Catalytic Conversion of CO_2 into Industrial Chemicals

Project Number 1022403

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NETL / DOE

U.S. Department of Energy
National Energy Technology Laboratory
Carbon Storage R&D Project Review Meeting
Transforming Technology through Integration and Collaboration
August 18-20, 2015

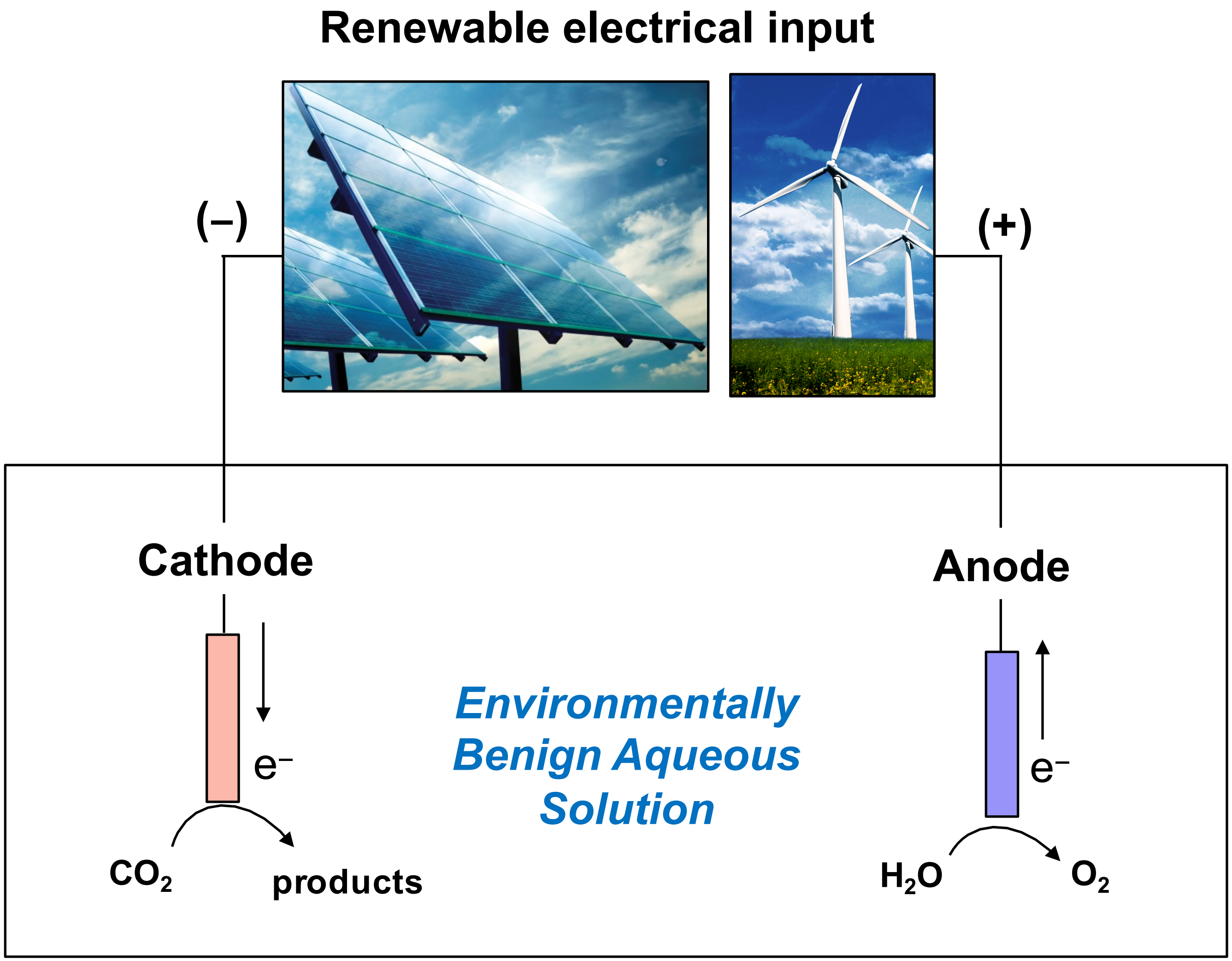
Executive Summary

1. NETL has developed benchmark CO_2 conversion technology
2. Electrochemical CO_2 conversion (ECC) operates at 85-100% efficiency ... no wasted electricity
3. Estimated tonne-per-day CO_2 conversion rates when coupled with current renewable energy sources (solar, wind, *etc.*)
4. The technology compares favorably to other CCUS technologies using NETL's CCUS Metrics (producing methanol from syngas)

