VIBRATIONALLY RESOLVED COLLISIONS OF HYDROGEN IONS AND MOLECULES

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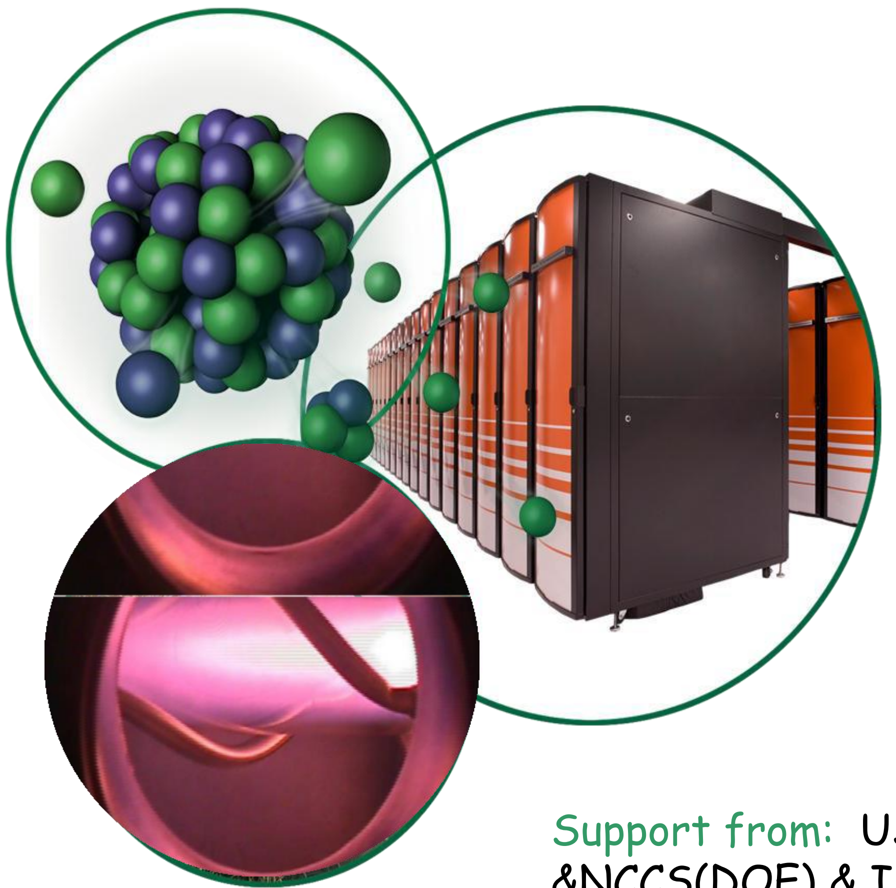

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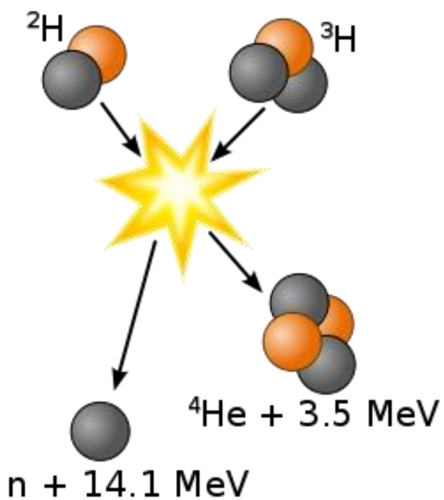
30th SPIG 2020, Virtual talk, August 24-28, Serbia

Basics of terrestrial fusion?

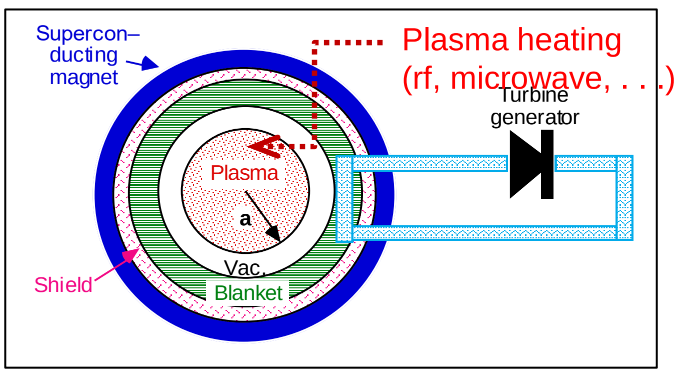


Fusion on earth (Controlled fusion!)

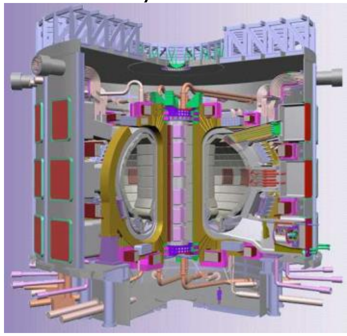
d-t fusion (more efficient)
T=150 mil K
Alpha-particles and neutrons carry most of the energy

Unlike nuclear fission where energy is volume-distributed

Schematic magnetic fusion reactor



ITER, DEMO



- Plasma-material interactions limit performance in present non-DT experiments

Atomic physics for magnetically confined fusion: Where does it meet the planetary science?

- 17 Mev per d+t fusion in plasma core (> 50 mil. K) ; 80% transferred by n to Li blanket which fuel t; 20% carried by α, 1/4 supports the plasma, rest needs to be exhausted by e, p, α via atomic inelastic processes:

- SOL plasma (50-300 eV), absence of neutrals and molecules, electron-impurity ion processes, radiative plasma cooling

Divertor region, 50 - 1 eV, $10^{14\,-15}$ cm^3, H, H_2 dominant, He, $He^{+,++}$, impurities;neutral particle transport, helium removal, recombination, collision with surfaces:

Key for thermal power exhaust problem

Planetary science is in energy a lower, partially overlapping region of collision energies!

1.Typical for the divertor **region** is formation of the molecules, particularly $\mathbf{H_2}$, $\mathbf{H_2^+}$, (if carbon facing plasma material), vib-rot excited, metals, inert gases,…

2. Huge increase of the cross sections (as n^4 for charge transfer) necessitates **electronically excited** atomic and molecular states!!!

3. **Vibrationally resolved** collisions for volume plasma recombination schemes **MAR and MAD** for hydrogen and hydrocarbons; For infrared emission plasma diagnostics; For CR models of H2/D2 plasma.

