

THE SCHWINGER VARIATIONAL PRINCIPLE TO ELECTRON-MOLECULE COLLISIONS

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ABSTRACT

We calculated differential cross sections for scattering of low-energy electrons by CH₄ and SiH₄ molecules. The calculations employed the Schwinger variational principle with plane waves as a trial basis set (J.L.S. Lino, M.A.P. Lima, Braz. J. Phys. 30, 432 (2000)). Our differential cross sections are found to be in good agreement with experimental data and theoretical results.

1. INTRODUCTION

The process of scattering of low-energy electrons by molecules plays an important role in the description of cold plasmas that are currently used in technological applications [1]. For example, the dissociation cross sections of molecules of the gas are fundamental in plasma etching and plasma enhanced vapor deposition [2]. It follows that the knowledge of elastic and inelastic cross sections for a wide range of molecular systems is a very important subject. Several methods have been developed as the Schwinger multichannel method (SMC) [3], the Kohn variational method [3] and R-Matrix [3]. We have previously discussed the Schwinger variational principle (SVP) for electron-molecule collisions and to account for polarization effects and multichannel coupling (due to inelastic processes involving energetically open electronic excited process), were introduced modifications into the SVP and created the so-called Schwinger multichannel method (SMC) [3]. The main limitation of the SMC method resides on what makes it a general method: the expansion of the scattering functions is done in a L^2 basis (Cartesian Gaussian functions) and this is effective only for short-range potentials. An important development of the method would be to allow inclusion of plane waves (PW) in the scattering basis. Recently we have presented some studies of the Schwinger variational principle with plane waves as a trial basis set (SVP-PW) where we have tested the Born-Ochkur approximation to include the effect of electron exchange [4-7]. In this paper we present elastic differential cross sections for e^- -CH₄, and e^- -SiH₄ scattering.

2. FORMALISM

Details of the Schwinger variational principle have been discussed extensively elsewhere [5-8]. Here we will review a few steps in the development, which are essential to the present discussion.

In the SVP for electron-molecule elastic scattering, the bilinear form of the scattering is

$$f(k_f, k_i) = - (1/2\pi) \{ \langle S_{kf} | V | \Psi^{(+)} \rangle + \langle \Psi^{(-)} | V | S_{ki} \rangle - \langle \Psi^{(-)} | V - VGV | \Psi^{(+)} \rangle \} \quad (1)$$

Here $|S_{ki}\rangle$ is the input channel state represented by the product of a plane wave k_i times, the initial (ground) target state. $|S_{kf}\rangle$ has an analogous definition, except that the plane wave points to k_f , V is the interaction between the incident electron and the target, G (or $G^{(+)}$) is the projected Green's function [8]. The scattering states $|\Psi^{(+)}\rangle$ and $\langle\Psi^{(-)}|$ are products of the target wave function $|\phi\rangle$ and one-particle scattering wave function. The initial step in our SVP calculations is to expand the one-particle scattering wave functions as a combination of plane waves. So, for elastic scattering, the expansion of the scattering wave function is done in a discrete form as

$$|\Psi^{(+)}\rangle = \sum a_m(k_m) |\phi k_m\rangle$$

$$\langle\Psi^{(-)}| = \sum a_n(k_n) \langle\phi k_n| \quad (2)$$

The inclusion of these definitions in Eq.(1) and the application of a stationarity condition with respect to the coefficients, gives the working form of the scattering amplitude:

$$f(k_f, k_i) = - (1/2\pi) \times [\sum \langle S_{kf} | V | \phi k_m \rangle (d^{-1})_{mn} \times \langle k_n \phi | V | S_{kf} \rangle]$$

where:

$$d_{mn} = \langle \phi k_m | V - VGV | \phi k_n \rangle \quad (3)$$

We have implemented a set of computational codes to evaluate all matrix elements. The Green's function and its associated discontinuities have been examined and treated in

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a similar way as in the subtraction method [9-11]. We have considered the effect of including exchange in the SVP-PW by replaning first Born approximation f_{FBA} by $f_{\text{FBA}} + g$ where “g” is the Born-Ochkur exchange amplitude [12] and our main interest is to check if the SVP-PW plus Born-Ochkur approximation is capable of describing the structures in the differential cross sections (DCS).

