Complete collision data set for electrons scattering on molecular hydrogen and its isotopologues

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Overview

- MCCC method : fixed-nuclei (FN) approach

  Cross sections obtained with the FN MCCC method

- MCCC method : adiabatic nuclei (AN) approach

  Vibrationally-resolved cross sections from AN MCCC

  Accessing MCCC collision data: MCCC database

- Example: modeling - Collisional Radiative Model for H_2
- Scattering from the excited states ($n=2$: $a\ ^3\Sigma_g^+$, $c\ ^3\Pi_u$,…)
- Isotopic and vibrational-level dependence of H_2 dissociation by electron impact
- Conclusions

MCCC method: fixed-nuclei (FN) approach

- Born-Oppenheimer approximation
- Fixed-nuclei approximation, R = fixed

→ Solve for the electronic wave function

- Diagonalization of the target Hamiltonian H_T in a Sturmian (Laguerre) basis

→ modeling of *infinite* number of bound & continuum states with a *finite* number of pseudostates

$$\langle \phi_f | H_T | \phi_i \rangle = \varepsilon_f \delta_{fi}$$

- N-state multi-channel expansion

$$\Psi_i^{(+)}(\mathbf{x}_p, \mathbf{x}_t) = \mathcal{A} \sum_{n=1}^{N} F_n(\mathbf{x}_p)\ \phi_n(\mathbf{x}_t)$$

- Solve integral LS equation for the T matrix

$$T_{fi}(\vec{k}_f, \vec{k}_i) = V_{fi}(\vec{k}_f, \vec{k}_i) + \sum_{n=1}^{N} \int d^3k \frac{V_{fn}(\vec{k}_f, \vec{k}) T_{ni}(\vec{k}, \vec{k}_i)}{E + i0 - \varepsilon_n - k^2/2}$$

- Cross sections

$$\sigma_{fi}(R) \propto \left| T_{fi}(R) \right|^2$$

Why electron-molecule is difficult: no central potential

→ multi-channel expansion + projectile partial wave expansion lead to a very large size of coupled equations, to solve need fast computers, effective parallelization, etc….

Cross sections for electron scattering from H_2

FN single-centre spherical coordinate MCCC approach

Established convergence in cross sections by performing: 491, 427, 259, 92, 9-state close-coupling

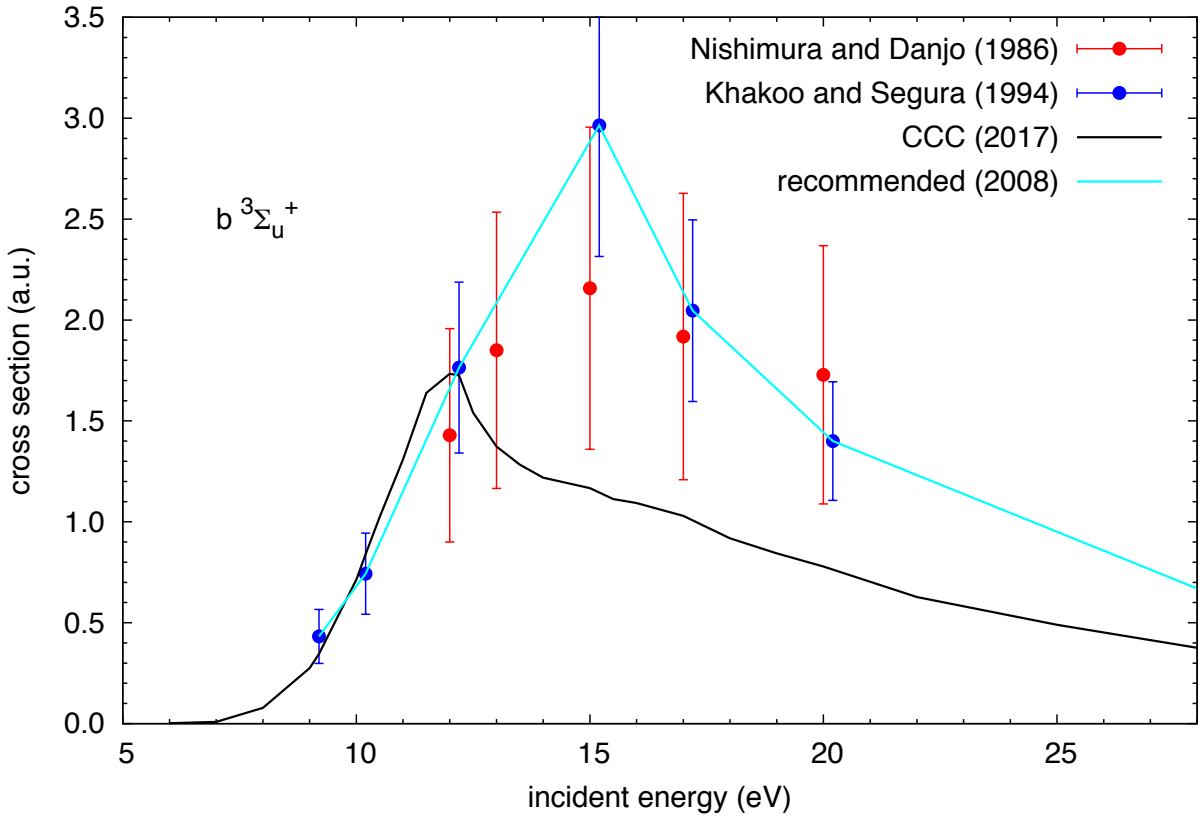
- total cross section, total ionization cross section, stopping power
- elastic scattering (ICS, DCS)
- excitation cross sections (ICS, DCS) for
  - $b\ ^3\Sigma_u^+$, $a\ ^3\Sigma_g^+$, $c\ ^3\Pi_u$, $e\ ^3\Sigma_u^+$, $h\ ^3\Sigma_g^+$, $d\ ^3\Pi_u$, $i\ ^3\Pi_g$, $j\ ^3\Delta_u$
  - $B\ ^1\Sigma_u^+$, $C\ ^1\Pi_u$, $EF\ ^1\Sigma_g^+$, $B'\ ^1\Sigma_u^+$, $D\ ^1\Pi_u$, $B''\ ^1\Sigma_u^+$, $D'\ ^1\Pi_u$, $H\ ^1\Sigma_g^+$, $GK\ ^1\Sigma_g^+$, $I\ ^1\Pi_u$, , $J\ ^1\Delta_g$

Scarlett *et al*., Phys. Rev. A **96** (2017) 062708
Zammit *et al*., Phys. Rev. A **95** (2017) 022708
Zammit *et al*., Phys. Rev. Lett. **116** (2016) 233201

Often found large disagreement with previous experimental and theoretical results

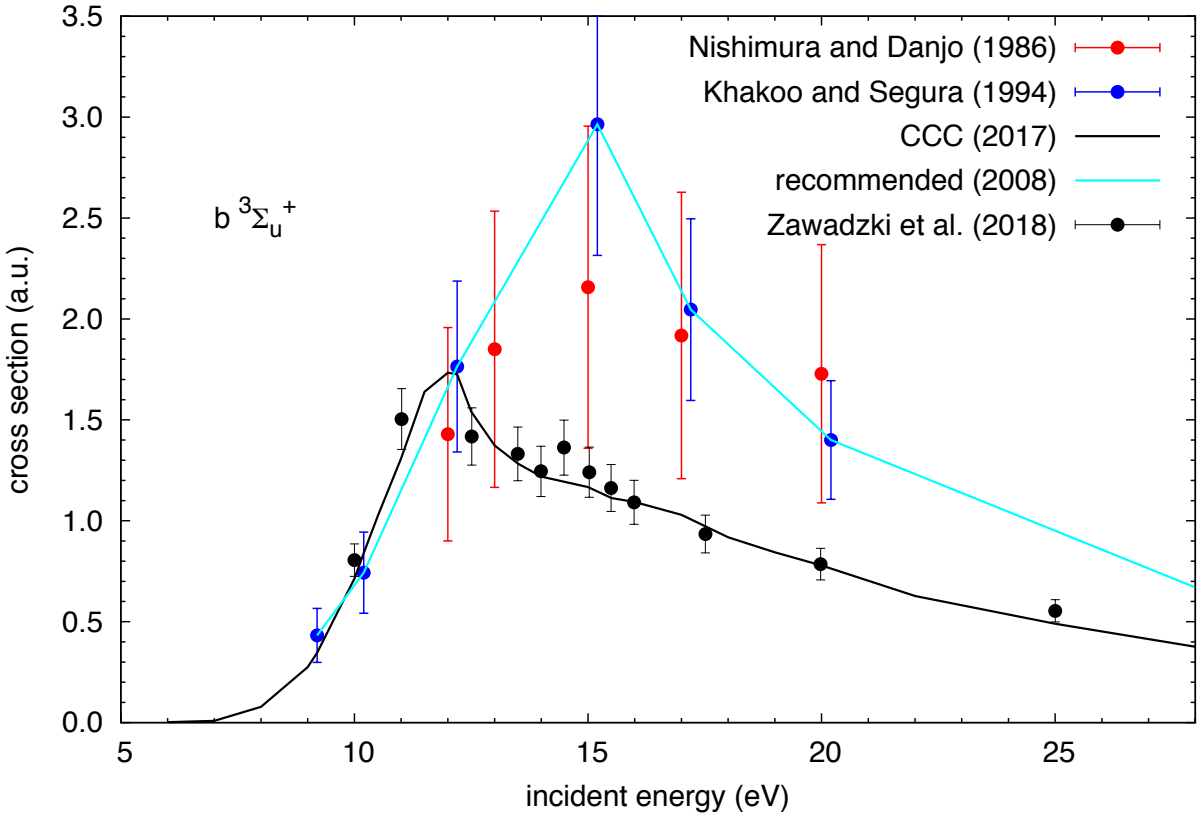
Cross sections for the b $^3\Sigma_u^+$ state

