

NATIONAL LABORATORY CHEMICAL SYNTHESIS CAPABILITIES Computational design, synthesis, scale-up, and people

A key strength of the National Laboratories is their multi-disciplinary teams of computational scientists, chemists, materials scientists, physicists, and engineers who address the design, synthesis, scale-up, and production of novel materials for a wide variety of applications. There are many mechanisms available to facilitate collaborations with National Laboratories to address challenges in chemical synthesis.





Unique resources are available for preparation of novel reaction environments for chemical synthesis. Hollow carbon nanospheres can be prepared to contain gold catalyst for reductions

Carbonizatio emplat Wavelength / nn

Tandem catalyst having multiple metal-metal oxide interfaces have been synthesized for chemical synthesis by sequential reactions. For example, ethylene hydroformylation with hydrogen and carbon monoxide formed in situ by methanol decomposition

Porous polymers

architectures from

atomic to macroscale can create

unique reaction

environments

with controlled



Novel Reactors for Scale-up

Novel reactors can be constructed to scale up chemical synthesis. Here, sunlight heats a ceramic reactor to convert carbon dioxide and water to syngas (H₂ and CO)



A full-scale plant was built by Archer Daniels Midland Company to produce propylene glycol from renewable sources based on a new chemical catalyst



Computational Synthesis

Computer-aided structure-based design is used to create chemical structures with predetermined functionality. A simple ligand was designed that self-assembled into capsules and selectively incorporated sulfate, rivaling nature's sulfate binding protein



Computational methods are used to uncover reaction mechanisms which aid in the design of new functional materials for energy applications



ENERGY Office of Science

Novel ab initio calculations combined with NMR measurements uncover the role of proton relays and water in hydrogen oxidation



Chemical Synthesis

transformations of carbon-containing molecules

National laboratories possess key strengths in the

Nanomaterials can be functionalized precision and tailored properties for selective reactions, such as the oxidation of alcohol Lawrence Livermor





