OAK RIDGE National Laboratory

ORNL Capabilities and Relevant Research

*BETO workshop: Leveraging First Generation Bioethanol Production
September 25-26, 2019 @ Ames, Iowa

Michelle K. Kidder, Maggie Connatser, Sam Lewis Sr., Tim Theiss

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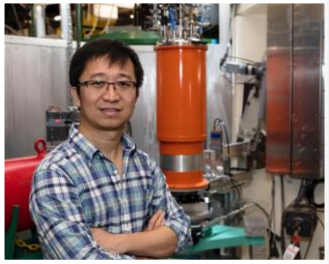

Building Technologies Research and Integration Center

Carbon Fiber Technology Facility

Center for Nanophase Materials Sciences

High Flux Isotope Reactor

Manufacturing Demonstration Facility

National Transportation Research Center

Spallation Neutron Source

Oak Ridge Leadership Computing Facility

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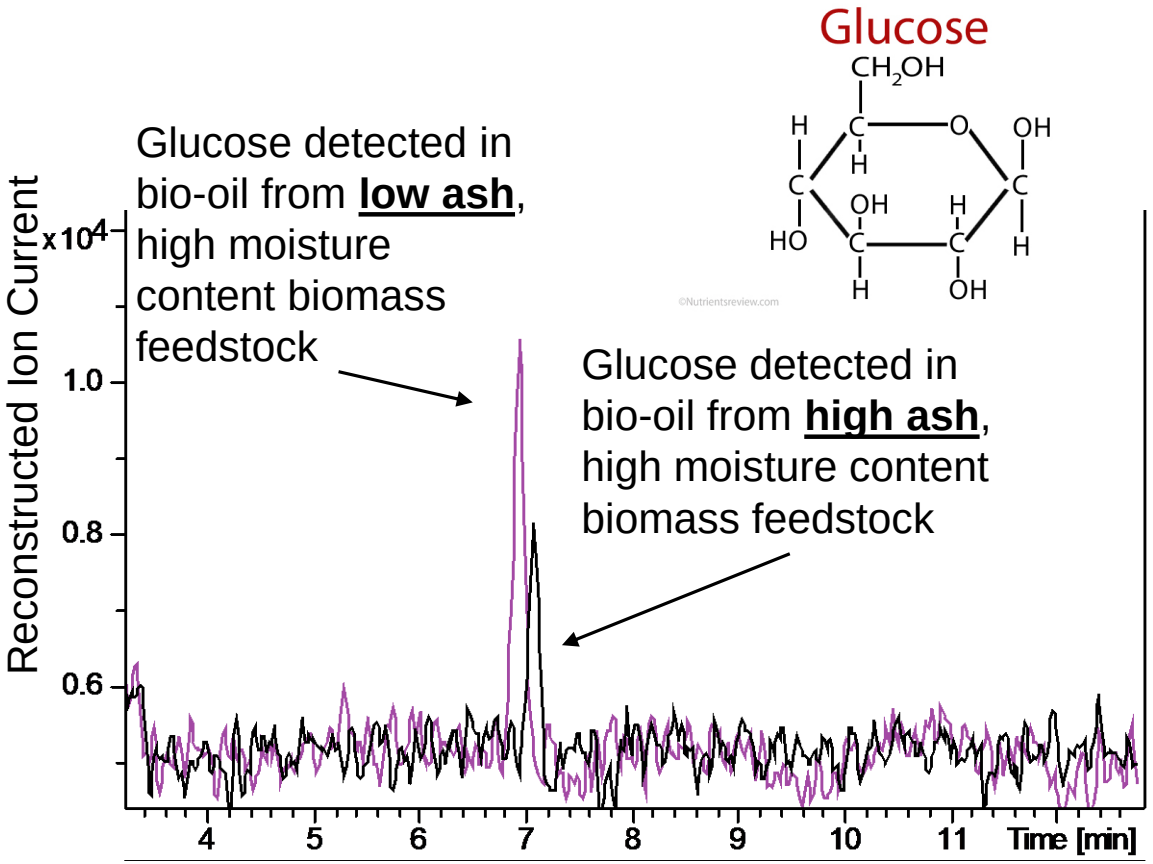
Preliminary Sugar Determination Via CE-ESI-MS

Samuel A. Lewis, Sr.; R. M. Connatser

- Corn fibers contain more recalcitrant molecular backbones than pure corn cellulosic materials
- Fragmented fiber product will also be a mixture 5-membered and 6-membered sugars
- ***Determining relative constituent ratio of xylonic (5-membered) to gluconic (6-membered) sugars could indicate whether the intermediate product stream is yielded preferentially from the plant fiber or other plant residuals***
- Capillary electrophoresis (CE) with electrospray ionization into a Q-TOF mass spec (ESI-MS)
  - CE: a water-friendly analytical separation technique for larger/less volatile analytes such as sugars
  - ESI-MS: less energetic ionization of the analytes separated and coming from the CE allows better structurally descriptive detection of intact sugar ions



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Design of hybrid materials for CO_2 capture and conversion

Michelle K. Kidder; Luke Daemen (NSD), Eugene Mamontov (NSD), Anibal Ramirez-Cuesta (NSD), Gernot Rother (CSD), Vimal Ramanuj, Stephan Irle (CNMS), Michael Cheshire (CSD)

