

PROCESE DE CIOCNIRE ION MOLECULAR-ELECTRON IN PLASME RECI

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institutia: Universitatea din Bucuresti, Facultatea de Chimie

director proiect: prof MAGDA FIFIRIG

Rezumat

IN ACEST PROIECT SUNT ANALIZATE PROCESELE DE CIOCNIRE DINTRE ELECTRONI DE ENERGIE JOASA SI IONI MOLECULARI, PROCESE IMPORTANTE IN UNELE PLASME RECI DE INTERES TEHNOLOGIC. IN CADRUL TEORIEI DEFECTULUI CUANTIC MULTICANAL SUNT EFECTUATE CALCULE TEORETICE SI NUMERICE PENTRU SECTIUNILE EFICACE SI RATELE PROCESELOR CE AU LOC LA CIOCNIREA ELECTRON-ION MOLECULAR: RECOMBINAREA DISOCIATIVA, EXCITAREA VIBRATIONALA, DEZEXCITAREA VIBRATIONALA SI EXCITAREA DISOCIATIVA. EVALUAREA CONTINE: I) DEPENDENTA SECTIUNII EFICACE SI A RATELOR DE ENERGIA ELECTRONULUI INCIDENT PENTRU DIFERITE CONFIGURATII ROVIBRATIONALE, II) CONTRIBUTIA DIFERITELOR SIMETRII MOLECULARE, III) COMPARATIA CU REZULTATELE EXPERIMENTALE PRECUM SI CU ALTE REZULTATE TEORETICE. SCOPUL CALCULELOR IL REPREZINTA FURNIZAREA DE DATE DE INTRARE PENTRU CALCULELE FOLOSITE LA MODELAREA CINETICII SI DINAMICII PLASMELOR RECI DE INTERES IN UNELE APLICATII INDUSTRIALE.

Echipa de cercetare

Cercetatori cu experienta:

prof. Fifirig Magda

lect. dr. Stroe Marius Cristian

lect. dr. Duca Mariana

Tineri cercetatori:

Varlan Aurica

Tudorache Diana (septembrie 2007-septembrie 2008)

Mihailescu Alexandru (septembrie 2009-septembrie 2010)

Importanta domeniului

Studiul dinamicii proceselor care au loc in plasmale reci se bazeaza pe cunoasterea sectiunilor eficace si a ratelor de recombinare si excitare disociativa (procesele responsabile pentru distrugerea ionilor moleculari din aceste plasmale) precum si a celorlalte procese competitive ce au loc in timpul ciocnirii electron-ion molecular. Numarul mare de aplicatii industriale in care sunt folosite plasmale reci mentine un interes constant pentru studiul teoretic si experimental al proceselor de ciocnire electron-ion molecular.

Obiectivele proiectului

- elaborarea modelului teoretic de calcul al sectiunilor eficace pentru excitarea disociativa (DE) (cazul nerotational)
- scrierea programelor de calcul al sectiunilor eficace pentru excitarea disociativa (cazul nerotational)
- elaborarea modelului teoretic de calcul al sectiunilor eficace pentru excitarea disociativa (cazul rotational)
- scrierea programelor de calcul al sectiunilor eficace pentru excitarea disociativa (cazul rotational)
- calcule numerice de obtinere a sectiunilor eficace de excitare disociativa pentru H_2^+ , DT^+ si HD^+
- elaborarea modelului teoretic pentru recombinarea disociativa (DR) cu metoda TDWP
- scrierea programelor de calcul al sectiunilor eficace pentru recombinarea disociativa cu metoda TDWP
- diseminarea rezultatelor

Activitatile proiectului

documentare

dezvoltarea modelelor teoretice

realizarea codurilor numerice

testarea si optimizarea codurilor scrise

efectuarea de calcule numerice

compararea rezultatelor proprii cu alte rezultate teoretice si cu rezultate experimentale din literatura

diseminarea rezultatelor

Implicarea tinerilor cercetatori in proiect

Varlan Aurica

a efectuat activitate de documentare

a efectuat calcule de chimie cuantica de determinare a curbelor de energie potentiala pentru HCO^+ , CH_2^+ si CH_3^+ cu ajutorul programului MOLPRO (in timpul stagiului de cercetare la Universitatea Provence Aix-Marseille I in perioada 2.03-16.04.2009)

a efectuat calcule de chimie cuantica de determinare a curbelor de energie potentiala pentru ionul molecular CH^+ in timpul stagiului de cercetare la Universitatea Provence Aix-Marseille I in perioada 1-31.07.2010

a invatat sa utilizeze codurile numerice elaborate in cadrul grantului

a evaluat sectiunile eficace pentru DR, DE, SEC si IC pentru H_2^+

a prezentat 2 comunicari orale: "Curbe de energie potentiala pentru recombinarea dissociativa a HCO^+ , CH_2^+ si CH_3^+ " la Sesiunea de comunicari stiintifice studentesti a Facultatii de Chimie a Universitatii din Bucuresti, mai 2009, si "Competition between reaction channels in electron collisions of vibrationally excited H_2^+ " la Sesiunea de comunicari stiintifice studentesti a Facultatii de Chimie a Universitatii din Bucuresti, mai 2010

a participat la redactarea a 2 articole "Competition between reaction channels in electron collisions of vibrationally excited H_2^+ ", A. Varlan, M. Duca and M. Fifrig, *Mol. Phys.*, **108**, 2093-2104 (2010), si in curs de redactare "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. Fifrig

Tudorache Diana (septembrie 2007-septembrie 2008)

a efectuat activitate de documentare

a studiat metoda MQDT de evaluare a sectiunilor eficace pentru DR

S-a inscris la doctorat in Franta in septembrie 2008 si a parasit echipa de cercetare.

