}{\pi}\tan(\eta)U,$$

MQDT: The formalism



The reaction zone

Frame Transformation

4. **Asymptotic region**

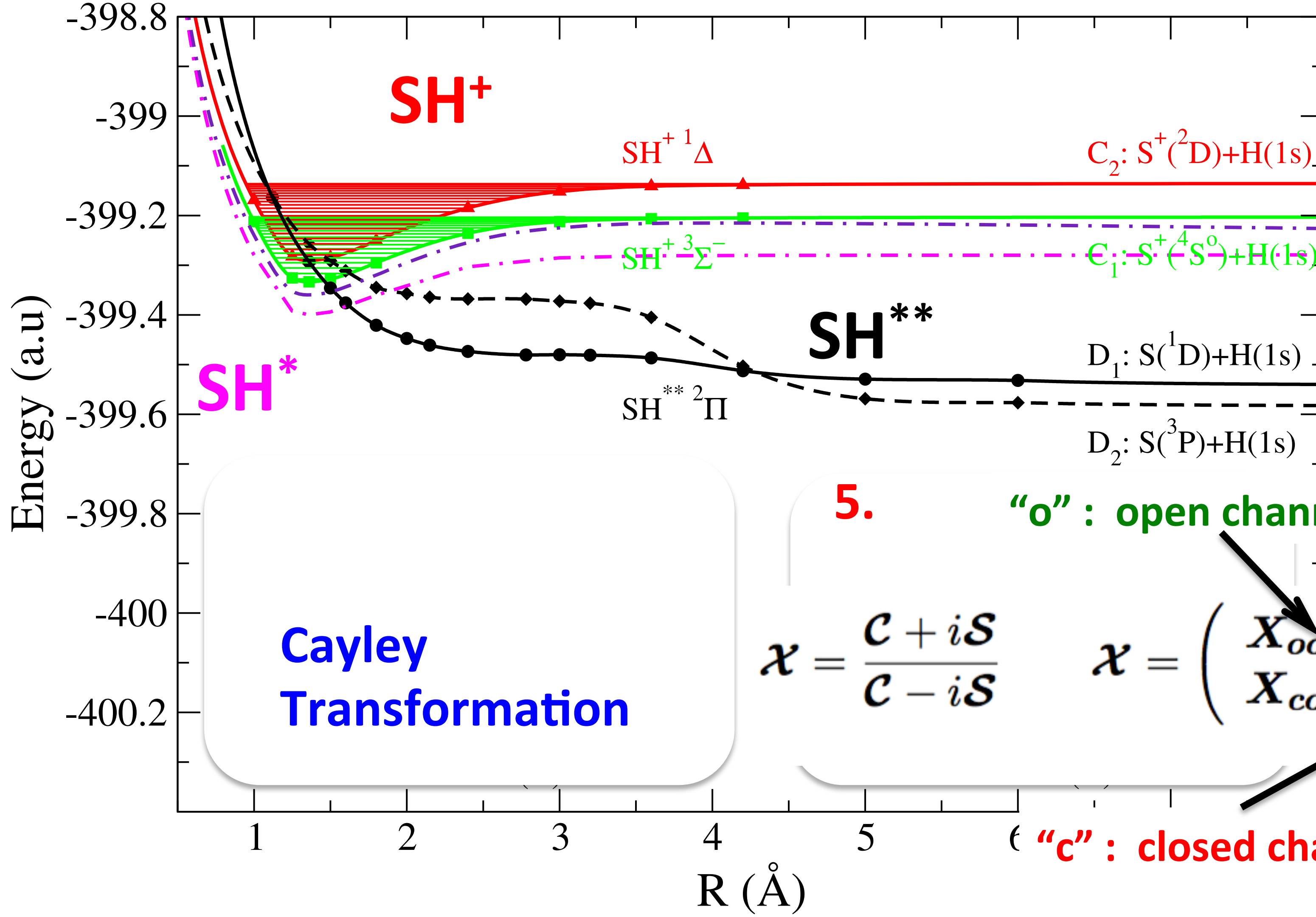
$$\mathcal{C}_{v^+_{c_\beta},\Lambda\alpha} = \sum_{v_{c_\beta}} U^\Lambda_{v_{c_\beta},\alpha} \left\langle \chi_{v^+_{c_\beta}}(R) \left| \cos\left(\pi\mu^\Lambda_{c_\beta}(R)+\eta^\Lambda_\alpha\right)\right| \chi_{v_{c_\beta}}(R)\right\rangle$$

$$\mathcal{C}_{d_j,\Lambda\alpha} = U^\Lambda_{d_j,\alpha}\cos\eta^\Lambda_\alpha$$

$$\mathcal{S}_{v^+_{c_\beta},\Lambda\alpha} = \sum_{v_{c_\beta}} U^\Lambda_{v_{c_\beta},\alpha} \left\langle \chi_{v^+_{c_\beta}}(R) \left| \sin\left(\pi\mu^\Lambda_{c_\beta}(R)+\eta^\Lambda_\alpha\right)\right| \chi_{v_{c_\beta}}(R)\right\rangle$$

$$\mathcal{S}_{d_j,\Lambda\alpha} = U^\Lambda_{d_j,\alpha}\sin\eta^\Lambda_\alpha,$$

MQDT: The formalism



Cayley Transformation

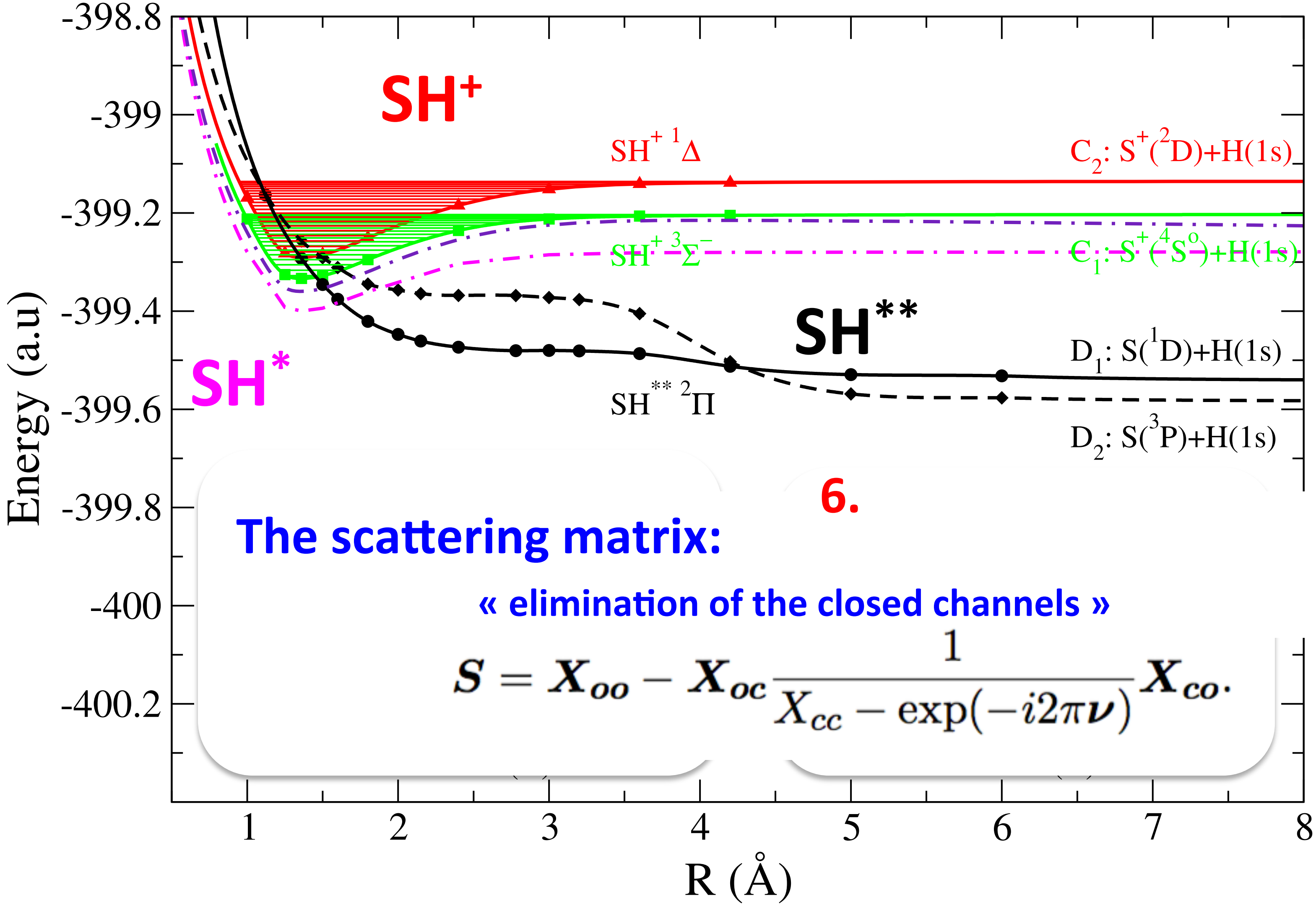
5.

$$\mathcal{X} = \frac{\mathcal{C} + i\mathcal{S}}{\mathcal{C} - i\mathcal{S}} \qquad \mathcal{X} = \begin{pmatrix} X_{oo} & X_{oc} \\ X_{co} & X_{cc} \end{pmatrix}$$

“o” : open channels

“c” : closed channels

MQDT: The formalism



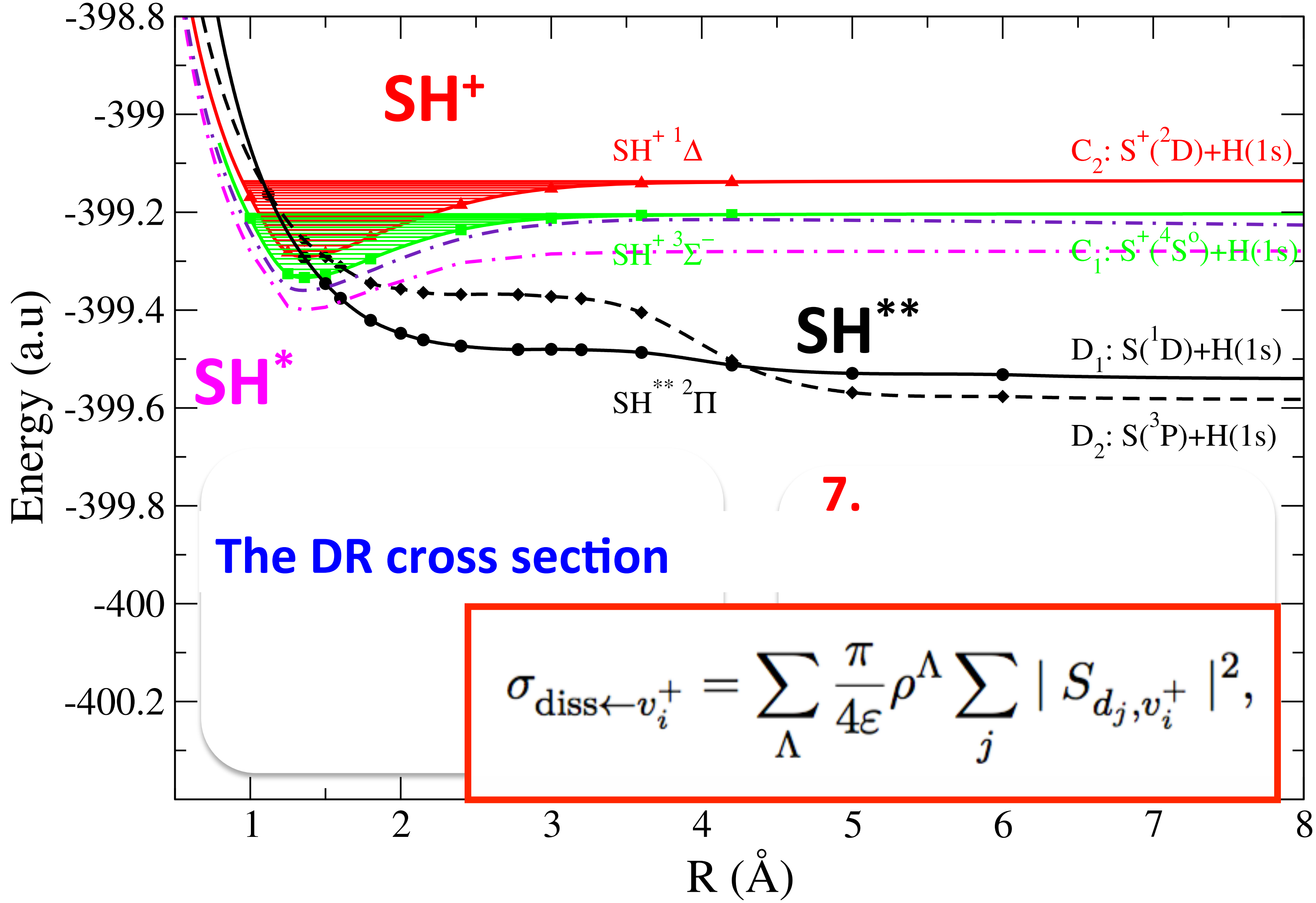
6.

