

Investigation of low energy electron interaction with silane molecules

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Synopsis Total and momentum transfer cross sections are calculated for the scattering of electrons from SiH_4 molecules in electron energy region of 0.1 – 20 eV. A parameter-free spherical optical potential (SOP) approach in the fixed nuclei approximation is applied. The present calculated results are compared with the available other calculations and the experimental measurements. The quantitative features of the scattering parameters (such as Ramsauer - Townsend minimum and shape resonance structure) as observed in experiments, are well reproduced in this study.

Knowledge of scattering cross sections for interaction of electrons with silane (SiH_4) molecules are very important in many fields of research including industries, space science, surface modification technique and even in fundamental chemistry. In the silicon hydrides, particularly silane (SiH_4) is the most important constituent used frequently in low temperature plasmas. It is also required in the fabrication of micro electronic devices and semi conducting component [1]. They are also used as surface coating agents for surface modification and as coupling agent for adhesion promotion between dissimilar materials [2]. In the glass industry [3], SiH_4 is used for the deposition of silicon - based layers, especially for car heat reflective windshields manufacturing that allow light but not heat to penetrate the glass.

Many groups have investigated the total cross sections for electron collisions with a large number of polyatomic molecules [4, 5]. In the present study, our aim here is to carry out *ab initio* calculations for the total (TCS) and the momentum transfer cross sections for electron scattering from SiH_4 molecules in the energy range 0.1 – 20 eV. A variable phase approach using parameter free spherical optical potential (SOP) model has been employed here. The projectile - target interaction is represented by a sum of three local and real terms, namely the static, the exchange and polarization potentials. All these potentials can be generated easily once the target charge density $\rho(\mathbf{r})$ is known. We determine $\rho(\mathbf{r})$ from a single-centre wave functions with enough terms in the expansion of each bound orbital. $\rho(\mathbf{r})$ is expanded in terms of symmetry – adapted functions belonging to the totally symmetry 1A_1 irreducible representation of the molecular point group. Present calculated TCS are compared with the available theoretical

calculations and experimental measurements in the energy region 0.1 – 1.0 eV (see Figure 1). The quantitative feature such as Ramsauer – Townsend minimum is well reproduced in the present study. The details of the results will be presented in the conference.

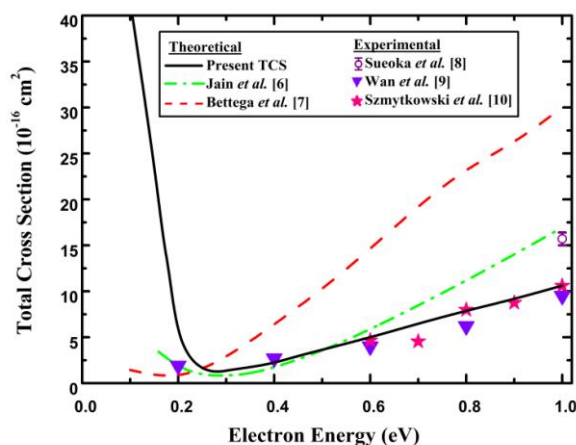


Figure 1. TCS for $e - \text{SiH}_4$ scattering in the energy range 0.1 – 1.0 eV.

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