Mihailescu Alexandru (septembrie 2009-septembrie 2010)

a efectuat activitate de documentare

a invatat sa utilizeze codul numeric pentru calculul rotational

a evaluat sectiunile eficace pentru H_2^+ si D_2^+

participa la redactarea unui articol "Rotational effects in electron impact dissociation of hydrogen molecular ions" autori: M Stroe, A Mihailescu si M Fifrig

Aspecte originale si contributii

- expresia analitica pentru matricea K asociata procesului de ciocnire a ionilor moleculari biatomici cu electroni a caror energie este mai mare decat energia de disociere a ionului molecular.
Rezultate publicate in "Dissociative Excitation in Electron Collisions with HD^+ ", M. Fifrig and M. Stroe, Phys. Scr. 78 (2008) 065302.
- coduri numerice originale de calcul a sectiunilor eficace de excitare disociativa (si ale celorlalte procese competitive) atat pentru cazul nerotational cat si pentru cel rotational.
- rezultate numerice noi (obtinute cu codurile numerice proprii) pentru sectiunile eficace si ratele de excitare disociativa (si ale celorlalte procese competitive) pentru H_2^+ si izotopomerii sai. Rezultate raportate in cele 6 articole publicate sau acceptate in perioada 2008-2010.
- comparatia intre rezultatele teoretice si cele experimentale pentru o distributie Franck-Condon a starilor vibrationale ale ionului H_2^+ .
Rezultate raportate in "Competition between reaction channels in electron collisions of vibrationally excited H_2^+ ", A Varlan, M. Duca and M. Fifrig, *Mol. Phys.*, **108**, 2093-2104 (2010).

Articole realizate in timpul grantului

Articole publicate:

- [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* acceptata 2010.

Articole in curs de redactare

- [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

Rezultate analitice

In cadrul metodei defectului cuantic multicanal (Multi-Channel Quantum Defect Theory, MQDT) adaptata pentru studiul recombinarii disociative (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) am dezvoltat un model teoretic pe baza caruia se pot calcula sectiunile eficace pentru procesele ce au loc la ciocnirea electron-ion molecular atunci cand energia electronilor este superioara energiei de disociere corespunzatoare starii electronice fundamentale. Acest model presupune includerea explicita a continuumurilor vibrationale asociate starilor electronice $1s\sigma_g$ si $2p\sigma_u$ ca si canale de ionizare.

Calculule MQDT incep cu evaluarea matricii de reactie K (o matrice de tip $N \times N$, N fiind numarul total de canale). Aceasta matrice este determinata in 2 etape. In

prima etapa se construiesc blocuri de tipul K_{dd} (o submatrice de tipul $N_d \times N_d$ cu N_d numarul de canale dissociative), K_{dv} (o submatrice de tipul $N_d \times N_v$, N_v fiind numarul de canale de ionizare asociate starii electronice fundamentale, egal cu suma dintre numarul de nivele vibrationale si numarul de stari discretizate asociate continuumului vibrational al starii electronice fundamentale), K_{dw} (o submatrice de tipul $N_d \times N_w$ cu N_w numarul de stari discretizate asociate continuumului vibrational al primei stari excitate a ionului molecular), K_{vv} (o submatrice de tipul $N_v \times N_v$), K_{vw} (o submatrice de tipul $N_v \times N_w$), si K_{ww} (o submatrice de tipul $N_w \times N_w$). Aceasta etapa corespunde unei ordonari a canalelor de ionizare dupa afilierea la corurile ionice. Astfel, matricea K are structura

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

In ecuatia (1), indicele v indexeaza canalele de ionizare asociate corului ionic $1s\sigma_g$, in timp ce w pe cele asociate corului ionic $2p\sigma_u$.

Folosind reprezentarea spectrala a operatorului Green, expresia elementelor de matrice $K_{d_i d_j}$ corespunzatoare interactiei dintre canalele de disociere d_i si d_j ($1 \leq d_i, d_j \leq N_d$) este

$$K_{d_i d_j} = V_{d_i d_j} + \sum_d \mathcal{P} \int d\mathcal{E} \frac{V_{d_i d} V_{d d_j}}{E - (E_d + \mathcal{E})} + \sum_v \mathcal{P} \int d\varepsilon \frac{V_{d_i v} V_{v d_j}}{E - (E_v + \varepsilon)} + \sum_w \mathcal{P} \int d\varepsilon' \frac{V_{d_i w} V_{w d_j}}{E - (E_w + \varepsilon')}, \quad (2)$$

unde \mathcal{P} este partea principala. Presupunand interactii independente de energie avem

$$K_{d_i d_j} = \sum_v V_{d_i v} V_{v d_j} I(E_v), \quad (3)$$

unde

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

Similar, elementele matricii K corespunzatoare interactiilor dintre canalele de ionizare w_i si w_j asociate corului $2p\sigma_u$, sunt de tipul

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

Blocul K_{wd} este construit din elementele de matrice definite de

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

Elementele matricii K corespunzatoare interactiei dintre canalele de ionizare v_i si v_j ($1 \leq v_i, v_j \leq N_v$), asociate corului ionic $1s\sigma_g$ sunt date de

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

Primul termen din ecuatia (7) poate fi exprimat in forma alternativa

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

unde $R_{<} = \min(R, R')$ si $R_{>} = \max(R, R')$, iar W este Wronskian-ul lui F_d si G_d (solutiile ecuatiei Schrödinger pentru potentialul disociativ).

