REACTIVE MOLECULAR CATION-ELECTRON COLLISIONS OF INTEREST FOR COLD PLASMAS

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Short presentation

THE AIM OF THIS PROJECT IS TO INVESTIGATE THE REACTIVE COLLISIONS BETWEEN SLOW ELECTRONS AND MOLECULAR CATIONS WHICH ARE RELEVANT PROCESSES IN SOME LOW-TEMPERATURE PLASMAS OF TECHNOLOGICAL INTEREST. IN THE FRAMEWORK OF MULTI-CHANNEL QUANTUM DEFECT THEORY (MQDT) WE HAVE PERFORMED THEORETICAL AND NUMERICAL CALCULATIONS FOR THE CROSS-SECTIONS AND RATE COEFFICIENTS FOR THE COMPETING PROCESSES (DISSOCIATIVE RECOMBINATION, VIBRATIONAL EXCITATION, VIBRATIONAL DE-EXCITATION OR DISSOCIATIVE EXCITATION) WHICH TAKE PLACE IN ELECTRON-MOLECULAR ION COLLISIONS. THE EVALUATION CONTAINS: I) THE DEPENDENCE OF THE CROSS SECTION AND RATE COEFFICIENTS ON THE ENERGY OF THE INCIDENT ELECTRON FOR DIFFERENT ROVIBRATIONAL CONFIGURATIONS, II) THE CONTRIBUTION OF THE DIFFERENT SYMMETRIES III) THE COMPARISON WITH THE EXPERIMENTAL RESULTS AND OTHER THEORETICAL RESULTS. THE ULTIMATE GOAL OF OUR CALCULATIONS IS TO PROVIDE INPUT DATA FOR THE KINETICS MODELLING OF THOSE NON-EQUILIBRIUM PLASMAS RELEVANT IN SOME PRESENT INDUSTRIAL APPLICATIONS.

Research team

Experienced researchers:

- prof. Fifirig Magda
- lect. dr. Stroe Marius Cristian
- lect. dr. Duca Mariana

Early-stage researchers:

- Varlan Aurica
- Tudorache Diana (september 2007-september 2008)
- Mihailescu Alexandru (september 2009-september 2010)

The importance of the subject

Dissociative recombination and excitation are the most important destruction mechanisms of molecular ions in the low temperature plasmas whose modelling is based on the knowledge of the cross sections and rate coefficients of the dissociative recombination and the related processes. The great number of the industrial and technological applications assisted by low temperature plasmas determines a constant interest in the study of the reactive molecular ion-electron collisions.

Project objectives

Elaboration of a MQDT theoretical model for dissociative excitation in the non-rotational case

Elaboration of a MQDT theoretical model for dissociative excitation in the rotational case

Elaboration of a computer program coded in Fortran 77 for dissociative excitation (DE) and related processes (dissociative recombination DR, vibrational excitation or inelastic collision IC, vibrational de-excitation or superelastic collision SEC and elastic scattering) in the non-rotational case

Elaboration of a computer program coded in Fortran 77 for dissociative excitation and related processes in the rotational case

Elaboration of a computer program coded in Fortran 77 based on a time dependent wave packet (TDWP) approach

Systematic computations for hydrogen molecular ion H_2^+ and its isotopomers

Project activities

documentation

elaboration of the theoretical model

elaboration of the numerical codes

testing and optimisation

computing

comparison with the experimental results and other theoretical results

publication

Early-stage researchers

Varlan Aurica

activities and results:

- documentation
- computations of potential curves for HCO^+, CH_2^+ and CH_3^+ using MOLPRO during a research stage at University of Provence Aix-Marseille I (2.03-16.04.2009)
- computations of potential curves for CH^+ using MOLPRO during a research stage at University of Provence Aix-Marseille I (1-31.07.2010)
- learn how to use DE numerical codes
- computations of DR, DE, SEC and IC cross sections for H_2^+
- 2 oral presentations: "Potential curves for dissociative recombination of HCO^+, CH_2^+ and CH_3^+" Faculty of Chemistry, University of Bucharest (May 2009), "Competition between reaction channels in electron collisions of vibrationally excited H_2^+" Faculty of Chemistry, University of Bucharest (May 2010)
- 2 papers "Competition between reaction channels in electron collisions of vibrationally excited H_2^+", A. Varlan, M. Duca and M. Fifirig, *Mol. Phys.*, **108**, 2093-2104 (2010), and in preparation "Potential energy curves of HCO^+, HCO, CH_2^+, CH_2, CH_3^+ and CH_3, relevant for dissociative recombination", A Varlan, D Hagebaum-Reignier and M. Fifirig

Tudorache Diana (september 2007-september 2008) activities:

- documentation
- learn how to use DR numerical codes based on MQDT approach

Since September 2008, she is a PhD student in France.

Mihailescu Alexandru (september 2009-september 2010) activities and results:

- documentation
- learn how to use DE numerical code for rotational case
- computations of DR and DE cross sections for H_2^+ and D_2^+
- a paper in preparation "Rotational effects in electron impact dissociation of hydrogen molecular ions" autori: M Stroe, A Mihailescu si M Fifirig

Originality and contributions

original theoretical approach to study dissociative excitation of diatomic molecular ions

original numerical codes for the computation of DE cross section for diatomic molecular ions

new numerical results for DE and related processes of H_2^+ and its isotopomers

Scientific results - papers

[1] "Dissociative Excitation in Electron Collisions with HD^+", M. Fifirig and M. Stroe, Phys. Scr. 78 (2008) 065302.

[2] "Electron-Induced Dissociation in H_2^+, HD^+ and HT^+", M. Stroe and M. Fifirig, Phys. Lett. A 373 (2009) 4152.