CO_2 Conversion

- **Utilize CO_2 emissions as an untapped chemical resource**
- **CO_2 conversion must be carbon neutral (or negative)**
  - Consume more CO_2 than produced
  - Must use carbon-friendly energy (solar, wind, etc.)
- **Catalytic approaches**
  - Thermochemical
  - Photochemical
  - Electrochemical
- **Electrochemical CO_2 conversion is most promising**
  - High efficiency
  - Carbon neutral
  - Renewable energy compatible

Electrochemical CO_2 Conversion



CO_2 reduction catalyst drives the reaction

Benefit to the Program

- Sustainable and environmentally responsible utilization of existing fossil fuel resources.

- Supplement current strategies for CO_2 Storage at the national, regional, basin, and formation scale.

Project Outline

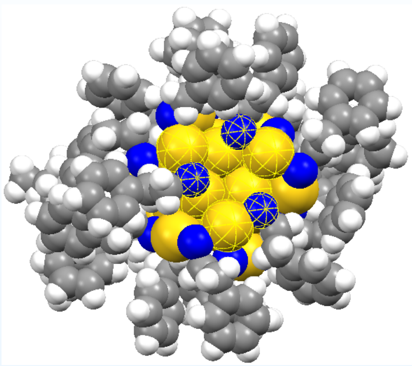
1. **Catalyst design, synthesis and characterization (2010-)**
   - Small-scale studies to identify promising materials
   - Experimental and computational
   - Identify reaction rates, product selectivity and reaction mechanisms

2. **Lifetime testing and scalability studies (2014-2015)**
   - Evaluate promising catalysts in “larger” bench-scale reactors
   - Identify scaling challenges
   - Longer-term testing
   - Provide metrics for techno-economic screening analysis

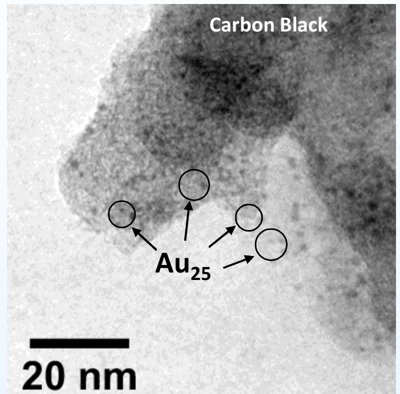
3. **Techno-economic screening analysis (2015)**
   - Collaboration between ORD and OPPB
   - Identify target products, market shares and industrial-scale viability
   - Performance benchmarks for future technologies

