Goal:
Utilize core computational capabilities across the US DOE national labs to enable and accelerate the development of new materials and optimize process scale-up to advance the bioenergy economy.

Approach:
In close collaboration with experimentalists, model conversion at atomic, meso, and process scales to translate bioenergy conversion from discovery to end-process stages.

Impacts:
• Actionable info towards accelerating catalyst formulation development
• Critical characterization of mass & heat transfer to enable optimal catalyst particle design
• Scalable catalytic conversion processes for a wide range of reactor designs