[3] "Electron Induced Processes in H_2^+, D_2^+ and T_2^+", M. Stroe and M. Fifirig, J. Phys. B: At. Mol. Opt. Phys. 42 (2009) 205203.

[4] "Dissociative Excitation of HD^+, D_2^+, and DT^+ by Electron Impact", M. Duca and M. Fifirig, Cent. Eur. J. Phys. 8 (2010) 87.

[5] "Competition between reaction channels in electron collisions of vibrationally excited H_2^+", A. Varlan, M. Duca and M. Fifirig, *Mol. Phys.*, **108**, 2093-2104 (2010).

[6] "Dissociation and vibrational excitation of cold HD^+ by electron impact", M Stroe and M. Fifirig, *Eur. Phys. J. D* accepted 2010.

Papers in preparation:

[1] "Dissociation of H_2^+ ions by collisions with electrons", M Fifirig and M. Stroe

[2] "Potential energy curves of HCO^+, HCO, CH_2^+, CH_2, CH_3^+ and CH_3, relevant for dissociative recombination", A Varlan, D Hagebaum-Reignier and M. Fifirig

[3] "Dissociation of vibrationally excited D_2^+ by slow electrons", M Stroe and M. Fifirig

[4] "Effects of molecular rotation in HD^+ dissociative excitation", M Stroe and M. Fifirig

[5] "Rotational effects in electron impact dissociation of hydrogen molecular ions", M Stroe, A Mihailescu and M. Fifirig

Analytical results

In the framework of the Multi-Channel Quantum Defect Theory (MQDT) adapted to dissociative recombination process (A. Giusti-Suzor, J. Phys. B: At. Mol. Phys. 13 (1980) 3867, S.L. Guberman and A. Giusti-Suzor, J. Chem. Phys. 95 (1991) 2602) we have developed an approach yielding the cross sections for all the competitive processes taking place in the reactive collisions between hydrogen molecular cations and electrons of energy above the dissociation threshold of the electronic ground state. It consists of the inclusion of the vibration continua of the two lowest electronic states $1s\sigma_g$ and $2p\sigma_u$ as explicit ionization channels.

Our theoretical procedure starts with the evaluation of the reaction matrix K which is evaluated in two steps. First, it is constructed from blocks of the type K_{dd} (a $N_d \times N_d$ submatrix of K, N_d being the dissociation channels), K_{dv} (a $N_d \times N_v$ submatrix of K, N_v being the ionization channels associated with $1s\sigma_g$ ionic core), K_{dw} (a $N_d \times N_w$ submatrix of K, N_w being the ionization channels associated with $2p\sigma_u$ ionic core), K_{vv} (a $N_v \times N_v$ submatrix of K), K_{vw} (a $N_v \times N_w$ submatrix of K), and K_{ww} (a $N_w \times N_w$ submatrix of K) corresponding to an arrangement of the ionization channels after their affiliation to the electronic cores. So, K matrix has the structure

$$K^{(2)} = \begin{pmatrix} K_{dd} & K_{dv} & K_{dw} \\ K_{vd} & K_{vv} & K_{vw} \\ K_{wd} & K_{wv} & K_{ww} \end{pmatrix} \tag{1}$$

In Eq. (1) v indexes the ionization channels built on the $1s\sigma_g$ ionic core, while w those associated with $2p\sigma_u$ ionic core.

Taking into account the spectral representation of the Green operator the expression of the elements $K_{d_id_j}$ corresponding to the interactions between the dissociation channels d_i and d_j ($1 \leq d_i, d_j \leq N_d$), is

$$\begin{aligned} K_{d_id_j} = V_{d_id_j} + \sum_d \mathcal{P} \int d\mathcal{E} \frac{V_{d_id}V_{dd_j}}{E-(E_d+\mathcal{E})} \\ + \sum_v \mathcal{P} \int d\varepsilon \frac{V_{d_iv}V_{vd_j}}{E-(E_v+\varepsilon)} + \sum_w \mathcal{P} \int d\varepsilon' \frac{V_{d_iw}V_{wd_j}}{E-(E_w+\varepsilon')} \ , \end{aligned} \tag{2}$$

where $\mathcal{P}$ is the principal part integral. In the above equation only the matrix elements V_{vd} of the interaction operator are nonnull. Assuming the energy-independent electronic interactions we have

$$K_{d_id_j} = \sum_v V_{d_iv}V_{vd_j} I(E_v) \ , \tag{3}$$

where

$$I(E_v) = \mathcal{P} \int_{\varepsilon_a}^{\varepsilon_b} \frac{d\varepsilon}{E-(E_v+\varepsilon)} = \ln \left| \frac{E-(E_v+\varepsilon_a)}{E-(E_v+\varepsilon_b)} \right| \ . \tag{4}$$

Similarly, the K matrix element corresponding to the interactions between the ionization channels w_i and w_j associated with the $2p\sigma_u$ core, is

$$K_{w_iw_j} = \sum_v V_{w_iv}V_{vw_j} I(E_v) \ , \quad 1 \leq w_i, w_j \leq N_w \ . \tag{5}$$

The block K_{wd} is constructed by elements defined by

$$K_{wd} = K_{dw} = \sum_v V_{dv} V_{vw} I(E_v) \ , \quad 1 \leq w \leq N_w \ , \quad 1 \leq d \leq N_d \ . \tag{6}$$

The K matrix element corresponding to the interactions between the ionization channels v_i and v_j ($1 \leq v_i, v_j \leq N_v$), built on the $1s\sigma_g$ core, is

$$K_{v_i v_j} = \sum_d \mathcal{P} \int d\mathcal{E} \frac{V_{v_i d}(\mathcal{E}) V_{d v_j}(\mathcal{E})}{E - (E_d + \mathcal{E})} + \sum_w V_{v_i w} V_{w v_j} I(E_w) \ . \tag{7}$$

First term in (7) can be expressed in the alternative form

$$\sum_d \frac{1}{W} \int \int \chi_{v_i}(R) V_{v_i d}(R) F_{d,k}(R_<) G_{d,k}(R_>) V_{d v_j}(R') \chi_{v_j}(R') \, dR \, dR' \ , \tag{8}$$

where W is the Wronskian of F_d and G_d, with G_d the irregular solution of the nuclear Schrödinger equation in the dissociative potential, lagging in phase by $\pi/2$ with respect to F_d. $R_<$ and $R_>$ denote the lesser and the greater, respectively, of R and R'.