4. **High rotational temperatures** of hydrogen molecules indicated!!!

5.Tritium co-deposition in tokamaks (with carbon, with tungsten around grain boundaries, too) closely linked with the plasma **chemistry**

Why does fusion/plasma needs accurate atomic physics theory?

Answering the general question: What is the sensitivity of the plasma modeling to the uncertainty of atomic data

Simulations done by David Coster, IPP Garching
(considered CT, ionization, dielectronic recombination at H^+)

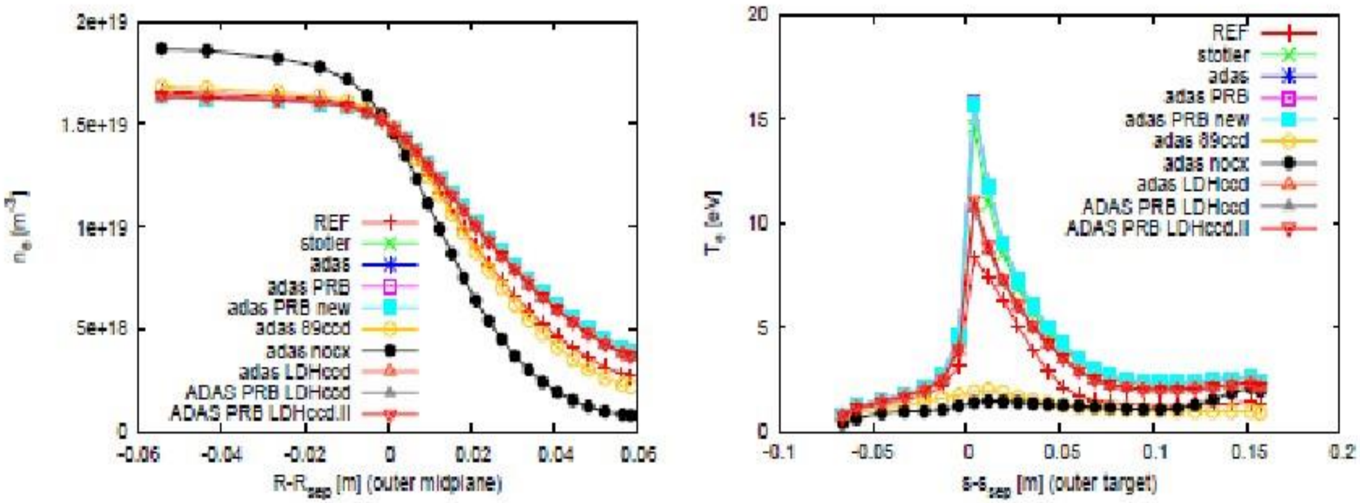


FIGURE 1. Effect of changing the atomic physics on SOLPS solutions of the electron temperature at the outer midplane (left) and outer target (right).

D. Coster et al, AIP Conf. Proc. 1125(1), 112 (2009)

Also:

D. Reiter et al, Phys. Scr. **T138, 014014 (2009) Hydrocarbon sens analysis**

And because :

For these kind of data (vib-rot-elec excit.,isotop.):

*Experiments difficult:

Impossible? Missing !

*Quality theoretical data: Sparse !

And: It is 21[st] century

$H^+ + H_2$ is the most fundamental ion-molecule system

We should know all about it

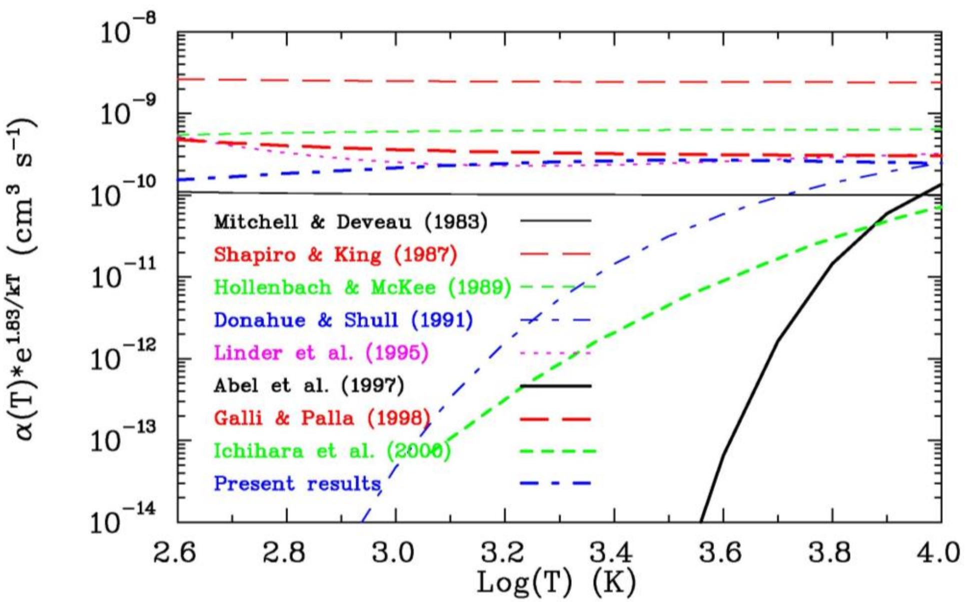
Do not know well this only (3+2)-body system?

Electronically, rovibrationally excited processes????

Also Because 2):

Example :Astrophysical applications

- **CT in H^++H_2** in the **early universe (0.1meV-10 eV)**;
- **Two-body association** (hydrogen plasma) in collapse of **interstellar clouds.**



[a bad example from astrophysical modeling community (can happen to Fusion community too)

Savin et al, ApJL (2004)]
CT in H^++H_2(v=0)

Data "produced" as fitted the need of a particular plasma-radiative model

These cannot be called scientific data!!! However a critical evaluation and recommendation can lead to the DATA!

Need for comprehensive, critically evaluated data;
Communication between various communities (theory, experimental, atomic,plasma

WHAT IS NEEDED?

Vibrationally excited: *Infrared emission plasma diagnostics.
*CR models of H2/D2 plasma.
*Lack of quantitative analysis in molecular spectr.

Rotationally : High rotational temperatures of H_2 indicated?

Electronically excited : *Huge increase of the cross sections (as n^4 for CT)
*For a complete H/H2 CR model, Hα diagnostics,
*Fulcher-band diagnostics for H_2.

