Calculations of electron and positron scattering from vibrationally excited H^{2+} and H_2

2015 J. Phys.: Conf. Ser. 635 072047

(http://iopscience.iop.org/1742-6596/635/7/072047)

XXIX International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC2015) IOP Publishing
Journal of Physics: Conference Series **635** (2015) 072047 doi:10.1088/1742-6596/635/7/072047

Calculations of electron and positron scattering from vibrationally excited H_2^+ and H_2

Mark C. Zammit [1], **Jeremy S. Savage, Dmitry V. Fursa, and Igor Bray**

Department of Physics, Astronomy and Medical Radiation Sciences, Curtin University, GPO Box U1987, Perth, WA 6845, Australia

Synopsis Electron and positron scattering from the vibrationally excited H_2^+ and H_2 molecules were investigated using the adiabatic-nuclei convergent close-coupling method. Converged results are presented for a range of vibrationally excited states.

Collision data of electron and positron scattering from vibrationally excited molecules is particularly important in the modelling of fusion plasmas and in the calculation of gas and soft-condensed (biological) matter transport properties. Recent scattering studies indicate a large dependence on the initial vibrational state of the molecule [1, 2]. Utilising the *ab initio* adiabatic-nuclei convergent close-coupling (CCC) method, formulated in both the spherical [1] and spheroidal coordinate systems, we investigate electron scattering from vibrationally excited H_2^+ and positron scattering from vibrationally excited H_2. Converged results in both the multichannel and partial-wave expansions are presented over a broad energy range for elastic, vibrational excitation, electronic excitation, grand total and total ionisation cross sections.

In Fig. 1 we present dissociative excitation (DE) cross sections for electron scattering from H_2^+ in the initial vibrational state v_i. The DE cross sections have a major dependence on v_i. For example, at 20 eV the $v_i = 9$ DE cross section is 500% larger than the $v_i = 0$ state. As v_i increases the DE cross sections monotonically increase and the cross section peak shifts to lower energies.

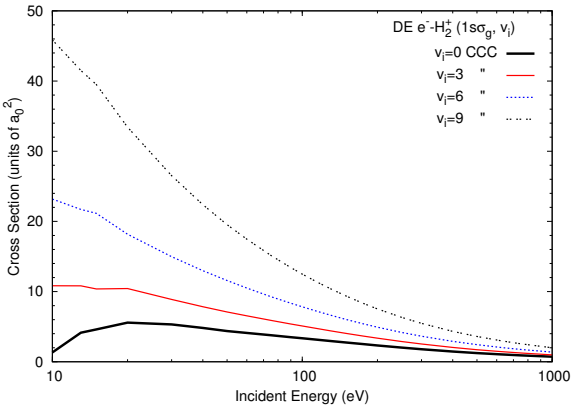

Figure 1. Dissociative excitation (DE) cross sections for electron scattering from H_2^+ in the vibrational state v_i.

The $0 \rightarrow 1$ vibrational excitation cross section for positron scattering from H_2 is presented in Fig. 2. Results are calculated directly from the adiabatic-nuclei approximation and are in excellent agreement with the measurements of Sullivan *et al.* [3].

Our preliminary results of positron scattering from H_2 in the initial vibrational state $v_i = 1$ indicate a major dependence on v_i in the low-energy region. At 3 eV the $v_i = 1$ grand total cross section is approximately 25% larger than the $v_i = 0$ cross section.

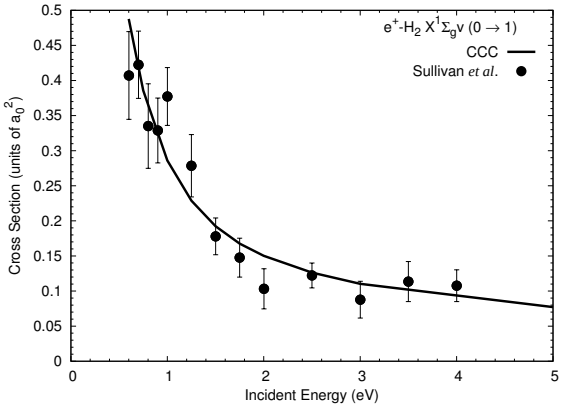

Figure 2. Vibrational $0 \rightarrow 1$ excitation cross section for positron scattering from H_2. Adiabatic-nuclei convergent close-coupling (CCC) results are compared with the measurements of Sullivan *et al.* [3].

References

[1] M. C. Zammit *et al.* 2014 *Phys. Rev. A.* **90** 022711

[2] M. C. Zammit *et al.* 2013 *Phys. Rev. A.* **88** 062709

[3] J. P. Sullivan *et al.* 2002 *Nucl. Instr. Meth. B.* **192** 3

[1] E-mail: mark.zammit@postgrad.curtin.edu.au