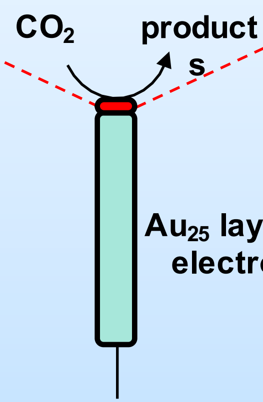
Electrocatalytic CO_2 Reduction

Fundamental tests in small scale reactor

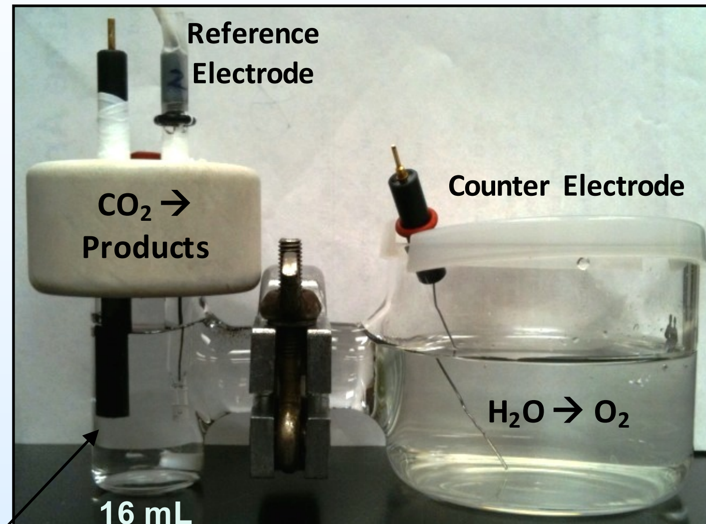


1 nm Au_{25} nano-catalyst





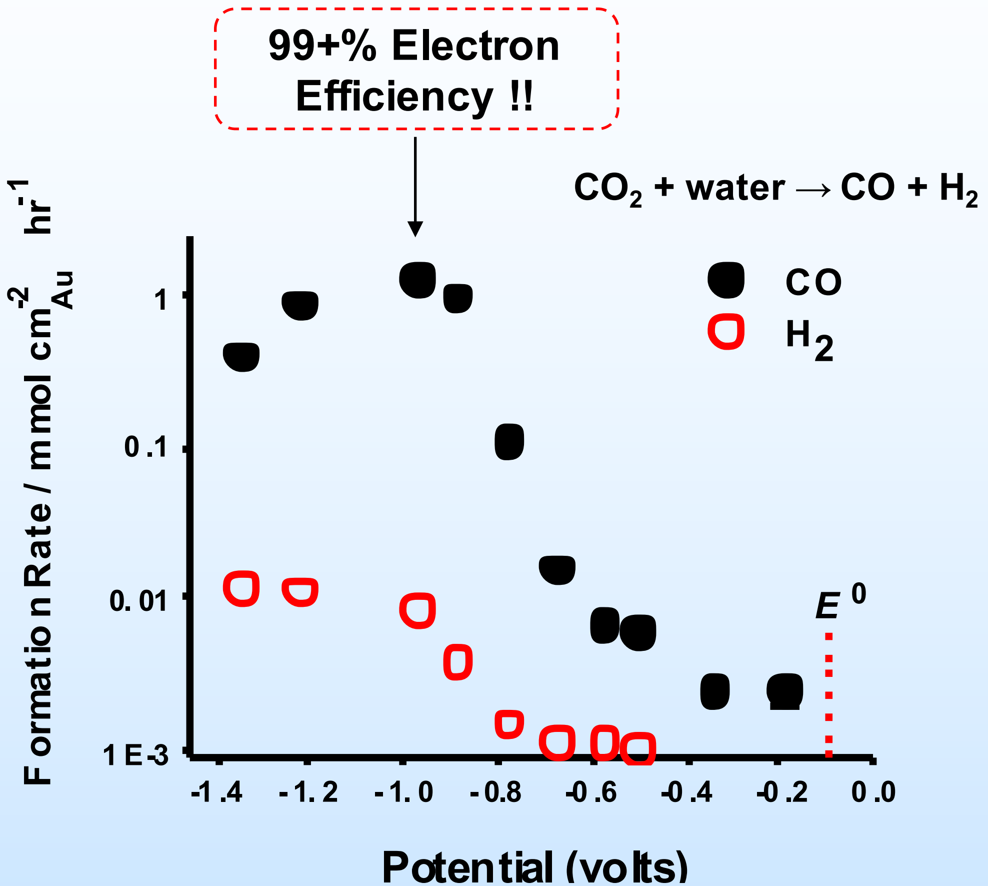
Sealed H-Cell Electrochemical Reactor



Au_{25} layer on
electrode

Electrocatalytic CO_2 Reduction

Au_{25} is the most active CO_2 conversion catalyst ever reported!



Performance Highlights

- 85-99+% Efficient .... No wasted electricity!
- 7-700 times more reactive than other catalysts
- CO_2 conversion within 100 mV of thermodynamic limit!
- Experiment and theory show negative charge increases CO_2 conversion rate

Kauffman et al *J. Am. Chem. Soc.* 2012; *J. Phys. Chem. Lett.* 2013; *Chemical Science* 2014, 5, 3151 // Two US patent applications, one patent pending