3. RESULTS

As a first application of our formulation we have calculated elastic differential cross sections (DCS) for electron-impact energies of 12.5, 15.4, and 30 eV for CH_4 , 7.5 and 15 eV for SiH_4 . We have used Hartree-Fock calculations to represent the ground state of Methane and Silane with the same Cartesian Gaussian basis set expansion used in previous calculations [13-15]. Figure 1 shows our DCS at 12.5 eV for electron-Methane and we have compared with experimental data [16] and theoretical cross sections as the Schwinger multichannel method [17]. As noted, at 12 eV the SVP-PW have a good agreement with experimental and theoretical results. In figure 2 (at 15.4 eV) for comparison we have also included the Schwinger variational iterative method (SVIM) using exchange plus polarization effects [17] and as observed our DCS agree well with the SIVM results. Figure 3 shows our DCS at 30 eV with experimental data [16] and the iterative Schwinger variational method [17]. The comparison between our results and theoretical and experimental results are very similar. For the SiH_4 in figure 4, we have shows DCS at 7.5 eV compared with the Schwinger multichannel method-SMC (using exchange effects) [18] and experimental data [19].

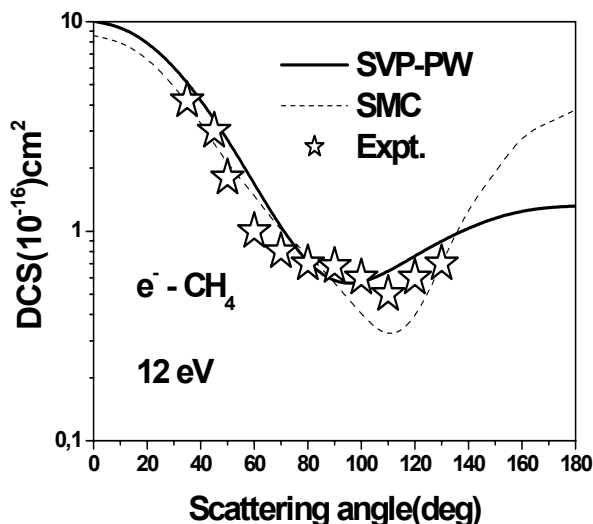


Figure 1 - Elastic differential cross sections for electron- CH_4 at 12 eV. Solid line (SVP-PW), Star (experimental results of Ref. [16]), Dashed line (Schwinger multichannel method of Ref [18]).

As observed, our results are very similar with experimental and theoretical results. In figure 5 we have shows DCS at 10 eV compared with experimental data [19] and theoretical results [20].

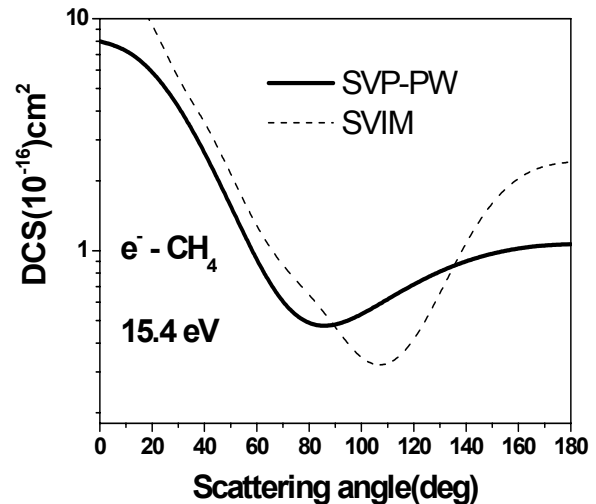


Figure 2 - Elastic differential cross sections for electron- CH_4 at 15.4 eV. Solid line (SVP-PW), Dashed line (Schwinger variational iterative method of Ref [18]).

