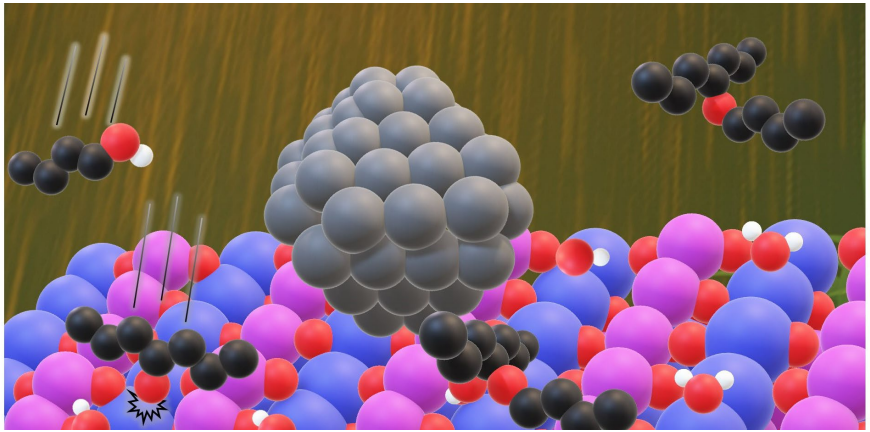
REGIONAL CARBON CONVERSION
US DEPT. OF ENERGY, FOSSIL ENERGY AND CARBON MANAGEMENT

Argonne NATIONAL LABORATORY 75 1946–2021

CARBON CONVERSION R&D ACTIVITIES AT ANL



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October 18
Minneapolis, MN

Argonne Major Research Initiatives

Facility

- Advanced Photo Source (APS)
- Argonne Leadership Computing Facility
- Center of Nanoscale Materials
- Materials Engineering Research Facility

Centers

- Joint Center for Electrical Energy Storage
- Advanced Materials for Energy Water Systems Center
- Water-AI Initiative
- Science for Circular Economy

Source: Argonne Lab Plan Summary document

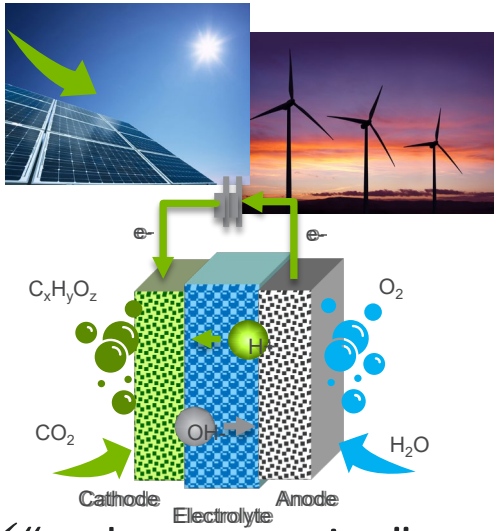
Carbon Conversion

Fundamental and applied Research and Development Opportunities

- **Circular Economy:** Development of methods for CO_2 capture/ Utilization
  - Catalytic Conversion of CO_2 to value added chemicals
    - Chemical/Photo or Electrochemical routes
    - Applied science/ engineering expertise (TEA, LCA) and facilities (MERF)
  - Discovery of new and improved catalysts
    - High throughput Experimentation
    - Role of AI/HPC to accelerate Catalyst Discovery
  - Waste Carbon to Sustainable Aviation fuels
    - New catalysts and conditions
  - Data science and AI
    - Catalyst and Materials Genome for Carbon Utilization

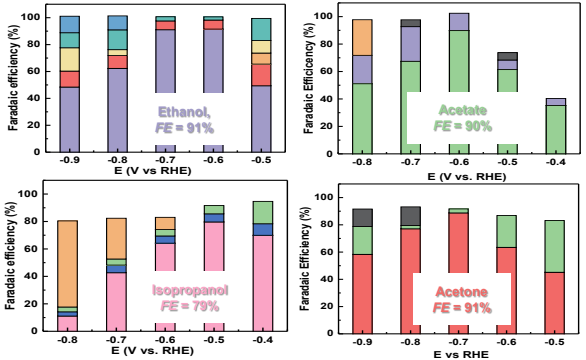
Carbon Negative Earth Shot "CO_2 Refinery" – A Technology of CO_2 conversion to chemicals

Concept of "CO_2 Refinery"



