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

CARBON CONVERSION
R&D ACTIVITIES AT ANL

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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 CO₂ capture/Utilization
  - Catalytic Conversion of CO₂ 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 “CO₂ Refinery” – A Technology of CO₂ conversion to chemicals

Concept of “CO₂ Refinery”

- “carbon-negative” manufacturing

CO₂RR Catalysis Science

- New electro-catalysts converts CO₂ to C₂ and C₃ -ethanol, isopropanol, acetone, at 80~90% selectivity through electrolysis at near ambient T.

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AI- Solvent Engineering

- Solvent Engineering for Efficient CO₂ Conversion
Materials for selective CO₂ reduction

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

Other Research directions:
✓ High entropy alloys for CO₂ conversion
✓ Photochemical conversion of CO₂
✓ Optimization of electrolytes for CO₂ electrochemical reactions
✓ Data-driven approach for next generation selective catalysts

(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.

Accelerate enabling technologies using computations and AI

Atomic, Mesoscale, reactor scale modeling

• 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
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Conversion

✓ The current state-of-the-art catalysts in eCO$_2$RR suffer largely from low reaction rates, insufficient C$_2+$ \textit{product selectivity}, high overpotentials, and \textit{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 \textit{accelerated} mechanistic understanding and performance outcome is critical to guide the future design of eCO$_2$RR catalysts that can play a significant role in closing the anthropogenic carbon loop.