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Double differential cross sections for liquid water ionization by impact of fast electrons.

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Synopsis A theoretical study for the single ionization of water molecules in liquid phase by electron impact at high energies is presented. Through a first order model, we compute multiple differential cross sections considering an asymmetric coplanar geometry. The wavefunctions for a single liquid water molecule are obtained in a realistic way by using a Wannier orbital formalism. We compare our results with experiments for the vapor phase and previous theoretical results obtaining a good qualitative agreement.

We study theoretically the single ionization of liquid water by energetic electrons through a first-order model. This reaction is important in many domains such as plasma physics, fusion experiments, astrophysics, and even in the study of ionizing collisions on living matter. As the latter is composed mainly of liquid water, the knowledge of its ionization reaction is crucial to understand the damage provoked to the living tissue by the ionizing radiations. Moreover, the low energy electrons (products of the ionization) are of importance in the mechanisms that lead to cell alteration [1]. As in track structure analysis the liquid phase in cells is often modeled as the gas phase, a more realistic description for the liquid is required. However, to obtain an appropriate description for ionization of liquid water is a difficult task. So, several approximations are required to describe the reaction.

Multiple differential cross sections give the most detailed information on the mechanisms involved in charge transfer reactions. Particularly, angular distributions of secondary electrons allow the determination of the preferential directions or energies for electron ejection following the ionization of the target.

Therefore, we compute double differential cross sections (DDCS) averaged on the molecule orientations and scattering angles for electron projectiles in a coplanar geometry. These DDCS describe the angular distribution of the ejected electrons at fixed incident and ejection energies. The model (see our previous work [2] for more details) uses an independent electron approximation, neglecting the exchange effects as we consider asymmetric collisions. The initial state of the molecule in the liquid phase is obtained through a Wannier technique [3]. The projectile is described by a plane wave whereas the ejected electron is described by a Coulomb wave taking into account its interaction with the residual target.

We compare our DDCS with calculations for vapor [4,5] as well as with experiments also for this phase [6,7]. Fig. 1 shows DDCS for ionization of a single water molecule. As can be seen, a good qualitative agreement is found but significant differences between gas an liquid are observed at low ejection angles.

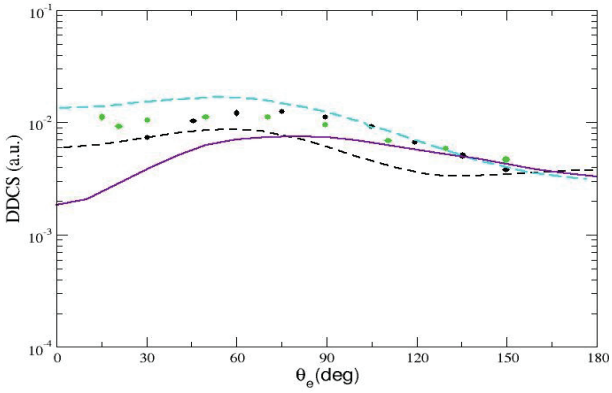

Figure 1. *DDCS for ionization of water molecules as a function of the ejection angle θ_e. Incident and ejection energies are E_i=500 eV and E_e=22 eV, respectively. For liquid, ▬, our results. For gas, ---, FBA calculations [4], ---, DWBA calculations [5], ●, experiments by Opal [6], ●, experiments by Bolarizadeh [7].*

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