The scattering matrix:

« elimination of the closed channels »

$$\boldsymbol{S} = \boldsymbol{X}_{oo} - \boldsymbol{X}_{oc}\frac{1}{\boldsymbol{X}_{cc} - \exp(-i2\pi\boldsymbol{\nu})}\boldsymbol{X}_{co}.$$

MQDT: The formalism

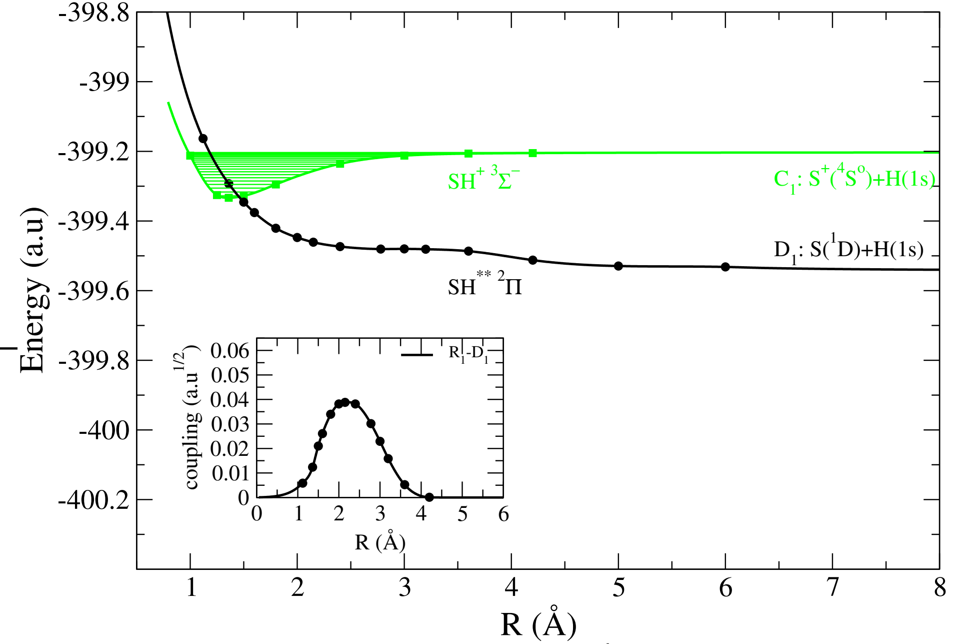


7.

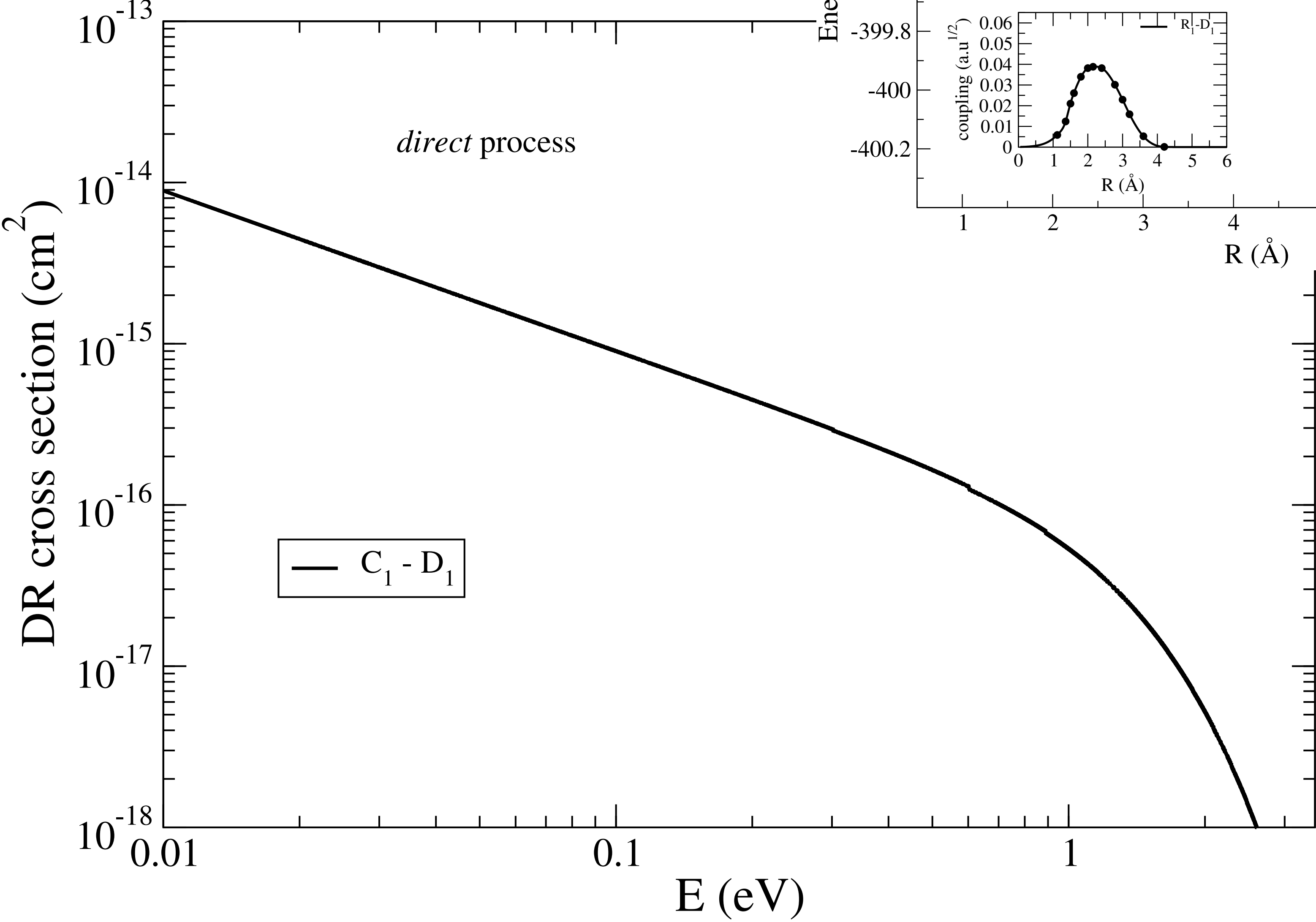
The DR cross section

$$\sigma_{\mathrm{diss}\leftarrow v_i^+} = \sum_{\Lambda} \frac{\pi}{4\varepsilon} \rho^{\Lambda} \sum_{j} \mid S_{d_j, v_i^+} \mid^2,$$

SH^+: DR xs

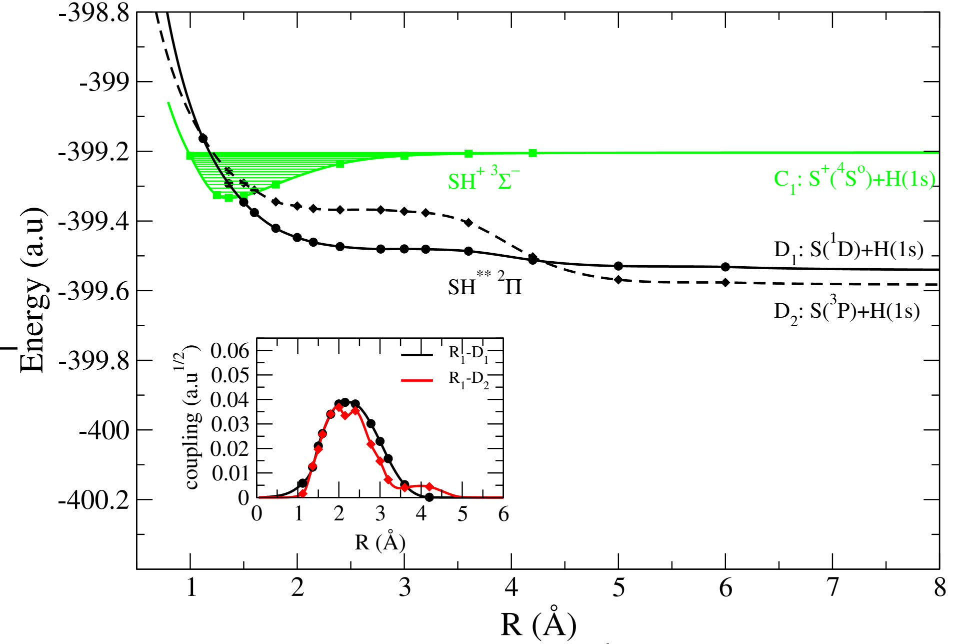


Energy (a.u)
R (Å)
$SH^{+\ 3}\Sigma^-$
C_1: $S^+(^4S^o)$+H(1s)
D_1: $S(^1D)$+H(1s)
$SH^{**\ 2}\Pi$
coupling ($a.u^{1/2}$)
R_1-D_1

