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Use Carbon Dioxide as a Soft Oxidant

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Project Summary

This project centers at using greenhouse gas carbon dioxide as a soft oxidant to convert ethane to ethylene (C_2H_4), a most produced and demanded intermediate in the chemical industry. A key to the project is to develop advanced nanocatalyst that exhibits high activity, selectivity and stability.

Ethylene, and other light alkenes such as 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 derived from crude oil. Multiple separation steps are required to obtain high purity ethylene, propylene and butanes. The oxidative dehydrogenation (ODH) of alkanes represents an alternative, energy efficient, and potentially more selective route. 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. In particular, using carbon dioxide (CO_2) as a soft oxidant to convert light alkanes to their corresponding alkenes has attracted considerable attention.

Two reactions of CO_2 with ethane may occur, including the ODH pathway shown in Equation (1) and dry reforming pathway in Equation (2). The two reactions occur simultaneously under reaction conditions.

$$CO_2 + C_2H_6 \leftrightarrow C_2H_4 + CO + H_2O \quad \ldots eqn(1)$$
$$2CO_2 + C_2H_6 \leftrightarrow 4CO + 3H_2 \quad \ldots eqn(2)$$

Equation (1) leads to the direct formation of ethylene oxide. CO and H2O can further go through water-gas-shift-reaction and generate CO_2 and H_2. The second independent reaction is called dry reforming of ethane, forming "Syngas" – a mixture of carbon monoxide and hydrogen. The syngas is also an important feedstock for the production of high chain fuel. 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.

Environmental Impacts: The use of CO_2 as the oxidant in the industrial scale can provide a promising route to achieve net-zero carbon emission. It could help to meet the environmental and societal challenges faced the world.

Student Primary Responsibilities:

- Perform catalyst performance evaluation
- Record and analyze data using standardized forms and lab notebooks
- Simulate the reaction equilibrium conversion using proper software
- 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 1 faculty, 1 senior researcher, 3 PhD students, 3 undergraduate researchers and 2-3 high school researchers during the summer. The RCEU undergraduate student will discuss research progress and plan for the next stage with the faculty on a daily basis. The lab activity will start with shadowing one of the PhD students in the group, and gradually lead to individual activity under supervision by the senior members in the group.

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. The RCEU student 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. The student is encouraged to submit their work to be published by the UAH undergraduate research journal – Perpetua.