Isotopic constitution : *D_2,T_2, HD, HT and DT, Sensitive on vib. energy levels
and excitation *Wherever internal energy plays role
("ion conversion").
*No data for excited molecules.
*Ex.:$\sigma_{pex}(D^+ + H_2 \rightarrow HD + H^+)$ » 10 $\sigma_{pex}(D^+ + HD \rightarrow D_2 + H^+)$.

WHAT HAVE WE DID WITH VIBRATIONAL RESOLUTION?

- Comprehensive QM calculations of cross sections,
- on the "same footing"
- 0.5-100 eV collision energy

$$H^+ + H_2(v_i) \leftrightarrow H^+ + H_2(v_f), v_{i,f} = 0\text{-}14$$ EXC

$$H^+ + H_2(v_i) \leftrightarrow H(1s) + H_2^+(v_f), v_i = 0\text{-}14, v_f = 0\text{-}19$$ CT

$$H^+ + H_2(v_i) \leftrightarrow H^+ + H + H, v_i = 0\text{-}14.$$ DISS

$$H + H_2^+(v_i) \leftrightarrow H + H_2^+(v_f), v_{i,f} = 0\text{-}19$$ EXC

$$H + H_2^+(v_i) \leftrightarrow H^+ + H_2(v_f), v_i = 0\text{-}19, v_f = 0\text{-}14$$ CT

$$H + H_2^+(v_i) \leftrightarrow H + H^+ + H, v_i = 0\text{-}19.$$ DISS

$$H^+ + H + H \leftrightarrow H^+ + H_2(v_f), v_f = 0\text{-}14.$$ ASSOC

$$H^+ + H + H \leftrightarrow H + H_2^+(v_f), v_f = 0\text{-}19$$ ASSOC

+ENERGY&ANGULAR SPECTRA (DISS)

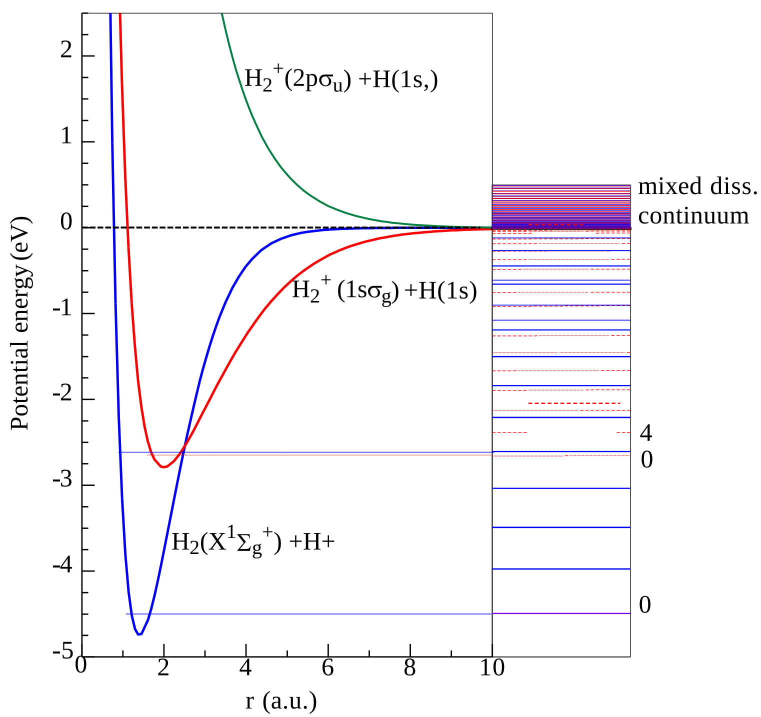
HOW?

By understanding the underlying physics FIRST (What to expect?)

Place of events: H_3^+

Two lowest electronic surfaces

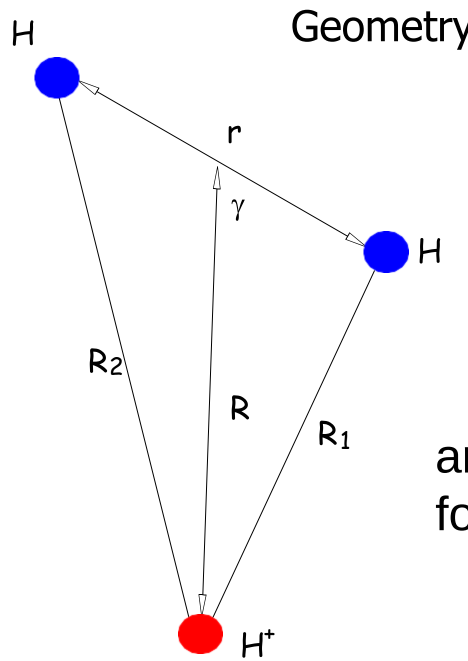
Fragments of H_3^+ (H_2, H_2^+, H, H^+)



At R = infinity

The approximation:
Sudden approximation for target rotations (IOSA): γ frozen

IOSA γ:"frozen"



and, similarly, for H+H_2^+

Jacoby coordinates

Cross sections averaged over γ

How did we approach for E< 10 eV?
Fully QM!!

- Diabatic representation for two electronic surfaces
- Large configuration space in r and R (40 a.u.)
- Dissociative continuum discretized in more than 800 states;

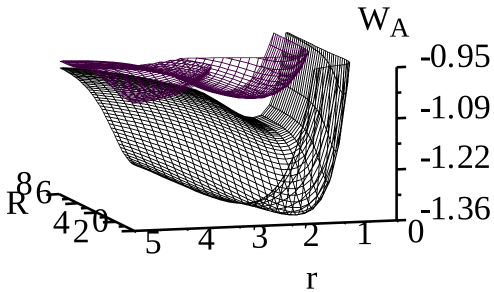
- Solve resulting Schrödinger equation by expanding in diabatic **vibrational basis** (bound + continuum)

