Development of New Methodology for Making Catalysts with Application to Production of Ammonia, Ethylene, Methanol, and Related Chemicals

Kick-off Meeting

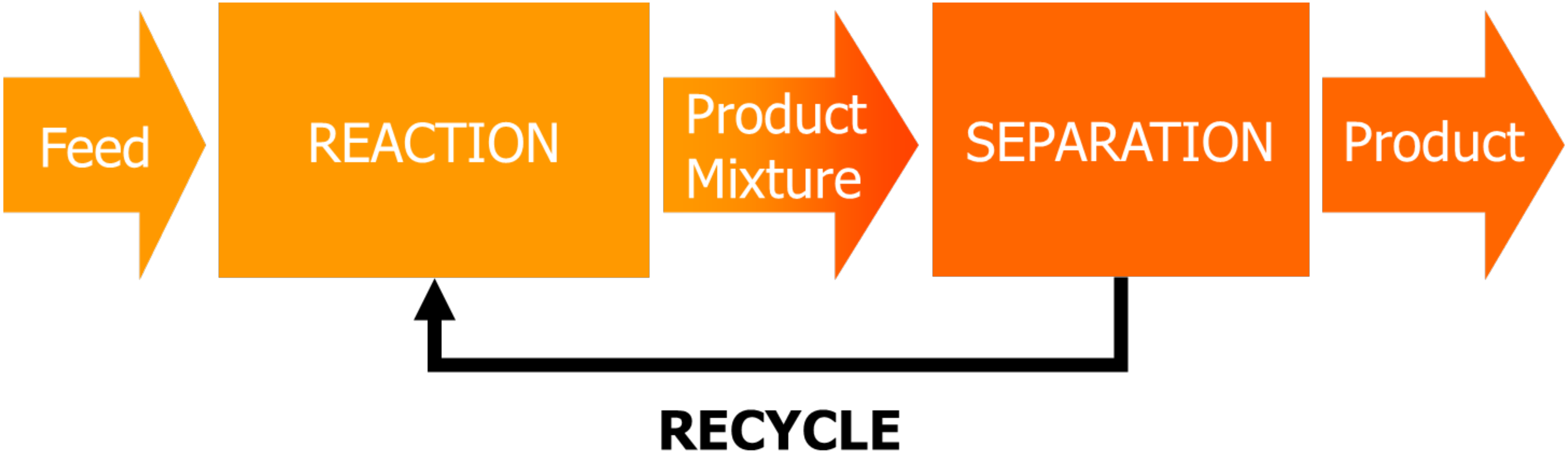
Idaho National Laboratory

March 8, 2017

Dr. Dickson Ozokwelu

Advanced Manufacturing Office

Why Catalysis? Possible Efficiency Gains

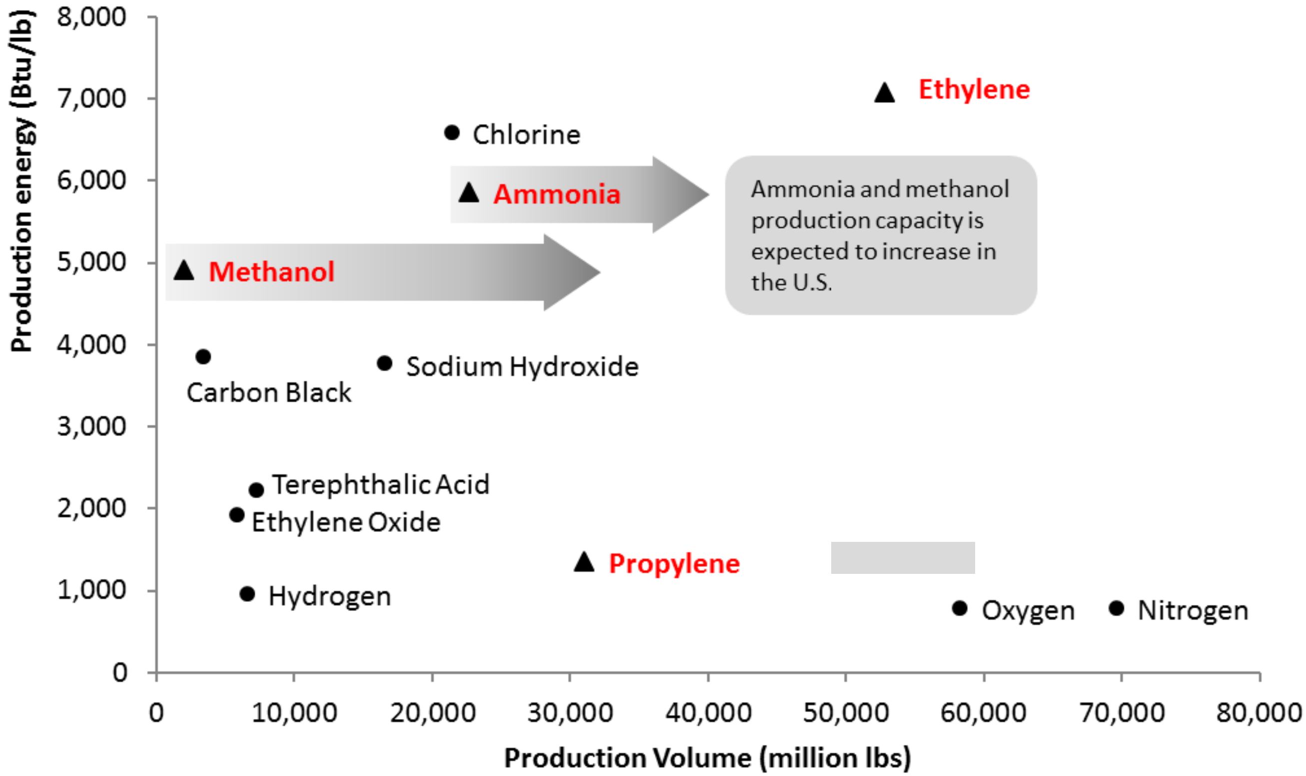


Low conversions and selectivity rates in Reaction phase

High energy intensity in Separations phase

★ Must Improve Reaction and Separation Efficiency ★

Catalysts: Global Impact