Interactia intre canalele disociative si cele de ionizare este descrisa de

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

In final, elementele matricii K corespunzatoare interactiei dintre canalele de ionizare asociate celor 2 coruri $1s\sigma_g$ si $2p\sigma_u$, sunt

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

Deoarece pragurile canalelor de ionizare sunt nivelele vibrationale si cele discretizate, ce sunt ordonate in raport cu energia, ultima etapa de determinare a matricii K consta in permutarea liniilor si coloanelor acesteia astfel incat liniile si coloanele noii matrici K sa corespunda ordonarii canalelor de ionizare dupa energiile totale asociate lor.

Legatura dintre zona de interactie si cea asimptotica este realizata de transformarea caracterizata de matricile \mathcal{C} si \mathcal{S} . Elementele matricii \mathcal{C} sunt date de

$$\mathcal{C}_{v+\alpha} = \sum_{l,v} U_{lv} \langle \chi_{v+} | \cos(\pi \mu_{1s\sigma_g, l} + \eta_\alpha) | \chi_v \rangle , \quad 1 \leq v \leq N_v , \quad (11)$$

$$\mathcal{C}_{w+\alpha} = \sum_{l,w} U_{lw} \langle \chi_{w+} | \cos(\pi \mu_{2p\sigma_u, l} + \eta_\alpha) | \chi_w \rangle , \quad 1 \leq w \leq N_w , \quad (12)$$

$$\mathcal{C}_{d\alpha} = U_{d\alpha} \cos \eta_\alpha , \quad 1 \leq d \leq N_d , \quad (13)$$

unde α ia valori de la 1 la N (numarul total de canale). $\mu_{1s\sigma_g, l}(R)$ sunt defectele cuantice pentru stările Rydberg asociate corului ionic $1s\sigma_g$ iar $\mu_{2p\sigma_u, l}$ sunt defectele cuantice asociate stării $2\Sigma_u$.

$\tan \eta_\alpha$ si U_α reprezinta valorile proprii si vectorii proprii corespunzatori matricii de reactie K

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

Blocurile $\mathcal{S}_{v+\alpha}$, $\mathcal{S}_{w+\alpha}$ si $\mathcal{S}_{d\alpha}$ ale matricii \mathcal{S} se obtin inlocuind functia cosinus cu functia sinus in $\mathcal{C}_{v+\alpha}$, $\mathcal{C}_{w+\alpha}$ si $\mathcal{C}_{d\alpha}$.

Cele 2 matrici \mathcal{C} si \mathcal{S} conduc la matricea de imprastiere X definita de

$$X = \frac{\mathcal{C} + i\mathcal{S}}{\mathcal{C} - i\mathcal{S}} . \quad (15)$$

Eliminarea canalelor de ionizare inchise conduce la matricea de imprastiere S

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

unde indicii o si c sunt asociati canalelor de ionizare deschise, respectiv inchise. Matricea diagonala ν ($c \times c$) are elementele nenule exprimate in uniti atomice prin $\nu_v = 1/\sqrt{2(E_v - E)}$ unde $E_v > E$.

Sectiunea eficace partiala pentru excitarea vibrationala in starea caracterizata de numarul cuantic vibrational, v^+ are expresia (in uniti atomice)

$$\sigma_{v^+ \leftarrow l v_i^+}^{sym}(\epsilon) = \frac{\pi}{4\epsilon} \rho |S_{v^+ \leftarrow l v_i^+}^{sym}|^2 \quad E_{v^+} > E_{v_i^+}, \quad (17)$$

unde ρ este raportul dintre multiplicatatile starilor electronice a moleculei neutre si a ionului molecular. Sumarea dupa indicii l si sym conduce la sectiunea eficace totala pentru excitarea vibrationala.

Sectiunea eficace pentru excitarea disociativa ($\sigma_{v_i^+}^{DE}$) este data de suma a 2 termeni, unul dintre ei corespunde excitarii vibrationale in continuumul vibrational al stari electronice fundamentale, iar celalalt corespunde excitarii vibrationale in continuumul vibrational al primei starii excitate. Fiecare dintre ei este obtinut prin sumarea tuturor contributiilor de tip (17) asociate nivelelor discretizate corespunzatoare.