Scarlett *et al.,* Phys. Rev. A **96** (2017) 062708
Zammit *et al.,* Phys. Rev. A **95** (2017) 022708



Cross sections for the b $^3\Sigma_u^+$ state

New time of flight (TOF) spectrometer at California State University, Fullerton

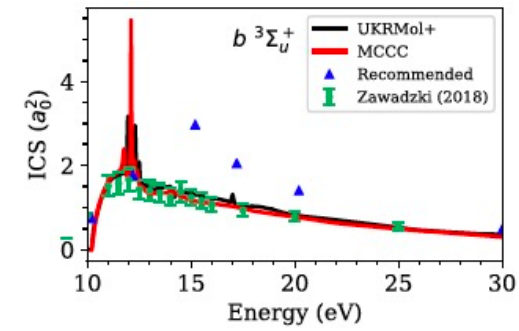


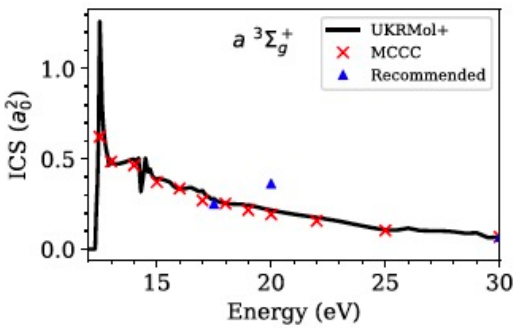
Zawadzki *et al.*, Phys. Rev. A **97** (2018) 050702(R)
Phys. Rev. A **98** (2018) 062704

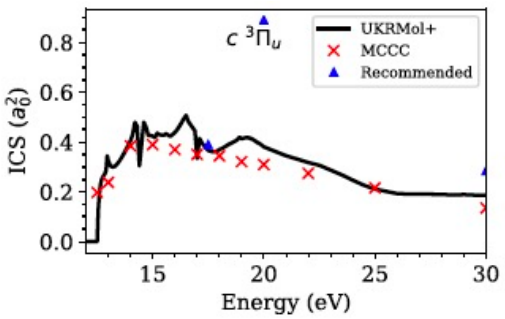
UKRMol+ and MCCC calculations: good agreement

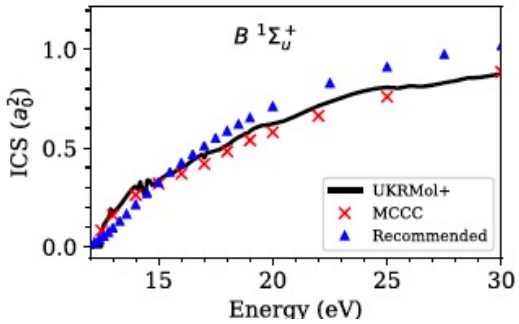
ICS

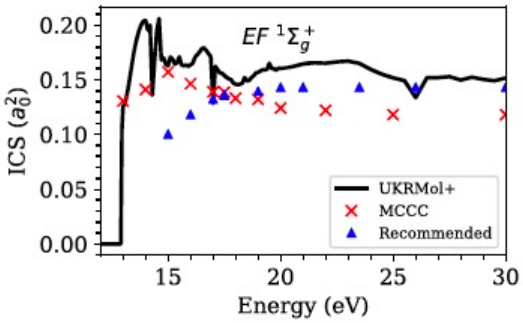
Meltzer *et al.*, J. Phys. B. **53** (2020) 145204

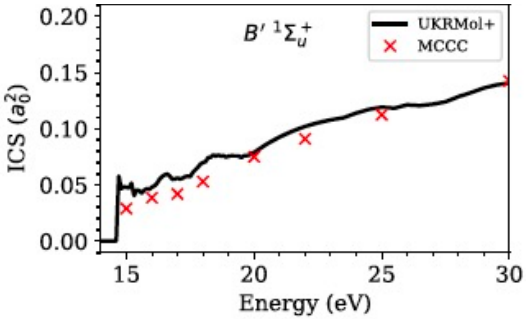




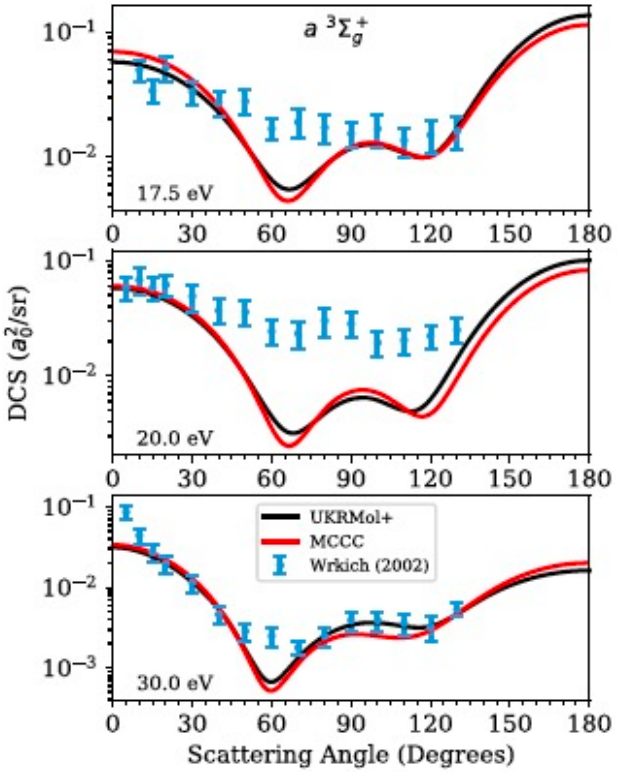




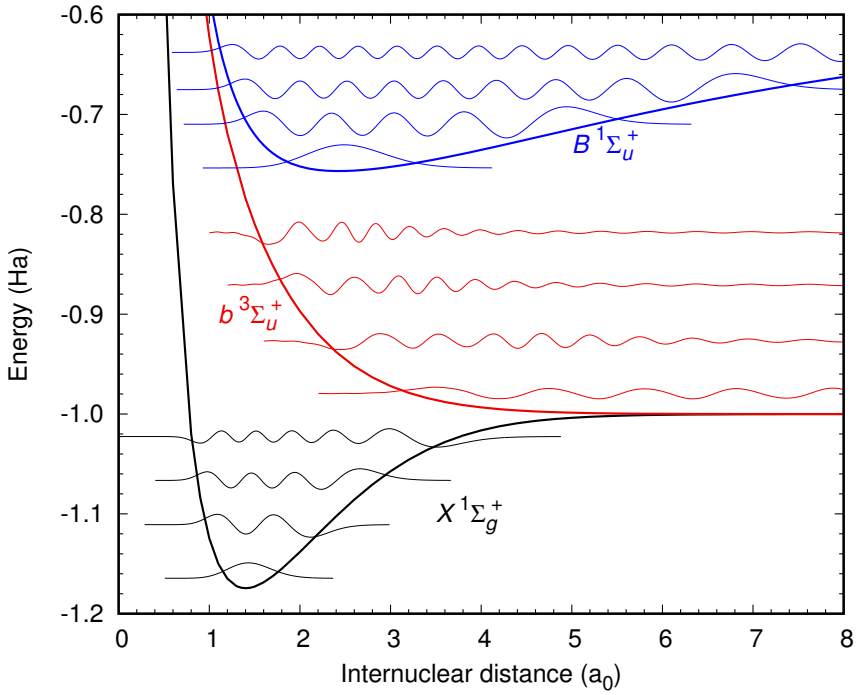




DCS



MCCC method: adiabatic nuclei (AN) approach



- AN T matrix

$$T_{f\mu,iv}(E) = \int dR \;\; \varphi_{f\mu}(R) T_{fi}(E;R) \;\; \varphi_{iv}(R)$$

- $\varphi_{n\mu}(R)$ are vibrational wave functions
- vibrationally-resolved cross sections

$$\sigma_{f\mu,iv}(E) \propto \left| T_{f\mu,iv}(E) \right|^2$$

  - computationally expensive (many R)
  - need high accuracy of FN model at large R