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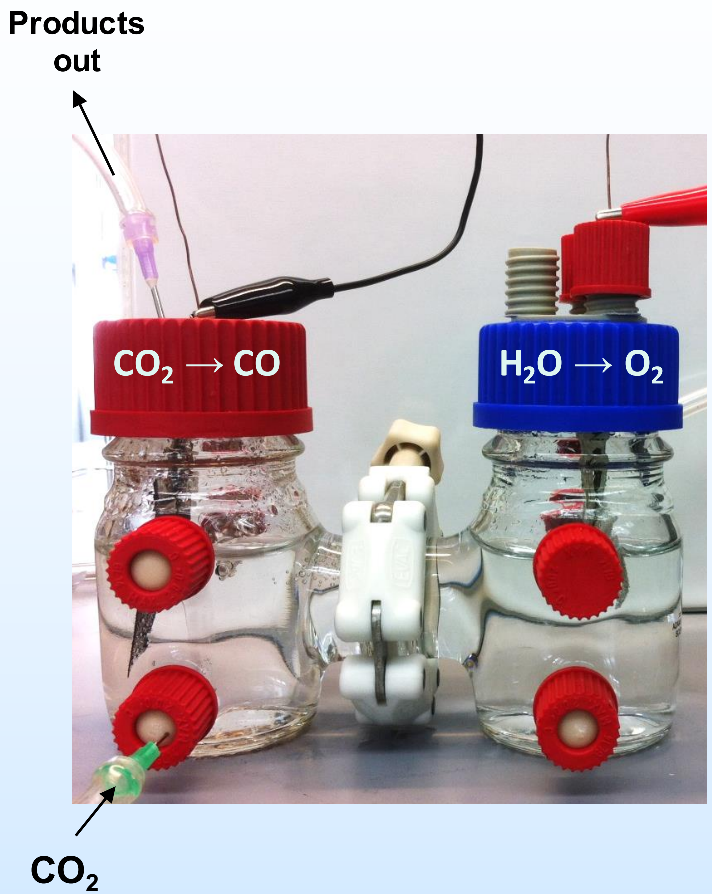
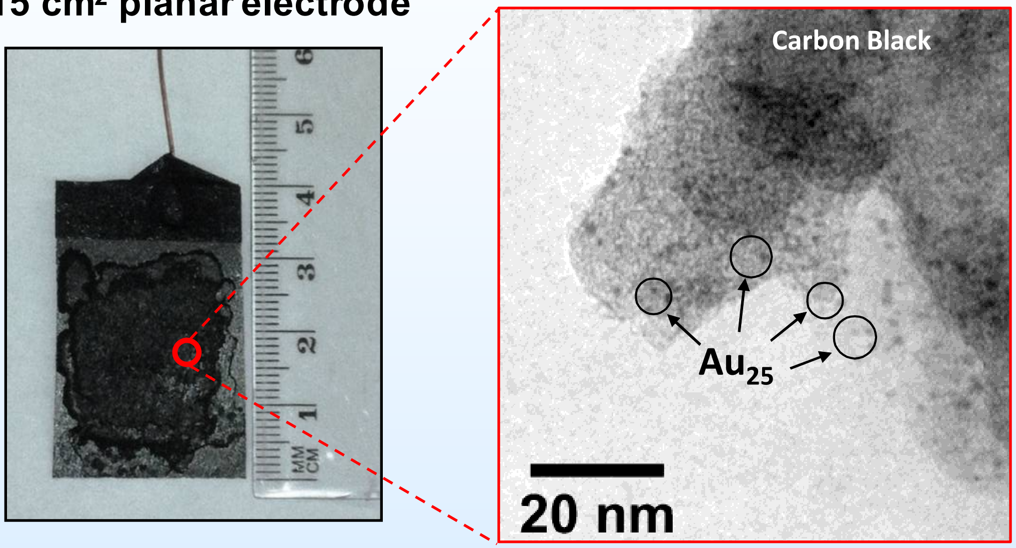
Scaling and Catalyst Lifetime

