NON-AUTOIONIZING Σ^- STATES OF MOLECULAR HYDROGEN

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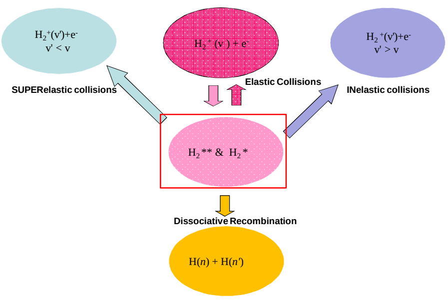
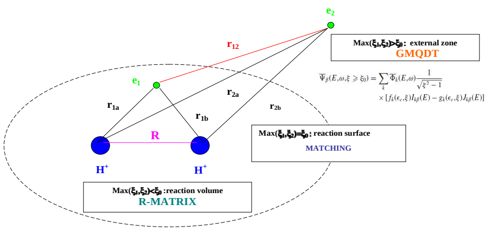
Introduction

The excited states of H_2 are involved in all the molecular processes



Halfium Model

In this work, we investigate Rydberg and doubly-excited states of the H_2 molecule. The molecule is treated in a collisional approach as consisting of a H_2^+ ionic core and an external electron which can be either in a Rydberg or continuum state.



$$\Psi_\beta = \sum_{ij} c_{ij}^\beta \bar{y}_{ij}$$

The configuration space is divided in two regions:
(i) Reaction volume: short range interactions
(ii) External zone : long range interactions

Formalism

The two-electron basis functions, of molecular hydrogen, is defined in the spheroidal coordonates as:

$$\bar{y}_{ij} = \bar{N}_{ij}\left\{\begin{array}{l}\left(\Phi_{i+}(\vec{r}_1)\Phi_{j-}(\vec{r}_2)+(-1)^s\left(\Phi_{i+}(\vec{r}_2)\Phi_{j-}(\vec{r}_1)\right)\right)+\left(-1\right)^q\\ \left(\Phi_{i-}(\vec{r}_1)\Phi_{j+}(\vec{r}_2)+(-1)^s\left(\Phi_{i-}(\vec{r}_2)\Phi_{j+}(\vec{r}_1)\right)\right)\end{array}\right.$$

q quantum number associated to σ_v operateur (σ_v corresponding to a reflection at a plane containing the nuclei) **[1], [7]**

Reaction volume: R-matrix

External zone: GMQDT

Matching on $\xi=\xi_0$

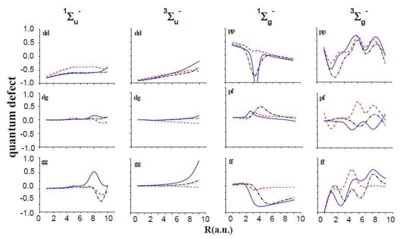
$$\left\{\begin{array}{l}\bar{u}_{k\beta}(\xi_0) = \langle\langle \bar{\Phi}_k(\omega)|\bar{\Psi}_\beta(\omega,\xi_0)\rangle\rangle = f_k(\xi_0)I_{k\beta} - g_k(\xi_0)J_{k\beta}\\ b_\beta \bar{u}_{k\beta}(\xi_0) = f_k'(\xi_0)I_{k\beta} - g_k'(\xi_0)J_{k\beta}\end{array}\right.$$

Short range reaction matrix: $\mathbf{K} = \mathbf{J}\mathbf{I}^{-1}$

Quantum defect: **[4] ,[5]** $\mu = \dfrac{1}{\pi}\arctan[\mathbf{K}]$

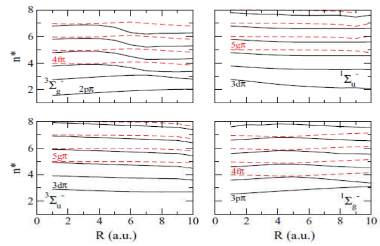
Results

Quantum defects μ(R): $U_n(R) = U^+(R) - \dfrac{1}{[n-\mu(R)]^2}$



The evolution of the quantum defect give us information about the bounding and anti-bounding states

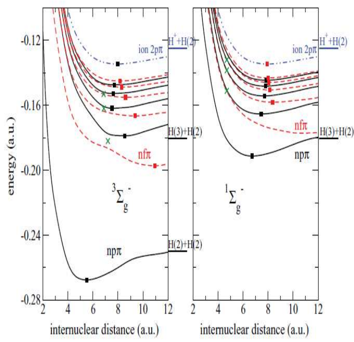
Effective principal quantum number for core excited Σ^- states of H_2



$$n^*(R) = n - \mu(R) \qquad n^* = \frac{1}{\sqrt{2\left(E_{2p\pi(H_2^+)} - E\right)}}$$

The avoided crossing between the p and f series

Energies of Σ^- states

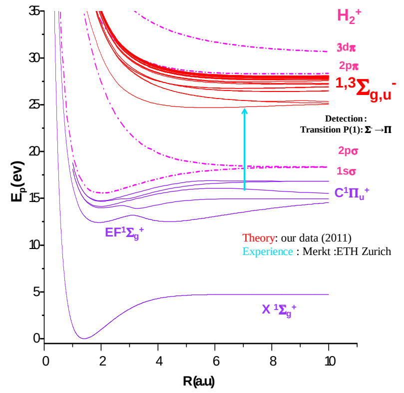


Non autoinising sates of H_2 situated at high energy (~25eV)

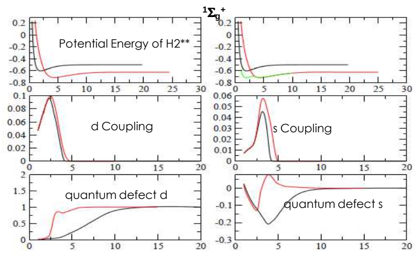
Our results are in good agreement with quantum chemical calculations **[3]** available only for the lowest state of each symmetry Σ^-

Conclusion and perspective

Potential energy curves of H_2^+ and H_2 : Position of Σ^- states

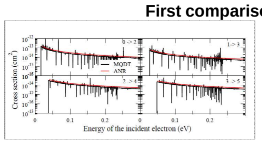


Sample of data used in the molecular processes computation

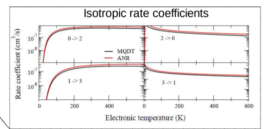


Comparison between our data in red and the previous data used

First comparison



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



Comparison of MQDT result (details of theory **[8]**) to Adiabatic Nuclear Rotation approximation (ANR) ones **[9], [10]**

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