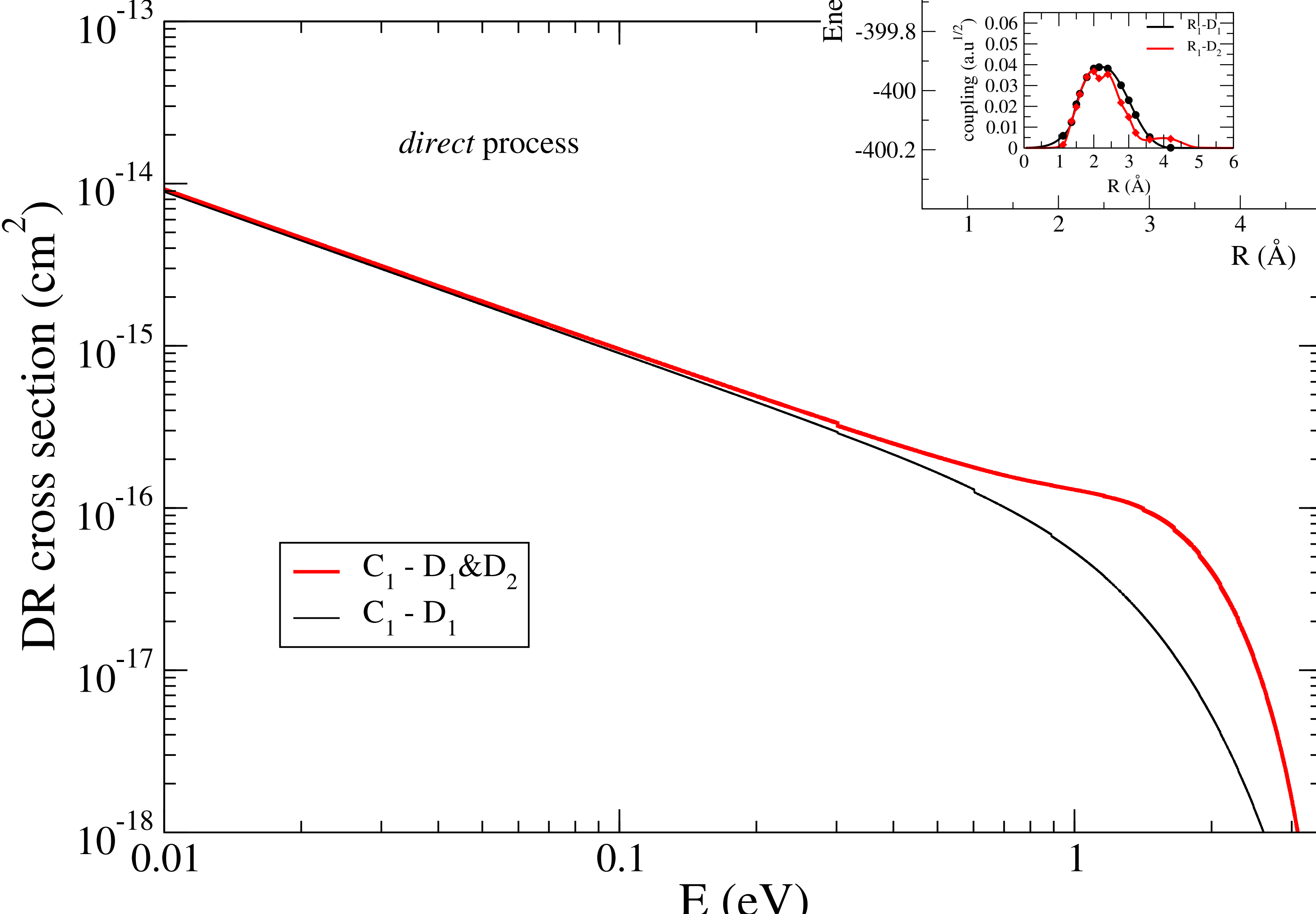


DR cross section (cm^2)
E (eV)
direct process
C_1 - D_1

SH^+: DR xs

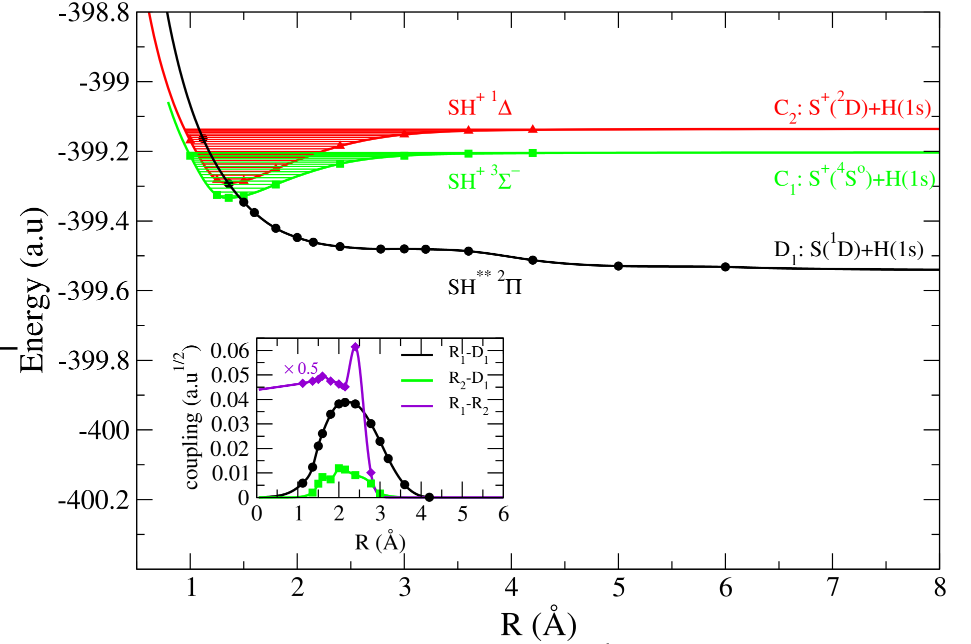


-398.8
-399
-399.2
-399.4
-399.6
-399.8
-400
-400.2
Energy (a.u)
SH+ 3Σ−
C1: S+(4So)+H(1s)
D1: S(1D)+H(1s)
SH** 2Π
D2: S(3P)+H(1s)
coupling (a.u−1/2)
0.06
0.05
0.04
0.03
0.02
0.01
0
0 1 2 3 4 5 6
R (Å)
R1-D1
R1-D2
1 2 3 4 5 6 7 8
R (Å)

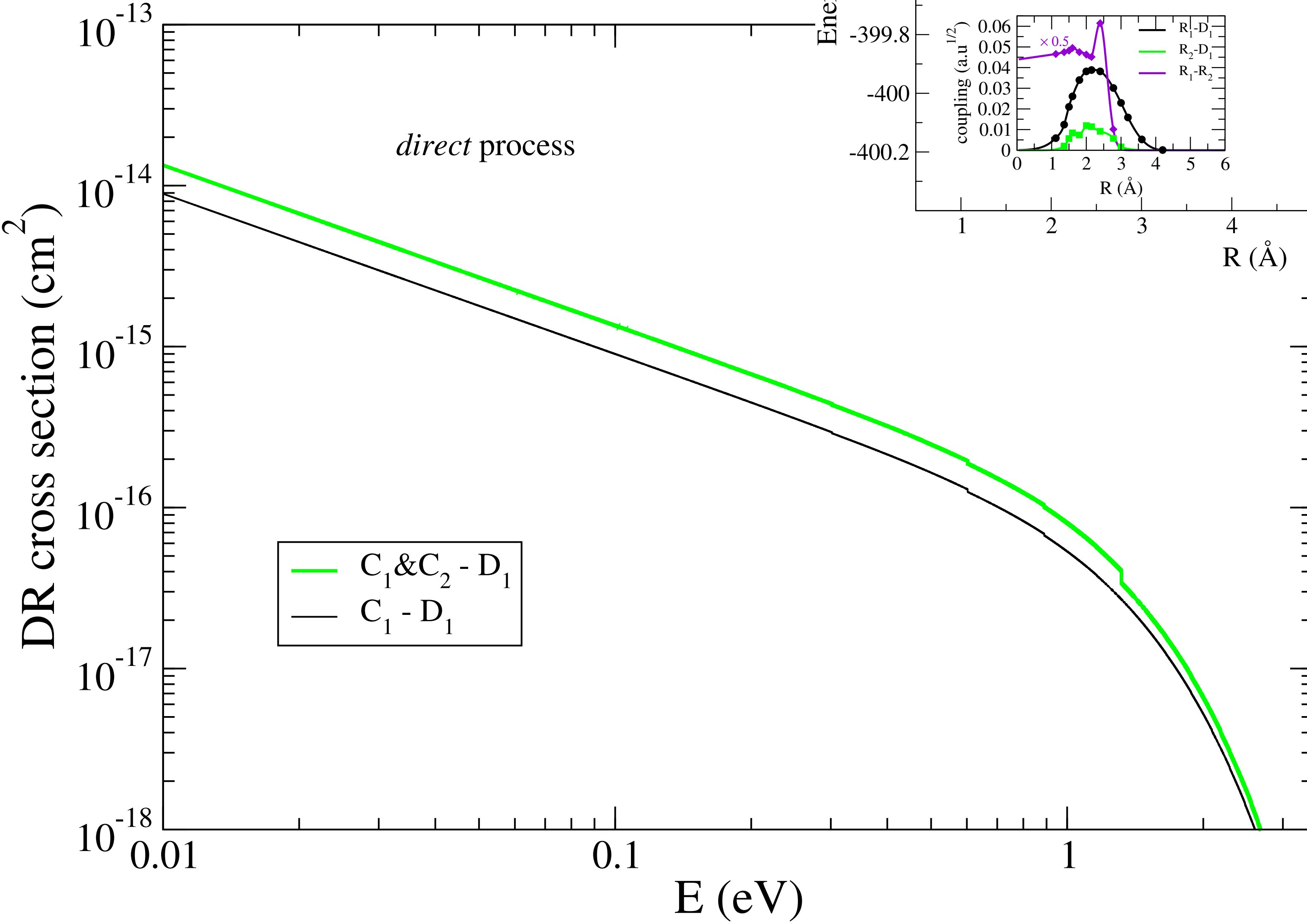


DR cross section (cm2)
10-13
10-14
10-15
10-16
10-17
10-18
direct process
C1 - D1&D2
C1 - D1
0.01
0.1
1
E (eV)

SH^+: DR xs

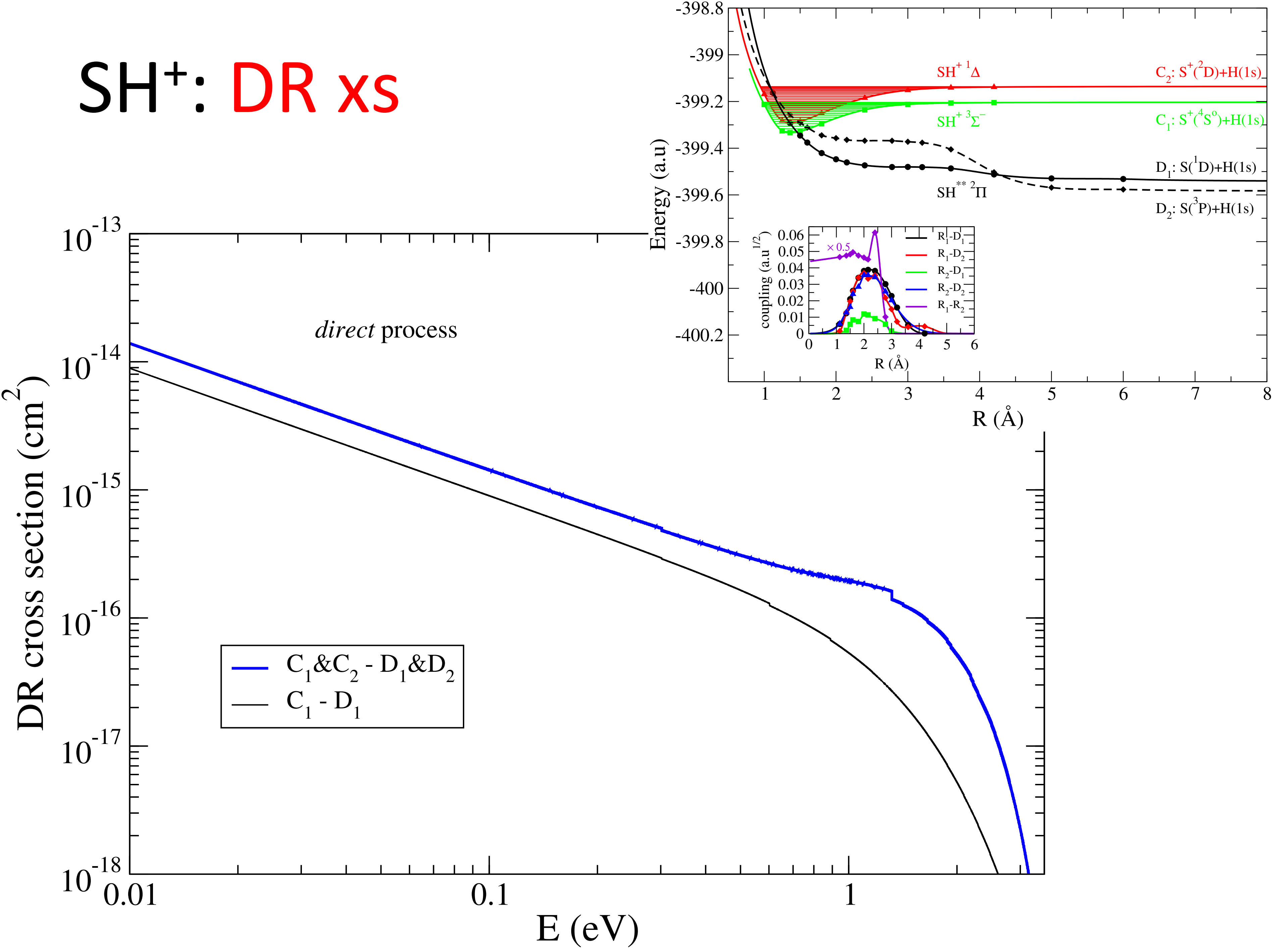


Energy (a.u)
R (Å)
$SH^{+\ 1}\Delta$
C_2: $S^+(^2D)$+H(1s)
$SH^{+\ 3}\Sigma^-$
C_1: $S^+(^4S^o)$+H(1s)
D_1: $S(^1D)$+H(1s)
$SH^{**\ 2}\Pi$
coupling (a.u$^{1/2}$)
× 0.5
R_1-D_1
R_2-D_1
R_1-R_2