Increased reactor volume by 10x and electrode area 150x



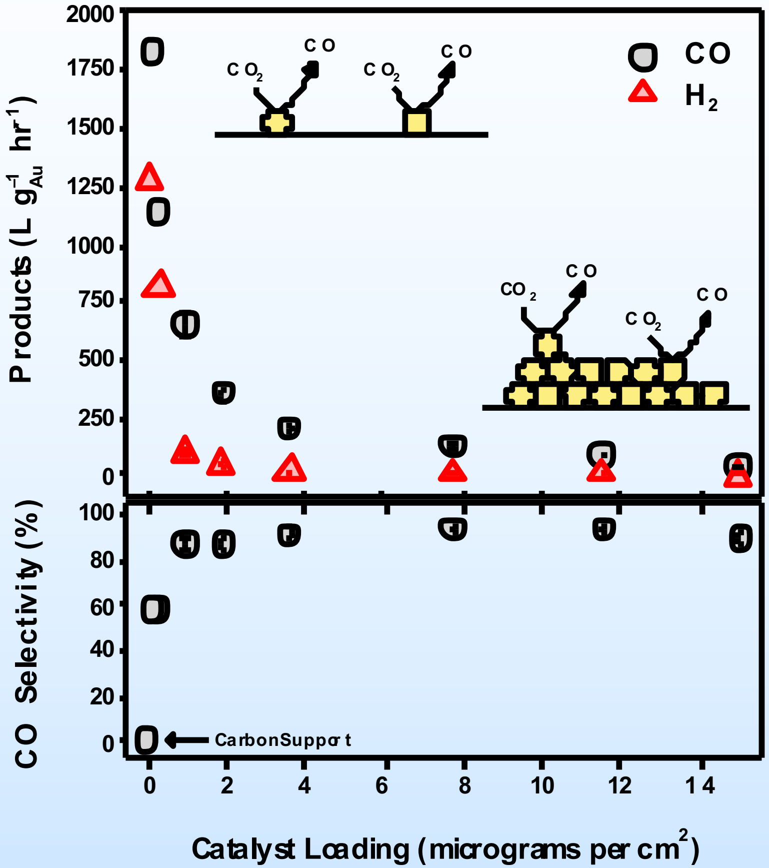
150 mL continuous flow reactor

~15 cm² planar electrode



A "Tunable" Chemical Reaction

Catalyst loading controls the reaction rate and CO to H_2 ratios

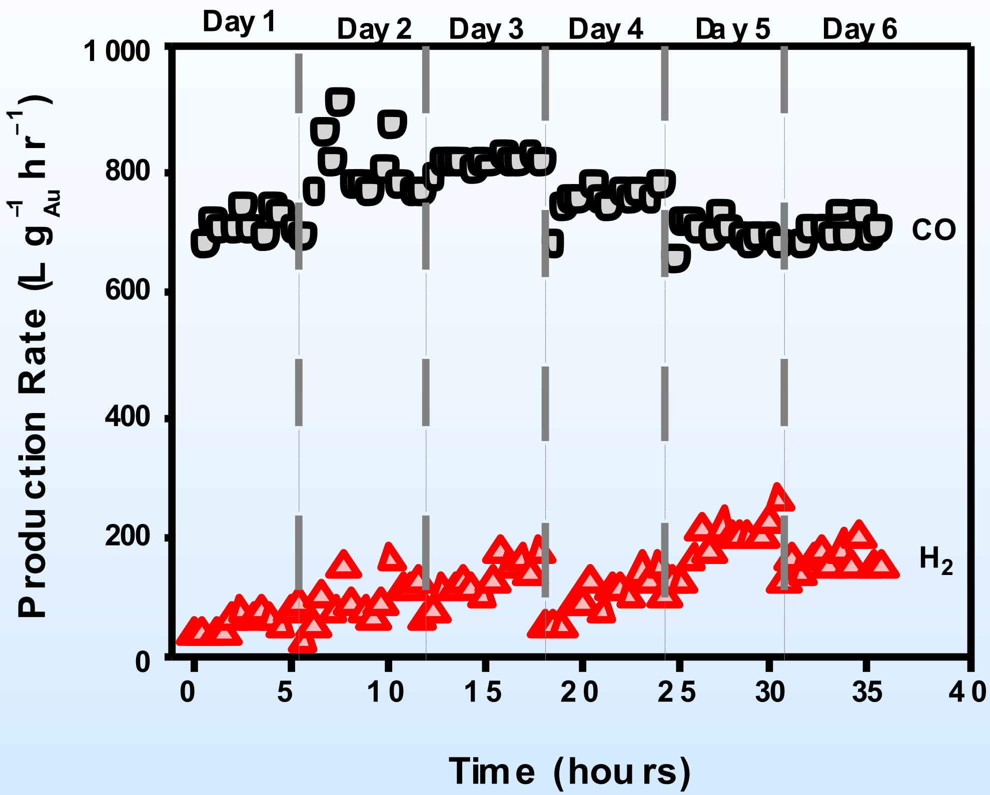


Performance Highlights

- Tune CO:H_2 ratio from 0-100% and everywhere in between!
- Target variety of down-stream products
- 50-fold tunability in reaction rate
- Operating voltage also controls reaction rate and products

