PROJECT FACTS

UNIVERSITY OF KENTUCKY CENTER FOR APPLIED ENERGY RESEARCH

CLEAN FUELS & CHEMICALS

Computational and Experimental Catalysis: Understanding Atomic-level Synthesis

UK's Center for Applied Energy Research (CAER) and the Center for Computation have joined forces to focus on heterogeneous catalysis with the goal of developing more efficient catalytic processes for energy production, usage and storage. The CAER provides experimental studies and in-depth nano- and sub-nanoscale investigations of a broad range of catalytic materials with industrial importance while the Computing Center's emphasis is on applying state-of-the-art computational software and hardware, thereby, providing a synergy for exploring the catalytic properties of nano-scale materials.

The project was initially based on recent advances in physical simulation algorithms and the advancement and availability of massively parallel computers without which many catalytic problems simply could not be embarked upon. The project first selected ceria as a model catalyst and is currently studying the oxidative potential of ultra-small ceria catalyst particles. High resolution TEM and EELS investigations are also part of the work and give insights into the physico-chemical properties of the synthesized ceria to which to compare the computational results. The computational efforts add important new dimensions to the understanding of heterogeneous catalysis and are expected to help at CAER to guide new synthesis approaches based on more detailed knowledge of atomic scale properties that lead to more precise atomic-level synthesis of materials. The overall goal is to develop computational tools that allow us to better model catalytic reactions and offer a fundamental basis for the design of new catalysts for energy production. A process that could greatly benefit from computational catalysis is the Fischer-Tropsch Synthesis (FTS) and the CAER currently has 23 CSTR reactors dedicated to FTS research.

PARTICIPANTS

UK CAER

UK Center for Computation

SPONSORS

KY EPSCOR
Tri-State Catalysis Society
Süd-Chemie Inc.

PROJECT VALUE

$50,000

CONTACT

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