8^{th} TcSUH STUDENT/POSTDOC SEMINAR

November 18, 2019 - 5:30 pm, HSC 102

Food and soft drinks will be served

Carbonate-assisted electrochemical methane conversion to methanol on Ni(111) and NiO(100): A density functional theory study

Qianyu Ning

TcSUH and Department of Chemical & Biomolecular Engineering

Abstract: Methane, an abundant resource in the U.S., has very strong C-H bonds, which makes it energy consuming to be activated. Thus, the development of catalysts to upgrade methane to higher value products is challenging but very desirable. Two major issues that current methane upgrading processes are facing are that high temperatures (up to 900 K) are required, and the short life time of the catalysts caused by sintering and coking. We aim to address these issues and pursue a low temperature process, which leverages the use of an electrochemical cell to convert methane to methanol.

The process uses carbonate anions (CO_3^{2-}) that are produced at the cathode and transferred to the anode. At the anode, carbonate anions deliver a single oxygen atom that can selectively oxidize methane to methanol. The fact that CO_3^{2-} reduction leads again to CO_2, which desorbs into the gas phase, is considered a key advantage of the proposed electrochemical process. The rate of CO_3^{2-} delivery can be controlled by adjusting the cell potential and current density. By simultaneously controlling the flow rate of CH_4 at the anode, we anticipate that the prevention of methane over-oxidation, such that a high yield of methanol can be achieved.

To obtain fundamental insights into the process, we have performed density functional theory (DFT) calculations on Ni(111) and NiO(100) and explicitly accounted for the effects of applied electric fields. Our results indicate that the interaction between the electric field and the surface dipole moment plays the dominant role in altering the binding behavior. Hence, the reaction enthalpies and activation barriers of certain elementary steps exhibit a strong dependence on the electric field. We have quantified the electric field effect for two distinct reaction pathways and the results show that a positive electric field lowers the activation barriers of most steps. Although the decrease of the activation barriers is small, we postulate that a properly tuned electric field can guide the reaction to proceed in the desired direction.

While the development of a viable process remains in its early stages, our results suggest that an electrochemical cell using CO_3^{2-} as an oxidant offers unique advantages for selectively upgrading methane to value-added products.

Bio: Ms. Qianyu Ning is currently a graduate student in Dr. Lars C. Grabow's group in the department of Chemical & Biomolecular Engineering and Texas Center for Superconductivity at University of Houston

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Persons with disabilities who require accommodations to attend this seminar should call 713-743-8213.

Development of REBCO film on the flexible ceramic substrate for cryogenic application

Sicong Sun

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Abstract: The microwave transmission line is an indispensable part of superconducting qubits quantum computers. The unique qubit coherence work function relies on a temperature hierarchal system which progressively lowers the temperature from Kelvin to millikelvin levels by a dilution refrigerator. The microwave transmission cables used between different temperature level qubits signal amplifiers need to cause less attenuation of signals transmitted between millikelvin and Kelvin temperature range. Therefore, the thermal resistance of these cables needs to be high. Here we propose REBCO superconducting coplanar strips on flexible YSZ (Yttria-Stabilized Zirconia) substrate for use as microwave transmission cables. The low-cost flexible YSZ can provide enough mechanical strength, similar thermal expansion coefficient as REBCO, and high-temperature roll-to-roll process capability which make it suitable as the substrate for this application. The engineering feasibility has already been demonstrated by growth of good quality REBCO thin film on flexible YSZ substrate and laser-patterned REBCO lines. The flexible-YSZ-based REBCO transmission lines are expected to show low dielectric loss tangent at cryogenic temperatures which make them suitable for transmission of high-quality signals between millikelvin and Kelvin levels and contribute to much less heating than the current discrete coaxial cables.

Bio: Mr. Sicong Sun is currently a graduate student in Dr. Venkat Selvamanickam's group in the department of Mechanical Engineering and Texas Center for Superconductivity at University of Houston.

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