Long-term Performance

Efficient and stable electrochemical CO_2 conversion

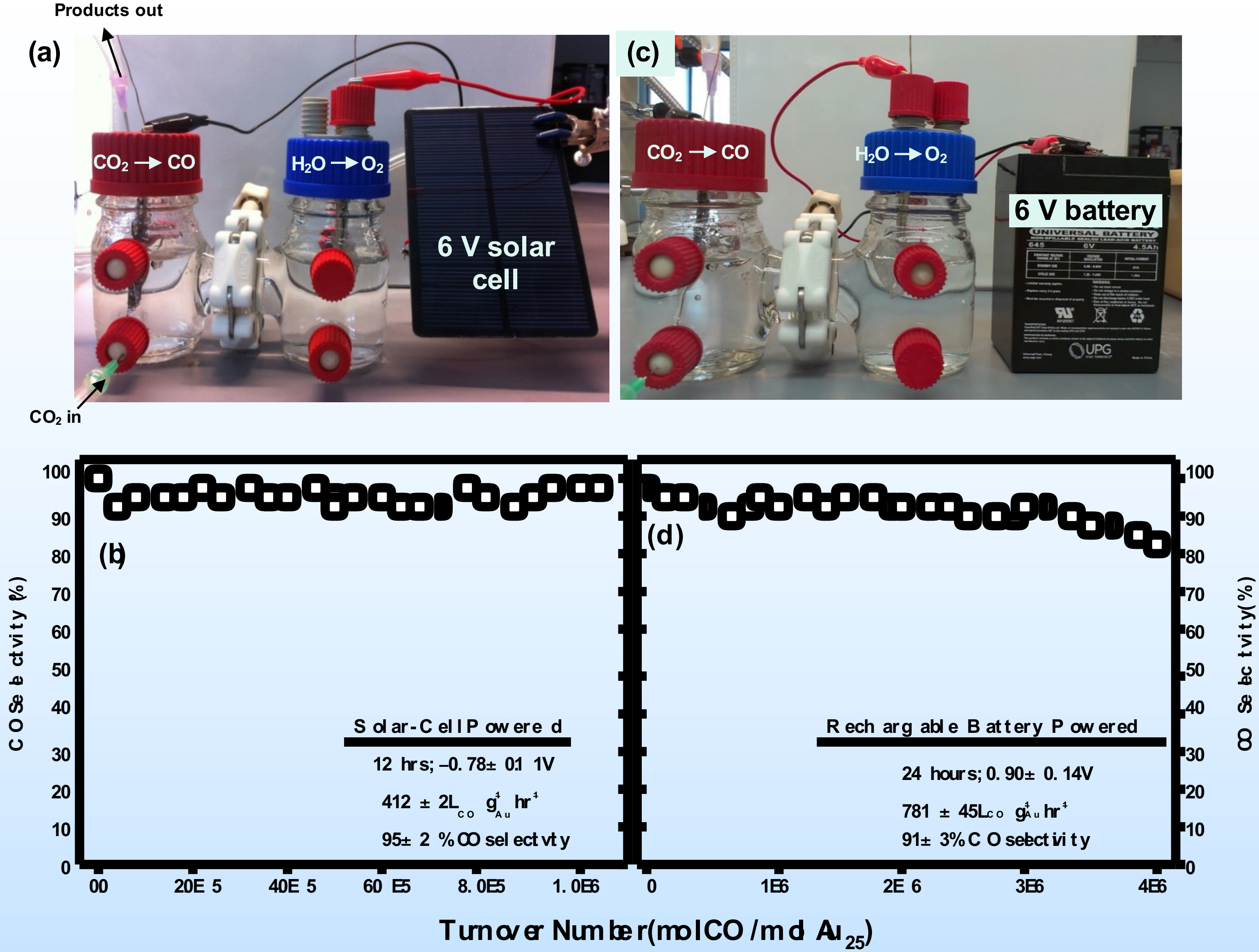


Performance Highlights

- 1.5 kg CO_2 per gram catalyst per hour
- 6+ million reactions per catalyst
- Extremely efficient (102 ± 6 %)
- Almost no wasted electricity

Kauffman et al. *ACS Applied Materials and Interfaces* **2015** 7, 15626-15632

Incorporating Renewable Energy



CO_2 Conversion Capacity

Estimates based on NETL experimental data

Solar power: 1.0 tonne CO_2 acre^{-1} day^{-1}
(assuming 16% efficiency)

One acre of solar panels can convert a metric tonne of CO_2 into CO, formaldehyde, methane or methanol every day.