- Catalysts are involved in 90% of all chemical manufacturing
- In 2010, total U.S. primary energy consumption in the chemical industry was 4.3 Quads
- Domestically in 2010, 559 TBtu were consumed by the 4 chemicals highlighted in red
- Savings Potential of **112-224 TBtu/yr.** (20%-40%)

Source: IEA (2013), MECS data.

A Transient Kinetic Approach to Catalytic Materials For Energy-Efficient Routes to Ammonia, Ethylene and Related Chemicals

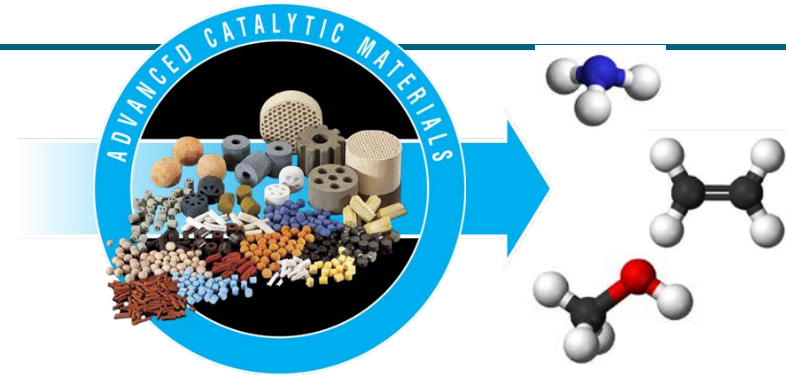
Chemical Catalysts Research and Testing
Idaho National Laboratory, Argonne National Laboratory

