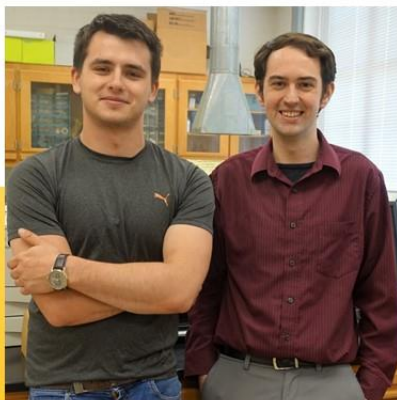




“Multiscale Modeling of a Functionalized Surface Catalyst for Hydrogen Peroxide Production”

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Hydrogen peroxide (HP) is a commodity chemical with a broad range of uses. The major environmental detriment of the life cycle of HP is the current industrial process used in HP synthesis; it is otherwise a “green” chemical in its applications. Reducing the environmental impact of HP synthesis through a new process would serve as a major improvement that would save energy and money. Computational modeling allows proposed materials such as surface catalysts to be studied for viability before any (sometimes costly) synthesis or thermodynamic characterization is carried out. The goal of this project is to model a simple surface catalyst for the production of hydrogen peroxide directly from hydrogen and oxygen gases, without the need for catalytic nanoparticles or multiphase reactors.