In cazul unei distributii de nivele vibrationale initiale, sectiunea eficace totala σ_{DE} este o suma de tipul

$$\sigma_{DE} = \sum_{v_i^+} p_{v_i^+} \sigma_{v_i^+}^{DE}, \quad (18)$$

unde $p_{v_i^+}$ (cu $\sum_{v_i^+} p_{v_i^+} = 1$) este populatia nivelului vibrational v_i^+ . Contributia relativa $q_{v_i^+}$ a nivelului vibrational initial v_i^+ la sectiunea eficace σ_{DE} are expresia

$$q_{v_i^+} = \frac{p_{v_i^+} \sigma_{v_i^+}^{DE}}{\sum_{v_i^+} p_{v_i^+} \sigma_{v_i^+}^{DE}}. \quad (19)$$

Rezultate numerice

Rezultatele numerice s-au obtinut utilizand codurile dezvoltate in cadrul proiectului. S-au folosit starile Rydberg ($1s\sigma_g$)($ns\sigma_g$) si ($1s\sigma_g$)($nd\sigma_g$) asociate corului ionic $1s\sigma_g$ (impreuna cu continuumurile asociate lor) si starile dublu-excite $^1\Sigma_g^+$, $^1,3\Pi_g$, $^1,3\Pi_u$, $^1,3\Sigma_u$ ce converg la starea excitata $2p\sigma_u$ a ionului molecular de hidrogen. Numarul cuantic orbital l pentru electronul extern implicat in autoionizarea in starea antibonding $^2\Sigma_u^+$ ia 2 valori: 1 si 3 pentru starile $^1\Sigma_g^+$ si $^1,3\Pi_g$, 0 si 2 pentru starile $^1,3\Sigma_u$, si 2 si 4 pentru starile $^1,3\Pi_u$. Datele moleculare de intrare sunt aceleasi cu cele utilizate intr-un calcul anterior (Stroe M, Florescu A, Fifrig M, Waffeu-Tamo F O, Ngassam V, Motapon O and Schneider I F, Rom. Rep. Phys. 57 (2005) 748). Datele moleculare pentru starile excitate construite pe corul ionic $2p\sigma_u$ au fost extrase din Tennyson (Tennyson J, Atomic Data and Nuclear Data Tables, 64 (1996) 253).

Rezultate numerice se refera la sectiunile eficace pentru excitarea disociativa (DE), recombinarea disociativa (DR), excitarea vibrationala sau ciocnire inelastica (IC), dezexcitare vibrationala sau ciocnire superelastica (SEC) si imprastiere elastica (ES) pentru H_2^+ si izotopomerii sai in Figs. 2-7. Contributiile diferitelor stari disociative la sectiunile eficace ale acestor procese sunt prezentate in Fig. 8, iar cele ale mecanismului indirect de excitare disociativa in Fig. 9. Compararea cu rezultatele din literatura este prezentata in Figs. 10-12. In cazul unei distributii Franck-Condon a starilor vibrationale initiale, contributiile diferitelor stari vibrationale sunt ilustrate in Fig. 12.

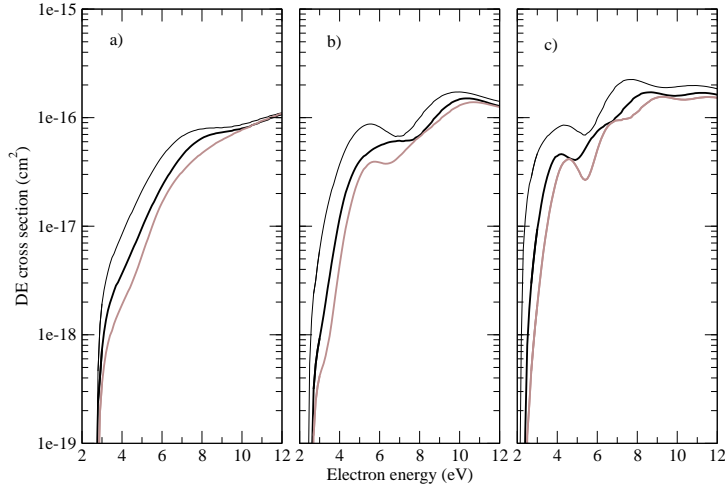


Figure 1: (a) Dissociative excitation cross sections of H_2^+ black thin solid line, D_2^+ black thick solid line, and T_2^+ grey thick solid line for $v_i^+ = 0$. (b) Same as (a) but for $v_i^+ = 1$. (c) Same as (a) but for $v_i^+ = 2$

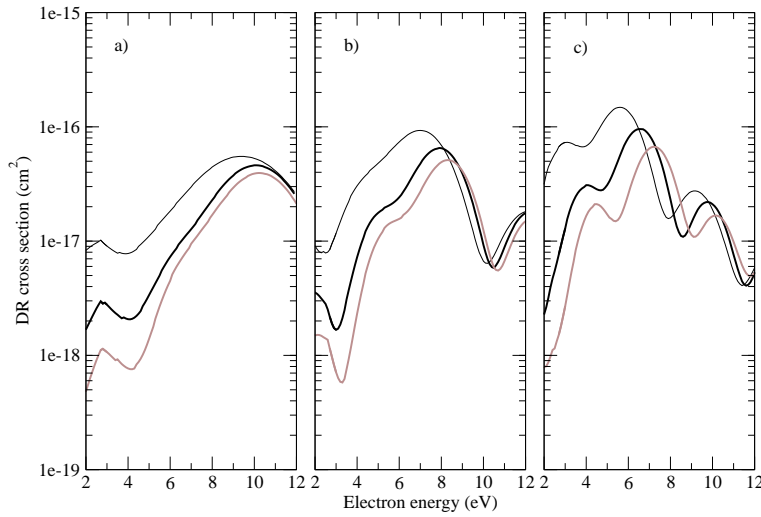


Figure 2: (a) Dissociative recombination cross sections of H_2^+ black thin solid line, D_2^+ black thick solid line, and T_2^+ grey thick solid line for $v_i^+ = 0$. (b) Same as (a) but for $v_i^+ = 1$. (c) Same as (a) but for $v_i^+ = 2$