Dr. Rebecca Fushimi, Idaho National Laboratory

U.S. DOE Advanced Manufacturing Office Technical Resources & Networking Forum
Washington, D.C.
June 15, 2017

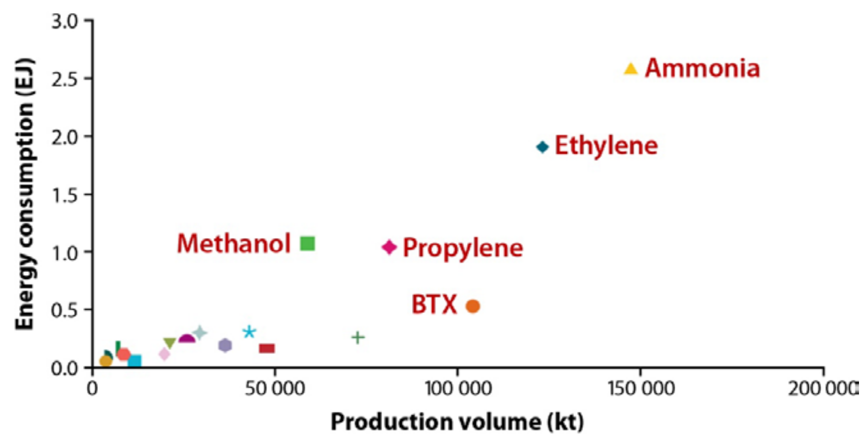
Project Objective

- A new paradigm for catalyst development based on transient kinetics



- Catalyst development is primarily trial-and-error to address:
  - Complex multistep reaction mechanism
  - Complex multicomponent, ill-defined materials

- New catalytic routes to ammonia, ethylene, etc.
  - Ammonia: 2% of the world's energy use
  - Ethylene: 30% energy saving with catalysis over current steam cracking practice

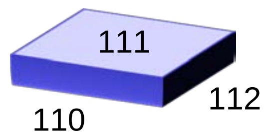


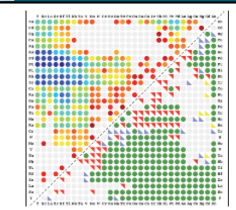
International Energy Agency, Technology Roadmap, Energy and GHG Reduction in the Chemical Industry via Catalytic Processes, 2013.

Technical Innovation

- Current practice of catalyst development

Surface Science	High-Throughput
– Detailed kinetics – Model materials	– Basic kinetics – Industrial materials





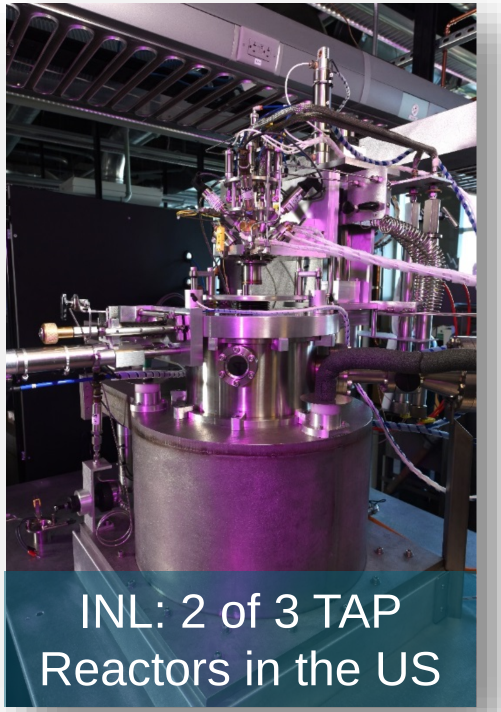
Curtarolo, Stefano, et al. *Nature materials* 12.3 (2013): 191-201.