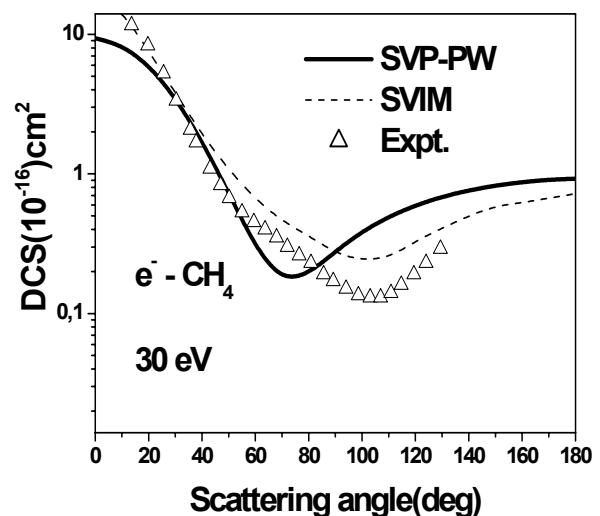


Figure 3 - Elastic differential cross sections for electron- CH_4 at 30 eV. Solid line (SVP-PW), Star (experimental results of Ref. [16]), Dashed line (Schwinger variational iterative method of Ref [18]).

4. CONCLUSION

We have presented calculations for elastic differential cross sections for CH_4 and SiH_4 by electron impact. Our results are, in general, in good agreement with experimental and

other theoretical methods. The present study helps to demonstrate the utility of SVP-PW to molecular systems.

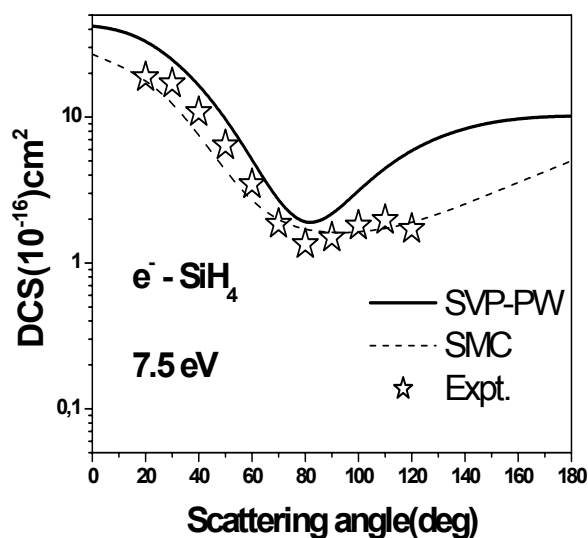


Figure 4 - Elastic differential cross sections for electron- SiH_4 at 7.5 eV. Solid line (SVP-PW), Star (experimental results of Ref. [19]), Dashed line (Schwinger multichannel method of Ref [20]).

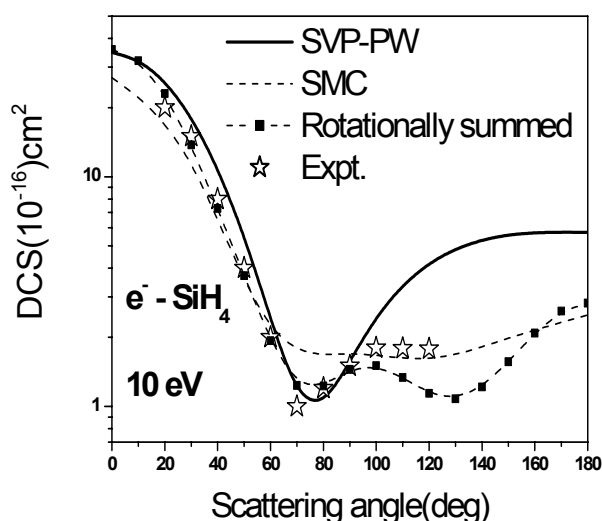


Figure 5 - Elastic differential cross sections for electron- SiH_4 at 10 eV. Solid line (SVP-PW), Star (experimental results of Ref. [19]), Dashed line (Schwinger multichannel method of Ref [18]), Dashed line with square (rotationally summed results of Ref. [19]).

5. ACKNOWLEDGEMENTS

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