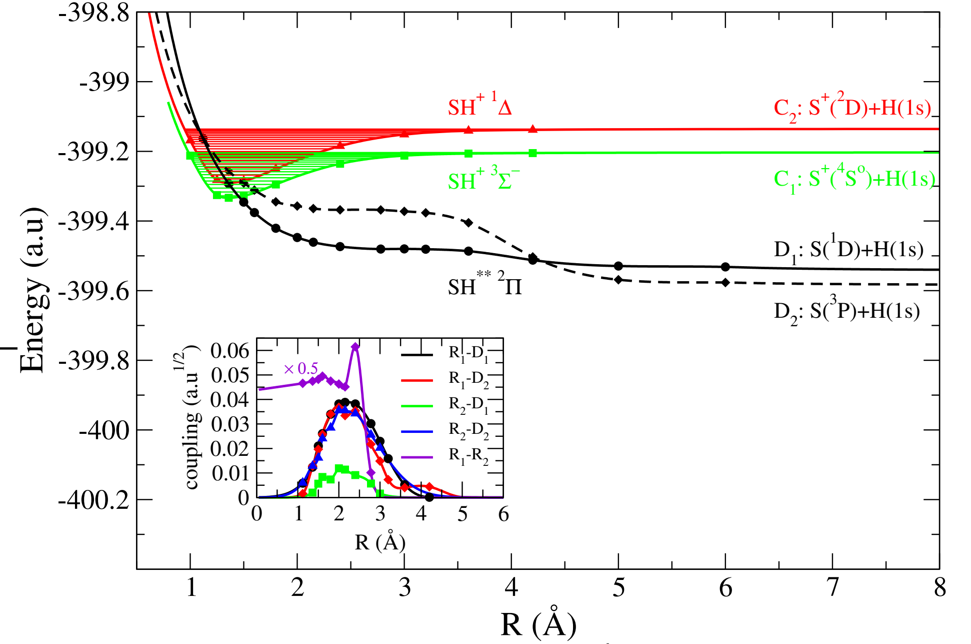
DR cross section (cm^2)
E (eV)
direct process
C_1&C_2 - D_1
C_1 - D_1

SH+: DR xs



DR cross section (cm²)
E (eV)
direct process
C1&C2 - D1&D2
C1 - D1
Energy (a.u)
R (Å)
SH+ 1Δ
SH+ 3Σ−
SH** 2Π
C2: S+(2D)+H(1s)
C1: S+(4So)+H(1s)
D1: S(1D)+H(1s)
D2: S(3P)+H(1s)
coupling (a.u1/2)
× 0.5
R1-D1
R1-D2
R2-D1
R2-D2
R1-R2

SH^+: DR xs



-398.8
-399
-399.2
-399.4
-399.6
-399.8
-400
-400.2
Energy (a.u)
SH+ 1Δ
SH+ 3Σ−
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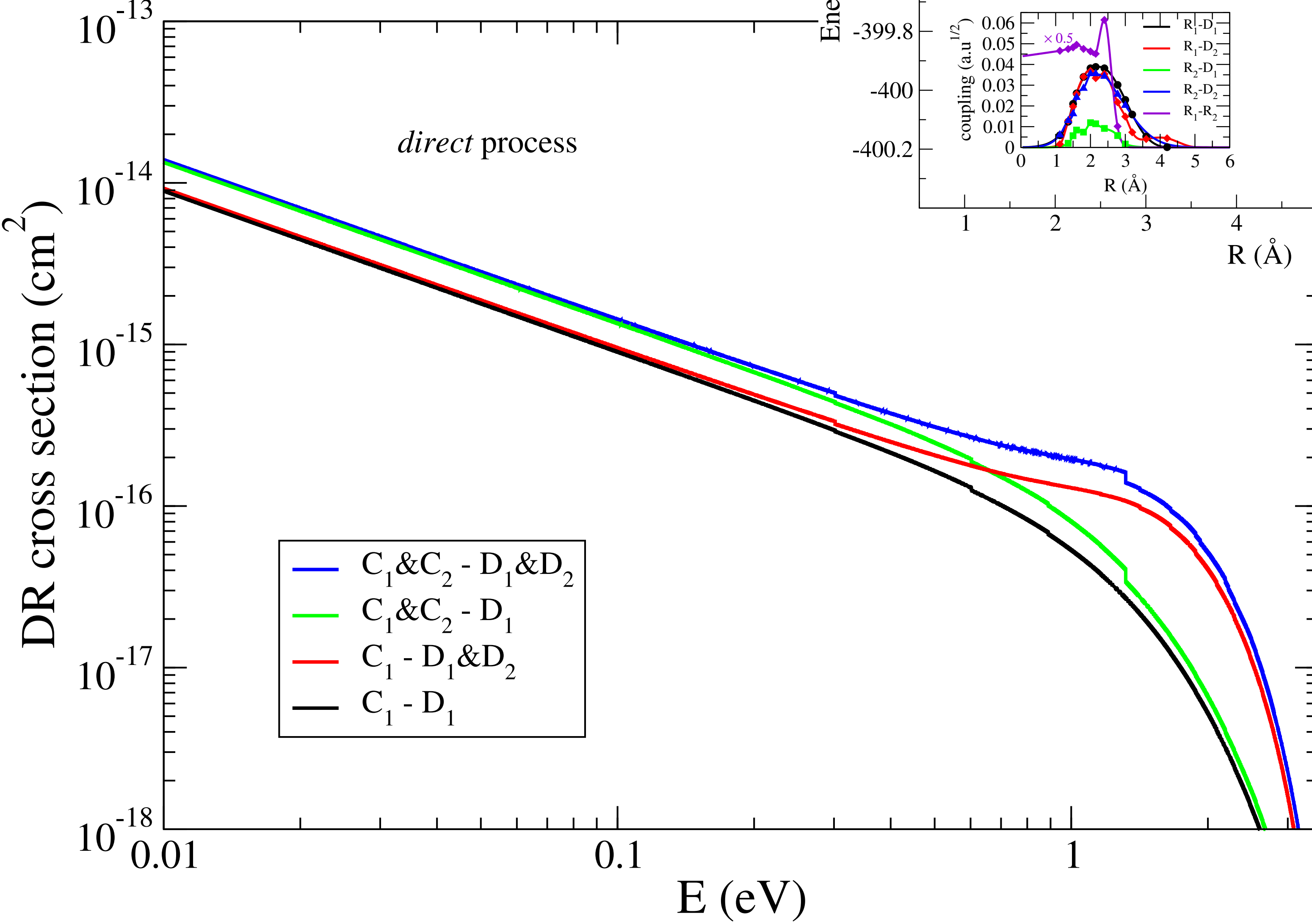
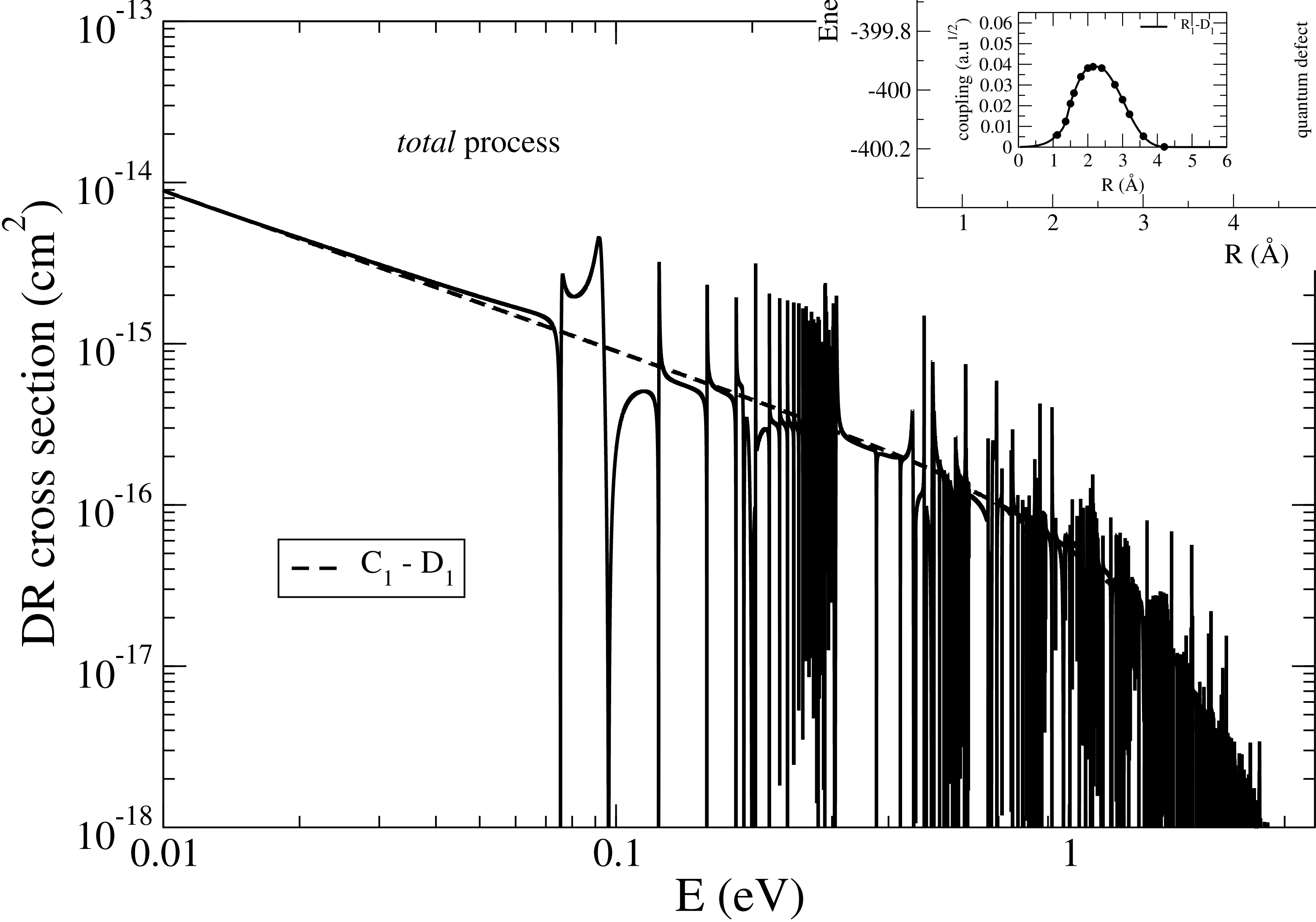
C1: S+(4So)+H(1s)
D1: S(1D)+H(1s)
D2: S(3P)+H(1s)
coupling (a.u1/2)
× 0.5
R1-D1
R1-D2
R2-D1
R2-D2
R1-R2
R (Å)
1
2
3
4
5
6
7
8
R (Å)

