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Theoretical elucidation of the molecular behavior of levoglucosan during biomass pyrolysis

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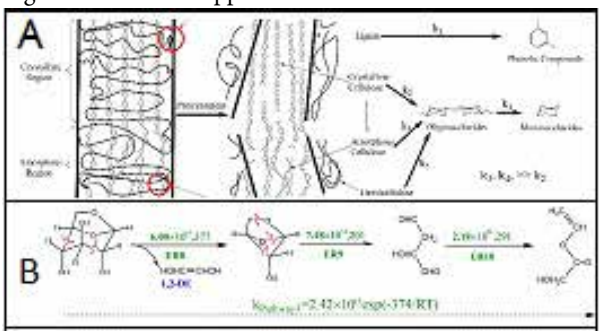
The bio-fuels and bio-chemicals derived from lignocellulosic biomass are popularly referred to as second-generation bio-fuels or bio-chemicals. As a valuable chemical material, levoglucosan is one important primary product during cellulose pyrolysis either as an intermediate or as a product. The fundamental investigation on the mechanism and kinetic modelling of the production of levoglucosan from lignocellulosic biomass has been carried out. Three available mechanisms for levoglucosan formation have been studied theoretically by performing density functional theory based calculations. Specifically, the molecular behaviour of levoglucosan has elucidated by revealing 14 reaction pathways, 26 elemental reaction steps, and the involved around 60 compounds act as intermediates, transition states, or products. By comparing with the activation energy obtained from the experimental results, it was concluded that levoglucosan chain-end mechanism fits better with the experimental data for the formation of levoglucosan. The variational transition state rate constants for every elementary reaction and every pathway were calculated. The first-order Arrhenius expressions for these elementary reactions and pathways were suggested. Furthermore, this research provides techno-economic assessment of the available routes for the production of levoglucosan and its derived products, and the paper will be concluded by identifying key challenges and future trends for second-generation bio-chemicals. It also confirms that Quantum Mechanics based simulation can reveal fundamental phenomena, which are difficult to be explored from traditional experimental techniques, and can be used to guide the experimental design and industrial application.



Fundamental insights of biomass fast pyrolysis. A. the overall process; B. one pathway levoglucosan decomposition obtained from atomic-level investigation. three elementary reactions are involved in this pathway

Biography

Xiaolei Zhang is a Lecturer at the Queen's University Belfast (QUB), UK since January 2015. She received a PhD in May 2013 from the Royal Institute of Technology (KTH), Sweden on the topic of quantum mechanics investigation of bioenergy systems and she has worked as a Researcher at University of Alberta, Canada on process modelling of bioenergy system for 14 months. Her rich international research achievements are reflected by the authored 20 peer-reviewed publications in leading international journals in the area of Energy, with over 200 citations and an H-index of 9 on Scopus; together with the delivery of 22 invited talks, lectures, and other conference contributions.

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