ChemCatBio Webinar Series

"Simulation and Modeling of Bioenergy Conversion from the Atomic to Process Scales"



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Wednesday, November 14, 2018
12– 12:45 p.m. MDT
Registration: https://attendee.gotowebinar.com/register/4000044587020583171

The Consortium for Computational Physics and Chemistry (CCPC) is a research project in ChemCatBio focused on accelerating catalyst discovery and enabling scale-up of new catalyst innovations in bioenergy. The CCPC is composed of Oak Ridge National Laboratory, Argonne National Laboratory, National Energy Technology Laboratory, the National Renewable Energy Laboratory, and Pacific Northwest National Laboratory. This webinar presentation will highlight modeling activities in the CCPC which span from atomic to meso and process scales. At the atomic scale, density functional theory calculations are used to guide experimental researchers and provide fundamental knowledge on binding energies and active catalyst sites. The meso scale models capture catalyst particle effects including mass transfer, heat transfer, and coking. Finally, process scale models are employed to understand conversion in reactors of various designs to enable scale up and prediction of optimal control conditions.

For more information, please visit our website at ChemCatBio.org or email us directly at Contact@ChemCatBio.org. ChemCatBio is funded by the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE) Bioenergy Technologies Office.