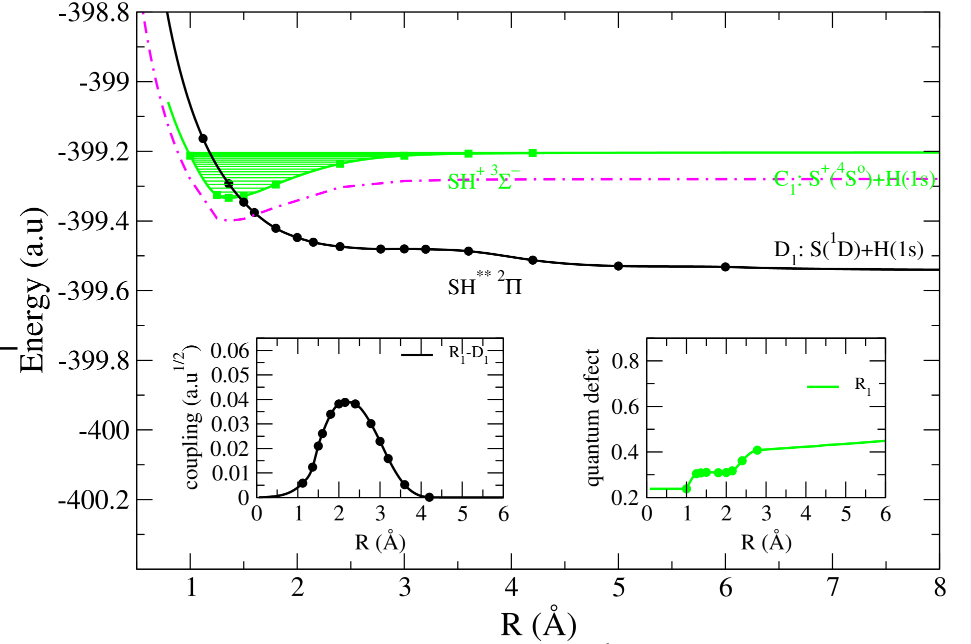


DR cross section (cm2)
10-13
10-14
10-15
10-16
10-17
10-18
direct process
C1&C2 - D1&D2
C1&C2 - D1
C1 - D1&D2
C1 - D1
0.01
0.1
1
E (eV)

SH^+: DR xs

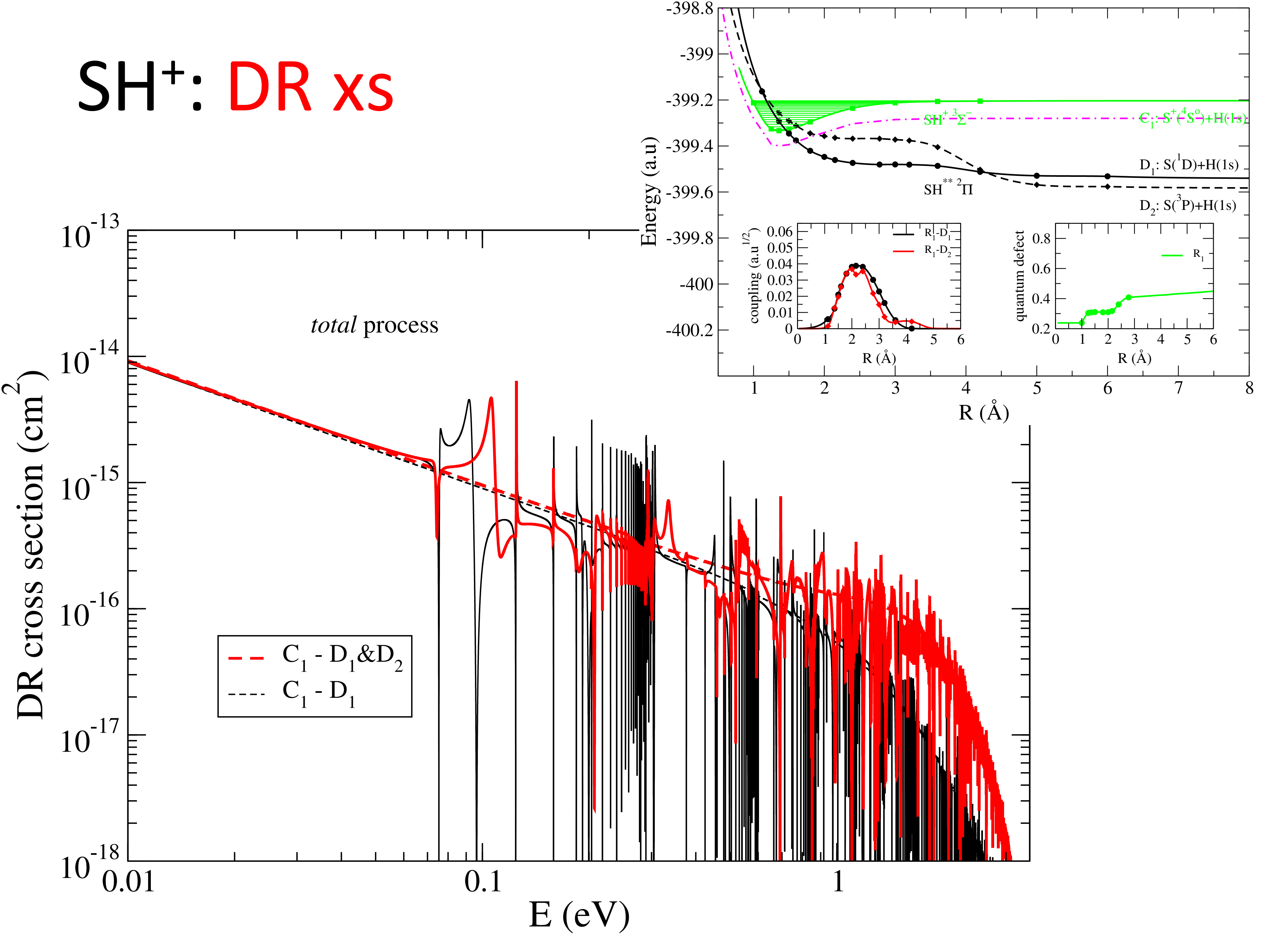


total process
C1 - D1
DR cross section (cm2)
E (eV)
0.01
0.1
1



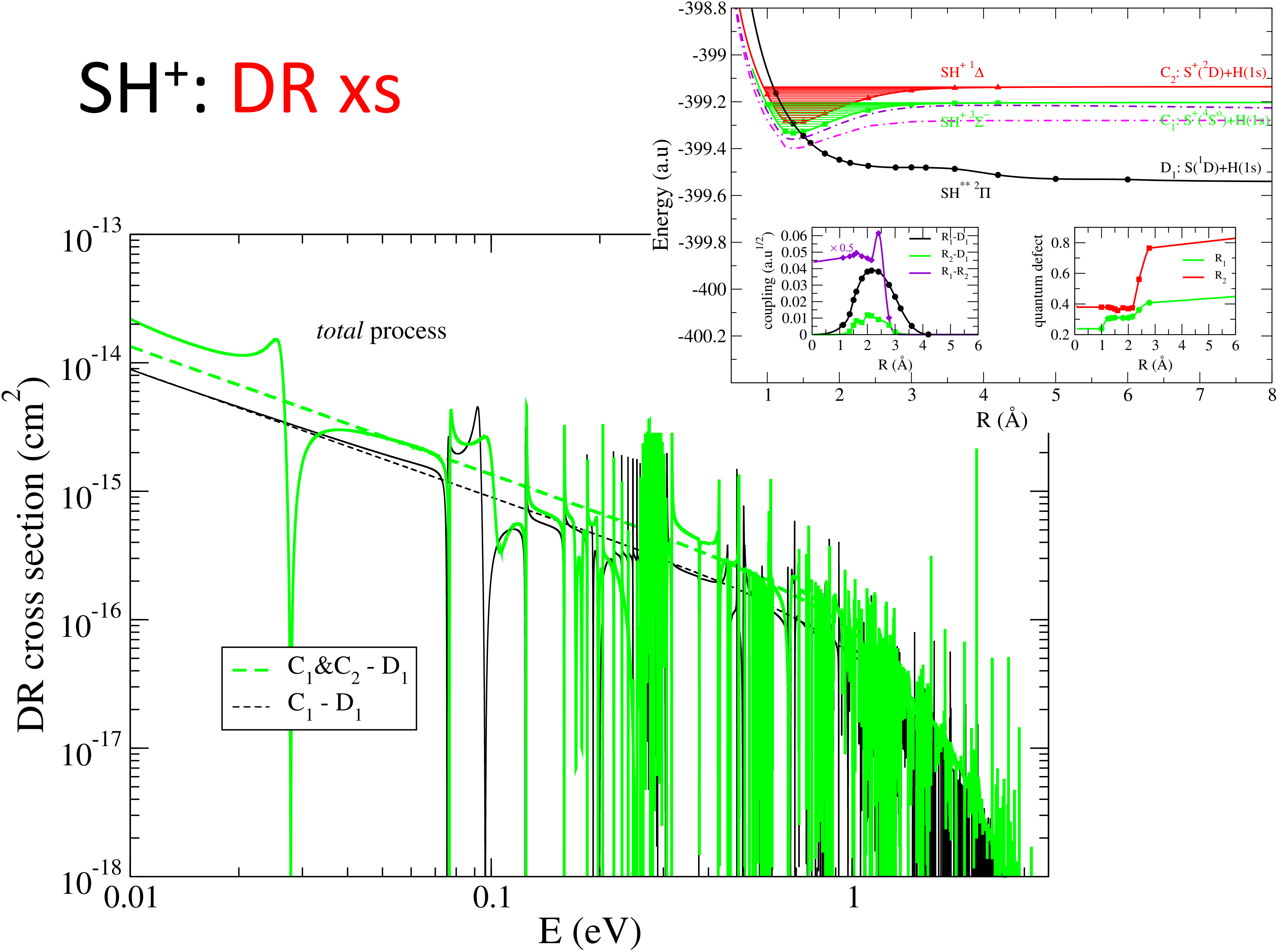
Energy (a.u)
R (Å)
SH+ 3Σ−
C1: S+(4So)+H(1s)
D1: S(1D)+H(1s)
SH** 2Π
coupling (a.u1/2)
R1-D1
quantum defect
R1

SH+: DR xs



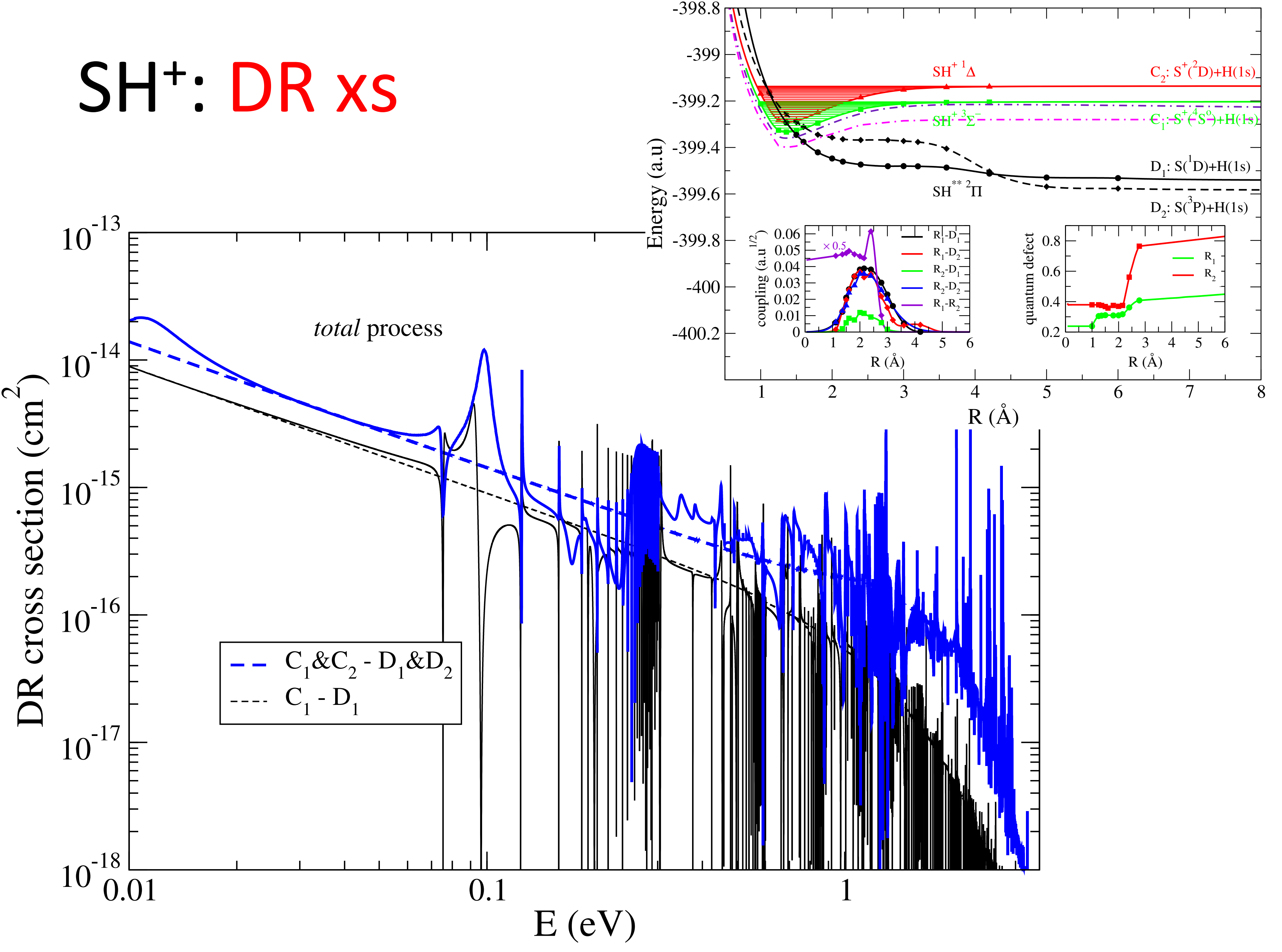
total process
C1 - D1&D2
C1 - D1
DR cross section (cm2)
E (eV)
Energy (a.u)
R (Å)
SH+ 3Σ−
C1: S+(4So)+H(1s)
D1: S(1D)+H(1s)
D2: S(3P)+H(1s)
SH** 2Π
coupling (a.u1/2)
R1-D1
R1-D2
quantum defect
R1