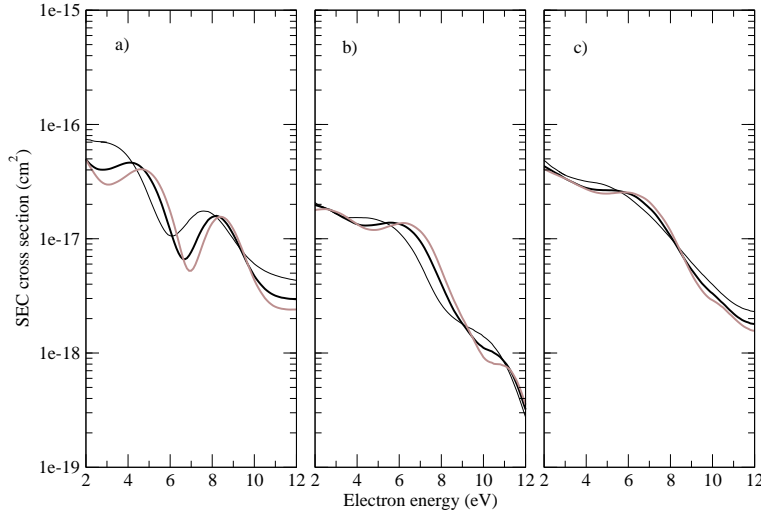


Figure 3: (a) Vibrational de-excitation cross sections of H_2^+ black thin solid line, D_2^+ black thick solid line, and T_2^+ grey thick solid line for the vibrational transition $2 \rightarrow 1$. (b) Same as (a) but for the vibrational transition $2 \rightarrow 0$. (c) Same as (a) but for the vibrational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

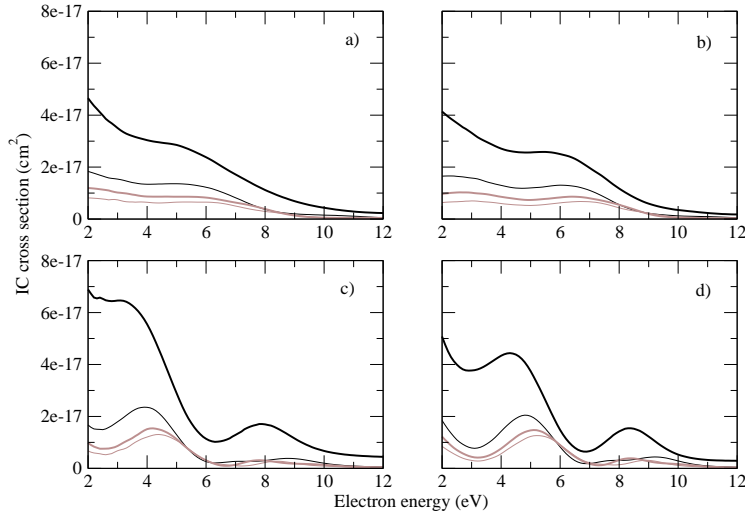


Figure 4: (a) Vibrational excitation cross sections of H_2^+ initially in the vibrational level $v_i^+ = 0$. Black thick solid line: vibrational transition $0 \rightarrow 1$, black thin solid line: vibrational transition $0 \rightarrow 2$, grey thick solid line: vibrational transition $0 \rightarrow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

