Molecular aspects of lignocellulosic biomass degradation: dynamics of enzymes and plant cell wall nanoarchitecture

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Lignocellulosic biomass from sugar-cane is a high-valued material for the obtention of biofuels. The best route for converting such biomass into fermentable sugars requires enzymatic catalysis, which is, however, the most expensive step of the whole process. To render such processes more efficient and economically viable, it is necessary to improve our understanding of the enzymatic digestability of cellulose and the molecular aspects associated with the nanoarchitecture of plant cell walls. In this talk, I discuss recent studies conducted at Unicamp aimed at elucidating the molecular mechanisms underlying the actions of cellulolitic enzymes and co-adjuvant proteins using molecular dynamics simulations and the interactions between the main components of cell walls.