Consortium for Computational Physics and Chemistry (CCPC)

A multi-scale problem … A multi-lab solution

OAK RIDGE National Laboratory · NREL National Renewable Energy Laboratory · NETL National Energy Technology Laboratory · Argonne National Laboratory · Pacific Northwest National Laboratory

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.

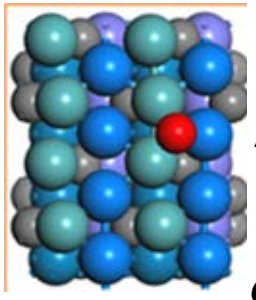
Approach:

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

Impacts:

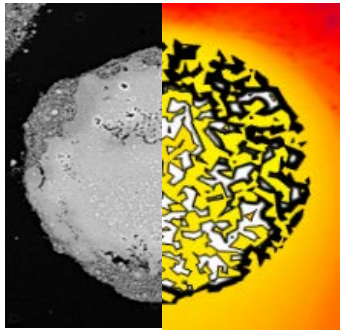
- Actionable info towards accelerating catalyst formulation development
- Critical characterization of mass & heat transfer to enable optimal catalyst particle design
- Scalable catalytic conversion processes for a wide range of reactor designs

Atomic Scale Catalysis Modeling



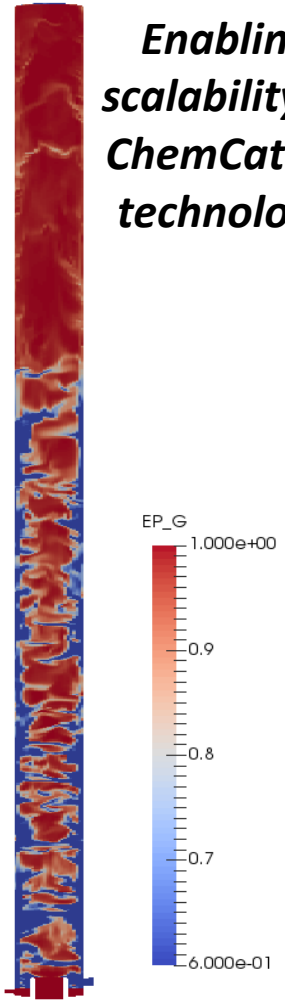
Accelerating ChemCatBio catalyst development

Meso Scale Particle Modeling



Addressing bio-complexity challenges

Process Scale Reactor Modeling



Enabling scalability of ChemCatBio technology