The interaction between the dissociation channels and the ionization channels built on $1s\sigma_g$ ionic core is described by

$$K_{vd} = K_{dv} = V_{dv} \ , \quad 1 \leq v \leq N_v \ , \quad 1 \leq d \leq N_d \ . \tag{9}$$

Finally, the elements of the block corresponding to the interactions between two ionization channels associated with the two molecular cores, $1s\sigma_g$ and $2p\sigma_u$, are

$$K_{wv} = K_{vw} = V_{vw} \ , \quad 1 \leq v \leq N_v \ , \quad 1 \leq w \leq N_w \ . \tag{10}$$

Since the ionization channel thresholds are the successive vibrational levels or discretized levels, which are ranked with respect to their energy, the last step in the construction of K matrix consists of the permutation of its lines and columns. The lines and columns of the new K matrix correspond to the natural arrangement of the ionization channels according to their energy.

In order to connect the interaction zone with the asymptotic one, we perform a frame transformation characterized by two matrices, $\mathcal{C}$ and $\mathcal{S}$. The elements of the matrix $\mathcal{C}$ are given by

$$\begin{aligned}
\mathcal{C}_{v^+\alpha} &= \sum_{l,v} U_{lv} \langle \chi_{v^+} \mid \cos(\pi \mu_{1s\sigma_g,l} + \eta_\alpha) \mid \chi_v \rangle \ , \qquad 1 \leq v \leq N_v \ , && (11) \\
\mathcal{C}_{w^+\alpha} &= \sum_{l,w} U_{lw} \langle \chi_{w^+} \mid \cos(\pi \mu_{2p\sigma_u,l} + \eta_\alpha) \mid \chi_w \rangle \ , \qquad 1 \leq w \leq N_w \ , && (12) \\
\mathcal{C}_{d\alpha} &= U_{d\alpha} \cos \eta_\alpha \ , \qquad 1 \leq d \leq N_d \ , && (13)
\end{aligned}$$

where α runs from 1 to N (the total numbers of channels) and $\mu_{1s\sigma_g,l}(R)$ and $\mu_{2p\sigma_u,l}$ are the quantum defects for Rydberg states built on $1s\sigma_g$ ionic core (along with the continuum lying above) and those at the ${}^2\Sigma_u$ threshold, respectively.

We have denoted by $\tan \eta_\alpha$ and by U_α, the real eigenvalue and the corresponding eigenvector of reaction matrix K

$$\sum_j \pi K_{ij} U_{j\alpha} = - \tan \eta_\alpha U_{i\alpha} \ , \qquad \alpha = \overline{1, N} \ . \tag{14}$$

The blocks $\mathcal{S}_{v^+\alpha}$, $\mathcal{S}_{w^+\alpha}$ and $\mathcal{S}_{d\alpha}$ of $\mathcal{S}$ matrix are obtained by replacing cosine function by sine function in $\mathcal{C}_{v^+\alpha}$, $\mathcal{C}_{w^+\alpha}$ and $\mathcal{C}_{d\alpha}$.

The two matrices $\mathcal{C}$ and $\mathcal{S}$ lead to the generalized "scattering" matrix defined by

$$X = \frac{\mathcal{C} + i\mathcal{S}}{\mathcal{C} - i\mathcal{S}} \ . \tag{15}$$

The elimination of the ionization channels below the energy threshold for the electron escape (the closed ionization channels) results in the physical scattering matrix

$$S_{oo} = X_{oo} - X_{oc}(X_{cc} - e^{-2i\pi\nu})^{-1}X_{co} \ . \tag{16}$$

where o and c denote the open and closed channel, respectively. The matrix ν is a $c \times c$ diagonal matrix having (in atomic units) the elements $\nu_v = 1/\sqrt{2(E_v - E)}$ with $E_v > E$.

The partial cross section for vibrational excitation in the state characterized by the vibrational quantum number v^+, has the expression (in atomic units)

$$\sigma^{sym}_{v^+\leftarrow lv_i^+}(\epsilon) = \frac{\pi}{4\epsilon}\,\rho\ \mid S^{sym}_{v^+\leftarrow lv_i^+} \mid^2 \qquad E_{v^+} > E_{v_i^+} \ , \tag{17}$$

where ρ is the multiplicity ratio between the electronic state of the molecule and the electronic state of the ion. The summation over the parameters l and sym leads to the total cross section for vibrational excitation.

The cross section for dissociative excitation ($\sigma^{DE}_{v_i^+}$) is the sum of two terms, one of them corresponds to the vibrational excitation in the ground state vibrational continuum and the other one to the vibrational excitation in the excited state vibrational continuum. Each of them is obtained by adding all the contributions of the type (17) associated with all discretized levels of the two vibrational continua.