SH+: DR xs



total process
C1&C2 - D1
C1 - D1
DR cross section (cm2)
E (eV)
SH+ 1Δ
C2: S+(2D)+H(1s)
SH+ 3Σ−
C1: S+(4So)+H(1s)
D1: S(1D)+H(1s)
SH** 2Π
Energy (a.u)
R (Å)
coupling (a.u1/2)
× 0.5
R1-D1
R2-D1
R1-R2
quantum defect
R1
R2

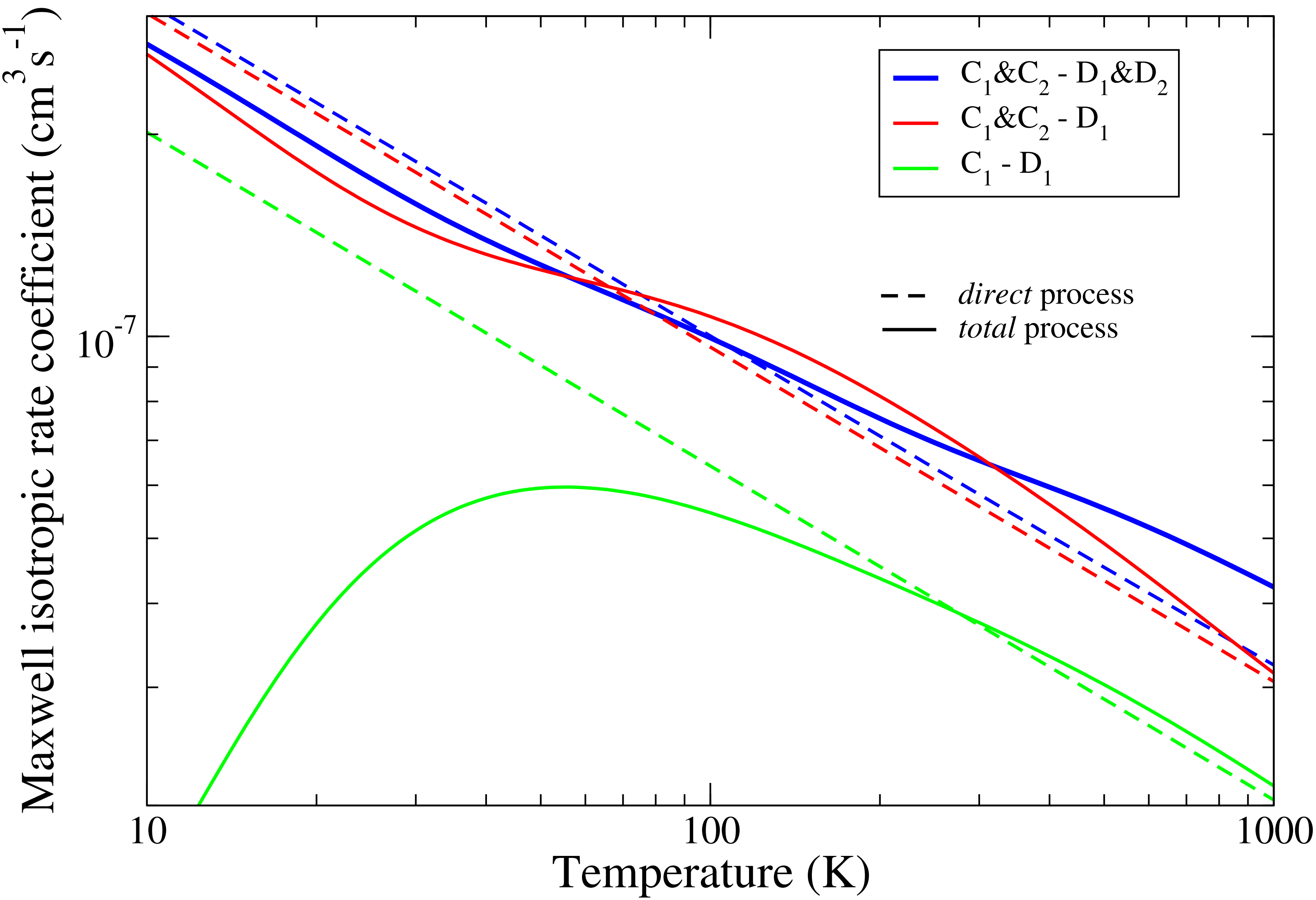
SH$^+$: DR xs



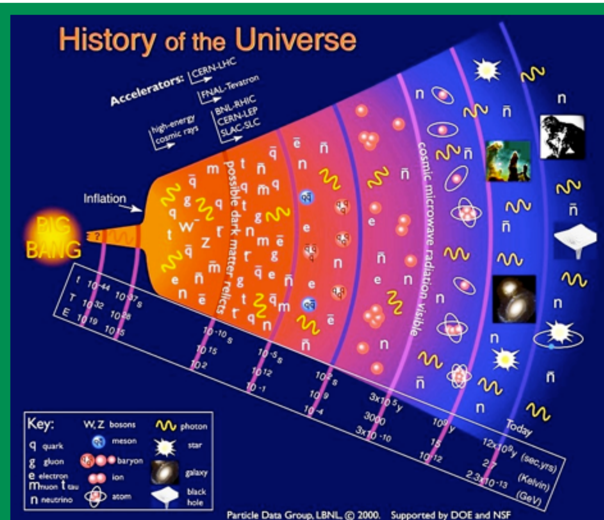
total process
C1&C2 - D1&D2
C1 - D1
DR cross section (cm2)
E (eV)
Energy (a.u)
R (Å)
SH+ 1Δ
SH+ 3Σ−
SH** 2Π
C2: S+(2D)+H(1s)
C1: S+(4So)+H(1s)
D1: S(1D)+H(1s)
D2: S(3P)+H(1s)
coupling (a.u1/2)
× 0.5
R1-D1
R1-D2
R2-D1
R2-D2
R1-R2
quantum defect
R1
R2

SH^+: DR rate

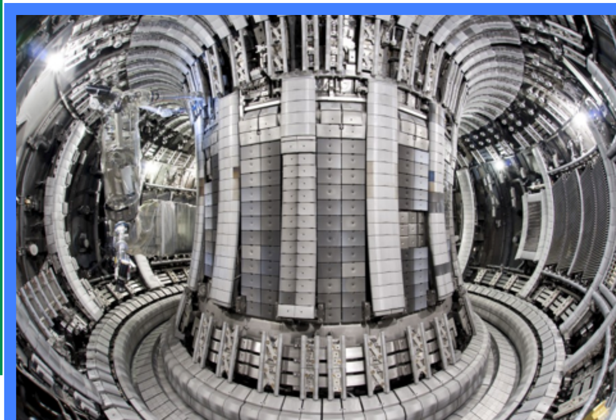
$$\alpha(T) = \left(\frac{m_e}{2\pi kT}\right)^{3/2} \int_0^\infty \sigma(v) v \exp\left(-\frac{m_e v^2}{2kT}\right) 4\pi v^2\, dv$$



Results: The most abundent molecule



H_2



Densities ~ 10^5- 10^7cm^{-3}
T ~ 30000 K – 0.003 K

Warm ionized medium (densities ~ 0.3 cm^{-3} - T ~ 10000 - 8000 K)
Warm neutral medium (densities ~ 0.3 cm^{-3} - T ~ 8000 K)
Cold neutral medium (densities ~ 30 cm^{-3} - T ~ 50 K)
Molecular clouds (densities > 100 cm^{-3}- T > 10 K)

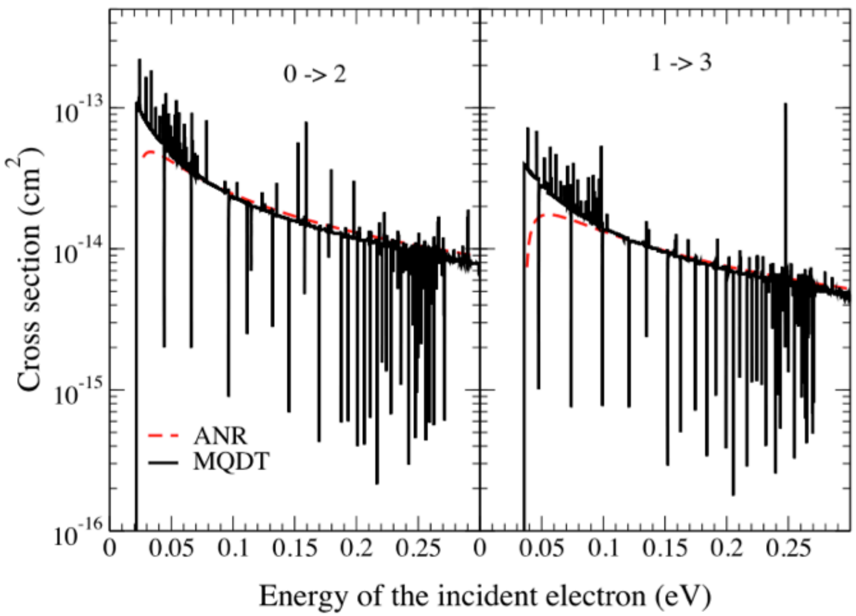
Some orders of magnitude :

* $n_e = 10^8$-10^{12} cm^{-3} (<10^{-2} and more often <10^{-5})
* $<\varepsilon_e>$ = 1-10 eV
* T_g = 300 - 6000 K
* 'T_v' = 1000 - 5000 K (molecular gases)

Results: The most abundant molecule @ *low temperatures*

➢ Rotational excitation

ANR: Faure & Tennyson MNRAS (2001)