Single-center spherical-coordinate formulation is inadequate

↓

Spheroidal-coordinate formulation of the MCCC method

Many FN calculations have to be performed on a grid of R → MCCC(210) model

Computationally efficient / feasible approach is required

MCCC method: spheroidal coordinate formulation

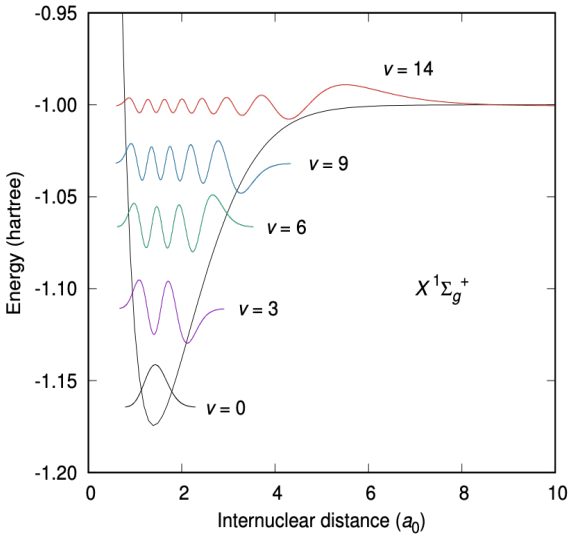
Target states

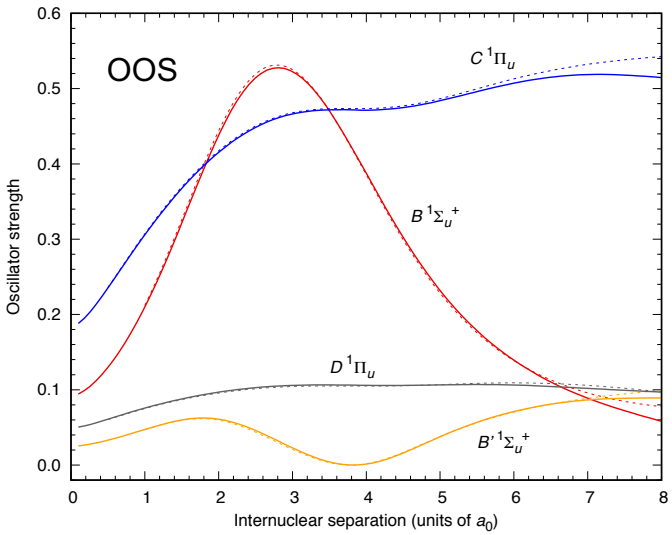
Very accurate target structure for *R* values spanned by first 10 H_2 vibrational levels

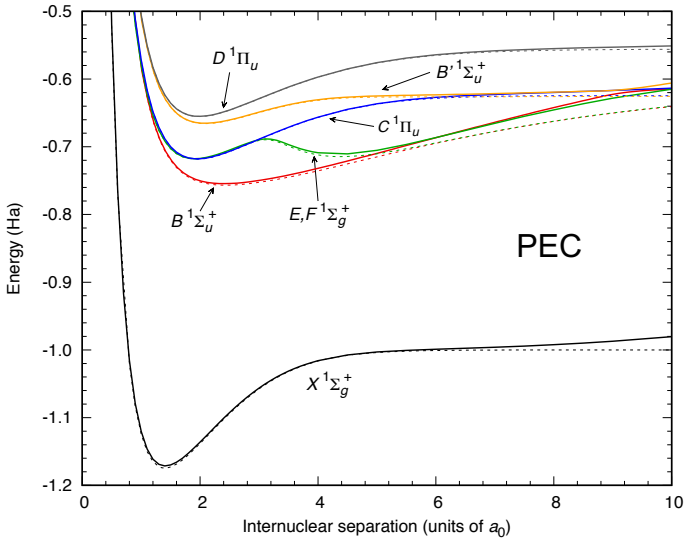
Still within 5% accuracy for larger *R*

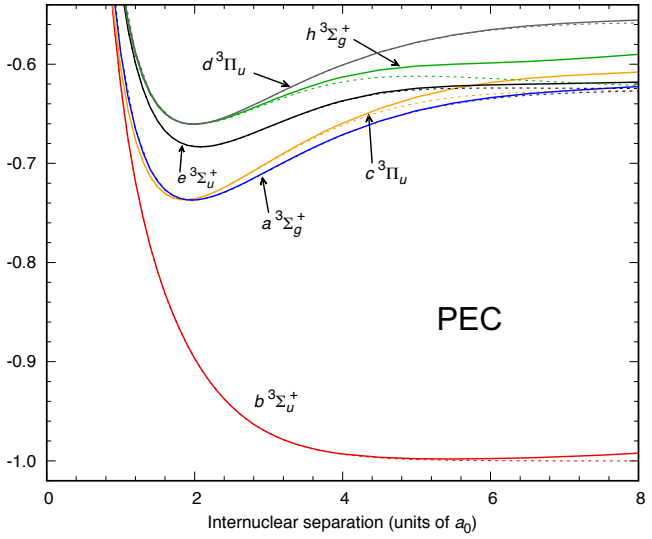
Solid lines: MCCC

Dashed lines: accurate (Wolniewicz et al)









MCCC(210) fully vibrationally resolved cross sections

Calculations have been performed for over 58,000 transitions in H_2 and its 5 isotopologues
includes dissociation cross sections

Scarlett et al., Atomic Data and Nuclear Data Tables, **137** (2021) 101361, **139** (2021) 101403

Scattering on all bound levels of the $X\ ^1\Sigma_g^+$ state

Data files per transition:

MCCC-el-H2-B1Su_vf=10.X1Sg_vi=0.txt

Analytic fits

$$\sigma(x) = \left(\frac{x-1}{x}\right)\left(\frac{A_0^2 \ln(x)}{x} + \frac{A_1}{x} + \frac{A_2}{x^2} + \frac{A_3}{x^3} + \frac{A_4}{x^4} + \frac{A_5}{x^5}\right)$$

In collaboration with Yu. Ralchenko (NIST)

Number of bound vibrational levels

State	Molecule					
	H_2	HD	HT	D_2	DT	T_2
Initial states → $X\ ^1\Sigma_g^+$	15	18	19	21	24	26
$B\ ^1\Sigma_u^+$	37	43	45	52	57	64
$EF\ ^1\Sigma_g^+$	33	38	40	47	51	57
$C\ ^1\Pi_u$	14	16	17	19	21	24
$B'\ ^1\Sigma_u^+$	9	11	12	13	15	16
$GK\ ^1\Sigma_g^+$	9	10	11	12	13	15
$I\ ^1\Pi_g$	4	4	5	5	6	7
$J\ ^1\Delta_g$	18	20	22	26	28	31
Final states → $H\ ^1\Sigma_g^+$	72	83	88	102	112	125
$D\ ^1\Pi_u$	18	21	22	25	28	31
$b\ ^3\Sigma_u^+$	0 (dissociative)					
$a\ ^3\Sigma_g^+$	19	22	23	27	30	34
$c\ ^3\Pi_u$	20	23	25	29	31	35
$e\ ^3\Sigma_u^+$	8	9	10	11	12	14
$h\ ^3\Sigma_g^+$	4	5	5	6	6	7
$d\ ^3\Pi_u$	20	23	25	29	32	35
$g\ ^3\Sigma_g^+$	19	22	23	27	30	33
$i\ ^3\Pi_g$	4	4	5	5	6	7
$j\ ^3\Delta_g$	18	21	22	26	28	32

Accessing MCCC data

All cross sections and fits available online

- **Atom. Data Nucl. Data Tables supplementary materials**

Complete collision data set for electrons scattering on molecular hydrogen and its isotopologues:

I. Fully vibrationally-resolved electronic excitation of $H_2(X\,^1\Sigma_g^+)$

Atomic Data and Nuclear Data Tables 137 (2021) 101361

II. Fully vibrationally-resolved electronic excitation of the isotopologues of $H_2(X\,^1\Sigma_g^+)$

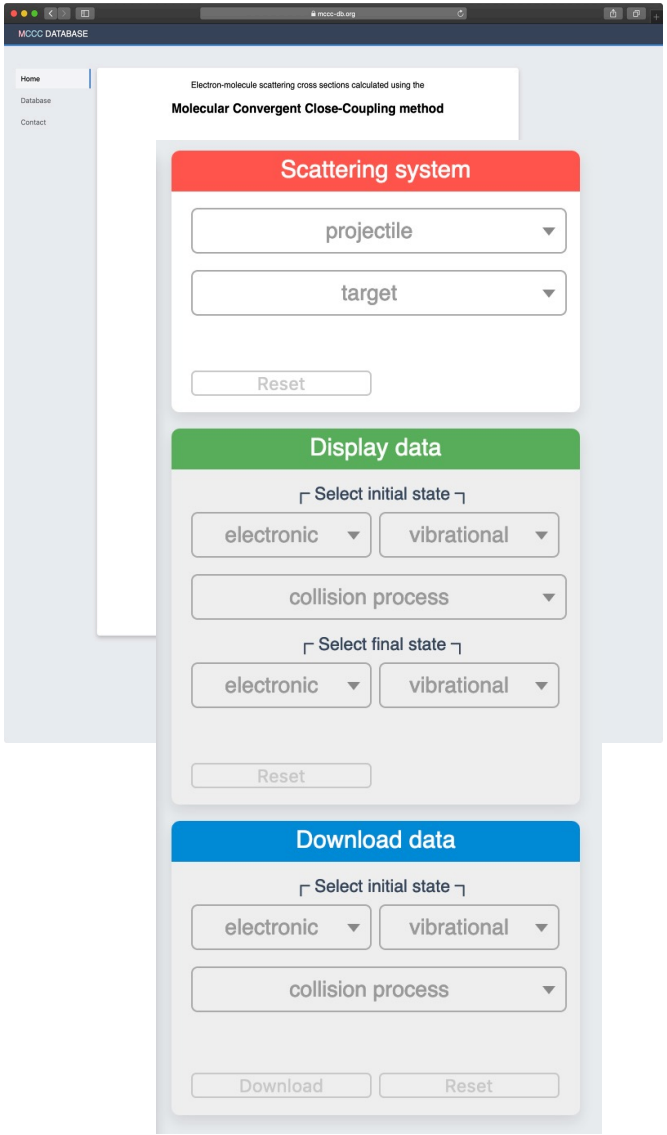
Atomic Data and Nuclear Data Tables 139 (2021) 101403