In the case of a mixture of different populations of the available vibrational states of the ground electronic state, the total DE cross section σ_{DE} is a sum over all the population-weighted cross sections from each vibrational state existing in the mixture

$$\sigma_{DE} = \sum_{v_i^+} p_{v_i^+}\sigma^{DE}_{v_i^+} \ , \tag{18}$$

where $p_{v_i^+}$ is the relative population ($\sum_{v_i^+} p_{v_i^+} = 1$) of the vibrational level v_i^+. The relative contribution $q_{v_i^+}$ of the vibrational state v_i^+ to the DE cross section has the expression

$$q_{v_i^+} = \frac{p_{v_i^+}\sigma^{DE}_{v_i^+}}{\sum_{v_i^+} p_{v_i^+}\sigma^{DE}_{v_i^+}} \ . \tag{19}$$

Numerical results

Using the above theoretical approach, our computations were performed with the $(1s\sigma_g)(ns\sigma_g)$ and $(1s\sigma_g)(nd\sigma_g)$ Rydberg states with the $1s\sigma_g$ ion core (along with the continuum lying above) and with the doubly-excited dissociative states ${}^1\Sigma_g^+$, ${}^{1,3}\Pi_g$, ${}^{1,3}\Pi_u$, ${}^{1,3}\Sigma_u$ converging

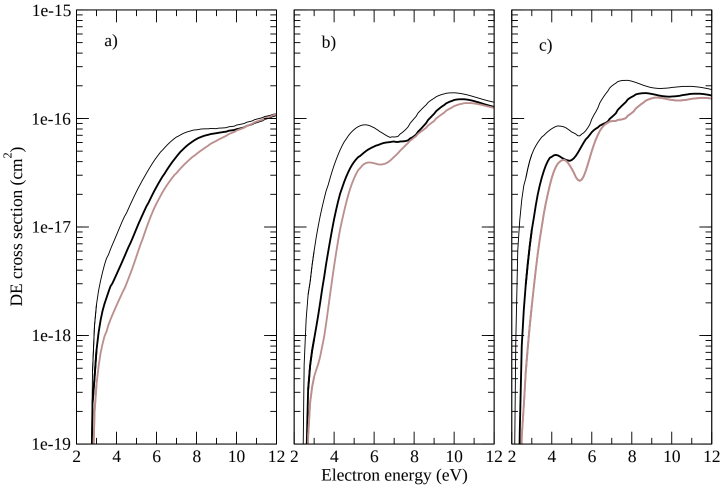

Figure 1: (a) Dissociative excitation cross sections of H_2^+ black thin solid line, D_2^+ black thick solid line, and T_2^+ grey thick solid line for $v_i^+ = 0$. (b) Same as (a) but for $v_i^+ = 1$. (c) Same as (a) but for $v_i^+ = 2$

to the $2p\sigma_u$ excited state of hydrogen molecular cations. The angular momentum quatum number l of the external electron implicated in the autoionization into the antibonding state ${}^2\Sigma_u^+$ has two values: 1 and 3 for ${}^1\Sigma_g^+$ and ${}^{1,3}\Pi_g$ states, 0 and 2 for ${}^{1,3}\Sigma_u$ states, and 2 and 4 for ${}^{1,3}\Pi_u$ states. The input quantities of the present MQDT computations are the same data as for the previous work regarding the DE of HD^+ (Stroe M, Florescu A, Fifirig M, Waffeu-Tamo F O, Ngassam V, Motapon O and Schneider I F, Rom. Rep. Phys. 57 (2005) 748). The molecular data for the excited states built on the $2p\sigma_u$ ionic core, firstly introduced in this study, are extracted from the numerical results reported by Tennyson (Tennyson J, Atomic Data and Nuclear Data Tables, 64 (1996) 253).

We report numerical results for DE and related processes for H_2^+ and its isotopomers in Figs. 2-7. Contributions of various dissociative states to the DR, DE, IC and SEC are presented in Fig. 8, while the contributions of the indirect DE mechanism to the DE cross section are shown in Fig. 9. Comparison with the experimental results is presented in Figs. 10-12. In the case of a mixture of vibrational states obeying a Franck-Condon distribution, the contributions of various vibrational states to the DE cross section are analysed in Fig. 12.

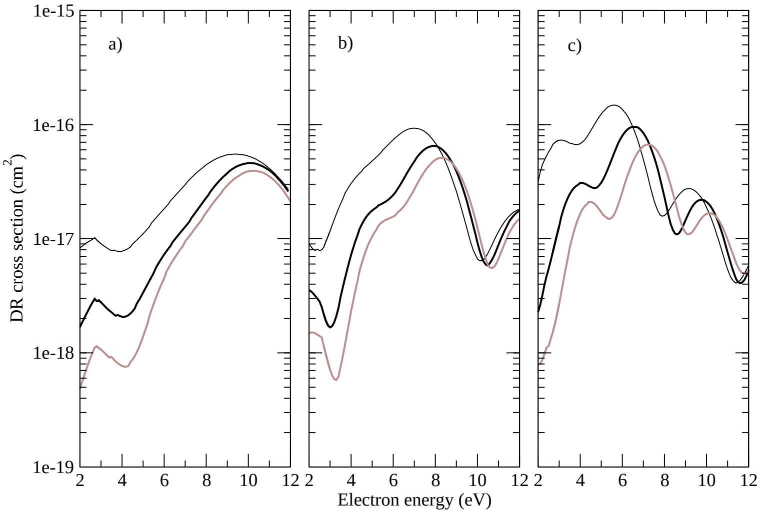

Figure 2: (a) Dissociative recombination cross sections of H_2^+ black thin solid line, D_2^+ black thick solid line, and T_2^+ grey thick solid line for $v_i^+ = 0$. (b) Same as (a) but for $v_i^+ = 1$. (c) Same as (a) but for $v_i^+ = 2$