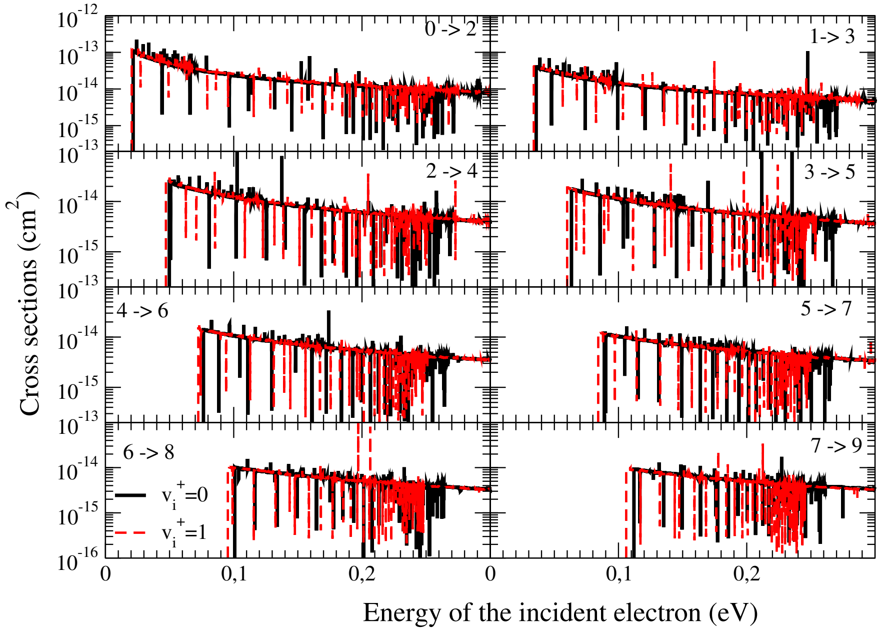
Monthly Notices of the ROYAL ASTRONOMICAL SOCIETY

MNRAS 455, 276–281 (2015) doi:10.1093/mnras/stv2329

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

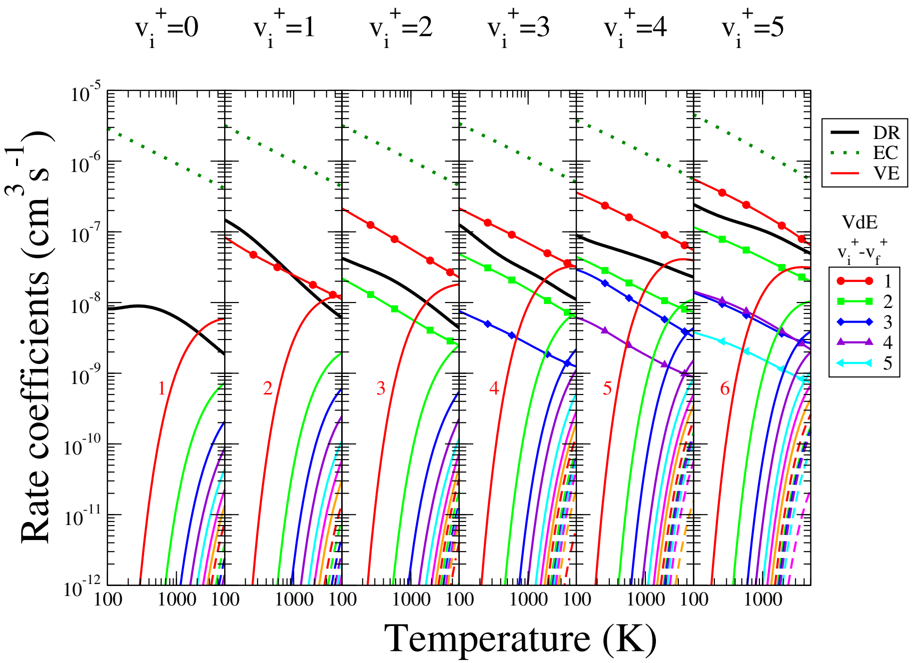
M. D. Epée Epée,[1] J. Zs Mezei,[2,3,4] O. Motapon,[1,5★] N. Pop[6] and I. F. Schneider[2,3★]

➢ Dissociative recombination



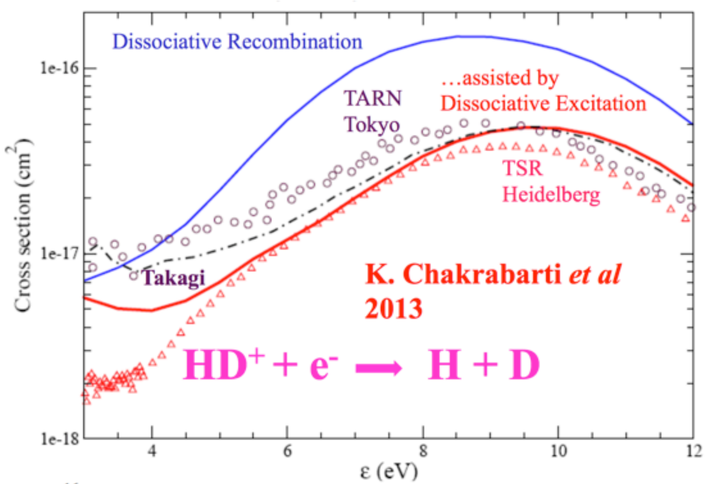
and its isotopoloques

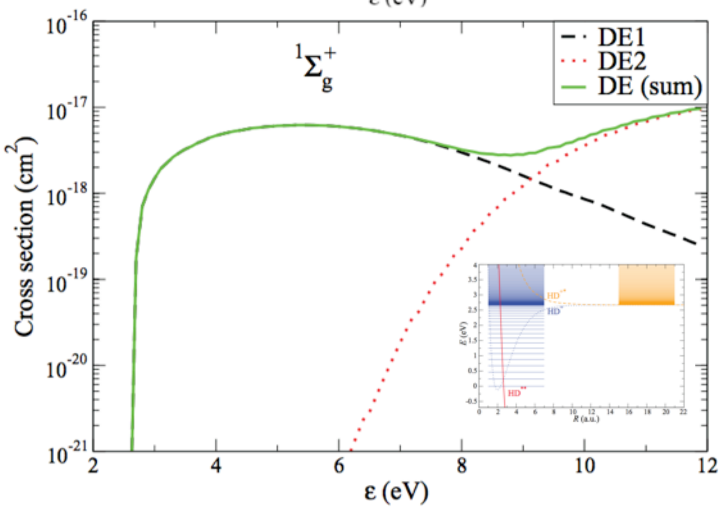
Results: The most abundant molecule
@ medium temperatures



in progress for its isotopoloques

Results: The most abundant molecule
@ high temperatures

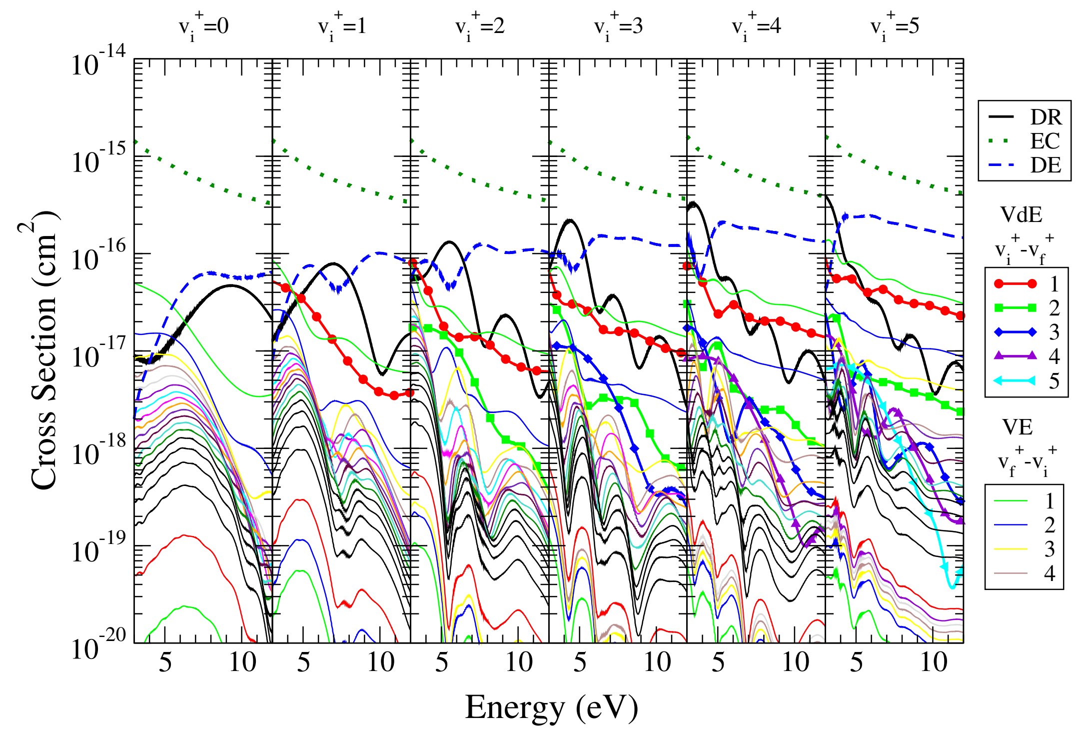




PHYSICAL REVIEW A **87**, 022702 (2013)

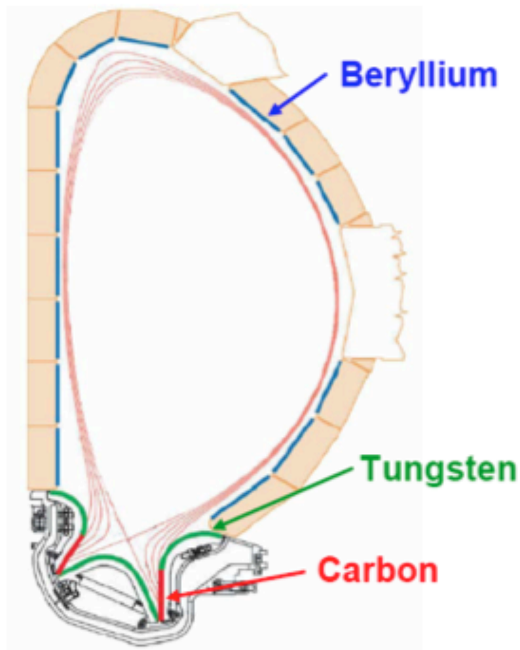
Dissociative recombination of electrons with diatomic molecular cations above dissociation threshold: Application to H_2^+ and HD^+

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]



in progress for its isotopoloques

Results: Molecules in fusion experiments



Wall materials

- ITER: Be, W and C
- ASDEX Upgrade: W
- ITER like wall of JET: Be, W
- Boronization of the walls (impurities, recycling)