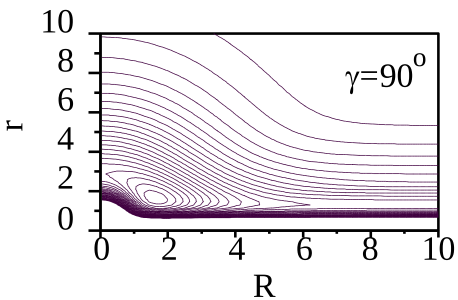
$$\left[-\frac{1}{2\mu}\left(\frac{\partial}{\partial R^2}+\frac{\partial}{\partial r^2}\right)I+\frac{l(l+1)}{2\mu R^2}I+\frac{j_0(j_0+1)}{2\mu r^2}I+\overline{W}(R,r,\gamma)-EI\right]\overline{\Psi}_l(R,r,\gamma)=0$$

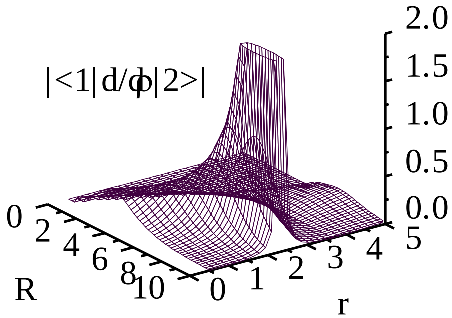
Resulting equation is a system of ordinary differential equations : Variable is R

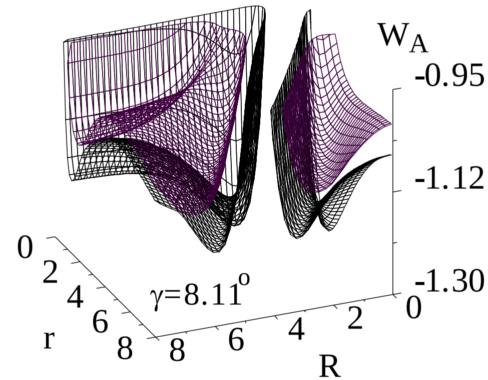
“Battle field of hydrogen molecule:
Two-electronic, strongly coupled potential-surfaces of H_3^+; Reactive

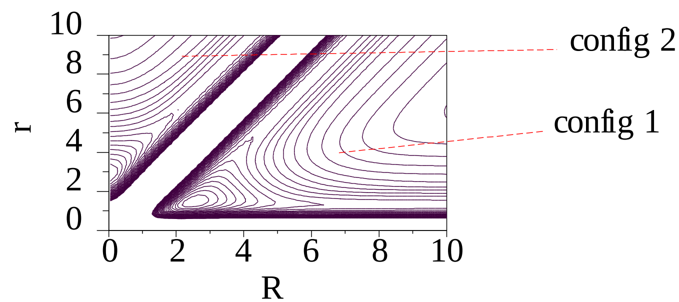
Physics highly dependent on projectile-diatom angle; Reactive at small γ

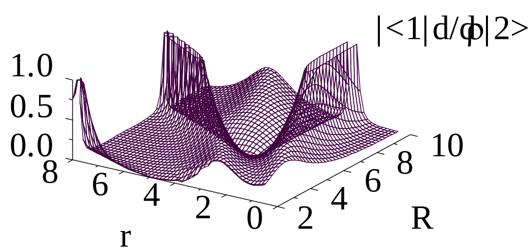










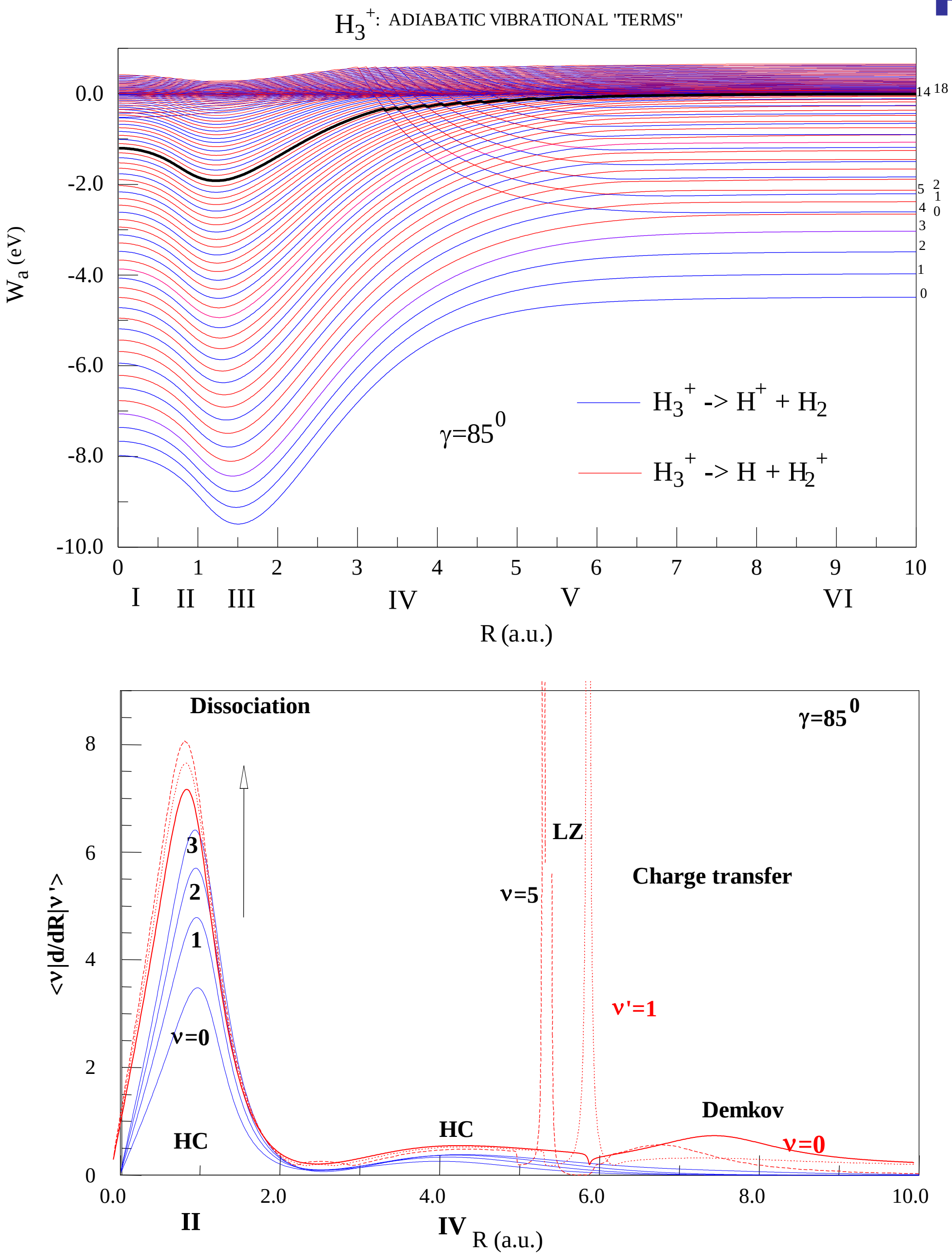


Violent coupling (CT)
Need trans to diabatic representation

Reactive at very large r for large γ
Need large config space (40 a.u.)

