Ionization of liquid water by fast electrons: a single and double differential study

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Synopsis Single and double differential cross sections for the ionization of liquid water molecules by fast incident electrons are computed. A first order model for asymmetric collisions in a coplanar geometry is developed. The condensed phase is described by a Wannier orbitals formalism. In order to scrutinize the differences between liquid and gas, we compare our calculations with experiments and theoretical results for the vapor phase. A good qualitative agreement and a trend for both phases is found.

Water molecules ionization is an important reaction in domains such as plasma physics, fusion experiments, astrophysics, and in the study of ionizing collisions on living matter. Moreover, secondary slow electrons (products of the ionization) are of importance in the mechanisms that lead to cell alteration [1]. As the living tissue is composed mainly of liquid water, it is important to describe this phase in a proper way.

In this work we study the single ionization of liquid water by energetic electrons employing a first-order model. As an appropriate description of this reaction is a difficult task, several approximations are required.

Previously, we calculated multiple differential cross sections [2] where a detailed information about charge transfer mechanisms of the reaction can be extracted. In this work, we compute single and double differential cross sections (SDCS and DDCS, respectively) averaged on the molecule orientations and scattering angles for electron projectiles under an asymmetric and a coplanar geometry. We present DDCS that give the angular distribution of the ejected electrons for fixed incident and ejection energies, and also SDCS as a function of the ejected energy. Our model is based on an independent electron approximation neglecting the exchange effects. This is justified at the high energies considered. Moreover, the initial state for a single molecule in the liquid phase is obtained through a Wannier technique [3]. Projectile and ejected electrons are described by a plane wave and Coulomb wave, respectively.

We compare our calculations for liquid water with theoretical results for vapor [4,5] as well as with experiments [6,7]. In Fig. 1 we show the DDCS for ionization of a single water molecule. We find that at this incident energy (500 eV) and ejected energy (100 eV), the cross sections for liquid are higher than the ones for the gas. We also have verified that this difference becomes smaller as the ejected energy decreases. However, this scenario is reverted when higher incident energies are considered (for instance, 1 keV). The same behavior is found for the SDCS.

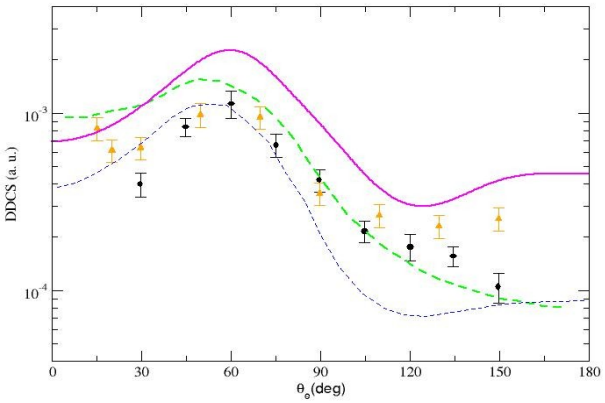

Figure 1. *DDCS for ionization of water molecules as a function of the ejection angle θ_e. Incident and ejection energies are E_i=**500** eV eV and E_e=100 eV, respectively. For liquid, ——, our results. For gas, - - -, FBA calculations [4], - - -, DWBA calculations [5], triangles, experiments by Bolarizadeh [6], circles, experiments by Opal [7].*

References

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