OVERCOMING RECALCITRANCE OF BIOBASED FEEDSTOCKS THROUGH CATALYTIC CONVERSIONS

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The challenges faced by the lignocellulose-to-ethanol conversion technologies are critically linked to the uncertainties of the physical properties of the feedstock. During the course of evolution, plant cell walls have become recalcitrant through architecture and design of its components to deal with environmental stress and pathogen attack. We present the results of extensive theoretical studies on lignocellulosic biomass that seek to obtain a molecular level understanding of recalcitrant properties of the cell wall components. Our studies probe these properties using computational techniques at different levels of resolutions comprising quantum chemical calculations, all atom and coarse-grained molecular dynamics simulations, polymer and statistical mechanical models and agent based and traditional kinetic models. We will discuss how such a multi-scale approach can give a coherent view of the molecular details of the biomass degradation problem.