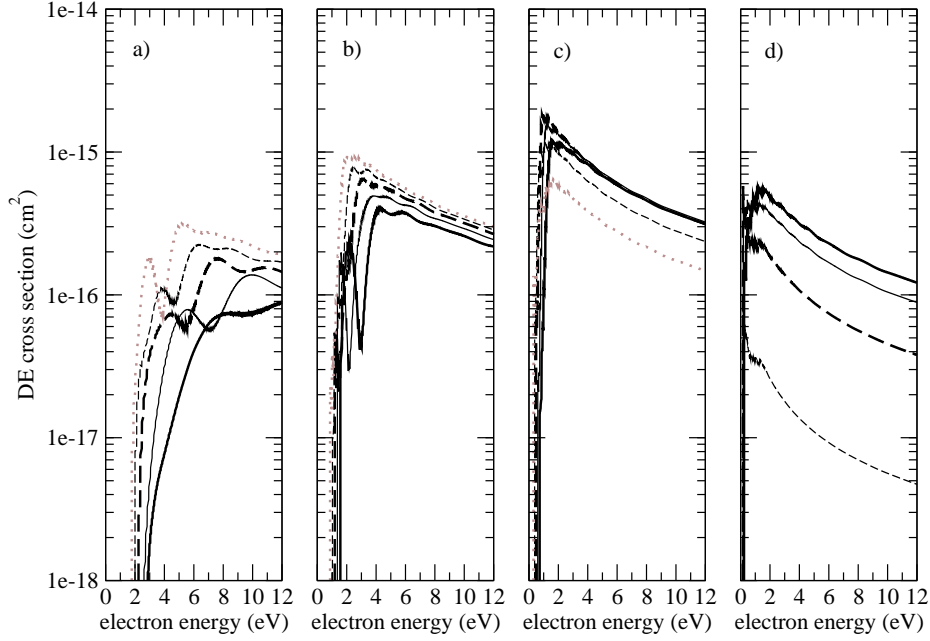


Figure 5: DE cross section ($\sigma_{v_i^+}^{DE}$) of the H_2^+ molecular ion initially in the electronic ground state and the vibrational state v_i^+ . Thick solid lines show our results for $v_i^+ = 0$ in panel (a), $v_i^+ = 5$ in panel (b), $v_i^+ = 10$ in panel (c), and $v_i^+ = 15$ in panel (d). 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).

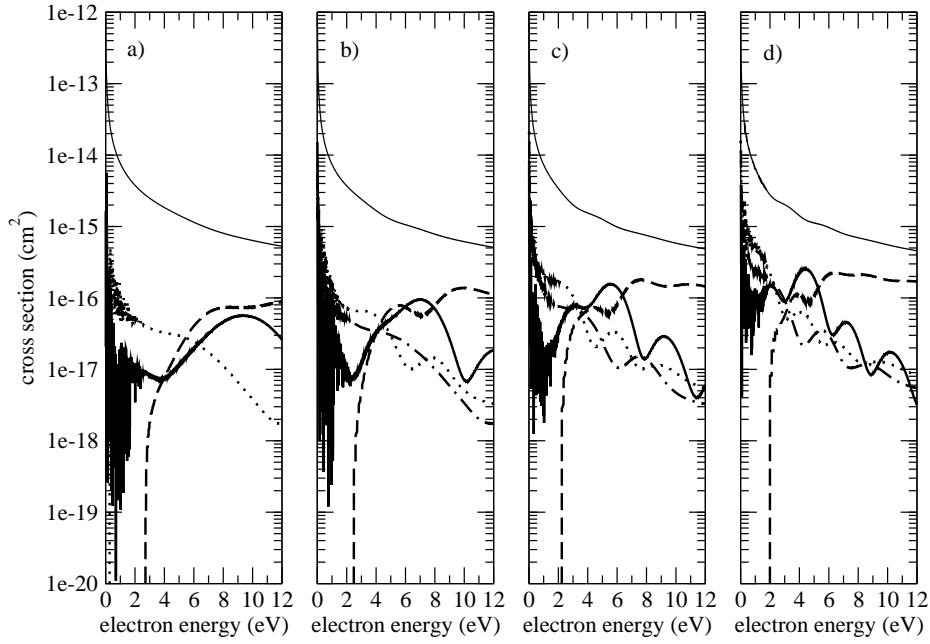


Figure 6: a): Cross sections of H_2^+ molecular ion initially in the electronic ground state and the vibrational state $v_i^+ = 0$ for dissociative recombination (DR) thick solid lines, for dissociative excitation (DE) thick dashed lines, for elastic scattering (ES) thin solid lines, for vibrational 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) $v_i^+ = 3$.

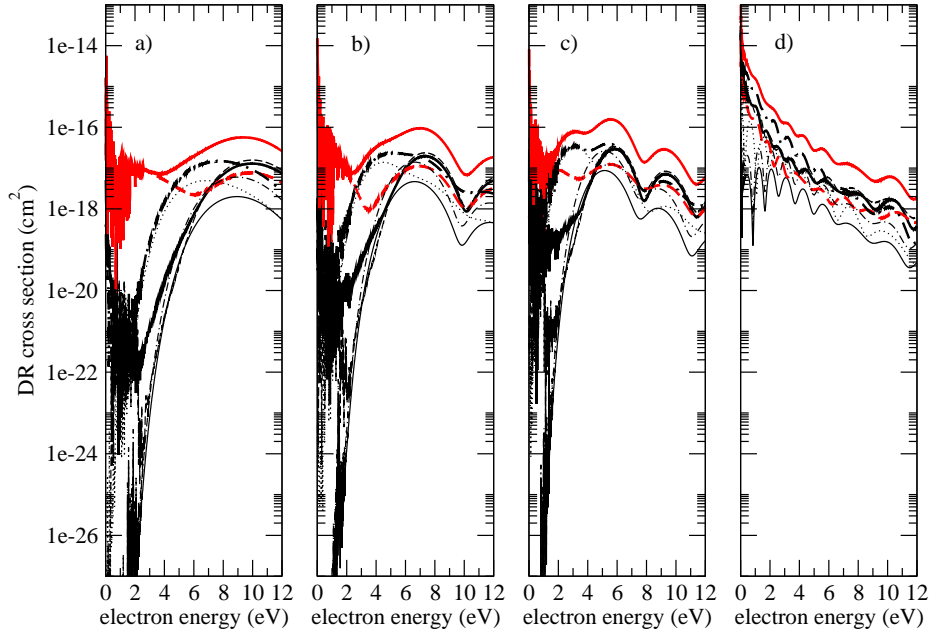


Figure 7: Contributions of various dissociative states to the DR cross section ($\sigma_{v_i^+}^{DR}$) of the H_2^+ molecular ion initially in the electronic ground state and the vibrational state: (a) $v_i^+ = 0$, (b) $v_i^+ = 1$, (c) $v_i^+ = 2$, and (d) $v_i^+ = 10$. Thick solid lines: $^1\Pi_g$ state, 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 $\sigma_{v_i^+}^{DR}$.