- **LXCat Database –** lxcat.net

- **IAEA hcdb: Atomic and Molecular Data for Fusion Energy Research**

  https://db-amdis.org/hcdb/

- **MCCC Database –** mccc-db.org



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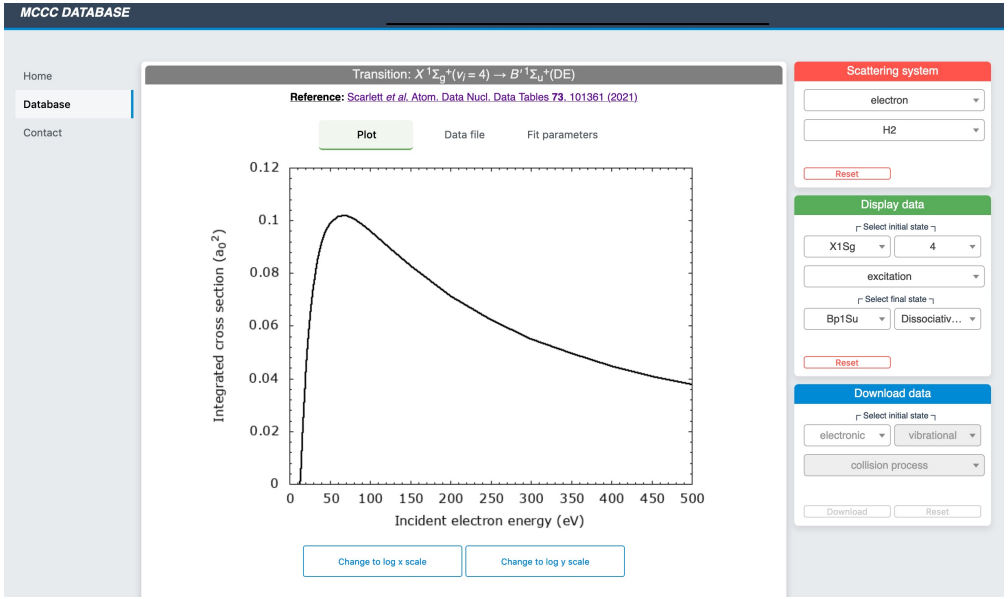
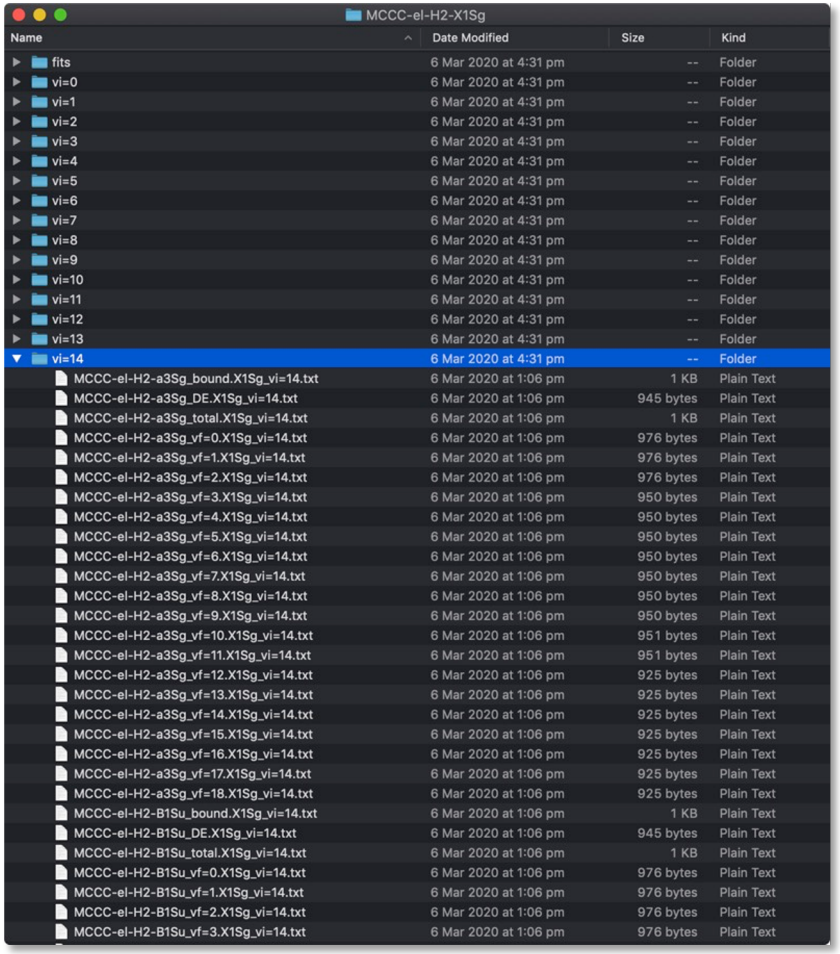


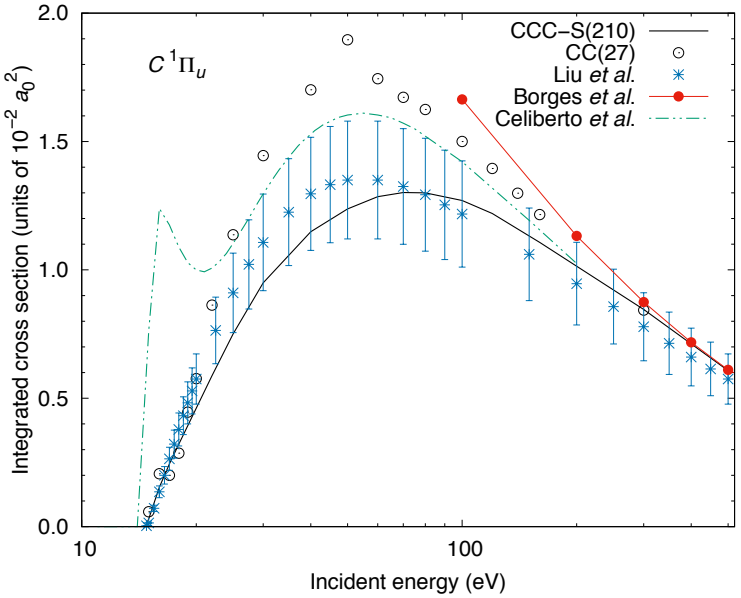


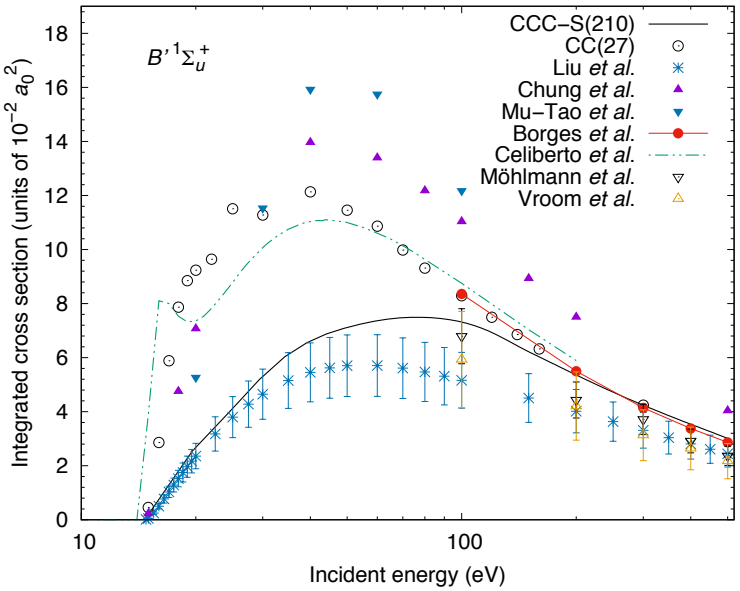
Dissociative excitation

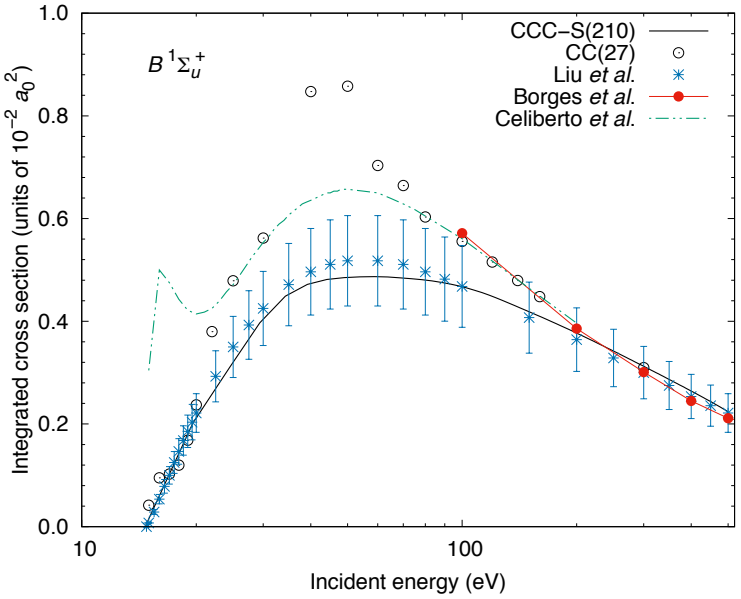
Tapley et al., Phys. Rev. A **98** (2018) 032701