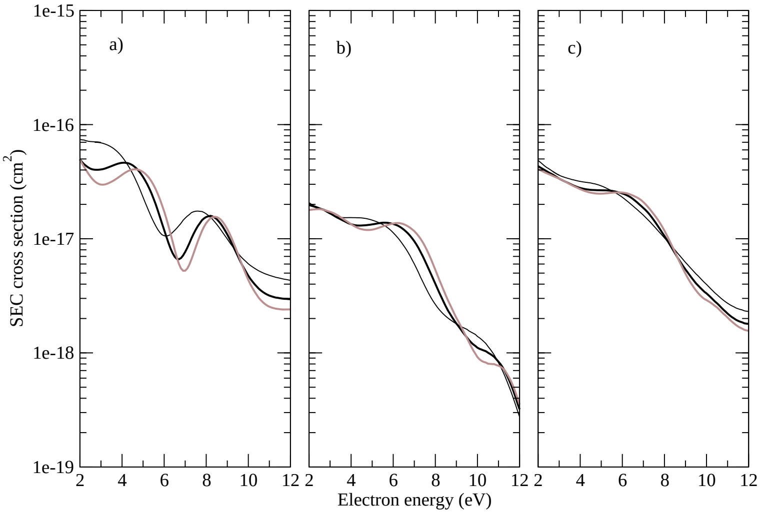

Figure 3: (a) Vibrational de-excitation cross sections of H_2^+ black thin solid line, D_2^+ black thick solid line, and T_2^+ grey thick solid line for the vibrational transition 2 → 1. (b) Same as (a) but for the vibrational transition 2 → 0. (c) Same as (a) but for the vibrational transition 1 → 0

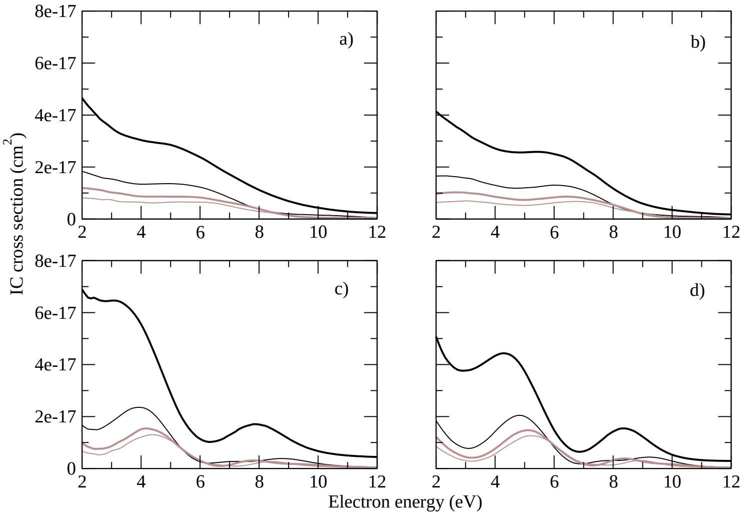

Figure 4: (a) Vibrational excitation cross sections of H_2^+ initially in the vibrational level $v_i^+ = 0$. Black thick solid line: vibrational transition 0 → 1, black thin solid line: vibrational transition 0 → 2, grey thick solid line: vibrational transition 0 → 3, grey thin solid line: vibrational transition 0 → 4. (b) Same as (a) but for D_2^+. (c) Same as (a) but for H_2^+ initially in the vibrational level $v_i^+ = 1$. Black thick solid line: vibrational transition 1 → 2, black thin solid line: vibrational transition 1 → 3, grey thick solid line: vibrational transition 1 → 4, grey thin solid line: vibrational transition 1 → 5. (d) Same as (c) but for D_2^+.

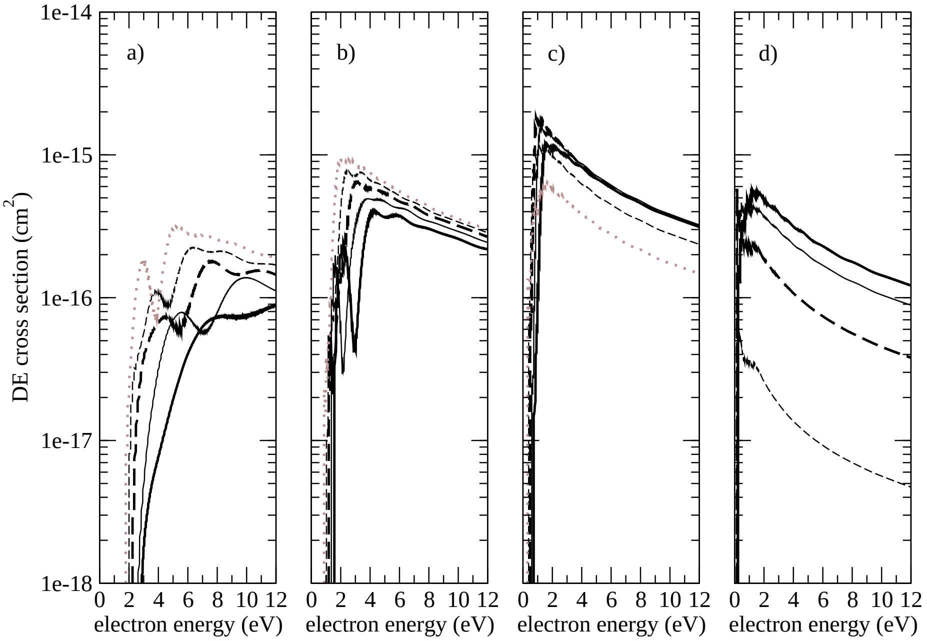

Figure 5: DE cross section ($\sigma^{DE}_{v_i^+}$) of the H_2^+ molecular ion initially in the electronic ground state and the vibrational state v_i^+. Thick solid lines show our results for $v_i^+ = 0$ in panel (a), $v_i^+ = 5$ in panel (b), $v_i^+ = 10$ in panel (c), and $v_i^+ = 15$ in panel (d). Thin solid lines display our results for $v_i^+ = 1$ in panel (a), $v_i^+ = 6$ in panel (b), $v_i^+ = 11$ in panel (c), and $v_i^+ = 16$ in panel (d). Thick dashed lines represent our results for $v_i^+ = 2$ in panel (a), $v_i^+ = 7$ in panel (b), $v_i^+ = 12$ in panel (c), and $v_i^+ = 17$ in panel (d). Thin dashed lines show our results for $v_i^+ = 3$ in panel (a), $v_i^+ = 8$ in panel (b), $v_i^+ = 13$ in panel (c), and $v_i^+ = 18$ in panel (d). Thick brown/grey dotted lines represent our results for $v_i^+ = 4$ in panel (a), $v_i^+ = 9$ in panel (b), $v_i^+ = 14$ in panel (c).