Wind Power: 1.6 tonnes CO_2 day^{-1} turbine^{-1}
(assuming 25% utilization)

A single 1 megawatt wind turbine can convert 1.6 metric tonnes of CO_2 into CO, formaldehyde, methane or methanol every day.

Batteries can power CO_2 conversion systems during periods without renewable energy.

Hankey, R.; Cassar, C.; Peterson, R.; Wong, P.; Knaub, J. Electric Power Monthly (Feb. 2015); U.S. Energy Information Administration; U.S. Dept. of Energy: http://www.eia.gov/electricity/monthly/ Table 1.1A.

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3. **Techno-economic screening analysis (2015)**
    - Electrochemical CO_2 conversion is cost competitive with other CCUS strategies
    - Target downstream $CO + H_2 \rightarrow$ methanol process.

Synergy Opportunities

– Collaboration between ORD and OPPB to evaluate promising CO_2 utilization strategies and estimate scalability and potential market share.
– Collaboration with other divisions to share capabilities (sensors, fuel cells, CCBTL, etc.)

Accomplishments to Date

- Demonstration of carbon-neutral CO_2 conversion system
- Demonstration that CO_2 conversion technology is cost-competitive with other CCUS technologies.
- Multiple publications, presentations and patent applications (one pending)

Comments / Questions?

WEDNESDAY, AUGUST 19, 2015

- **1:15 PM** Monitoring the Extent of CO_2 Plume and Pressure Perturbation - Bill Harbert
- **2:05 PM** Reservoir and Seal Performance - Dustin Crandall
- **3:45 PM** Monitoring Groundwater Impacts - Christina Lopano
- 5:30 p.m. **Poster Session (SubTER, NRAP, and EFRCs)**
  1. Kelly Rose - Evaluating Induced Seismicity with Geoscience Computing & Big Data – A multi-variate examination of the cause(s) of increasing induced seismicity events
  2. NRAP, EDX, and NATCARB Grant Bromhal, Bob Dilmore, Kelly Rose, Maneesh Sharma
  3. John Tudek- EFRC
  4. Sean Sanguinito NETL CO2 SCREEN)

THURSDAY, AUGUST 20, 2015

- **11:25 AM** Shales as Seals and Unconventional Reservoirs for CO_2– Robert Dilmore

https://edx.netl.doe.gov/carbonstorage/

NETL RESEARCH CARBON STORAGE PROGRAM

Appendix

– These slides will not be discussed during the presentation, but are mandatory

Organization Chart

Team Members: D. Kauffman, D. Alfonso, D.N. Tafel, C. Matranga

Task 8: Catalytic Conversion of CO2 into Industrial Chemicals (TTC: Kauffman)

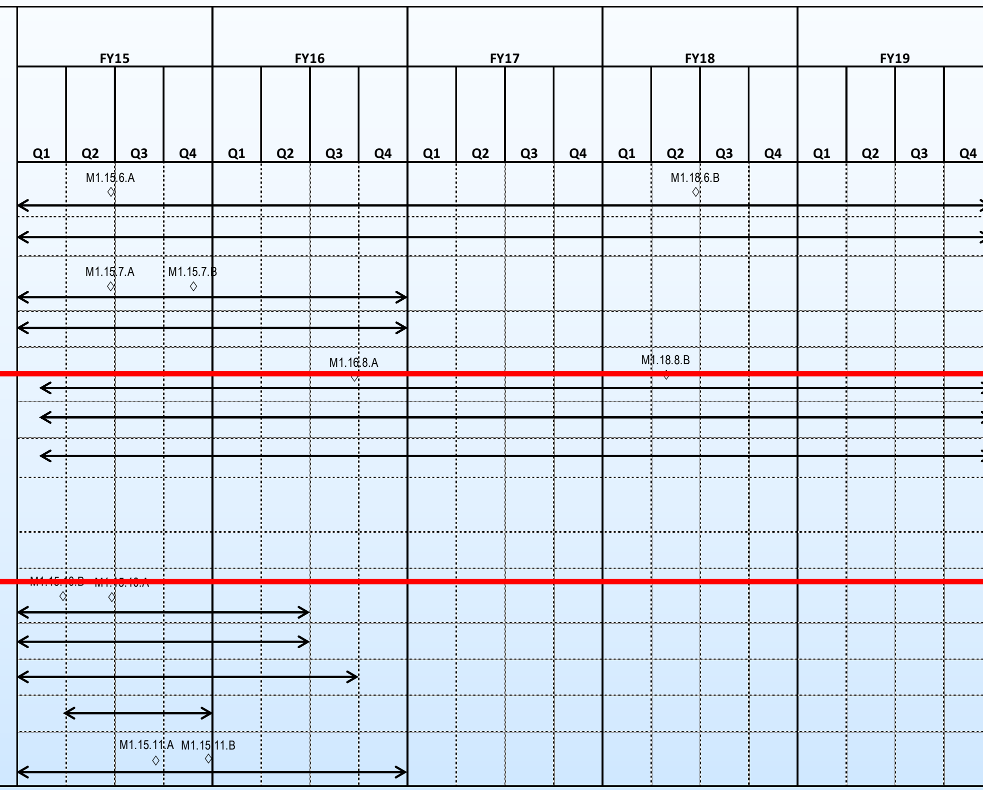
- **Subtask 8.1:** Novel Reactor Chemistry and Reactor Design (Kauffman)
- **Subtask 8.2** Design, Discovery, Synthesis, and Characterization of Novel Catalyst Systems for Catalytic CO_2 Conversion (Kauffman)

