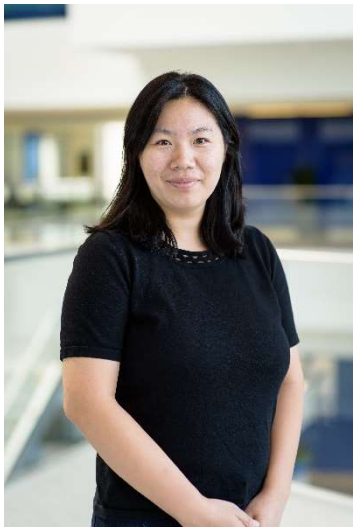
The CATALYSIS SOCIETY of Metropolitan New York
www.nycsweb.org

Wednesday, January 26th, 2022 at 4:00pm EST
Virtual Meeting: Zoom

Dr. Fanglin Che



Assistant Professor
Chemical Engineering
University of Massachusetts Lowell

CO_2RR Driven by Confined Organic-Inorganic Interfaces

Electrochemical CO_2 reduction reaction (CO_2RR) using renewable electricity represents a net zero-carbon pathway for sustainable and valuable hydrocarbon production. C_2 species (i.e., ethylene and ethanol) usually have a higher economic value especially in fuel industry than C_1 species. Copper (Cu) is considered as one of the most promising and low-cost metal catalysts for CO_2RR to generate C_2 species. However, Cu has two significant limitations with respect to CO_2RR-to-C_2: (1) CO_2 is a stable molecule containing two π bonds, which means a large overpotential is needed to activate CO_2, thus resulting in a low CO_2RR current density (2) CO_2 reduction over Cu produces a number of C_1 and C_2 products but there are not reliable strategies to control the selectivity to the desired C_2 species.

To mitigate the above challenges, we designed organic-inorganic interface for enhancing CO_2RR-to-C_2. DFT on thermodynamic energetics and microkinetic modeling on surface reaction rates demonstrated organic-inorganic interface could facilitate CO_2-to-C_2 through: (1) promoting CO_2 adsorption and activation by organic functional group; (2) inducing confinement effect and organic-inorganic hybrid active sites to enlarge the adsorption energy difference between CO^* and COH^*, thus favoring carbon-carbon (C-C) coupling; and (3) changing surfaces' dipole moment and polarizability to further favor the C-C coupling under the electrode/electrolyte interfacial electric field. This theoretical research provides an innovative picture of electrocatalysis at hybrid organic-inorganic interfaces, and specifically their roles in increasing the catalytic activity and selectivity. The outcomes of this study will be transformative to other electrocatalytic reactions that suffer from weak reactant adsorption and adsorption-sensitive selectivity (e.g., CH_4 conversion to methanol, nitrogen reduction reaction) and thermal catalysis.

Speaker Bio

Dr. Fanglin Che joined in Chemical Engineering department at University of Massachusetts Lowell as an Assistant Professor in September, 2019. Dr. Che earned her Ph.D. in Chemical Engineering at Washington State University in 2016, under the advisement of Professor Jean-Sabin McEwen. Her work is related to investigate electric field effects on methane steam reforming reaction over Ni-based catalysts. From 2017 to 2018, she worked on computational catalysis with Professor Edward Sargent at University of Toronto as a Postdoctoral Researcher. From October 2018 to July 2019, she worked on microwave heating effects on heterogeneous catalysis as a Postdoctoral Researcher in the Department of Chemical and Biomolecular Engineering at University of Delaware in Professor Dionisios G. Vlachos's laboratory. The overarching goal of Dr. Che's research at UMass Lowell is to advance the knowledge of revealing the fundamental science of chemical processes by providing a new paradigm of 'virtual lab' via building multi-scale (i.e., from atomic-femtosecond to pellet-second scales) and multi-physics (i.e., kinetics coupled with mass and heat transfer) computational models. A special focus is placed on understanding catalytic properties of field-induced chemistry, electrocatalysis, plasma catalysis, and microwave catalysis.

Zoom meeting number (access code): 842 5502 5995 | Meeting password: 938676 | Join Meeting

One tap mobile
+16465588656,,84255025995#,,,,*938676# US (New York)
+13126266799,,84255025995#,,,,*938676# US (Chicago)

Dial by your location
+1 646 558 8656 US (New York)
+1 312 626 6799 US (Chicago)
+1 301 715 8592 US (Washington DC)
+1 253 215 8782 US (Tacoma)
+1 346 248 7799 US (Houston)
+1 669 900 9128 US (San Jose)
Meeting ID: 842 5502 5995
Passcode: 938676
Find your local number: https://us02web.zoom.us/u/kcqSbAOzAx

Presentation	**4:00 PM**	**Annual Membership Dues**	**$35 (*Students* = $15)**

Deadline for reservations is **4:00PM Monday, January 24th, 2022**
To make your reservation, fill out the online form.