Materials Design from First Principles

Larry A. Curtiss, Argonne National Laboratory

ALCC 30M

Science and Approach

Reduce the significant chlorinated waste from producing propylene

- Subnanometer Ag clusters may provide pathways to overcome this waste problem.
- Structure of key molecule optimized and study completed on part of the process

Study the transformation of biofuels with efficient catalysts

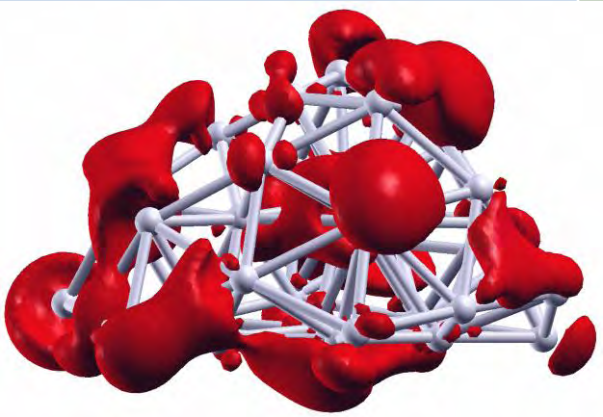
- Structure of ZrO_2 nanobowls in dry and hydroxylated alumina have been optimized
- In support of the Institute for Atomic-efficient Chemical Transformation (IACT), an Energy Frontiers Research Center (EFRC)
- J. Phys. Chem. C, 2011, 115 (44), pp 21785–21790

Key Impact

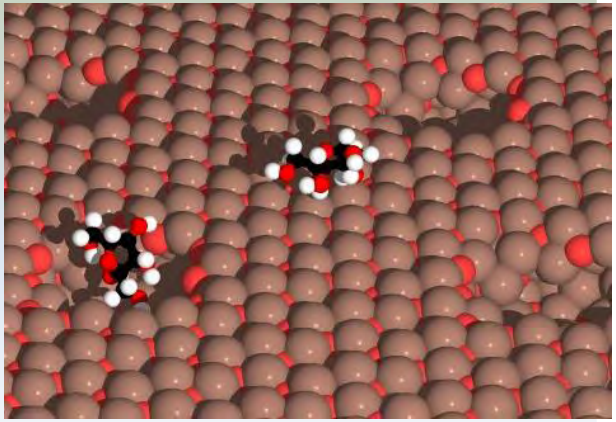
- Provide the fundamental understanding and predictions needed to design new materials for catalysis and energy storage

ALCF Contributions

- Significant time was spent mentoring 4 post-docs on using GPAW and how to use Intrepid
- Building off of significant effort on the performance and scalability of GPAW



Thirty-three atom silver cluster that is being studied as a new catalyst for propylene epoxidation.



Nanobowl in ZrO2 surface (1nm diam.) that is being studied for biomass conversion to fuels