Why is this so difficult?

Physics in direct channel



Extensively rich

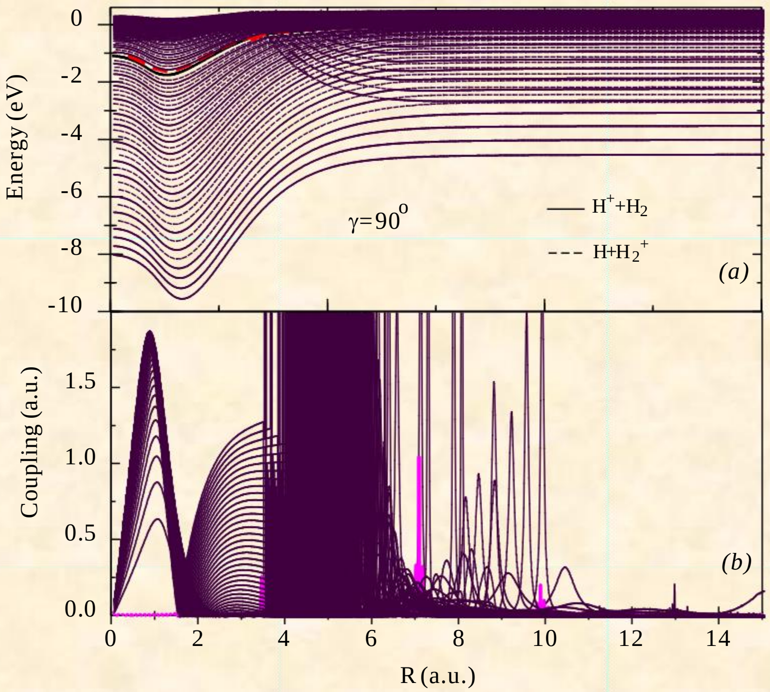
Dissociative continuum discretized

- We describe both electronic and nuclear motion quantum-mechanically
- Solve resulting Schrödinger equation by expanding in diabatic vibrational basis
- Several hundreds states to converge

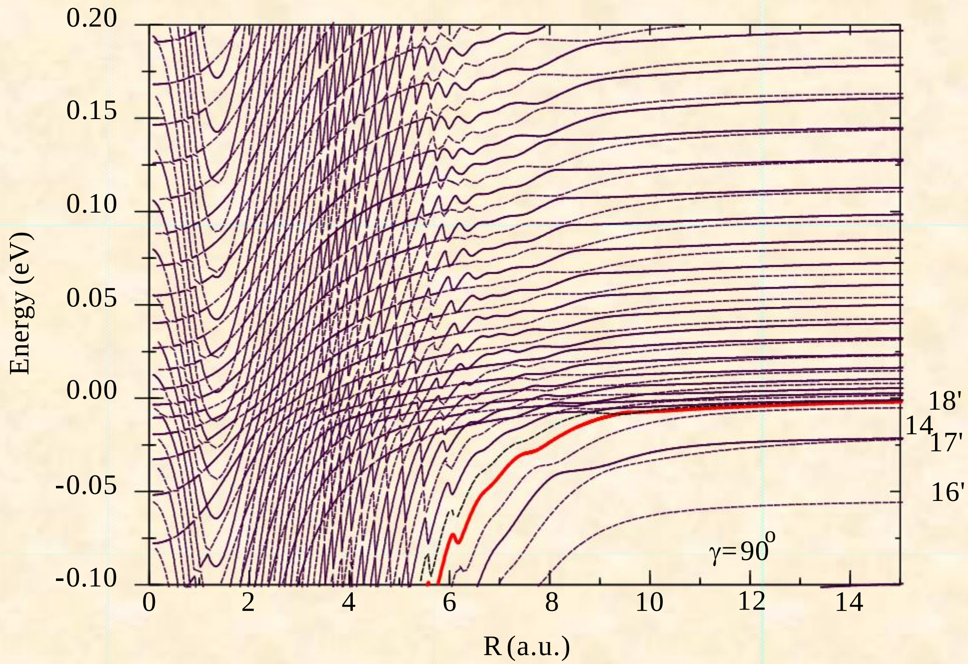
Too many states and processes!!!

Collision dynamics extensively rich (within both bound states and continuum)

Red line: Dynamically changing continuum edge.



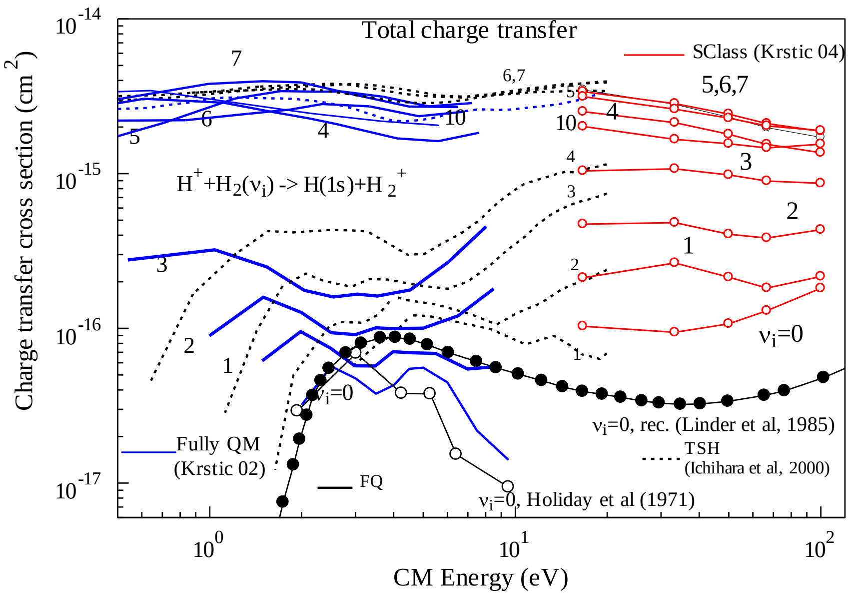
Adiabatic vibronic states and nonadiabatic couplings



