Oddělení spektroskopie,
Oddělení chemie iontů a klastrů
a Oddělení teoretické chemie
ÚFCH JH AV ČR

srdečně zvou všechny zájemce na **mimořádný seminář zahraničního hosta**,
na kterém promluví:

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(Department of Imaging and Applied Physics,

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na téma:

" Electron and positron scattering from molecular hydrogen and its ion"

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Juraj Fedor **Ondřej Votava**

Electron and positron scattering from molecular hydrogen and its ion

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The convergent-close-coupling (CCC) method has achieved considerable success in providing accurate collision data for electron and positron scattering from atoms and ions [1,2]. The fundamental strength of the method is its ability to account for coupling to the ionisation channels. The target continuum is incorporated to convergence utilising pseudostates obtained via diagonalisation of the target Hamiltonian in a complete Sturmian (Laguerre) basis. The CCC implementation for atoms is a complete scattering theory in the sense that it yields accurate elastic, excitation, and ionisation cross sections irrespective of the projectile energy.

The CCC method has recently been extended to model electron and positron collisions with molecules. For these types of collisions it is our aim to provide a comprehensive set of cross sections that are demonstratively convergent and valid over a wide range of incident energies. In this talk I will present results for three projects:

- electron scattering from hot (vibrationally excited) molecular hydrogen ion [3],

- electron scattering from molecular hydrogen [4],

- positron scattering from molecular hydrogen [5].

For e-H_2^+ and e^+-H_2 scattering we performed calculations in the adiabatic nuclei approximation and for e-H_2 scattering the fixed-nuclei approximation was utilised. Agreement with experimental results is very good for all cases. As a demonstration of the method we present electron-impact ionisation cross sections of H_2^+ and H_2 molecules in Fig. 1 and the grand total scattering cross section for positron scattering of H_2 in Fig.2.

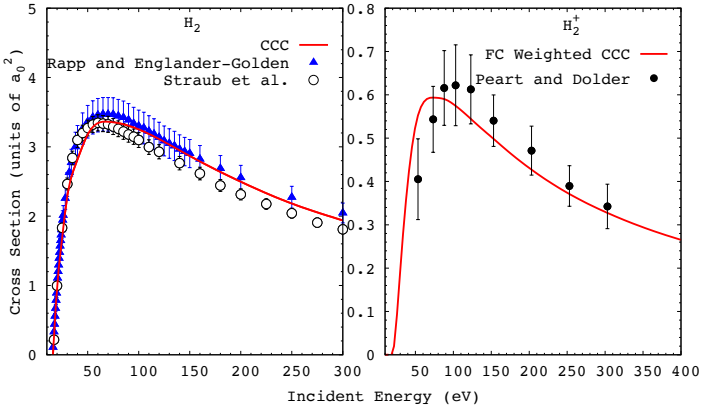

Figure 1. Ionisation cross sections for electron scattering from H_2 [4] and vibrationally excited H_2^+ [3].

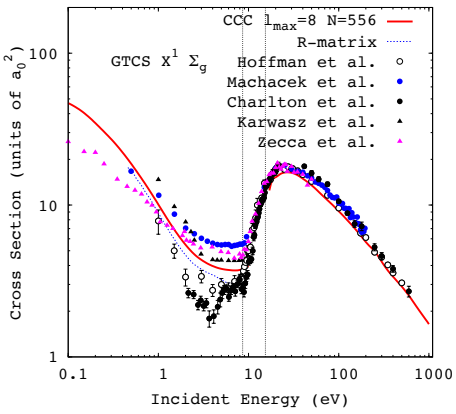

Figure 2. Grand total scattering cross section for positron scattering from H_2 [5].

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