Low temperatures in the plasma edge
⇒ formation of molecules

Recycling at the wall

H_2, D_2, T_2, HD, HT, DT

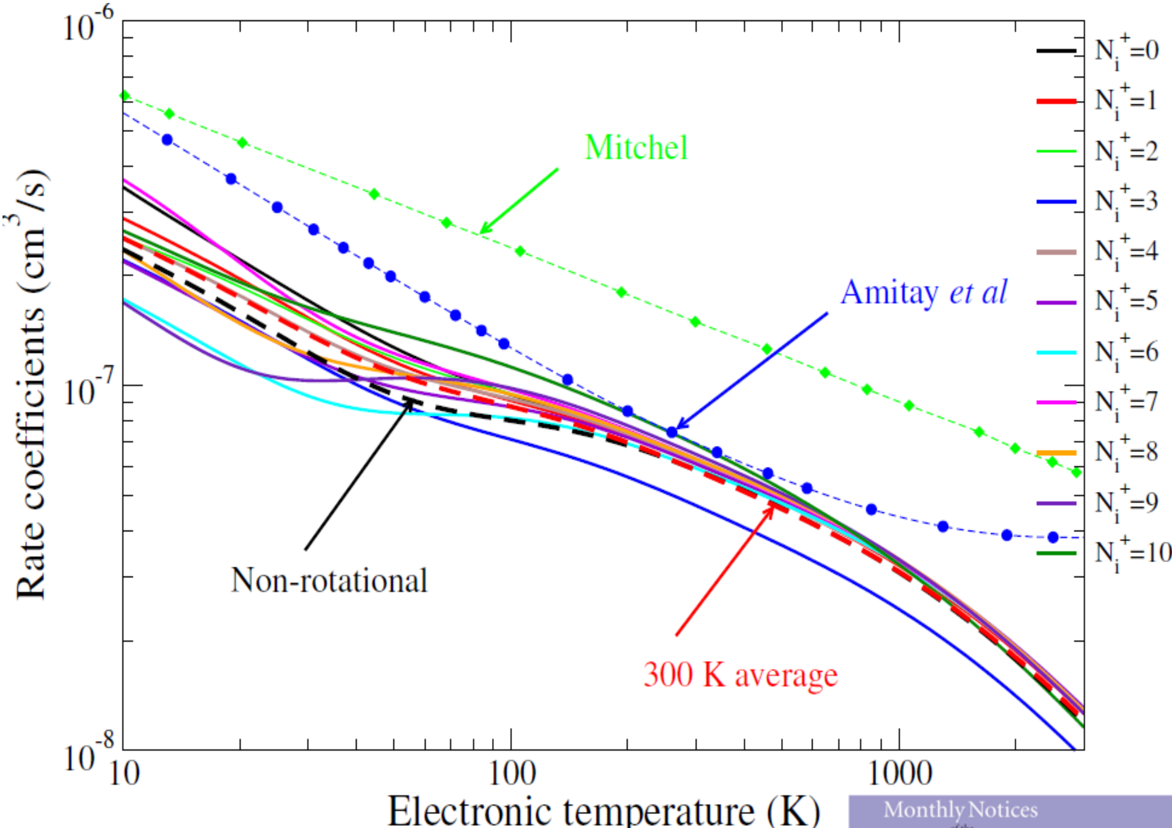
Plasma wall interaction

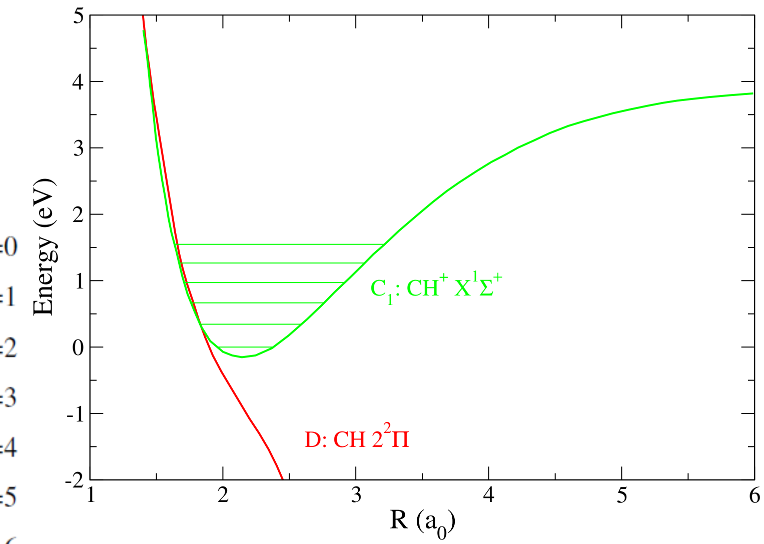
CH, CD, CT, C_2

BeH, BeD, BeT

BH, BD, BT

Results: CH^+





Dissociative recombination

@ low temperatures

Monthly Notices of the ROYAL ASTRONOMICAL SOCIETY

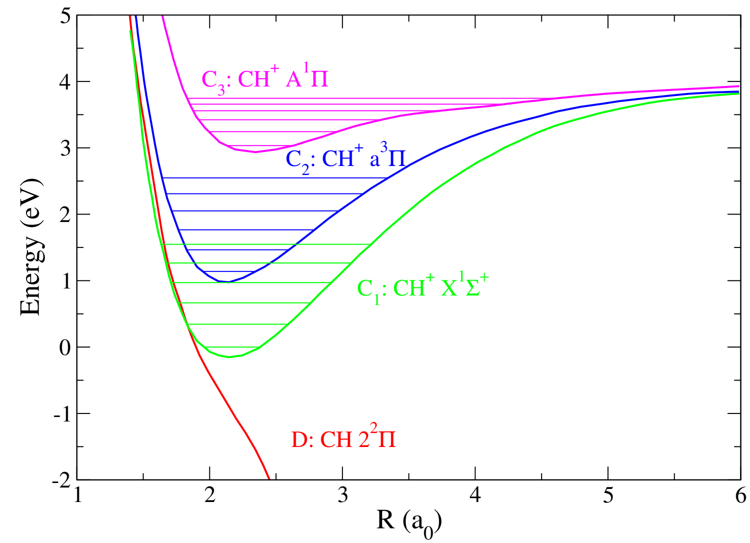
MNRAS **469,** 612–620 (2017) doi:10.1093/mnras/stx892

Advance Access publication 2017 April 11

State-to-state chemistry and rotational excitation of CH^+ in photon-dominated regions

A. Faure,[1★] P. Halvick,[2★] T. Stoecklin,[2] P. Honvault,[3] M. D. Epée Epée,[4] J. Zs. Mezei,[5,6,7,8] O. Motapon,[4,9] I. F. Schneider,[5,7★] J. Tennyson,[10] O. Roncero,[11] N. Bulut[12] and A. Zanchet[11]

Results: CH^+



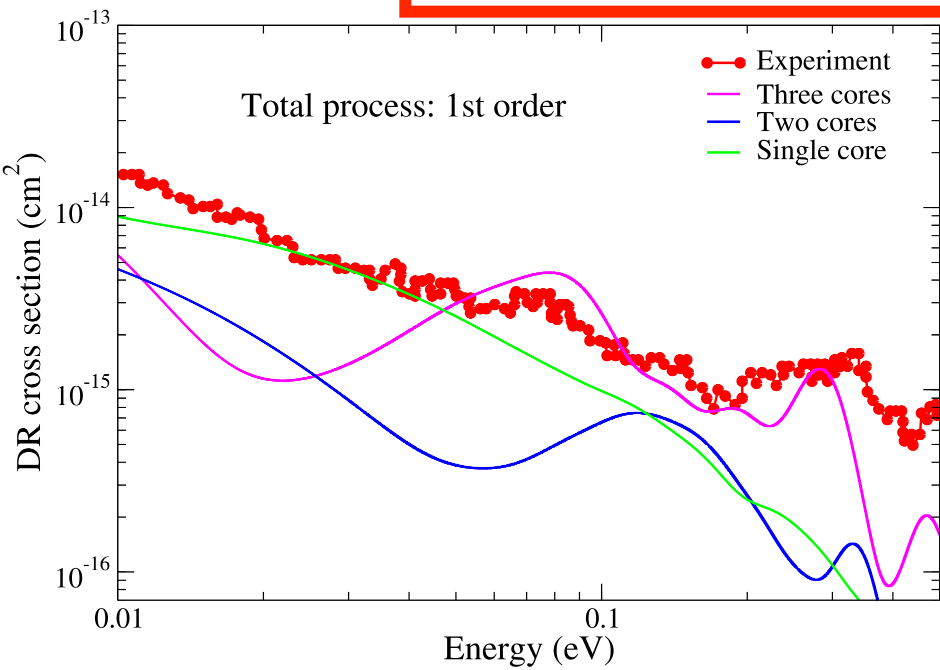
IOP Publishing Journal of Physics B: Atomic, Molecular and Optical Physics

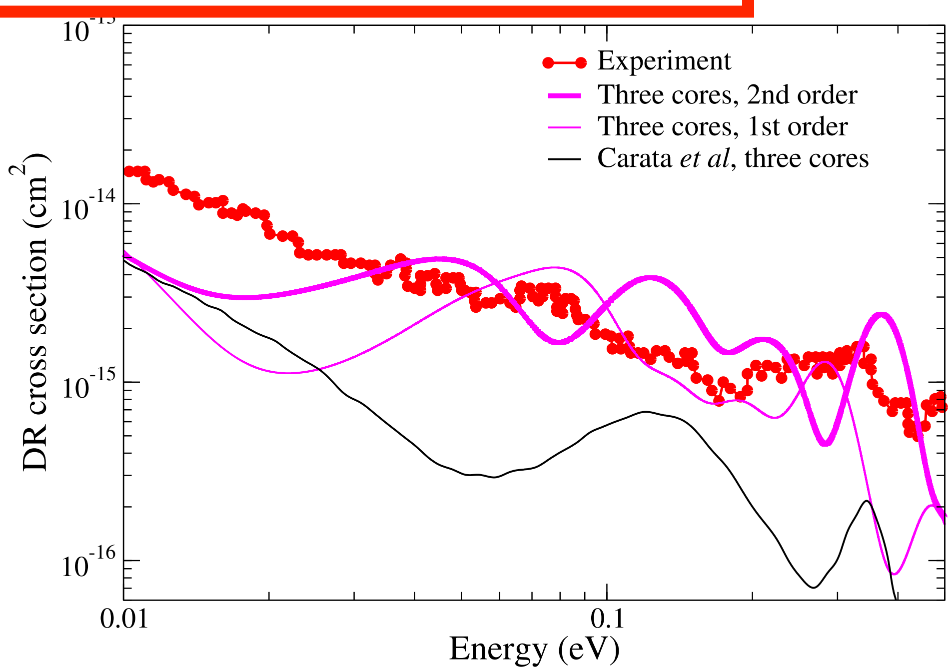
J. Phys. B: At. Mol. Opt. Phys. **00** (2018) 000000 (8pp)

Dissociative recombination of the CH^+ molecular ion at low energy

K Chakrabarti[1,2], J Zs Mezei[1,3,4], O Motapon[5], A Faure[6], O Dulieu[7], K Hassouni[3] and I F Schneid r[1,7]

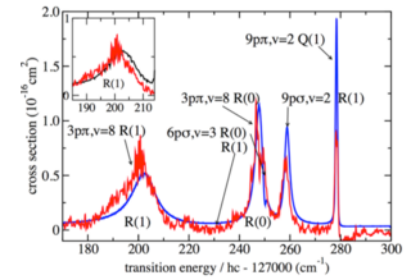
Poster of N. Pop *et al* and K. Chakrabarti *et al.*



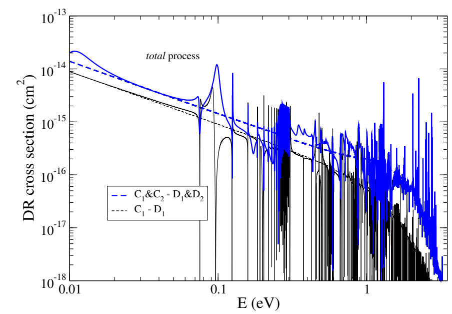


Conclusions

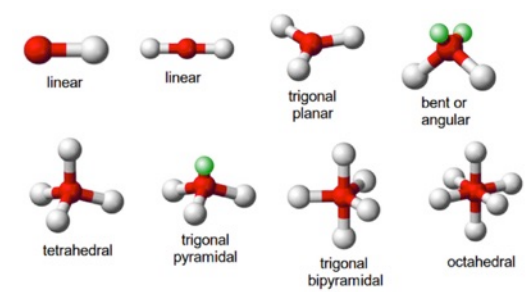
- MQDT: state-to-state calculations



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



- Data needs: di- and poly-atomics



In collaboration with

- I. F. Schneider, A. Abdoulanziz, F. Colboc, V. Laporta, Y. Moulane (Univ. du Havre)
- N. Pop (Politech. Univ. Timisoara), F. Iacob (West Univ. Timisoara), O. Motapon, M. D. Epee Epee (Univ. Douala), S. Niyonzima (Univ. of Burundi)
- J. Tennyson, D. A. Little (Univ. College London), K. Chakrabarti (Univ. of Kolkatta)
- D. Talbi (Univ. Montpellier), D. O. Kashinski (West Point), A. P. Hickman (Lehigh Univ.)
- Ch. Jungen, J. Robert, O. Dulieu (Univ. Paris Sud)
- Å. Larson (Stockholm Univ.), A. E. Orel (Univ. of California Davis), V. Kokoouline (Univ. of Central Florida)

PROGRAMME BLANC
Acronyme SUMOSTAI
EDITION 2009

SUperexcited MOlecular STates of Astrophysical Importance : dissociative recombination and spectroscopy

Thank you for the attention!

EnCoMix

ENUMPP

Projet :
LABEX EMC3-2014-PICOLIBS

EMoPlaF