$B'\,^1\Sigma_u^+$ state has the largest DE cross section
for scattering on $v = 0$ ground state $X\,^1\Sigma_g^+$

exp.: Liu et. al, J. Phys B **45** (2012)
IP: semiclassical impact-parameter method – Bari group
Celiberto et al., Atom. Data Nucl. Data Tables 77 (2001) 161
FBA: Borges et al., Phys. Rev. A 57 (1998) 1025

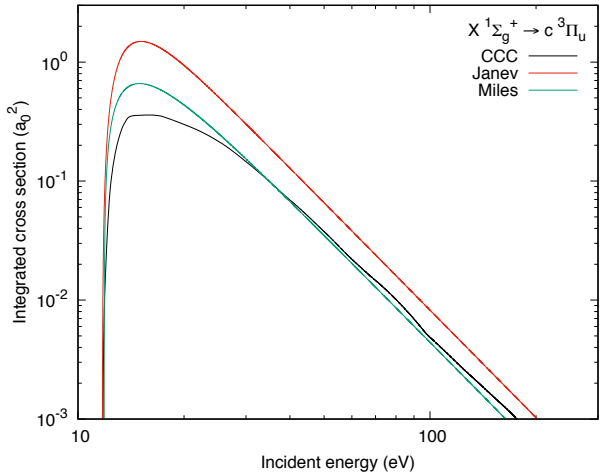


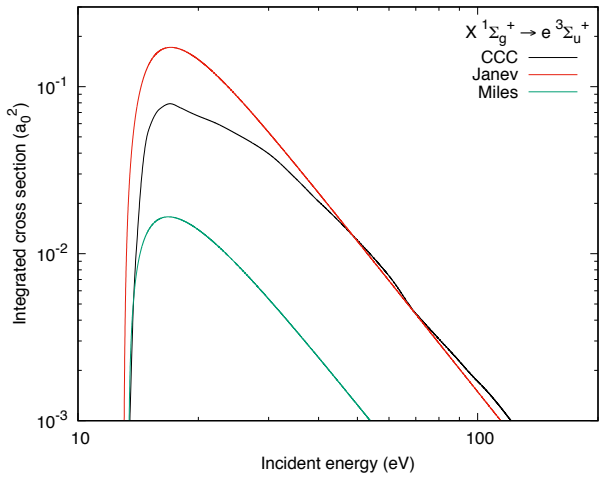


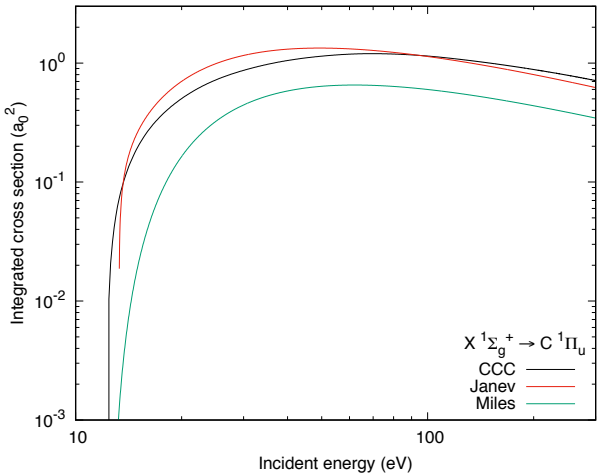


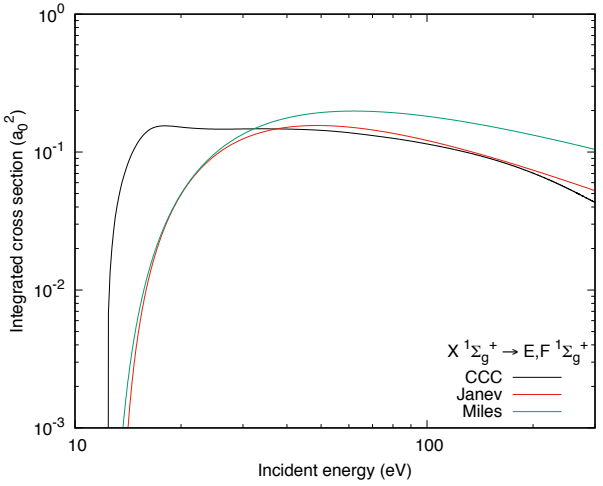
Collisions data & plasma physics applications: Janev & Miles comparisons

Miles, Thompson, Green, J. App. Phys. **43** (1972) 678; Janev, Reiter, Samm, JÜL-4105, Jülich, 2003 → used by Ursel Fantz & Dirk Wuenderlich (Garching) in their CR model









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https://doi.org/10.1088/1361-6463/abccf2

Application of molecular convergent close-coupling cross sections in a collisional radiative model for the triplet system of molecular hydrogen

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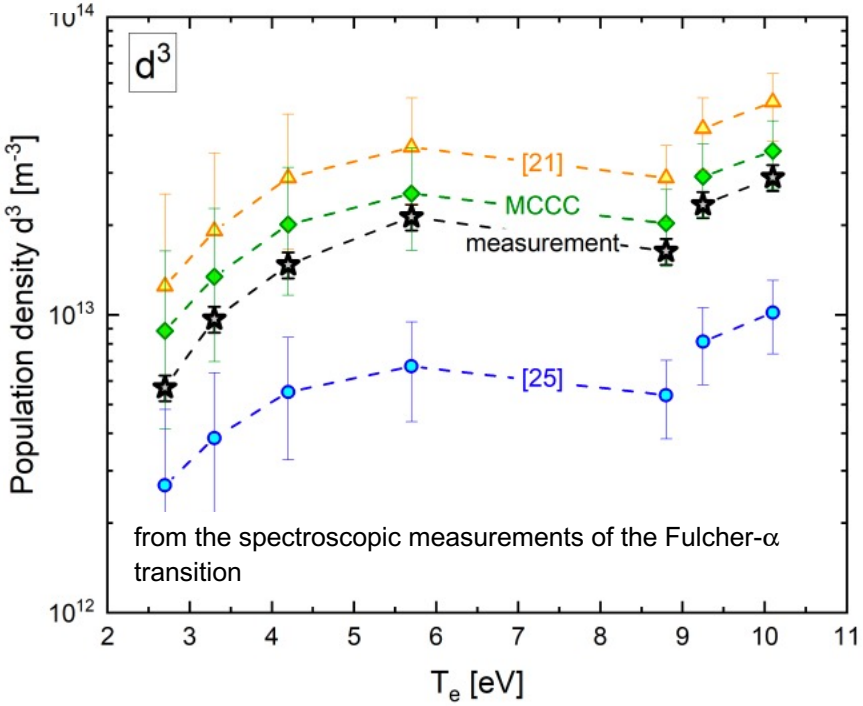
[2] Curtin Institute for Computation and Department of Physics, Astronomy and Medical Radiation Sciences, Curtin University, Perth, Western Australia 6102, Australia
[3] Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, United States of America

Comparison of measured population densities of the d^3 state to the ones calculated with the CR model Yacora H_2 using cross section from either Miles et al. [25], Janev et al. [21] or the MCCC data.

Significant differences in the simulation results depending on the collision dataset used →



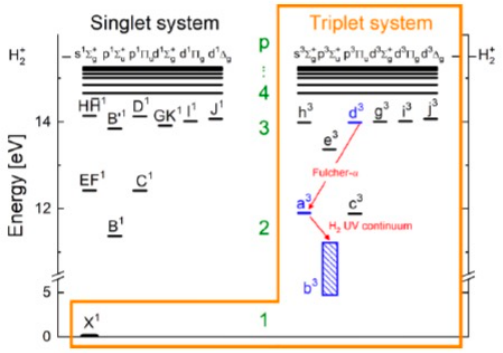
Further improvements:

- more accurate account of cascading from high level states
- use of vibrationally resolved cross sections
- use of rotationally resolved cross sections

