Abstract Submitted for the DAMOP12 Meeting of The American Physical Society

Low-Energy Electron Scattering by Sugarcane Lignocellulosic Biomass Molecules¹ ELIANE OLIVEIRA, CTBE/CNPEM, SERGIO SANCHEZ, MARCIO BETTEGA, UFPR, MARCO LIMA, CTBE/CNPEM, MAR-CIO VARELLA, USP — The use of second generation (SG) bioethanol instead of fossil fuels could be a good strategy to reduce greenhouse gas emissions. However, the efficient production of SG bioethanol has being a challenge to researchers around the world. The main barrier one must overcome is the pretreatment, a very important step in SG bioethanol aimed at breaking down the biomass and facilitates the extraction of sugars from the biomass. Plasma-based treatment, which can generate reactive species, could be an interesting possibility since involves low-cost atmospheric-pressure plasma. In order to offer theoretical support to this technique, the interaction of low-energy electrons from the plasma with biomass is investigated. This study was motived by several works developed by Sanche et al., in which they understood that DNA damage arises from dissociative electron attachment, a mechanism in which electrons are resonantly trapped by DNA subunits. We will present elastic cross sections for low-energy electron scattering by sugarcane biomass molecules, obtained with the Schwinger multichannel method. Our calculations indicate the formation of π^* shape resonances in the lignin subunits, while a series of broad and overlapping σ^* resonances are found in cellulose and hemicellulose subunits. The presence of π^* and σ^* resonances could give rise to direct and indirect dissociation pathways in biomass. Then, theoretical resonance energies can be useful to guide the plasma-based pretreatment to break down specific linkages of interest in biomass.

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