Dynamics in the dissociative continuum mimics discrete states dynamics

Verification of data in action: Calculations of various energy scales by different methods and comparison where they overlap

$$H^+ + H_2(v_i) \rightarrow H + H_2^+$$



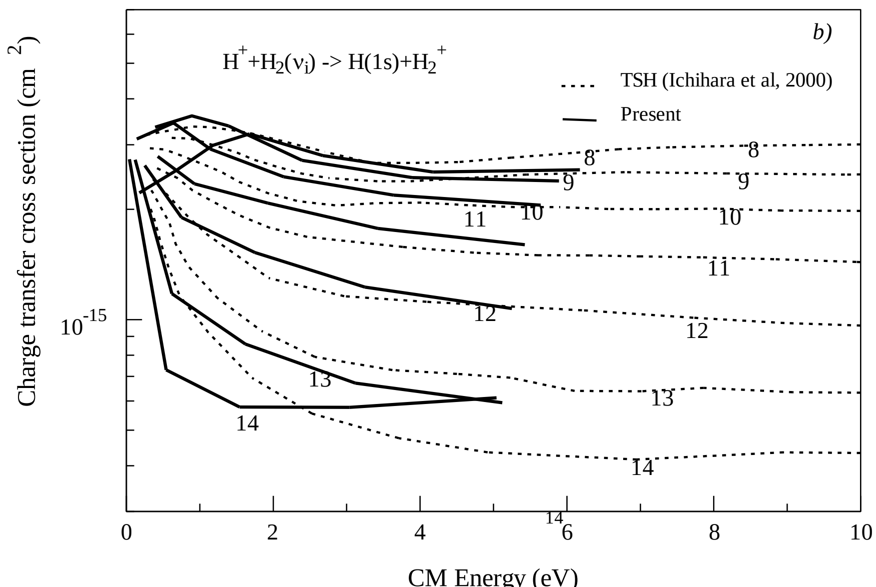


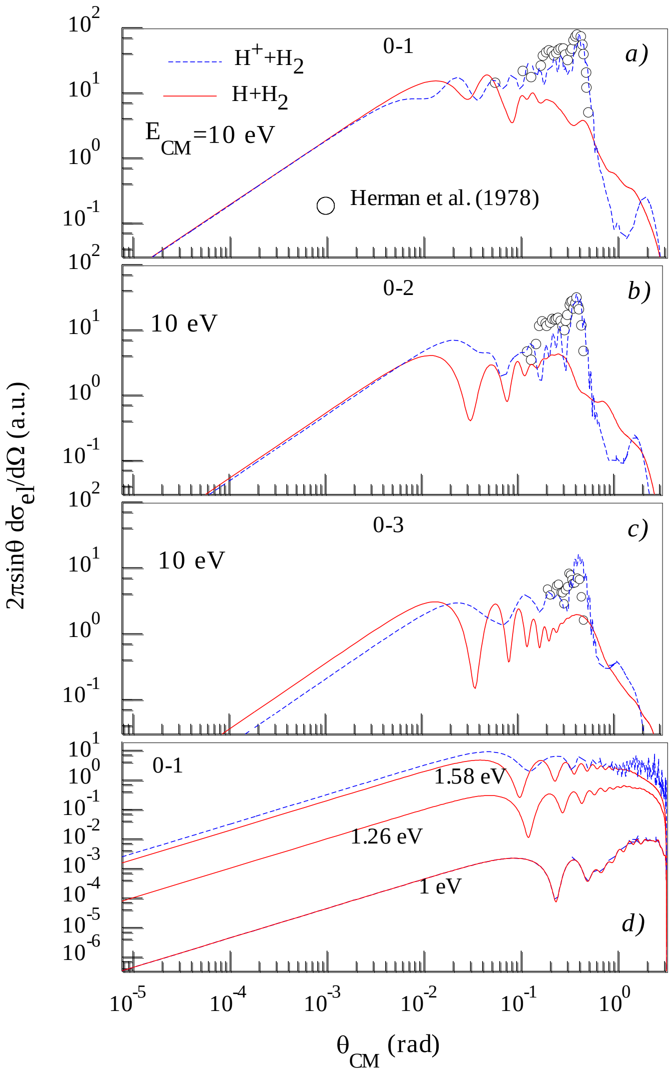
Fig. 1b)