Scattering from excited (n=2, v=0) electronic states

Vertical excitation energies at $R = 2$

State	R_m	Energy (Ha) Present	Energy (Ha) Ref.	ΔE (eV) Present	ΔE (eV) Ref.
		$n = 1$			
$X\ ^1\Sigma_g^+$	1.448	−1.1360	−1.1381[a]	−10.86	−10.90
$b\ ^3\Sigma_u^+$		−0.8967	−0.8971[b]	−4.347	−4.344
		$n = 2$			
$B\ ^1\Sigma_u^+$	2.518	−0.7503	−0.7521[c]	−0.364	−0.397
$c\ ^3\Pi_u$	2.022	−0.7369	−0.7375[b]		
$a\ ^3\Sigma_g^+$	1.928	−0.7357	−0.7361[b]	0.032	0.037
$C\ ^1\Pi_u$	2.016	−0.7177	−0.7182[d]	0.523	0.5237
$EF\ ^1\Sigma_g^+$	1.978	−0.7172	−0.7177[e]	0.536	0.538
		$n = 3$			
$e\ ^3\Sigma_u^+$		−0.6831	−0.6832[b]	1.465	1.478
$B'\ ^1\Sigma_u^+$		−0.6650	−0.6655[c]	1.957	1.959
$d\ ^3\Pi_u$		−0.6606	−0.6607[b]	2.077	2.089
$h\ ^3\Sigma_g^+$		−0.6602	−0.6606[b]	2.088	2.093
$GK\ ^1\Sigma_g^+$		−0.6599	−0.6604[e]	2.095	2.097
$g\ ^3\Sigma_g^+$		−0.6595	−0.6598[b]	2.106	2.113
$i\ ^3\Pi_g$		−0.6592	−0.6596[b]	2.115	2.120
$I\ ^1\Pi_g$		−0.6591	−0.6595[f]	2.117	2.121
$j\ ^3\Delta_g$		−0.6574	−0.6576[f]	2.164	2.173
$J\ ^1\Delta_g$		−0.6573	−0.6576[f]	2.166	2.174
$D\ ^1\Pi_u$		−0.6551	−0.6553[d]	2.226	2.235
$H\ ^1\Sigma_g^+$		−0.6547	−0.6549[e]	2.238	2.246



PHYSICAL REVIEW A 103, 032802 (2021)

Convergent close-coupling calculations of electrons scattering on electronically excited molecular hydrogen

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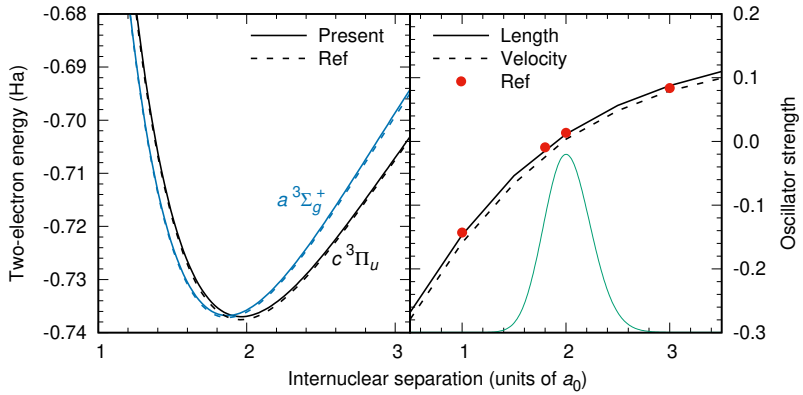


Excitation energies are relative to the $c\ ^3\Pi_u$ state

Example: the $c\ ^3\Pi_u(v=0)$ state

it is a metastable state
it is lower than $a\ ^3\Sigma_g^+(v=0)$ state
by 0.0228 eV

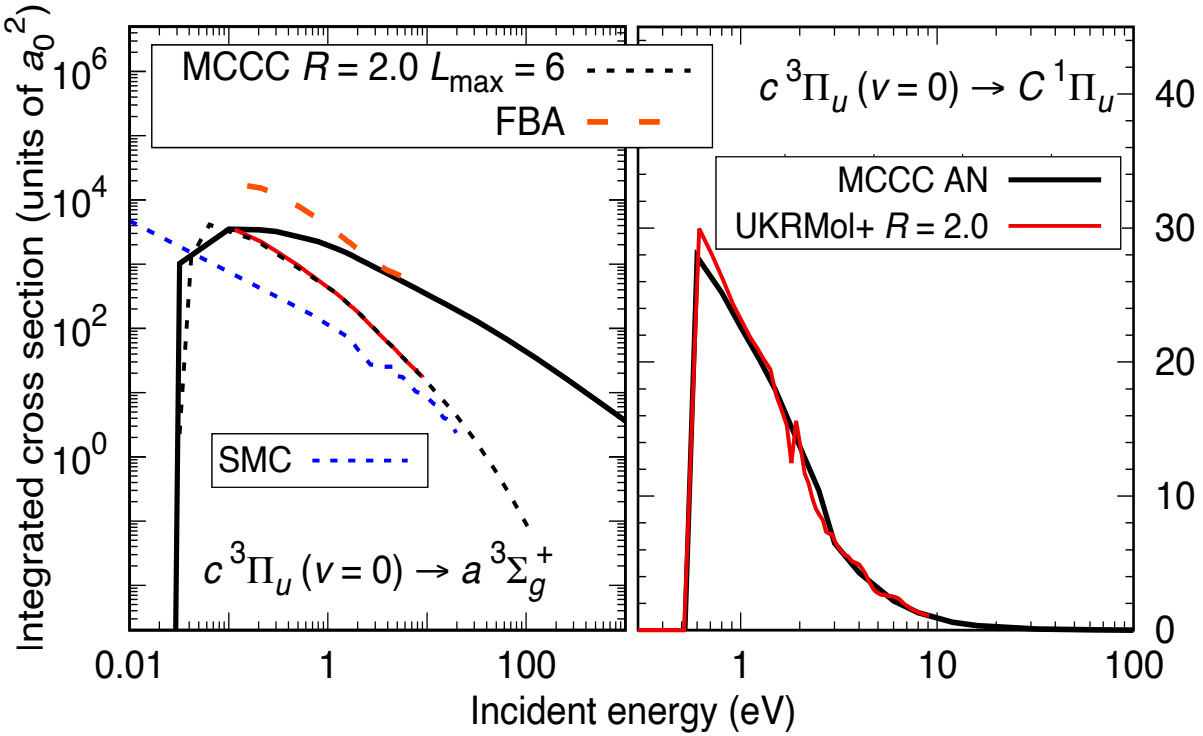
$c\ ^3\Pi_u \rightarrow a\ ^3\Sigma_g^+$ transition is by far the largest as it is a dipole allowed transition
small excitation energy means:

(a) large projectile partial wave expansion is required
(b) Born limit will be reached relatively fast
(c) target structure accuracy is very important

Scattering from excited (n=2, v=0) electronic states

Partial-wave convergence:

- Much slower than for scattering on ground state (L_{max} = 10)
- Many dipole-allowed transitions unconverged even with L_{max} = 25
- Even with Analytical Born Completion L_{max} = 20 is necessary
- Agreement with recent UKRMol+ calculations (L_{max} = 6) for dipole-forbidden and spin-exchange transitions, but not dipole-allowed transitions



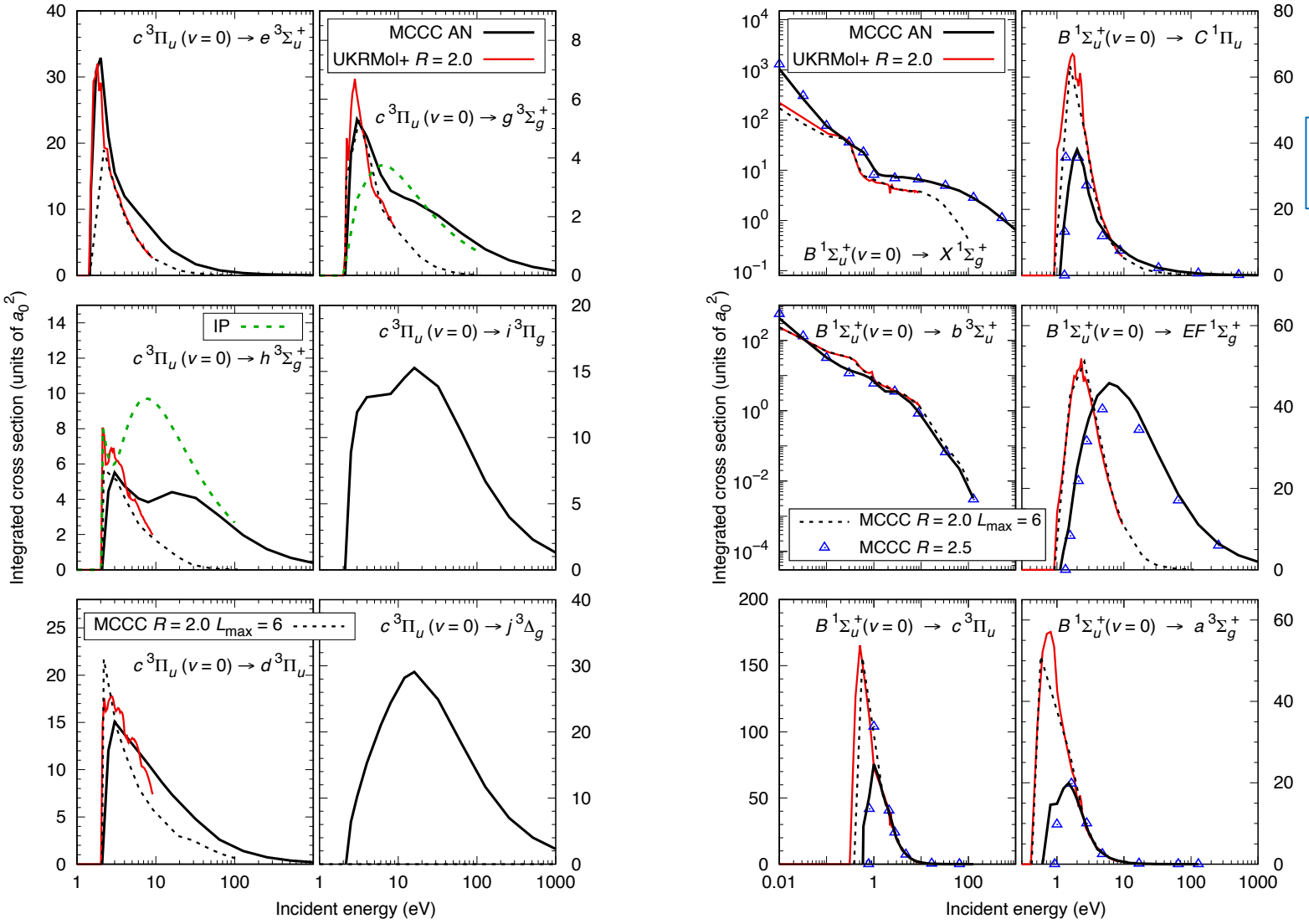
MCCC (AN): Scarlett et al., PRA **103** (2021) 032802

UKRmol+ (FN): Meltzer et al., J. Phys. B **53** (2020) 245203

SMC (FN): Sartori et al. Phys. Rev. A 55 (1997) 3243

FBA (FN): Rescigno & Orel (from IEEE Trans. Plasma Sci. PS-11, 266 (1983).)