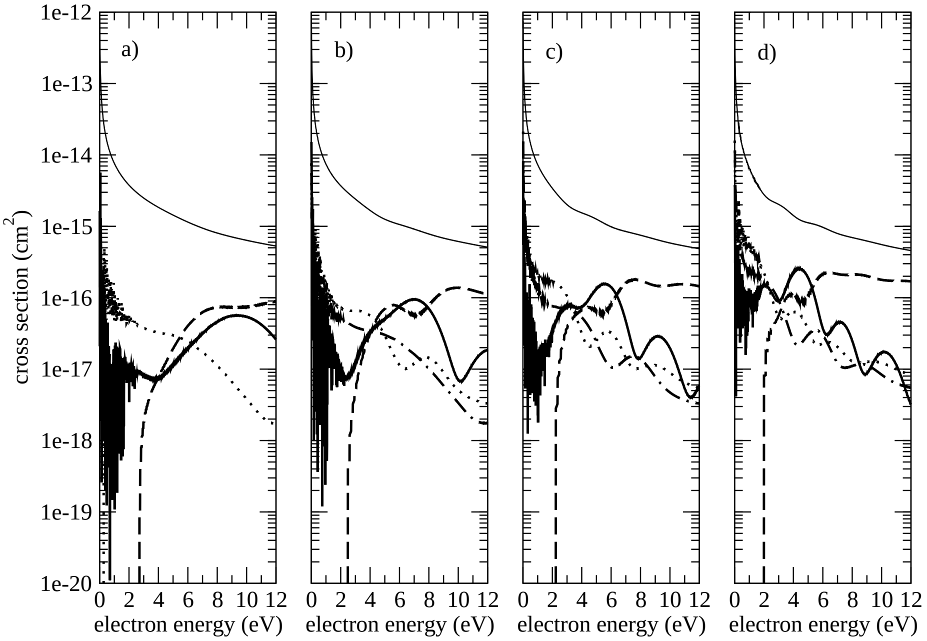

Figure 6: a): Cross sections of H_2^+ molecular ion initially in the electronic ground state and the vibrational state $v_i^+ = 0$ for dissociative recombination (DR) thick solid lines, for dissociative excitation (DE) thick dashed lines, for elastic scattering (ES) thin solid lines, for vibrational excitation (inelastic collision, IC, $v_i^+ \rightarrow v_i^+ + 1$): dotted lines and for vibrational de-excitation (superelastic collision, SEC, $v_i^+ \rightarrow v_i^+ - 1$) chain lines. (b): $v_i^+ = 1$, (c): $v_i^+ = 2$, and (d) $v_i^+ = 3$.

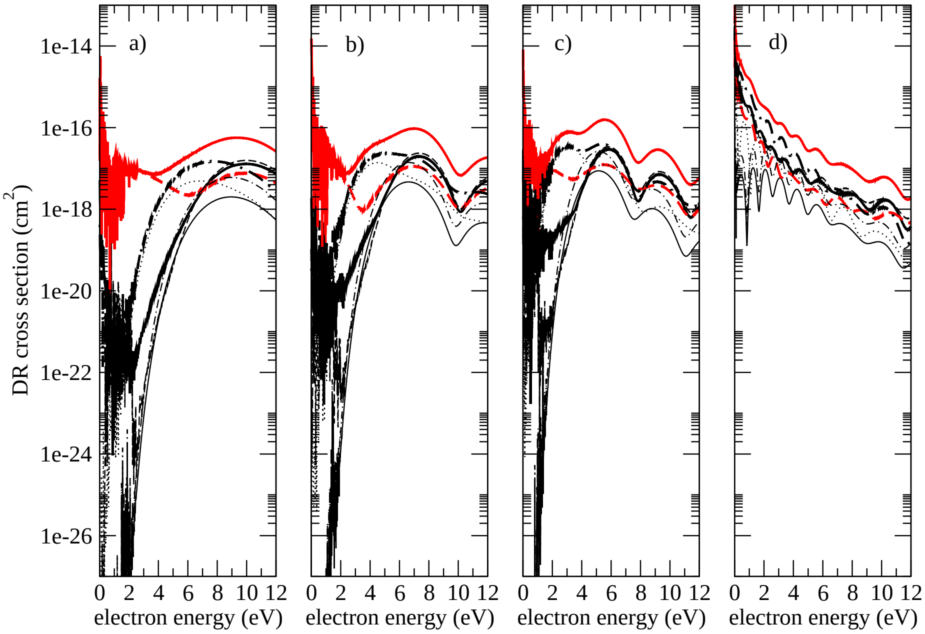

Figure 7: Contributions of various dissociative states to the DR cross section ($\sigma^{DR}_{v_i^+}$) of the H_2^+ molecular ion initially in the electronic ground state and the vibrational state: (a) $v_i^+ = 0$, (b) $v_i^+ = 1$, (c) $v_i^+ = 2$, and (d) $v_i^+ = 10$. Thick solid lines: $^1\Pi_g$ state, thin solid lines: $^1\Pi_u$ state, thick red/grey dashed lines: $^1\Sigma_g$ state, thin dashed lines: $^1\Sigma_u$ state, thick chain lines: $^3\Pi_g$ state, thin chain lines: $^3\Pi_u$ state, dotted lines: $^3\Sigma_u$ and thick red/grey solid lines: DR cross section $\sigma^{DR}_{v_i^+}$.

