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Electron Scattering by biomass molecular fragments

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The replacement of fossil fuels by biofuels from renewable sources may not be a definite answer for greenhouse gas emissions problems, but it is a good step towards a sustainable energy strategy. Few per cent of ethanol is being mixed to gasoline in many countries and in some of them, like Brazil, a very aggressive program has been developed, using, in large scale, flex fuel engines that can run with any mixture of gasoline and ethanol, including 100% ethanol. Important points are how to produce ethanol in a sustainable way and with which technology? Biomass is a good candidate to enhance the first generation (produced from Corn in USA and from sugarcane in Brazil) production towards the so-called second-generation ethanol, since it has cellulose and hemicellulose as source of sugars. In order to liberate these sugars for fermentation, it is important to learn how to separate the main components. Chemical routes (acid treatment) and biological routes (enzymatic hydrolysis) are combined and used for these purposes. Atmospheric plasmas can be useful for attacking the biomass in a controlled manner and low energy electrons may have an important role in the process. Recently, we have been studying the interaction of electrons with lignin subunits (phenol, guaiacol, p-coumaryl alcohol), cellulose components, β-D-glucose and cellobiose (β(1-4) linked glucose dimer) and hemicellulose components [2] (β-D-xylose). We also obtained results for the amylose subunits α-D-glucose and maltose (α(1-4) linked glucose dimer). Altogether, the resonance spectra of lignin, cellulose and hemicellulose components establish a physical–chemical basis for electron-induced biomass pretreatment that could be applied to biofuel production. In order to describe a more realistic system (where molecules are "wet"), we have obtained the shape resonance spectra of phenol-water clusters, as obtained previously from elastic electron scattering calculations. Our results, obtained in a simple model (phenol in the presence of one and two water molecules), indicate that the well-known indirect mechanism for hydrogen elimination in the gas phase is significantly impacted on by microsolvation, due to the competition between vibronic couplings on the solute and solvent molecules. This fact suggested how relevant the solvation effects could be for the electron-driven damage of biomolecules and the biomass delignification. We have also discussed microsolvation signatures in the differential cross sections that could help to identify the solvated complexes and access the composition of gaseous admixtures of these species. In a collaboration project involving Australia (within the Brazilian Science Without Borders program), Portugal, Spain and Brazil, we have focused on obtaining theoretical and experimental electronic excitation cross sections of phenol and furfural for 10-50 eV electron impact energies. Convergence on electronic multichannel coupling stands as the biggest challenge to obtain agreement between theory and experiments. In my presentation, I will discuss the current status of this project.