Single and Double differential cross sections for ionization of water molecules in the liquid state by fast electrons.

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Synopsis We compute double and single differentials cross sections for the ionization of water molecules in liquid phase by energetic incident electrons. Asymmetric collisions and a coplanar geometry are considered. We employ a first order model and describe the condensed phase through a formalism based on the Wannier orbitals. Comparison with the vapor phase, both experiments and theoretical results, are in a good qualitative agreement with our calculations and show the trend of different phases.

This work study the single ionization of liquid water by energetic electrons employing a first-order model. The ionization of water molecules is an important reaction in many domains such as plasma physics, fusion experiments, astrophysics, and even in the study of ionizing collisions on living matter. Moreover, secondary slows 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, is important to describe this phase in a properly way. However, as an appropriate description for ionization of liquid water is a difficult task, several approximations are required to describe the reaction.

In previous works [2] we calculate multiple differential cross sections which give the most detailed information about the mechanisms involved in charge transfer reactions. In particular, angular distributions of secondary electrons determine the preferential directions or energies for electron ejection following the ionization of the target. Now, we compute single and double differential cross sections (SDCS and DDCS, respectively) averaged on the molecule orientations and scattering angles for electron projectiles in a coplanar geometry. DDCS describe the angular distribution of the ejected electrons at fixed incident and ejection energies, while SDCS are in function of the ejected energy. In our simple model, based on the independent electron approximation, the exchange effects are neglected. The initial state of the molecule in the liquid phase is obtained through a Wannier technique [3]. The projectile electron is described by a plane wave whereas the ejected electron by a Coulomb wave considering its interaction with a residual target.

Comparison of liquid DDCS with calculations for vapor [4,5] as well as with experiments [6,7] show that for high incidents energies the cross sections for liquid result lower than the corresponding for the gas. Nevertheless, this is reverted when we consider lower incidents energies. The same behavior is found for the SDCS. In Fig. 1 we show the DDCS for ionization of a single water molecule. A good qualitative agreement is found and differences between gas an liquid are observed at low ejection angles.

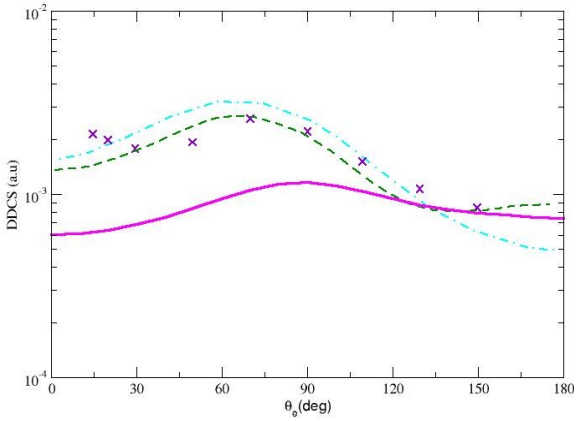

Figure 1. *DDCS for ionization of water molecules as a function of the ejection angle θ_e. Incident and ejection energies are E_i=1 KeV eV and E_e=40 eV, respectively. For liquid, ——, our results. For gas, - - -, FBA calculations [4], —·—, DWBA calculations [5], x, experiments by Bolarizadeh [6].*

References

[1] B. Boudaiffa *et al* 2000 *Science* **287** 1658
[2] M.L. de Sanctis *et al* 2012 *J. Phys. B* **45** 045206
M.L. de Sanctis *et al* 2015 *J. Phys. B* **48** 0155201
[3] P. Hunt *et al* 2003 *Chem. Phys. Lett*. **376** 68
[4] C. Champion *et al* 2002 *J. Chem. Phys.* **117** 197
[5] S. Houamer *et al* 2007 *J. E. S. and R. P.* **161** 38
[6] M.A. Bolorizadeh *et al* 1985 *Phys. Rev. A* **33** 882
[7] C. B. Opal *et al* 1972 *Atomic Data* **4** 209

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