Note comparison with Holiday's experiment :**Validation for v=1 and 0 only**

Also comparison with Ichihara semi-classical calculation,

and our semi-classical calculation

Validation in action: Comparison with experiment



Krstic, 1998

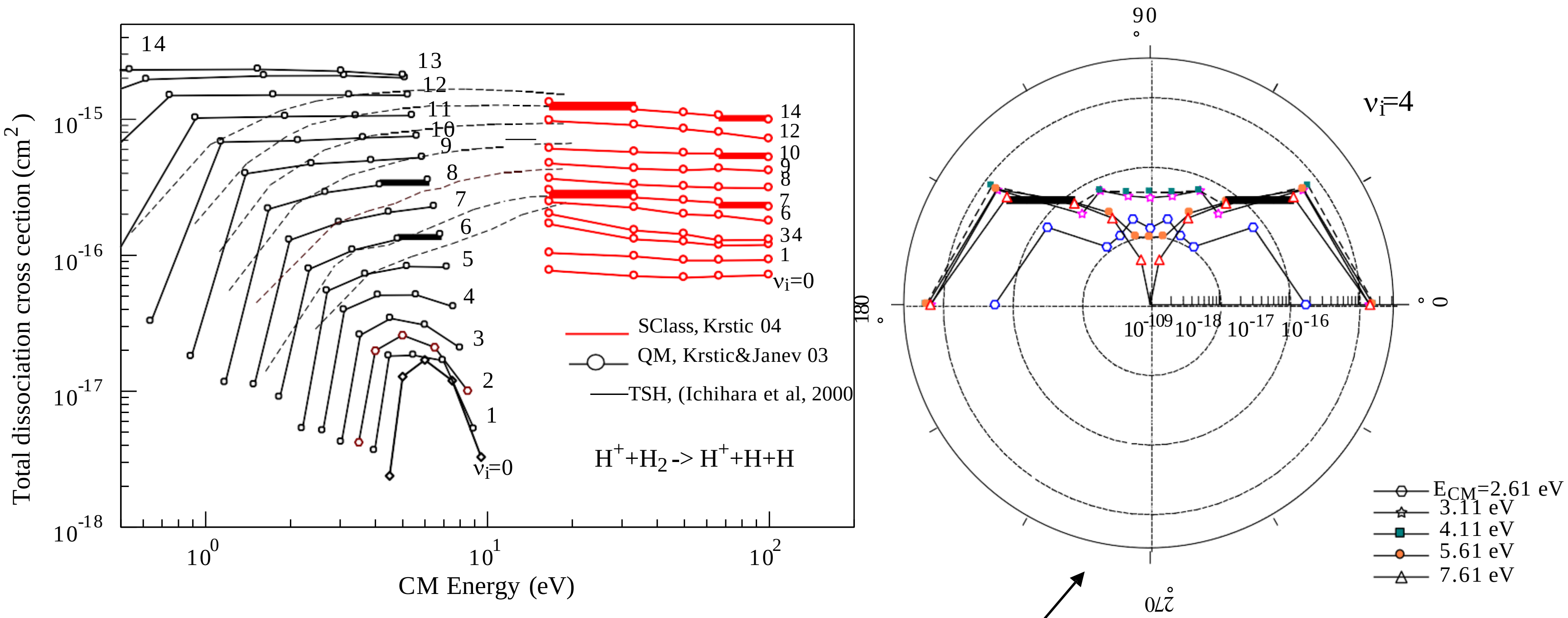
Vibrational excitation: Differential cross sections

More on comparisons with sparse experiments.

DCS for excitation to the first three vibrationally states from the ground state.

Excellent agreement! Partially validated!

Dissociation from various υ $H^{+}+H_2$



Total dissociation from vibrationally excited target
Direct; CT dissociation
Differential cross section (angular, momentum)

Collisionally assisted diatomic association (also known as three-body recombination)

Two atoms (or ion-atom) associate in presence of a third particle which “relaxes” the excess energy and momentum.

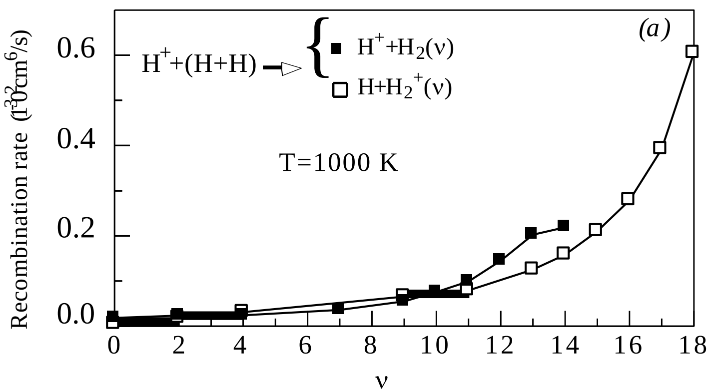
Possible processes:

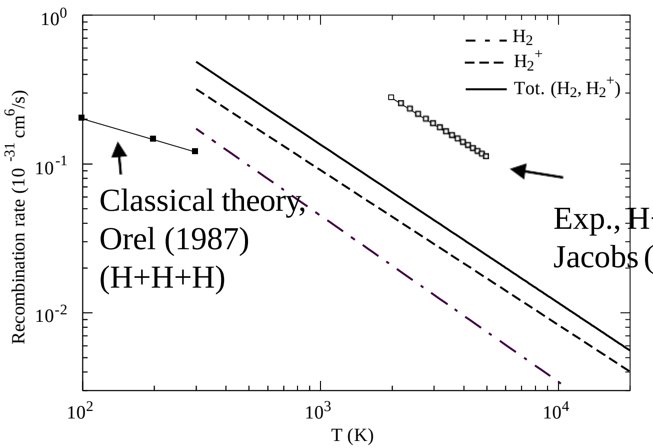
$H^+ + (H+H) \rightarrow H^+ + H_2$ direct association
$\rightarrow H + H_2^+$ charge transfer association

$H + (H^+ + H) \rightarrow H^+ + H_2$ charge transfer association
$\rightarrow H + H_2^+$ direct association

Range of values:
5×10^{-32}-6×10^{-34}
(200-20,000K)

