Theoretical investigation on electron-NH_3 scattering at low and intermediate energy range

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The development of a computational method capable to provide electron-molecule scattering cross sections in a wide energy range and independently of the molecular symmetry is of great interest. In the last decades several efforts have been done to reach this objective. It is well known that at intermediate energies numerous open inelastic scattering channels are responsible for the so called absorption effects. These effects play important roles on the collision dynamics and are substantially difficult to be taken into account with purely *ab-initio* methods. Therefore, a method that combines *ab-initio* with model potentials seems to present one of the most practical and efficient way for supplying electron-molecule scattering cross sections with such effects included.

EPolyScatD was originally developed by Lucchese *et al.* [1] and recently modified by our research group for inclusion of absorption effects [2]. The interaction potential is given by:

$$V_{opt} = V_{st} + V_{ex} + V_{cp} + iV_{ab},$$

where V_{st} , V_{ex} and V_{cp} are the static, the exchange, and the correlation-polarization components respectively. V_{ab} is the improved model absorption potential developed by our research group [3].

Very recently, our research group extended the EpolyScatD application for two polar molecules: methanol and ethanol [4]. In the present work, we present its application to another polar target: ammonia (NH_3). Calculated results of electron-NH_3 scattering cross sections are compared with theoretical and experimental existing data at low and intermediate energy range.

In the figure 1 we show our calculated differential cross sections (DCS) with selected experimental data. Additional results will be presented at the Conference.

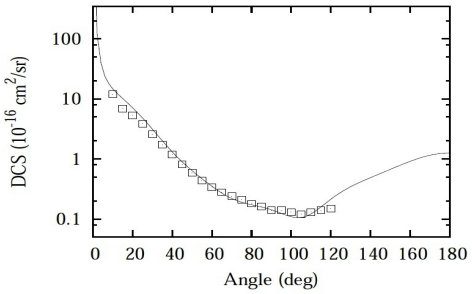

Fig. 1: DCS for elastic electron scattering by NH_3 at 30eV. Solid line, present results including absorption effects; open squares, experimental results of Alle *et al.* [5].

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