- Transient kinetics

Temporal Analysis of Products (TAP) Reactor System

- Detailed kinetics : Complex mechanism
- Industrial materials : Complex materials

Understanding *how* and *why* materials function



- Kinetic-Centric Informatics

Exploiting data science tools around microkinetics

- Experimental & Theoretical

- Accelerating the catalyst development

Technical Approach & Resources

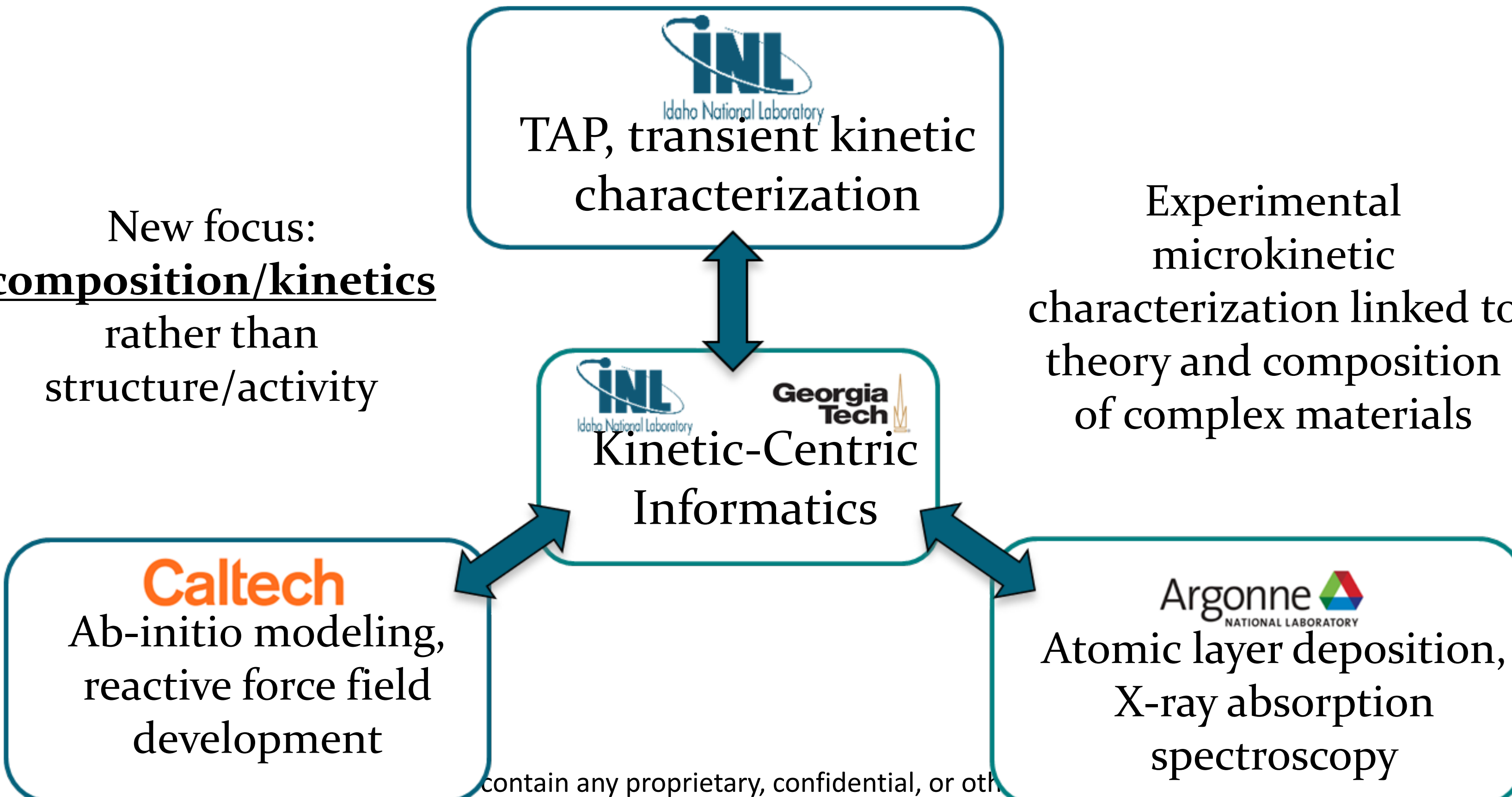
- A new paradigm for catalyst development:

  Transient kinetic experiments

- Kinetic-Centric Informatics tool:

  More meaningful connections from complex data sources

New focus:
<u>composition/kinetics</u>
rather than
structure/activity

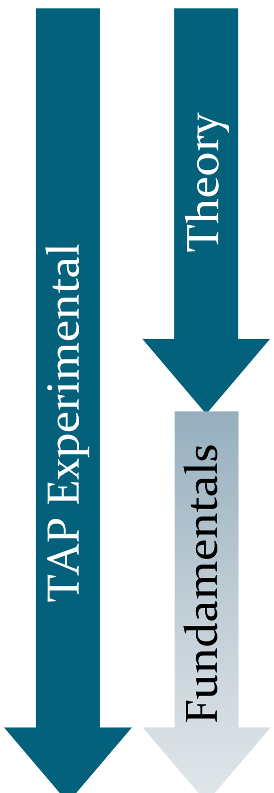


Experimental microkinetic characterization linked to theory and composition of complex materials

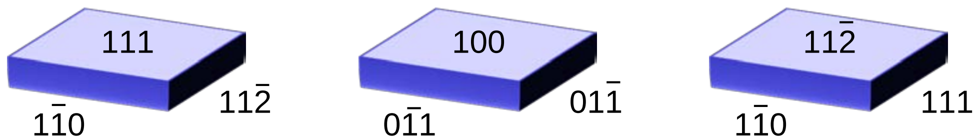
Technical Approach

- Ammonia synthesis from 200 to 20 bar

- Elementary reaction steps, N-N rupture, N-H formation
- Incremental surface coverage change, N, NH, H, etc.
- Material complexity

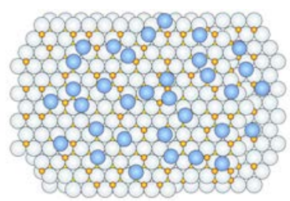


Fe Single Crystals

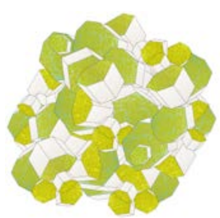


Polycrystalline Fe

Single site, Atomic cluster catalysts



Na, K, Ca Promoters



Commercial Catalysts

TAP + DFT

Experimental measurement theoretical predictions

- Enthalpies, ΔH
- Rate constants, k_{ads}, k_r

Brings new direction for applying combinatorial tools to the right problem

Measure of Success

- Moving catalyst development beyond trial-and-error
- Enduring benefit
  - A unique capability to support industrial research
  - Changing the way materials are studied and designed
- Measurement
  - Industry participation (CRADA and SPP Agreements)
  - Transition of early-research to industry

- Wide-adoption of TAP and understanding of transient kinetics
- Move beyond catalysis to other gas/solid reaction applications
  - Chemical sensors, advanced sorbents, photo and electrochemical systems, energetic reactions, materials characterization, etc.
- Adoption of more-efficient transient chemical processes
  - Redox mode, transport bed, switched feed, chemical looping

Program Engagement

- Industry Advisory Board
- CRADA, Cooperative Research and Development Agreements
- SPP, Strategic Partnership Projects
- Minimum 6 month engagement suggested for R&D
- CAES: Center for Advanced Energy Studies
  - CAES & INL Technical Assistance Program
  - Short-term proof-of-concept