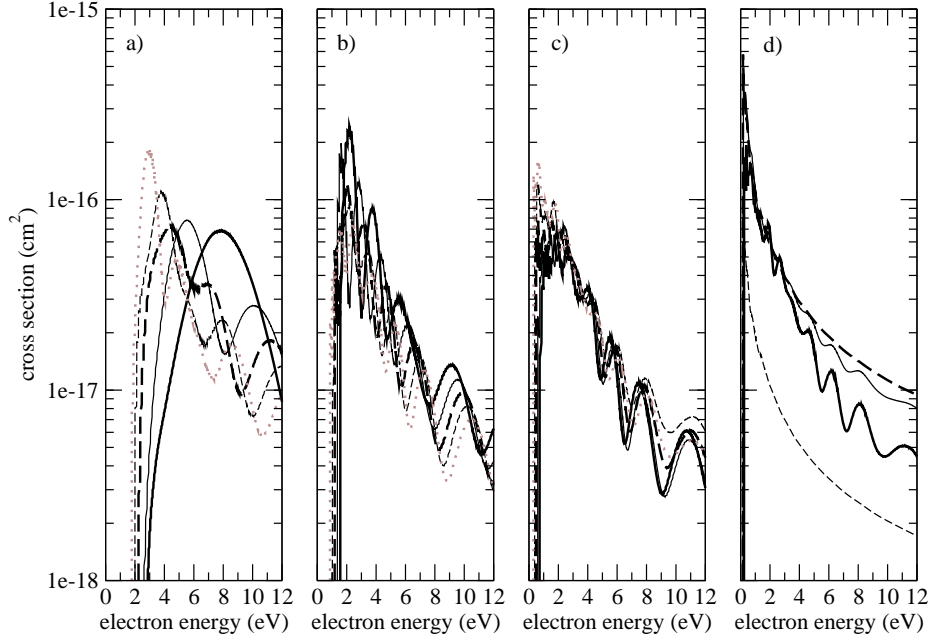


Figure 8: Indirect DE cross section ($\sigma_{v_i^+}^{DE1}$) of the H_2^+ molecular ion initially in the electronic ground state and the vibrational state v_i^+ . Thick solid lines show our results for $v_i^+ = 0$ in panel (a), $v_i^+ = 5$ in panel (b), $v_i^+ = 10$ in panel (c), and $v_i^+ = 15$ in 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).

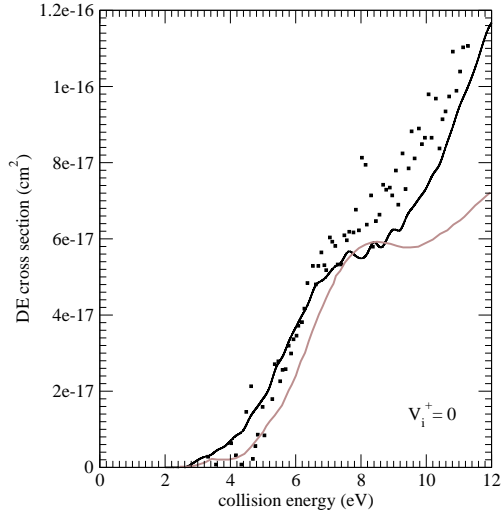


Figure 9: DE cross sections of HD^+ for $v_i^+ = 0$. Solid line: our results (M. Fifrig and M. Stroe, Phys. Scr. 78 (2008) 065302), squares: experimental results (Zajfman D and Amitay Z 1996 *Dissociative Recombination: Theory, Experiment and Applications III* (World Scientific) 114), grey full line: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

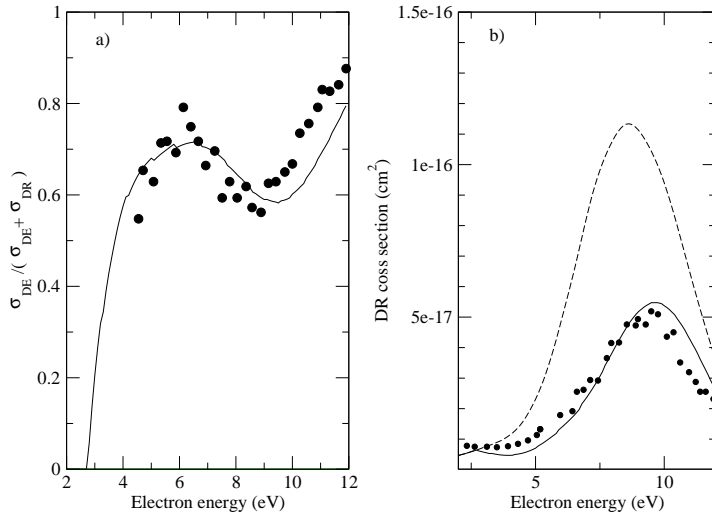


Figure 10: (a) The ratio (DE cross section)/(DE cross section+DR cross section) for HD^+ initially in the vibrational level $v_i^+ = 0$. Black solid line: our numerical results [M. Stroe and M. Fifrig, Phys. Lett. A 373 (2009) 4152], and black full circles: experimental results from ASTRID [L.H. Andersen, 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.

