Electron Interactions with Lignin Precursors: scenarios for plasma-based sugarcane biomass pretreatment

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Replace fossil fuels for biofuels from renewable sources is one way of contributing to reduction of the emission of greenhouse gases. In this scenery, production of ethanol from lignocellulosic biomass plays a very important role. Besides substituting gasoline, cellulosic bioethanol can be a good strategy to combat undesirable increase of both area occupied by sugarcane plantation and burning.

Lignocellulosic biomass is a heterogeneous organic polymer that consists of cellulose fibers embedded tightly within hemicellulose and lignin. Due to the complexity structure, it is necessary to submit the biomass to a pretreatment in order to break it down and, consequently, improving the efficiency of enzymatic hydrolysis. This pretreatment may be done through the use of a low-cost atmospheric-pressure plasmas, which can generate interesting reactive species for ethanol productions.

Is well known that DNA damage arises from dissociative electron attachment, a mechanism in which electrons are resonantly trapped by DNA subunits. Believing that a similar process can be possible in biomass, theoretical resonance energies can be useful for guide the plasma-based pretreatment to break down linkages of interest in lignocellulosic material.

Aiming at offering theoretical support to this pretreatment, we intend to study the interaction between the low-energy electrons of the plasma and the material under treatment. However, the complexity of biomass structure makes the description of the potential surfaces of the relevant metastable ions very computationally demanding, even for biomass subunits. Since phenol molecule is a precursor of monolignols, it can be an interesting prototype towards understanding the dissociation dynamics of biomass.

In this work we present elastic cross sections for electron scattering by phenol molecules obtained with the Schwinger Multichannel method. Our results indicate three resonances states that could provide dissociation pathways for biomass pretreatment.

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