Scattering from excited (n=2, v=0) electronic states

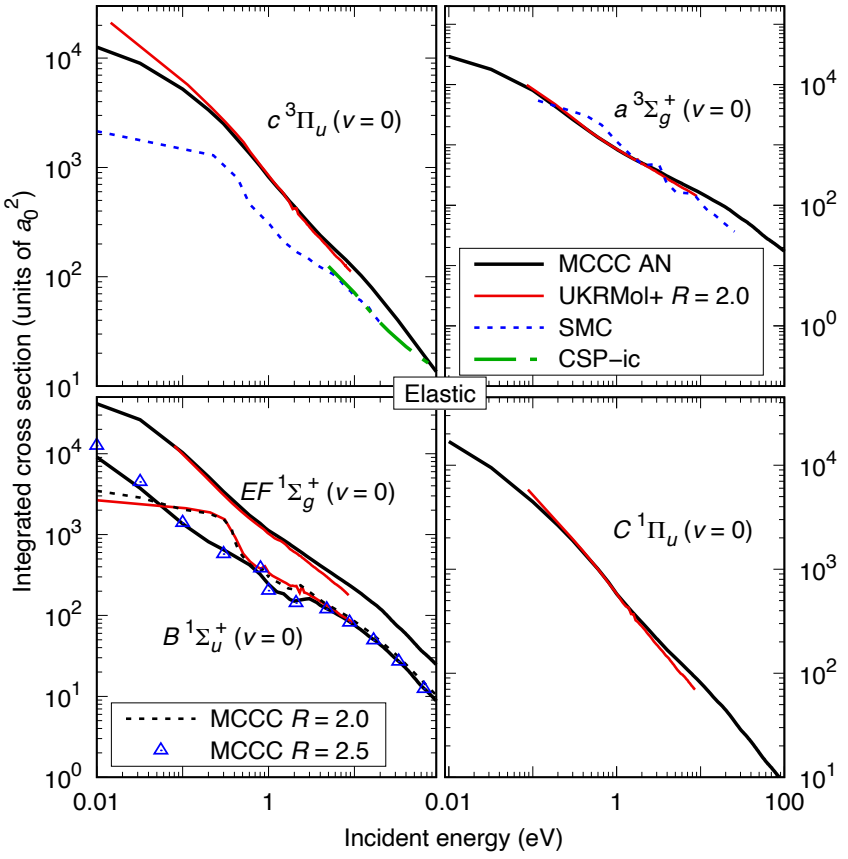


$B\,^1\Sigma_u^+$
$R_m = 2.52$

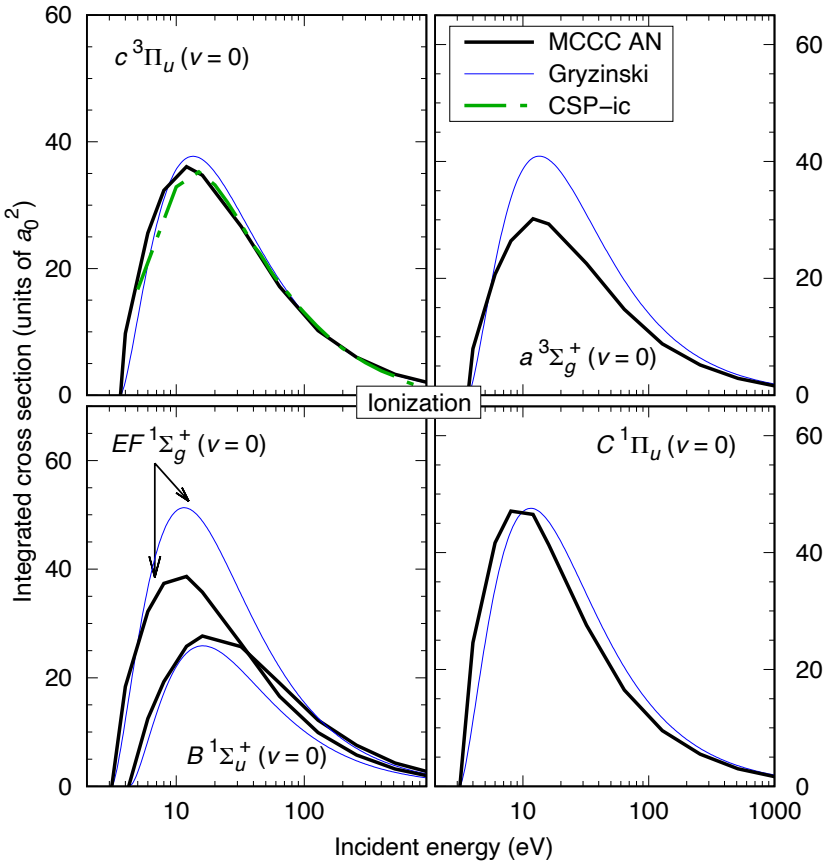
IP: Laricchiuta et. al., Phys. Rev. A **69** (2004) 22706

Scattering from excited (n=2, v=0) electronic states

Elastic scattering cross sections



Ionization cross sections



R = 2.0 used in FN UKRMol+ calculations does not accurately model scattering on more diffuse $B\ ^1\Sigma_u^+$ state (average R = 2.5)

CSP-ic.: Joshipura et al., J. Phys. B **43** (2010) 135207

Gryzinski: Wunderlich et al., Chem. Phys. **390** (2011) 75

Isotopic and vibrational-level dependence of H_2 dissociation by electron impact

Standard formula to calculate energy-differential cross section for dissociation (used in MCCC):

$$\frac{\mathrm{d}\sigma}{\mathrm{d}E_{\mathrm{out}}} = \frac{\pi}{k_{\mathrm{in}}^2} \sum_{\substack{\ell' m' \\ \ell m}} \left| \langle \nu_{E_{\mathrm{k}}} | T_{\ell' m', \ell m}(R; E_{\mathrm{in}}) | \nu_v \rangle \right|^2$$

$$E_k = E_{\mathrm{in}} - D_v - E_{\mathrm{out}}$$

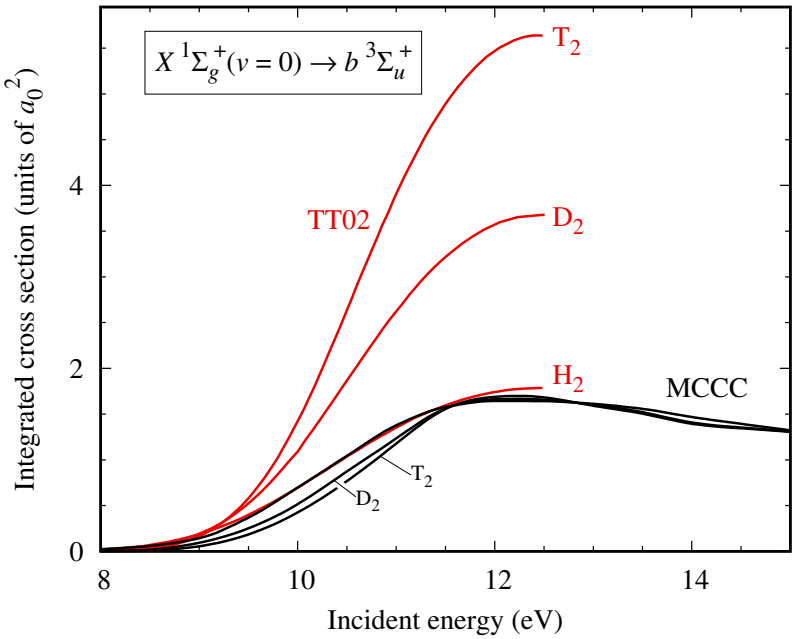
- ν_{E_k} energy-normalized continuum vibrational wave functions
- Isotopic dependence only from vibrational wave functions

$$\sigma = \int \frac{d\sigma}{dE_{\mathrm{out}}} dE_{\mathrm{out}}$$

Trevisan and Tennyson (J. Phys. B **34** (2001) 2935-2949) derived a different formula:

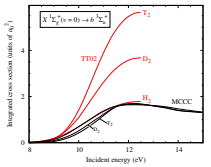
$$\frac{\mathrm{d}\sigma}{\mathrm{d}E_{\mathrm{out}}} = \frac{m_{\mathrm{H}}}{4\pi^3 m_{\mathrm{e}}} \frac{E_{\mathrm{k}}}{E_{\mathrm{in}}} \sum_{\substack{\ell' m' \\ \ell m}} \left| \langle \nu_{E_{\mathrm{k}}} | T_{\ell' m', \ell m}(R; E_{\mathrm{in}}) | \nu_v \rangle \right|^2$$

- Explicit mass dependence – cross sections scale with mass
- Explicit dependence on the energy of the dissociating fragments E_k
- Formula was applied in R-matrix calculations of H_2 dissociation cross sections which are widely used in plasma modelling applications



R-matrix calculations TT02: Trevisan and Tennyson, Plasma Phys. Control. Fusion **44** (2002) 1263-1276, 2217-2230

Isotopic and vibrational-level dependence of H_2 dissociation by electron impact



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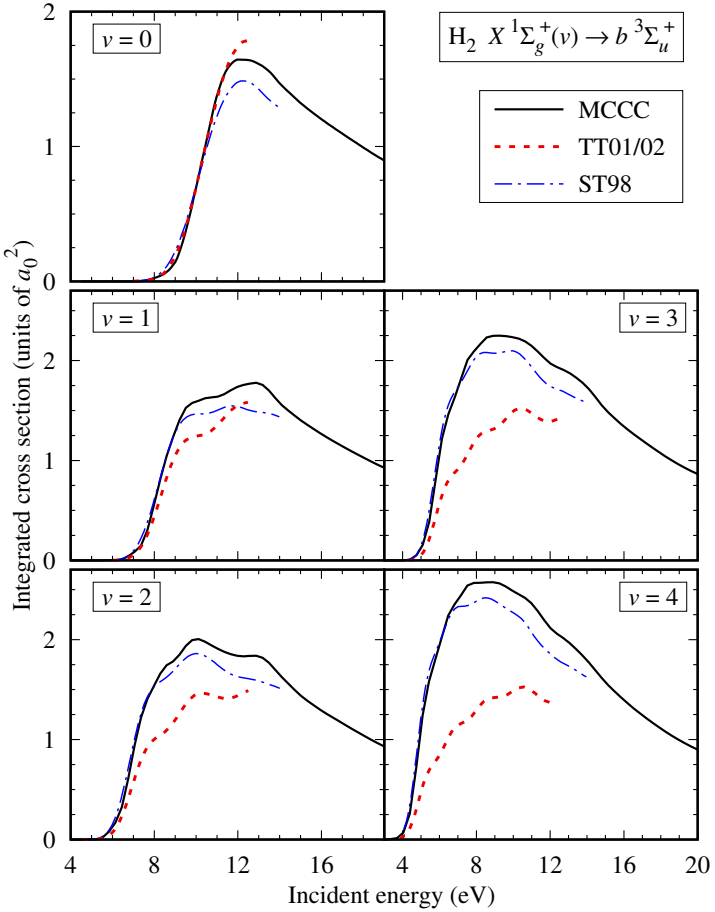

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Isotopic and vibrational-level dependence of H_2 dissociation by electron impact

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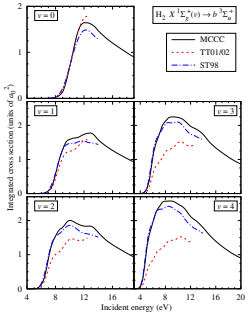

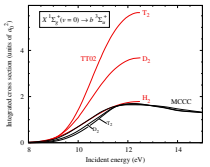

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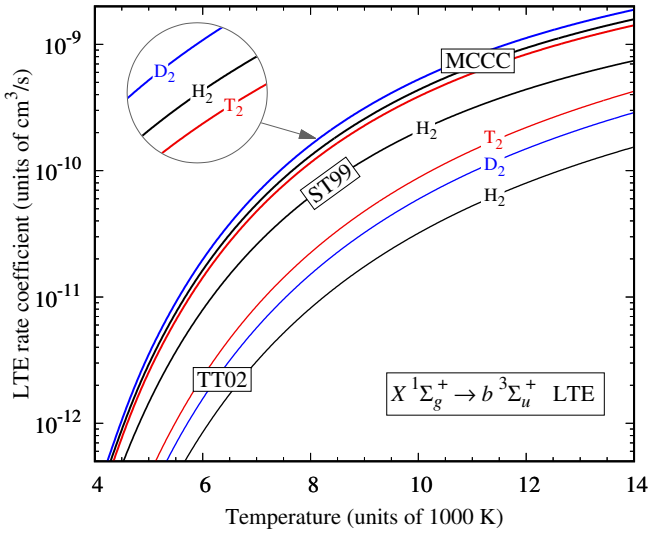


R-matrix calculations TT02: Trevisan and Tennyson, Plasma Phys. Control. Fusion **44** (2002) 1263-1276, 2217-2230

Isotopic and vibrational-level dependence of H_2 dissociation by electron impact

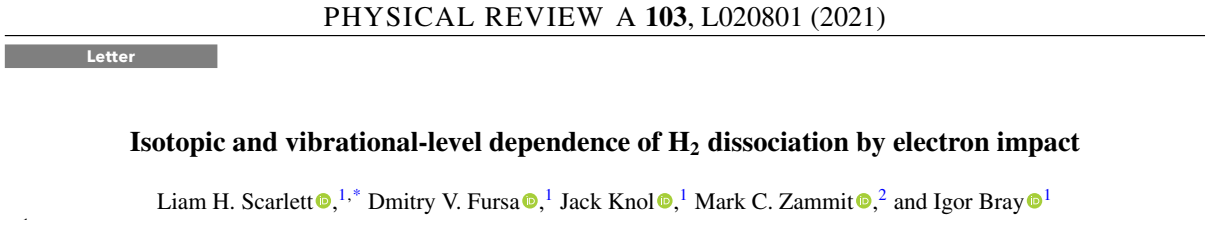
Which formula is correct?

$$\frac{\mathrm{d}\sigma}{\mathrm{d}E_{\mathrm{out}}} = \frac{\pi}{k_{\mathrm{in}}^2} \sum_{\substack{\ell' m' \\ \ell m}} \left| \langle v_{E_{\mathrm{k}}} | T_{\ell' m', \ell m}(R; E_{\mathrm{in}}) | v_v \rangle \right|^2$$

?

$$\frac{\mathrm{d}\sigma}{\mathrm{d}E_{\mathrm{out}}} = \frac{m_{\mathrm{H}}}{4\pi^3 m_{\mathrm{e}}} \frac{E_{\mathrm{k}}}{E_{\mathrm{in}}} \sum_{\substack{\ell' m' \\ \ell m}} \left| \langle v_{E_{\mathrm{k}}} | T_{\ell' m', \ell m}(R; E_{\mathrm{in}}) | v_v \rangle \right|^2$$

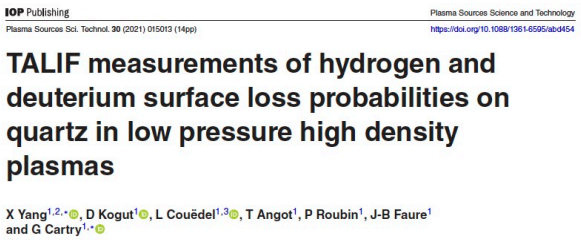
- In the paper we show that Trevisan and Tennyson's approach to deriving the dissociation cross section leads to the standard formula
- The differences in their formula are due to errors in the derivation


PHYSICAL REVIEW A **103**, L020801 (2021)

Letter

Isotopic and vibrational-level dependence of H_2 dissociation by electron impact

Liam H. Scarlett[1,*] Dmitry V. Fursa[1] Jack Knol[1] Mark C. Zammit[2] and Igor Bray[1]


IOP Publishing Plasma Sources Science and Technology

Plasma Sources Sci. Technol. **30** (2021) 015013 (14pp) https://doi.org/10.1088/1361-6595/abd454

TALIF measurements of hydrogen and deuterium surface loss probabilities on quartz in low pressure high density plasmas

X Yang[1,2,*], D Kogut[1], L Couëdel[1,3], T Angot[1], P Roubin[1], J-B Faure[1] and G Cartry[1,*]

Conclusions

- Large-scale close-coupling calculations for H_2 : produced a comprehensive dataset of e^--H_2 vibrationally resolved excitation cross sections: from the ground to n=2,3 excited electronic states, isotopically resolved dataset.
- Collisional Radiative Model for the triplet system of molecular hydrogen: using MCCC cross sections
- Produced a set of cross sections for H_2 transitions between electronically excited states
- Identified & resolved a major discrepancy for the isotopic and vibrational-level dependence of H_2 dissociation by electron impact

Thank you

- In preparation:
  - detailed data set of vibrationally resolved cross sections for H_2 for transitions between electronically excited states, + isotopologues (D_2, HD, …)
  - rotationally-resolved electron scattering on H_2 + isotopologues (D_2, HD, …)
    rovibrationally resolved cross sections
    polarization of radiation in Fulcher-α band emission ($d^3 \rightarrow a^3$)
  - vibrational close-coupling technique with exact account of coupling to electronic degrees of freedom
- Results available from LXCat and IAEA databases and MCCC database (mccc-db.org)