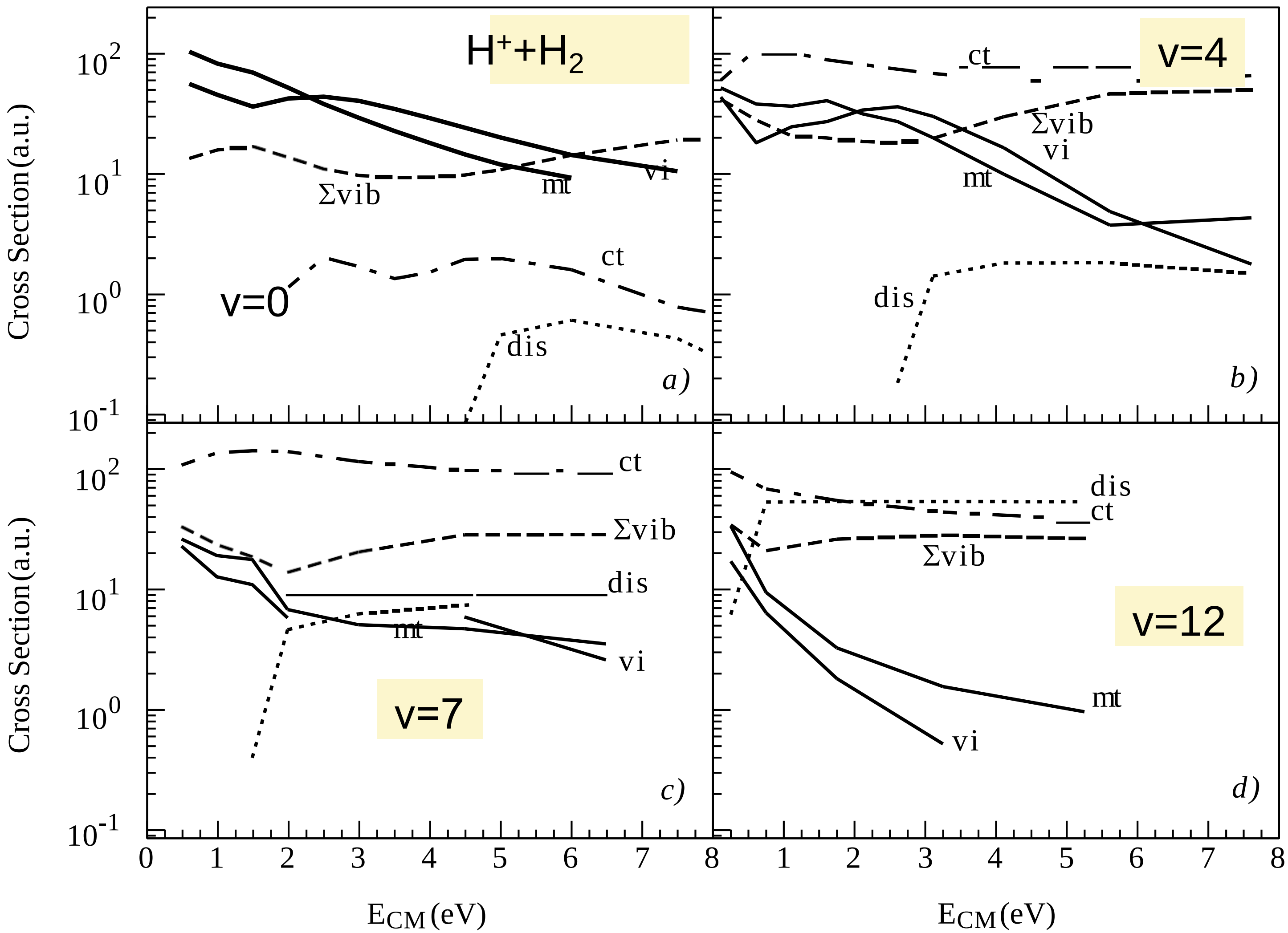
Krstic et al, JPBL 36, L249 (2003)

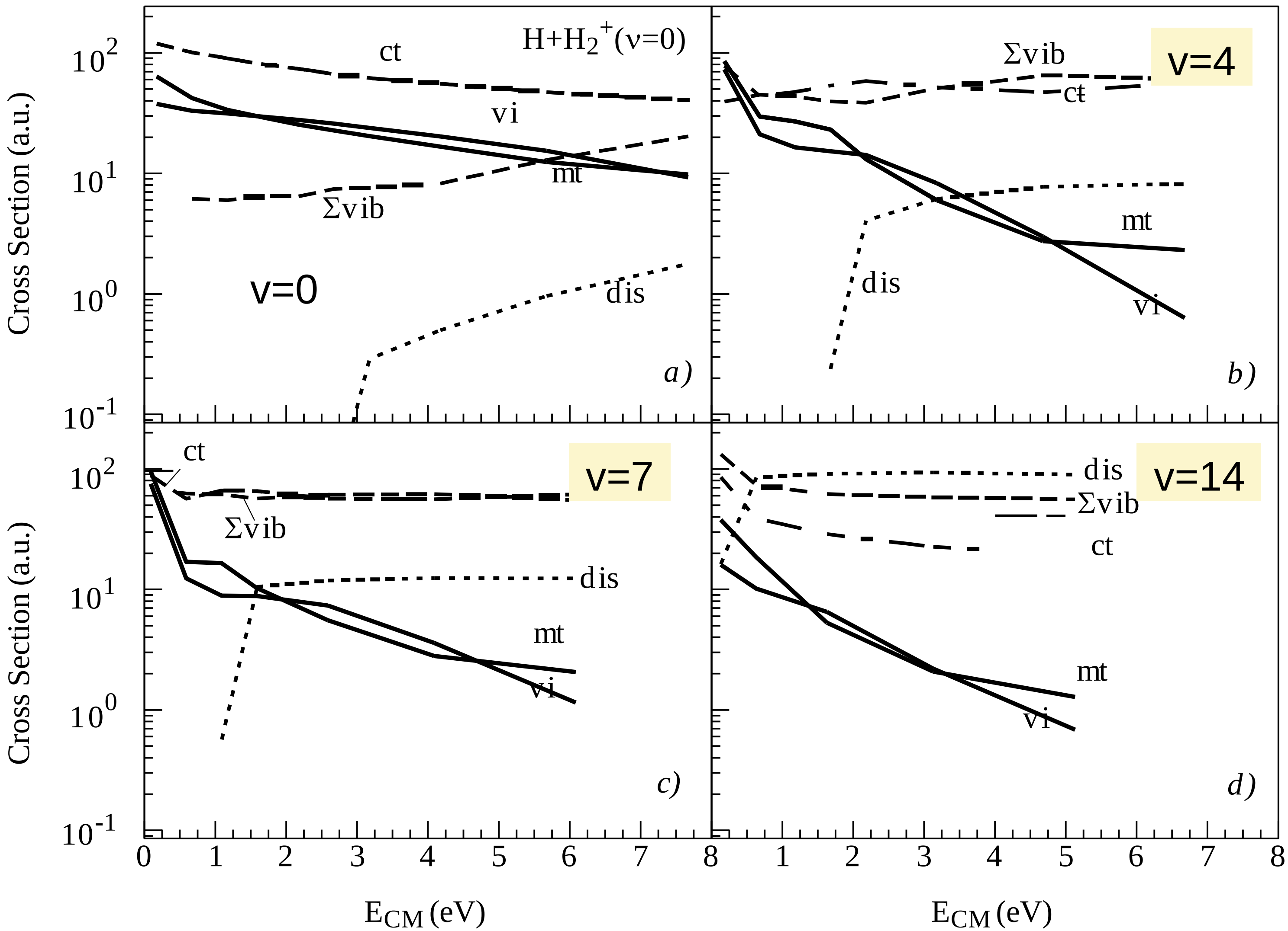




Dominance of the H2+ creation in both cases

"Interplay" of transport and inelastic processes




H+H2+(v=0)
ct
vi
mt
Σvib
dis
v=0
a)
v=4
Σvib
ct
mt
dis
vi
b)
v=7
ct
Σvib
dis
mt
vi
c)
v=14
dis
Σvib
ct
mt
vi
d)
Cross Section (a.u.)
ECM (eV)

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Thank You