Catalysis Development Tools, Research and Catalyst Technologies Network

Magdalena Ramirez/INL

U.S. DOE Advanced Manufacturing Office Technical Resources & Networking Forum
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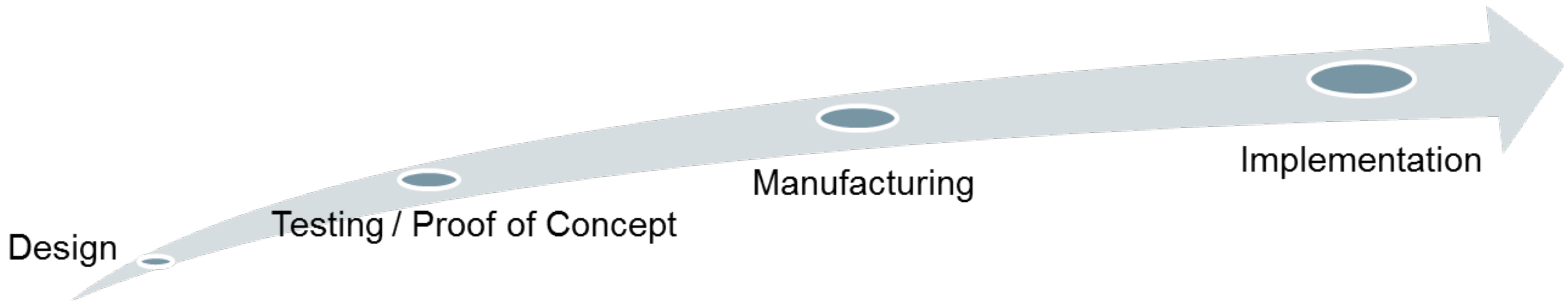
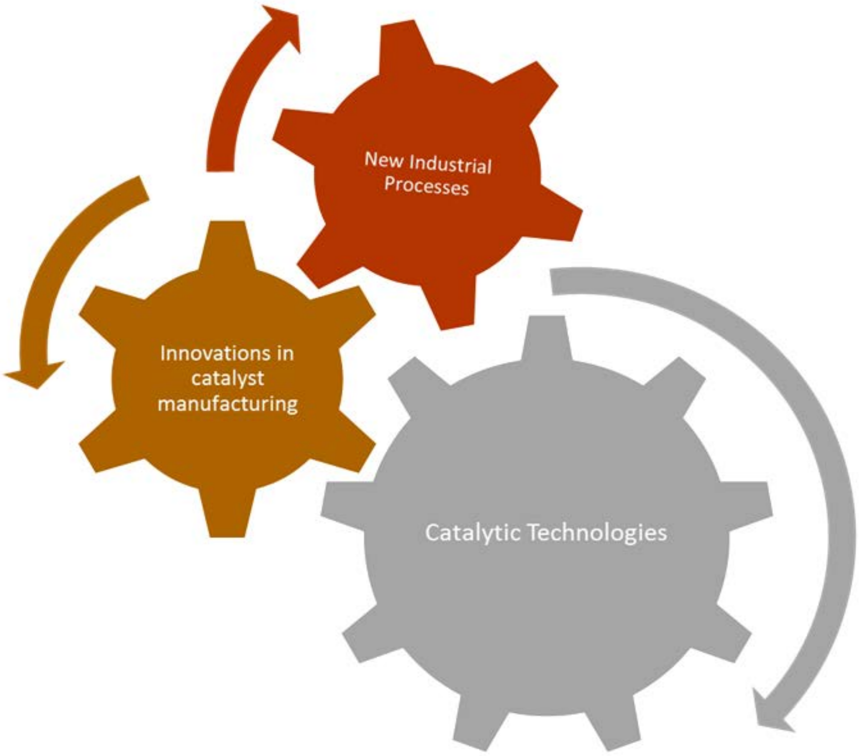
Program Introduction



- For research purposes, catalytic materials are prepared at lab-scale using careful and controlled synthetic methods, which are not typically represented in industrial manufacturing processes.
- The missing link: Scientific basis of catalysts manufacturing processes
- The Program will accelerate the path of R&D outcomes to industrial uses