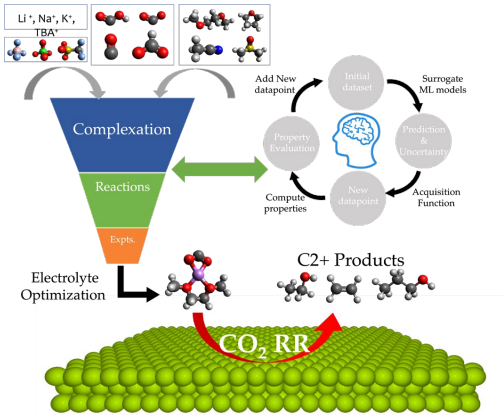
✓"carbon-negative" manufacturing

CO_2RR Catalysis Science



✓New electro-catalysts converts CO_2 to C_2 and C_3 -ethanol, isopropanol, acetone, at 80~90% selectivity through electrolysis at near ambient T.

AI- Solvent Engineering

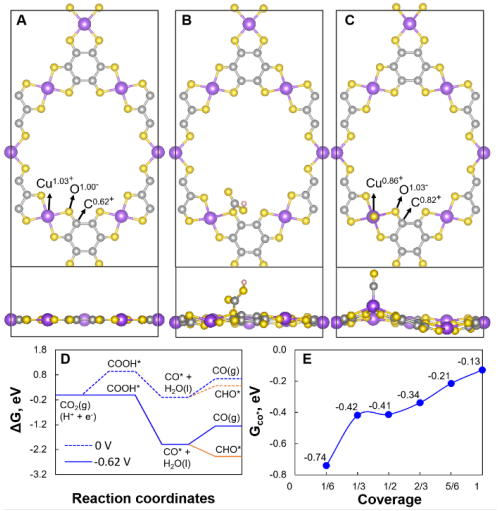


✓ Solvent Engineering for Efficient CO_2 Conversion

Di-Jia Liu, Argonne National Lab, djliu@anl.gov

Materials for selective CO_2 reduction

Two-Dimensional Conductive Cu-MOF (good TOF: 20.8 s-1)



(A) clean Cu-THQ surface, (B) COOH/ Cu-THQ, (C) CO/ Cu-THQ , (D) free energies for CO production on Cu-THQ, (E) BE(ads) of CO at different coverages on Cu-THQ.

Other Research directions:

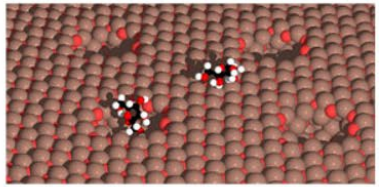
- ✓ High entropy alloys for CO_2 conversion
- ✓ Photochemical conversion of CO_2
- ✓ Optimization of electrolytes for CO_2 electrochemical reactions
- ✓ Data-driven approach for next generation selective catalysts

L. A Curtiss, A. Salehi-Khojin et al., Adv. Materials 33 (10), 2004393 (2021).

Accelerate enabling technologies using computations and AI

Atomic, Mesoscale, reactor scale modeling

IACT-EFRC (2009-13)



Institute for Atom-efficient Chemical Transformations

CCPC
Consortium for Computational Physics and Chemistry
U.S. DEPARTMENT OF ENERGY
BIOENERGY TECHNOLOGIES OFFICE

Argonne NATIONAL LABORATORY | Idaho National Laboratory | NETL NATIONAL ENERGY TECHNOLOGY LABORATORY | NREL Transforming ENERGY | OAK RIDGE National Laboratory | Pacific Northwest NATIONAL LABORATORY

A multi-scale problem ... A multi-lab solution

CCPC (2013-present)

2009 2010 2012 2013 2014 2015 2016 2017 2018 2019 2020 2021

- IACT was part of BES
- CCPC is part of ChemCatBio Consortium supported by EERE/BETO

https://www.energy.gov/eere/bioenergy/consortium-computational-physics-and-chemistry

TAKE HOME MESSAGES

Conversion

- ✓The current state-of-the-art catalysts in eCO_2RR suffer largely from low reaction rates, insufficient C_{2+} **product selectivity**, high overpotentials, and **industrial-scale stability**.
- ✓Overcoming the scientific/applied technical hurdles for commercial realization demands a holistic integration of catalytic designs, deep mechanistic understanding, and efficient process engineering.
- ✓Special emphasis on **accelerated** mechanistic understanding and performance outcome is critical to guide the future design of eCO_2RR catalysts that can play a significant role in closing the anthropogenic carbon loop.