

COMPUTATIONAL MODELING OF BIOMASS CONVERSION SYSTEMS

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Computational modeling offers a powerful, complementary approach to experiments, and often it can provide direct, molecular insights that enable new routes to design catalysts and processes. To examine fundamental problems of interest to biomass conversion, our group uses a suite of computational approaches including molecular dynamics, coarse-grained simulations, and quantum mechanical calculations. This talk will cover a survey of work from our group using these methods to understand cellulose structure at multiple length scales, to elucidate new pathways for engineering cellulase enzymes, and to understand lignin deconstruction mechanisms via catalytic or thermal processes. Several studies will be presented in detail on these topics where computational modeling has enabled new understanding.