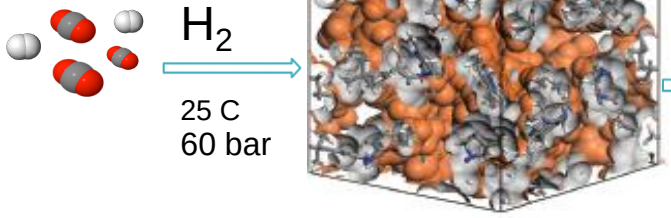
- *Deep dive, holistic approach to understand and predict best design of materials and processes for capture and conversion into hydrocarbons*

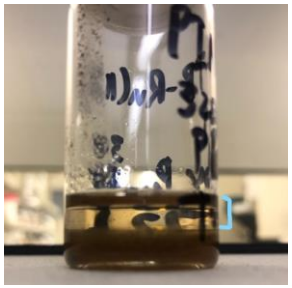
Technical concept: measure and simulate molecular view of key interactions responsible for CO_2/H_2 adsorption capacity, reactivity and transport *at relevant condition*

➢**Catalytic polymer for capture and conversion**

➢**Synthesis, characterizations, probe reactions**

Not limited to this reaction or product!!





Catalytic porous polymer

➢**Modeling and simulation**

- gas-solid multiphase flow and catalytic reaction inside porous polymer
- Sorption geometries

➢**Developing new experimental conditions for in-situ studies with neutrons**

- CO_2/H_2 in-situ reactions-intermediate formation
- Surface diffusion with pressure

- Patent disclosure submitted
- "Characteristics of flow through randomly packed solid and permeable particles using pore resolved simulations," in submission
- "Advancing the design of catalytic materials for CO2 conversion" in draft.

Electrochemical Conversion of CO_2 to Ethanol

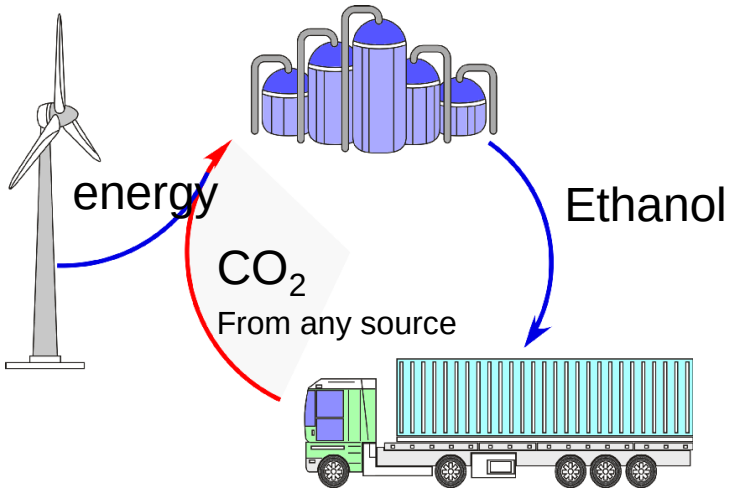
Adam Rondinone, et. al.; current BETO Seed funded

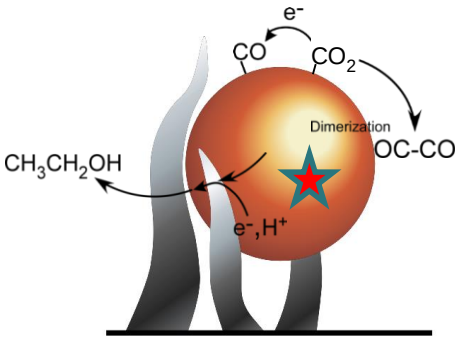
- A means to store electrical energy as a liquid.
- Alternative to battery/electric transportation
  - Carbon neutral
  - Not all consumers can accommodate electric cars – e.g. on street parking
- Better for commercial transport:
  - No long charge times or range issues
  - Much higher energy density

Full Reaction:

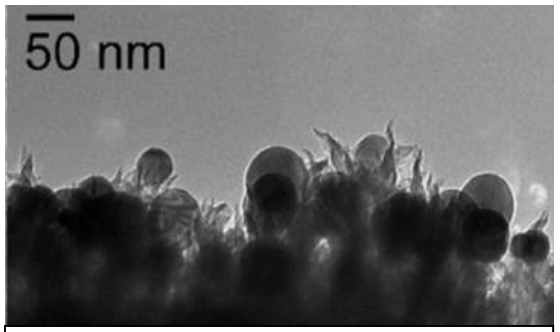
Cathode: $2CO_2 + 9H_2O + 12e^- \rightarrow C_2H_5OH + 12OH^-$

Anode: $12OH^- \rightarrow 12e^- + 6H_2O + 3O_2$





Conceptual illustration of reaction mechanism. Nanotechnology based sequential catalyst with unprecedented selectivity for ethanol



Electron micrograph of carbon nanospike/ copper nanoparticle electrode.

- Electrochemical catalyst for conversion of CO2 to ethanol. US Patent App. 16/098,306
- Song, Y.; et. al.; *Chemistry Select*, **2016**, *1*, 6055.