

# Seminar

Wednesday, December 6, 2017

11:00 AM – 206 Furnas Hall

## PhD Seminar

Chemical and Biological Engineering University at Buffalo

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**Advisor: Haiqing Lin**

### Highly Polar Polymers with Superior Membrane CO<sub>2</sub>/N<sub>2</sub> Separation Properties for Carbon Capture

Greenhouse gas CO<sub>2</sub> emissions to the atmosphere are believed to be the primary reason for the global warming. One effective way to mitigate CO<sub>2</sub> emissions is to capture CO<sub>2</sub> from post-combustion flue gas in coal-fired power plants. Membrane technology has been widely explored for this application due to its high energy-efficiency. Current membrane materials are often based on poly(ethylene oxide) (PEO) because the ether oxygens in PEO interact favorably with CO<sub>2</sub>, leading to high CO<sub>2</sub> solubility, and thus high CO<sub>2</sub>/N<sub>2</sub> selectivity. In this study, we demonstrate that polymers with higher ether oxygen content than PEO exhibit enhanced CO<sub>2</sub>/N<sub>2</sub> separation performance. Specifically, a family of polymers containing poly(1,3-dioxolane) (with an O:C ratio of 2:3, compared to 1:2 in PEO) were synthesized by photopolymerization of two macromonomers, poly(1,3-dioxolane) acrylate (PDXLA) and poly(1,3-dioxolane) ethyl ether acrylate (PDXLEA). The macromonomers and polymers were systematically characterized for chemical structures and physical properties using NMR, DSC, FTIR, XRD, etc. Pure-gas solubility and pure and mixed-gas permeability were determined as a function of pressures and temperatures. These highly polar polymers exhibit CO<sub>2</sub>/N<sub>2</sub> separation properties above the upper bound in the Robeson' plot. For example, a copolymer prepared from PDXLA and PDXLEA (1:1) exhibits a CO<sub>2</sub> permeability of 840 Barrers with a CO<sub>2</sub>/N<sub>2</sub> selectivity of 54 at 35°C, which are the best among those reported in the literature. The relationship between polymer structure and gas transport properties will also be discussed in this presentation.

**Hanguang Zhang**

**Advisor: Gang Wu**

### Design of Atomically Dispersed Iron Catalysts for the Electrocatalysis of Oxygen in Fuel Cells

Fuel cells can convert the chemical energy of hydrogen fuel with oxygen into electricity to power vehicles without emission for future transportation. The high cost of platinum (Pt) catalyst used for oxygen reduction reaction (ORR) in fuel cells is one of the bottlenecks for the widespread deployment of fuel cell vehicles. Fe-N-C catalysts, produced by high-temperature pyrolysis of iron, nitrogen and carbon precursors together, have been identified as the promising alternatives with highly active Fe-N-C sites as well as earth-abundant and low-cost elements to replace Pt catalysts. However, it remains a grand challenge to prepare Fe-N-C catalysts with uniform morphology and abundant Fe-N-C active sites to achieve high ORR activity due to the presence of inactive Fe species in catalysts. In this talk, I will present our design of Fe-N-C catalysts with atomically dispersed Fe from well-defined Fe-containing metal-organic framework (MOF) precursors via controlled synthesis. Such MOF precursors allow us to prepare morphology-preserved catalysts and to precisely control (i) the Fe content to avoid the formation of inactive Fe agglomerates and (ii) particle size of catalysts to produce high-performance Fe-N-C catalysts for ORR. The observation of exclusive atomic-level Fe-N-C active sites will be discussed in high-performance ORR catalysts. These catalysts with controlled composition and morphology also enable us to investigate: (i) the structure-performance relation of catalysts for the design of future catalysts and (ii) the formation of active sites during high-temperature pyrolysis to understand the origin of Fe-N-C active sites.



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