Molecular recipes save time and money for clean fuel development

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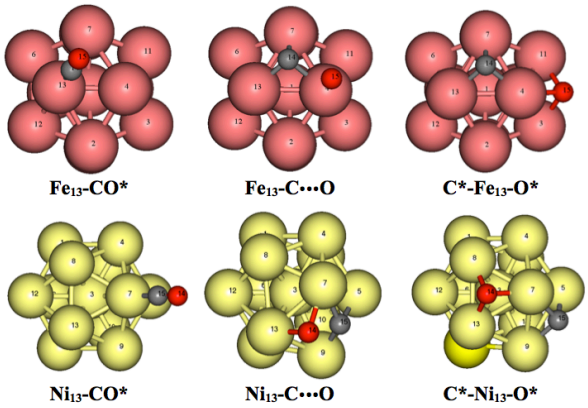
Outcome: Research with metal alloys has led to the development of catalysts that can be used in the development of liquid fuels that are produced in a “clean” process without emitting greenhouse gases.

Using Louisiana’s world-class computational tools, a team of Louisiana Tech University computational scientists led by Dr. Daniela Mainardi, has developed a computer program to help screen and identify the best “recipe” of materials for further studies by experimental scientists in the lab. For example, the team’s program predicts that a core-shell catalyst with a nickel core and an iron outer shell is a better candidate for fuel production than the reverse, an iron core and nickel shell.



Carbon monoxide splitting to form liquid fuels: Two catalyst reactions are shown with iron (top row) and nickel (bottom row). The first picture in each set corresponds to carbon monoxide adsorbed on the catalyst material, the middle one corresponds to an intermediate state, and finally the last picture is the carbon monoxide molecule split into carbon and oxygen on the material’s surface.

Credit: Daniela Mainardi, Institute for Micromanufacturing, Louisiana Tech University.

Impacts/Benefits: Computational research has tremendous advantages for discovery because it greatly speeds up testing times and the experiments can be conducted virtually without a physical laboratory and expensive materials. Narrowing down the best materials will ensure fuel research and generation will happen in the most effective way. The recipe is guiding the design of modified and new materials and continued research on the synthesis of fuels.

Background: When a mixture of carbon monoxide and hydrogen gas is introduced to the right material (the catalyst), it causes a reaction and recombines to form liquid fuels. This chemical reaction is known as the Fischer-Tropsch process.