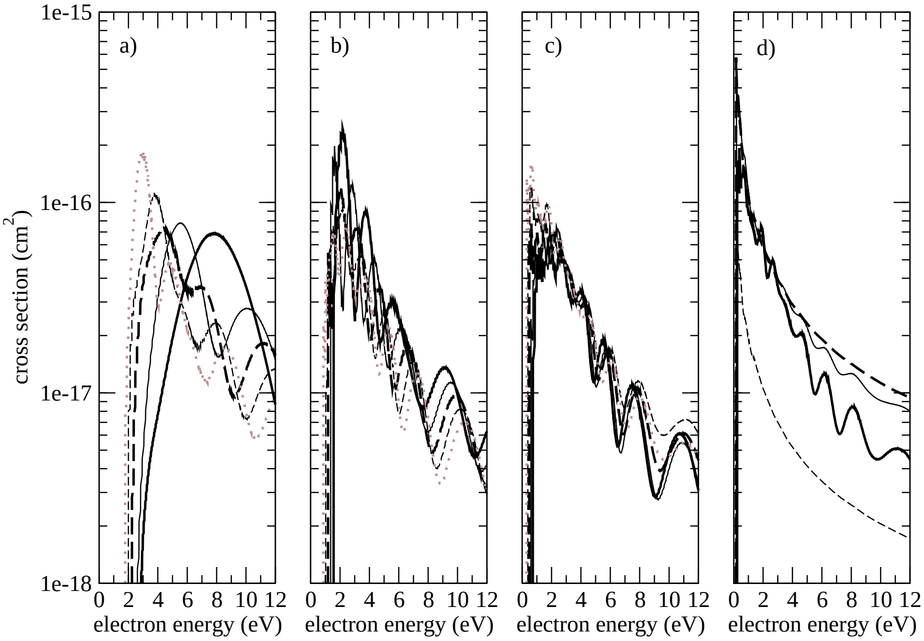

Figure 8: Indirect DE cross section ($\sigma^{DE1}_{v_i^+}$) of the H_2^+ molecular ion initially in the electronic ground state and the vibrational state v_i^+. Thick solid lines show our results for $v_i^+ = 0$ in panel (a), $v_i^+ = 5$ in panel (b), $v_i^+ = 10$ in panel (c), and $v_i^+ = 15$ in panel (d). Thin solid lines display our results for $v_i^+ = 1$ in panel (a), $v_i^+ = 6$ in panel (b), $v_i^+ = 11$ in panel (c), and $v_i^+ = 16$ in panel (d). Thick dashed lines represent our results for $v_i^+ = 2$ in panel (a), $v_i^+ = 7$ in panel (b), $v_i^+ = 12$ in panel (c), and $v_i^+ = 17$ in panel (d). Thin dashed lines show our results for $v_i^+ = 3$ in panel (a), $v_i^+ = 8$ in panel (b), $v_i^+ = 13$ in panel (c), and $v_i^+ = 18$ in panel (d). Thick brown/grey dotted lines represent our results for $v_i^+ = 4$ in panel (a), $v_i^+ = 9$ in panel (b), $v_i^+ = 14$ in panel (c).

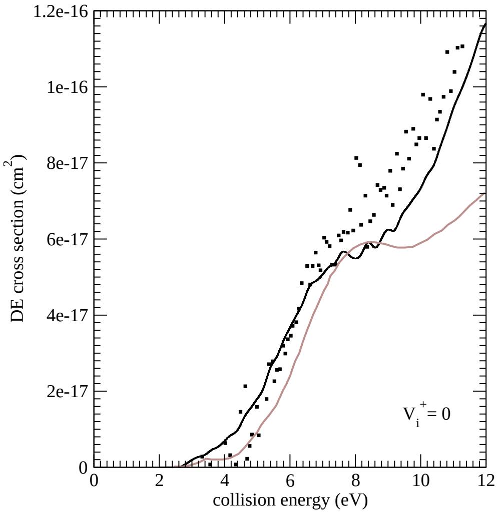

Figure 9: DE cross sections of HD^+ for $v_i^+ = 0$. Solid line: our results (M. Fifirig and M. Stroe, Phys. Scr. 78 (2008) 065302), squares: experimental results (Zajfman D and Amitay Z 1996 *Dissociative Recombination: Theory, Experiment and Applications III* (World Scientific) 114), grey full line: Takagi's theoretical results (Takagi H, Phys. Scripta, T96 (2002) 52).

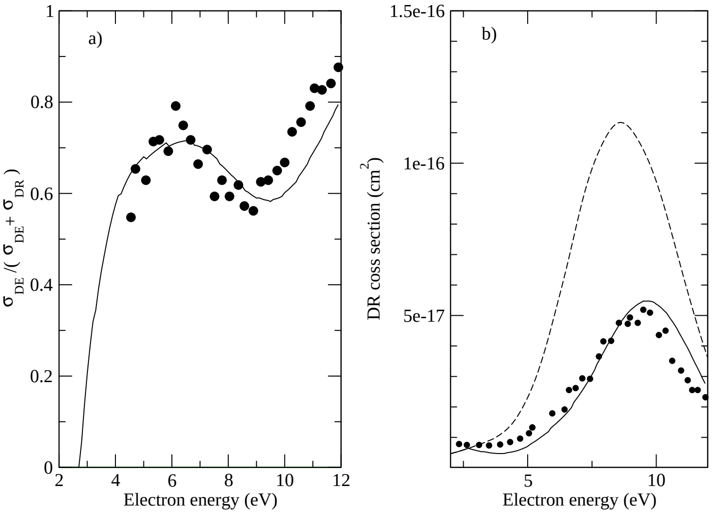

Figure 10: (a) The ratio (DE cross section)/(DE cross section+DR cross section) for HD^+ initially in the vibrational level $v_i^+ = 0$. Black solid line: our numerical results [M. Stroe and M. Fifirig, Phys. Lett. A 373 (2009) 4152], and black full circles: experimental results from ASTRID [L.H. Andersen, P.J. Johnson, D. Kella, H.B. Pedersen and L. Vejby-Christensen, Phys. Rev. A 55 (1997) 2799]. (b) HD^+ DR cross section as a function of the colliding electron energy. Black solid line: present results, black broken line: computation without the inclusion of the vibrational continua as explicit ionization channels, and black full circles: experimental results from ASTRID.

