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Project Summary

Light alkenes such as ethylene, propylene and butenes are among the most produced chemicals and building blocks for many polymers and a number of chemical intermediates. The main process for the production of the light alkenes is steam cracking of hydrocarbons, particularly naphtha. Naphtha steam cracking provides a range of distribution of alkenes. Multiple separation steps are required to obtain high purity ethylene, propylene and butanes. As steam cracking is highly endothermic, it requires high temperature to overcome the thermodynamic limitations, making steam cracking suffer from coking and high energy consumption. Therefore, new processes to produce light alkenes are desired.

The oxidative dehydrogenation (ODH) of alkanes represents an alternative, energy efficient, and potentially more selective route (compared to the current methods). The reaction is exothermic and produces specific alkenes. Recent domestic shale gas and tight oil boom in recent years not only changes our dependence on imported energy, but it also potentially increases the availability of C1-C4 alkanes as feedstock, making ODH of light alkanes even more attractive.

The primary goal of this proposed research is to test the hypothesis that the oxidative dehydrogenation of light alkanes can be achieved at a much high conversion and selectivity with the use of inverse, monolayer oxide/metal catalysts. We focus our attention on the ODH of ethane using monolayer MgO and FeO_x-based thin film supported metal nanoparticles.

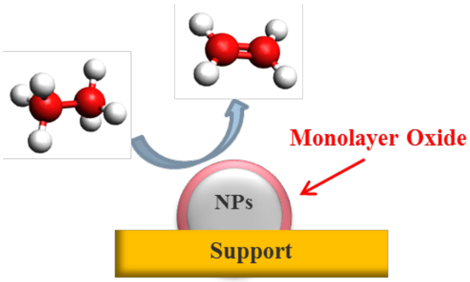

Figure 1. A schematic of ethane ODH to produce ethylene by using monolayer oxide supported on metal nanoparticles.

This hypothesis is built on the surface science studies on inverse model catalysts. The premise is that the inverse oxide/metal catalysts can exhibit collective properties that are superior to their bulk counterparts due to possible factors caused by the oxide/metal contacts, including but not limited to, electron charge transfer, modified HOMO-LUMO character, and lattice epitaxy effect. These factors can be affected by the choice of oxide/metal pairs, the coverage and dispersion of the monolayer oxide, the diameter of the underlying metal nanoparticles, and the degree of lattice mismatch between the oxide and the metal. We aim at obtaining understandings on these factors and provide a collective interpretation for rational design of new generation ODH catalysts.

Project Impacts

Energy Impacts: The current industrial pathway to generate olefin are endothermic and thus suffer from high-energy consumption (reaction temperatures > 873 K), low yield of olefins at low temperatures due to thermodynamic limitation, and catalyst deactivation by extensive coking. ODH reaction is an alternative pathway to olefin production with several advantages: exothermic, thermodynamically unrestricted, operation at much lower temperatures, and minimized coke deposition on catalysts. The reaction temperature can be lowered to 573 – 823 K range. Substantial energy savings (up to 30%) can therefore be realized by ODH thanks to the low reaction temperature and the elimination of the catalyst de-coking step.

Economic Impacts: The US ranks 5th and 4th in the world in terms of proved natural gas reserve and recoverable shale gas, respectively. In the State of Alabama, in addition to the 2,261 billion cubic feet of proved natural gas reserve, the Black Warrior basin and Appalachian thrust belt of Alabama contain gas shale plays with gas resources that may exceed 800 trillion cubic feet (original gas-in-place). Currently, most of the natural gas is used to generate heat and electricity. If the proposed research is successful, it can potentially lead to radically transform of the chemical industry of ethylene production, significantly increasing the economic attractiveness of this natural gas resource in the US and the state of Alabama.

Student Primary Responsibilities:

- Perform catalyst performance evaluation
- Record and analyze data using standardized forms and lab notebooks
- Assist in writing reports describing procedures used
- Assure all job activities adhere to UAH Environmental, Health and Safety requirements.

Qualifications

- Major in chemical/mechanical/environmental engineering, chemistry, and physics
- Ability to work in a group setting
- Effective communication with the advisor and coworkers
- Strong computer capabilities including Microsoft Office, PowerPoint and Excel

Mentor Supervision and Interaction

Our multi-disciplinary research group currently consists of 4 graduate students, 2 undergraduate researchers and occasionally high school researchers during the summer. The RCEU undergraduate student will start their everyday research activities with one of the graduate students in the group. This does not reflect any lack of interest on my part in your project; it is rather an attempt to ensure that you will always have ready access to qualified, expert advice without necessarily having to hunt me down. It is also very important that graduate students have the opportunity to develop their own mentoring skills. Besides lab activities,

Individual Meeting. A definite schedule of individual meetings and team meetings is adopted weekly in our group. The group member will meet with the mentor in an informal fashion to discuss recent progress.

Group Meeting. Our group holds weekly group meetings. The perspective student will participate in the group meeting and be able to interact with graduate students and faculty members. He/She is expected to present in the group meeting, covering literature review and research progress.

Assessment

The minimum requirement for the RCEU student is to at least present at UAH by the end of the program and submit their work to be published by the UAH undergraduate research journal –Perpetua.