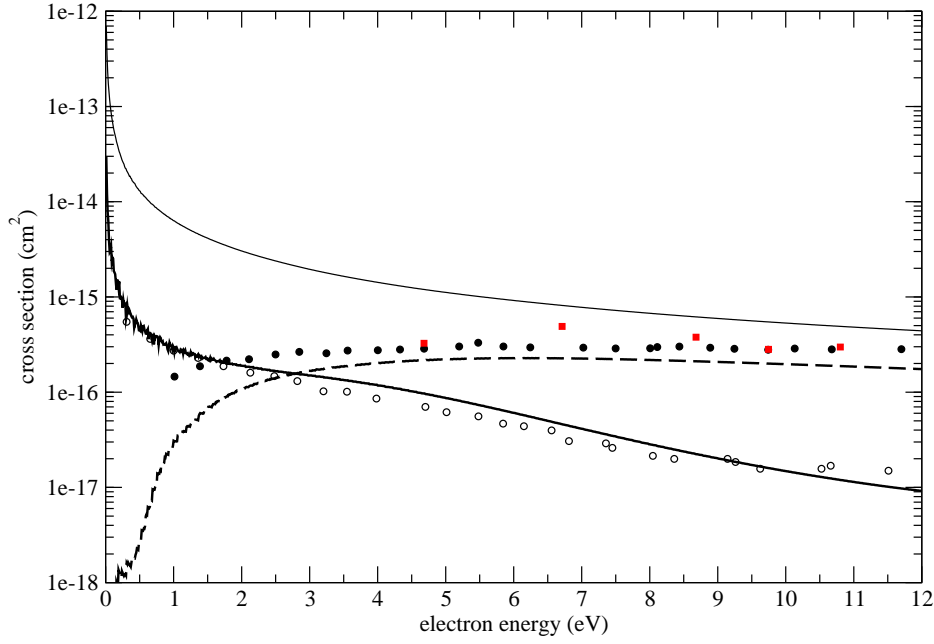


Figure 11: Cross sections of vibrationally excited H_2^+ assuming a Franck-Condon distribution of the vibrational levels of its ground electronic state, for DR: thick solid lines, for DE: thick dashed lines and for elastic scattering thin solid lines. Lines represent our results, open circles the experimental 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.

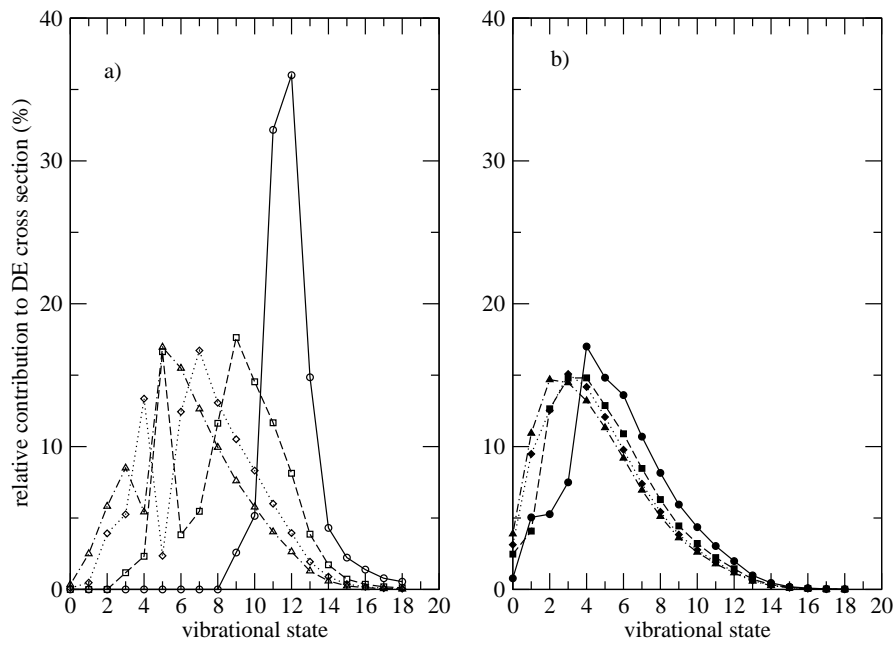


Figure 12: Relative contribution of each vibrational state v_i^+ to the total DE cross section. a) Circles: $E = 1$ eV, squares: $E = 2$ eV, diamonds: $E = 3$ eV, and triangles: $E = 4$ eV. b) Full circles: $E = 5$ eV, full squares: $E = 7$ eV, full diamonds: $E = 9$ eV, and full triangles: $E = 11$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