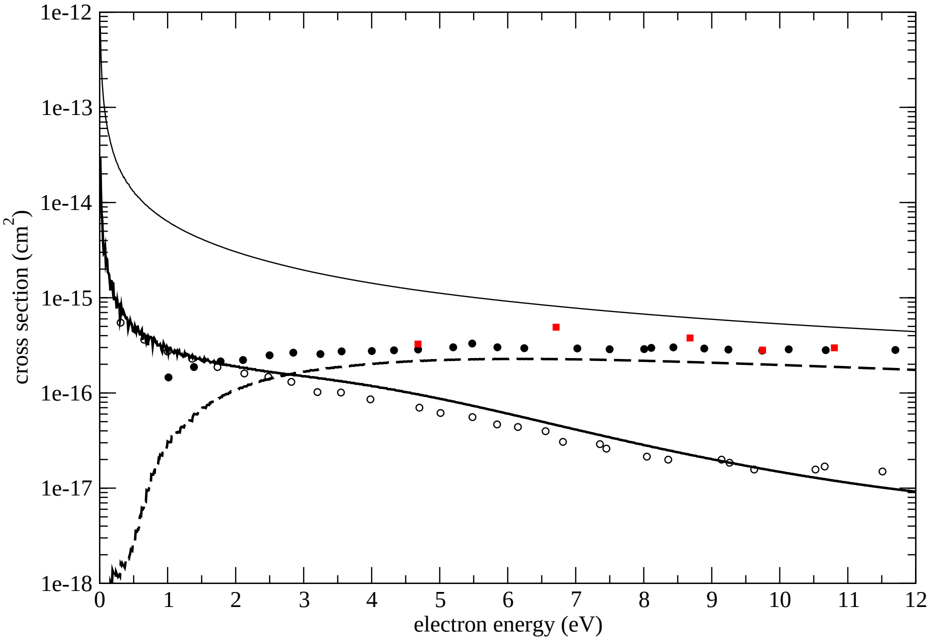

Figure 11: Cross sections of vibrationally excited H_2^+ assuming a Franck-Condon distribution of the vibrational levels of its ground electronic state, for DR: thick solid lines, for DE: thick dashed lines and for elastic scattering thin solid lines. Lines represent our results, open circles the experimental DR results reported by Andersen et al [L.H. Andersen, P.J. Johnson, D. Kella, H.B. Pedersen and L. Vejby-Christensen, Phys. Rev. A 55 (1997) 2799] and full circles and red/grey full squares the experimental DE results reported by Andersen et al and by Abdellahi El Ghazaly et al [M.O. Abdellahi El Ghazaly, J. Jureta, X. Urbain and P. Defrance, J. Phys. B: At. Mol. Opt. Phys. 37 (2004) 2467], respectively.

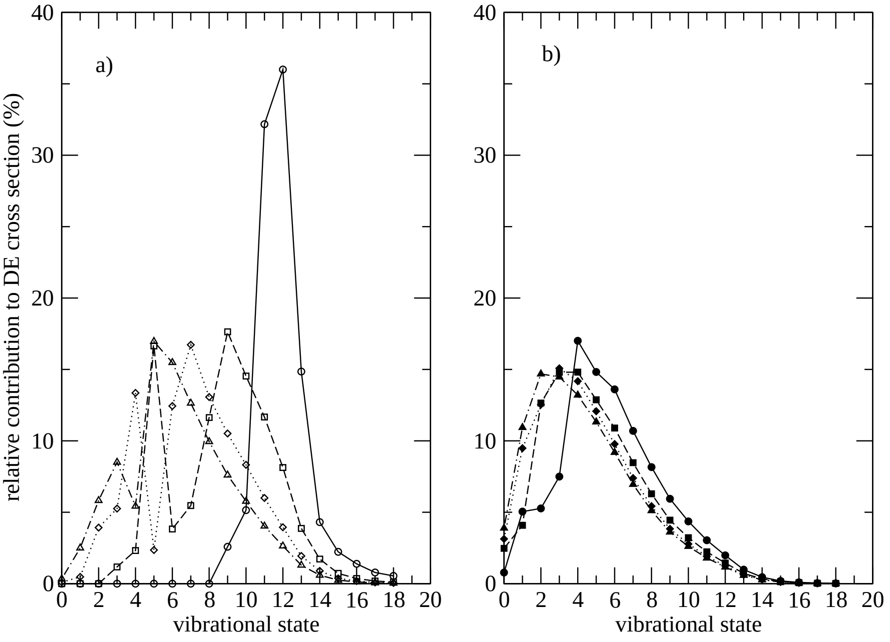

Figure 12: Relative contribution of each vibrational state v_i^+ to the total DE cross section. a) Circles: $E = 1$ eV, squares: $E = 2$ eV, diamonds: $E = 3$ eV, and triangles: $E = 4$ eV. b) Full circles: $E = 5$ eV, full squares: $E = 7$ eV, full diamonds: $E = 9$ eV, and full triangles: $E = 11$ eV.