Task 9: Evaluation of CO_2 Use and Re-Use Strategies (TTC: Kauffman)

- Collaboration with OPPB for techno-economic screening studies

Gantt Chart

FY15 Carbon Storage (Project Period: 10/01/14 – 09/30/19)	**Project Dates** For each Task, Subtask, Sub-subtask of your WBS **Start** Reflects the date the work is scheduled to begin	**Finish** Reflects the date the work is scheduled for completion
6. Energy Data eXchange/National Carbon Sequestration Database and Geographic Information System Geospatial Resources	**10/1/2014**	**9/30/2019**
6.1 Energy Data eXchange/National Carbon Sequestration Database and Geographic Information System	10/1/2014	9/30/2019
7. Monitoring the Extent of CO_2 Plume and Pressure Perturbation	**10/1/2014**	**9/30/2016**
7.1 Knowledge and Technology Gap Identification	10/1/2014	9/30/2016
8. Catalytic Conversion of CO_2 to Industrial Chemicals	**11/15/2014**	**11/14/2020**
8.1 Novel Reaction Chemistries and Reactor Development for Scalability Assessments	11/15/2014	11/14/2020
8.2 Design, Discovery, Synthesis, and Characterization of Novel Catalyst Systems for Catalytic CO_2 Conversion	11/15/2014	11/14/2020
9. Evaluation of CO_2 Use and Re-Use Strategies	**TBD**	**TBD**
9.1 CO_2 Use and Re-Use Strategy Evaluation		
10. SubTER - Induced Seismicity with Big Data	**10/1/2014**	**3/30/2015**
10.1 Data Gathering	10/1/2014	3/30/2015
10.2 Development of Data Mining Techniques	10/1/2014	6/30/2015
10.3 Data Mining	1/1/2015	9/30/2015
11. Perfluorocarbon Tracers (PFT) Analysis to Support SW Partnership	**10/1/2014**	**9/30/2016**



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- **D. Kauffman**, D. Alfonso, C. Matranga, H. Qian, R. Jin "Experimental and Computational Investigation of Au_{25} Clusters and CO2: A Unique Interaction and Enhanced Electrocatalytic Activity" *J. Am. Chem. Soc.* **2012**, *134*, 10237-10243. Available online: http://dx.doi.org/10.1021/ja303259q

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- **D. Kauffman**, D. Alfonso, C. Matranga, P. Ohodnicki, X. Deng, R. C. Siva, C. Zeng, R. Jin, "Probing Active Site Chemistry with Differently Charged Au_{25}^q Nanoclusers (q = -1, 0, +1). Chem. Sci. **2014**, *5*, 3151. Available online: http://dx.doi.org/10.1039/c4sc00997e

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- **D. Kauffman**, D. Alfonso, D. N. Tafen, J. Lekse, C. Wang, X. Deng, J. Lee, H. Jang, J-S. Lee, S. Kumar, C. Matranga "Electrocatalytic Oxygen Evolution with an Atomically Precise Nickel Complex" *Submitted and currently under review.*

- 10+ presentations delivered at international scientific conferences.