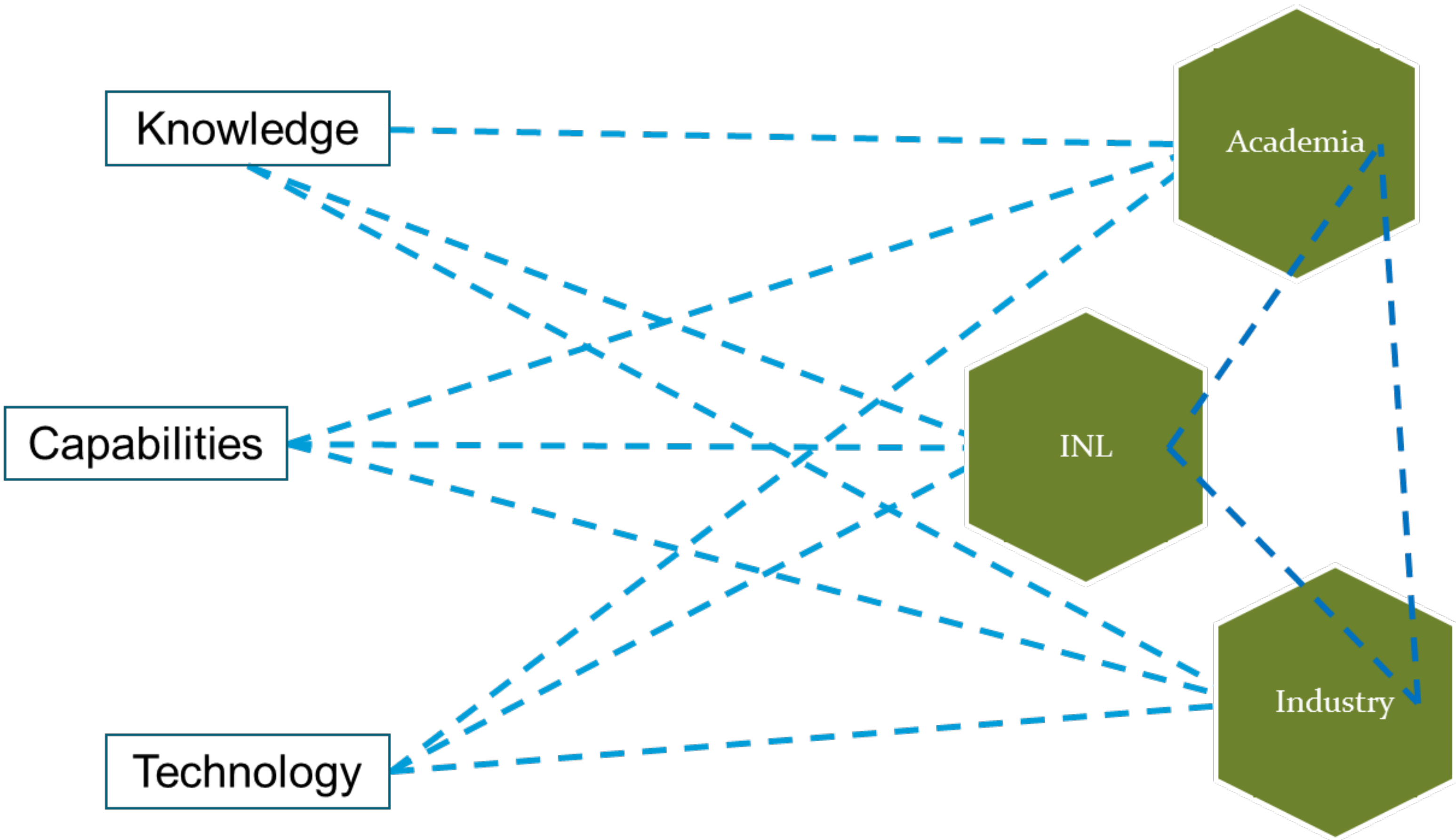
Catalytic Technology Network, CTN

Catalytic technologies to enable cleaner and more efficient manufacturing



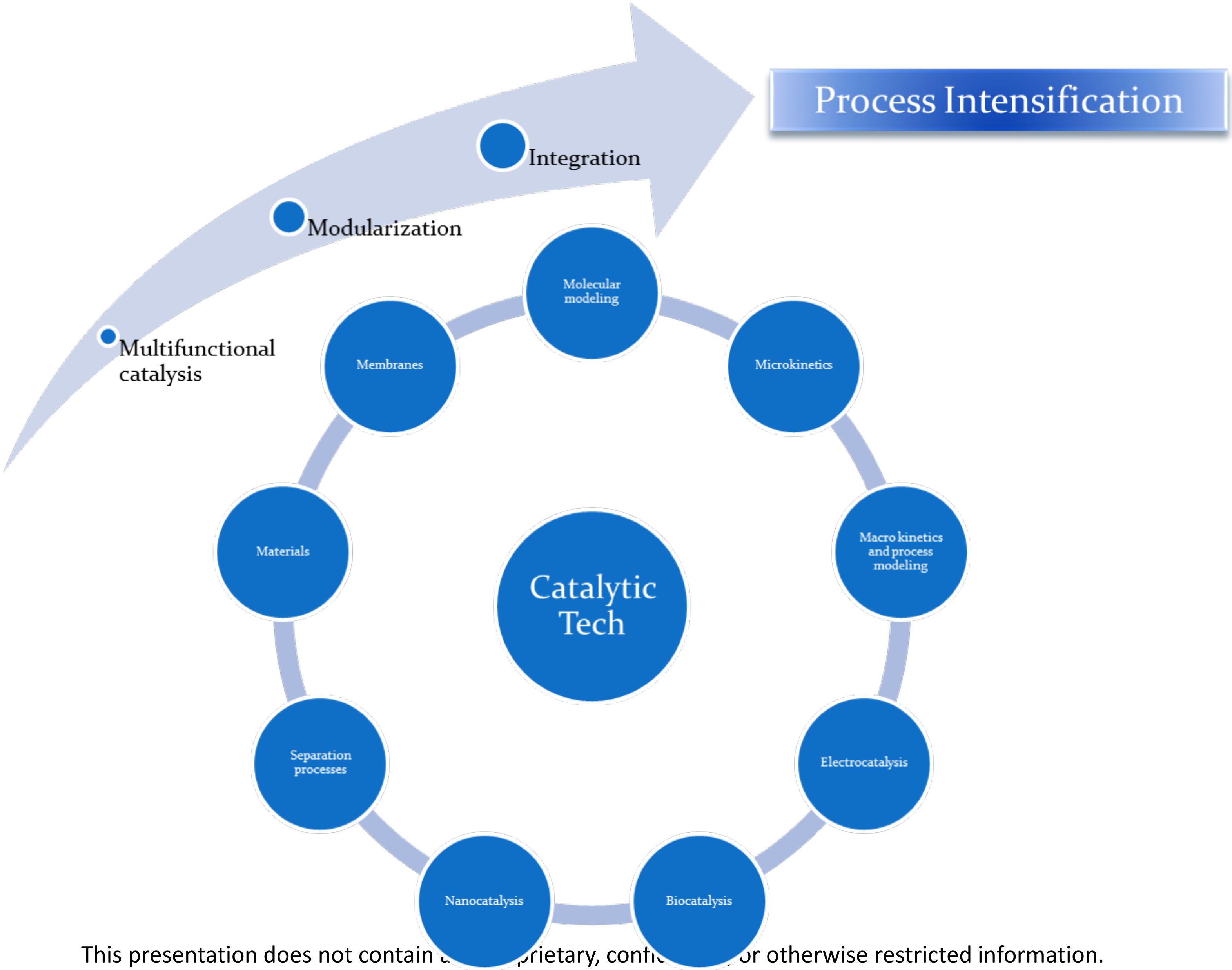
- A world-class **catalytic technologies network,**
- providing more energy efficient and cleaner manufacturing methods,
  - for catalytic materials
  - and for fuels/chemicals through catalytic processes.

The Network



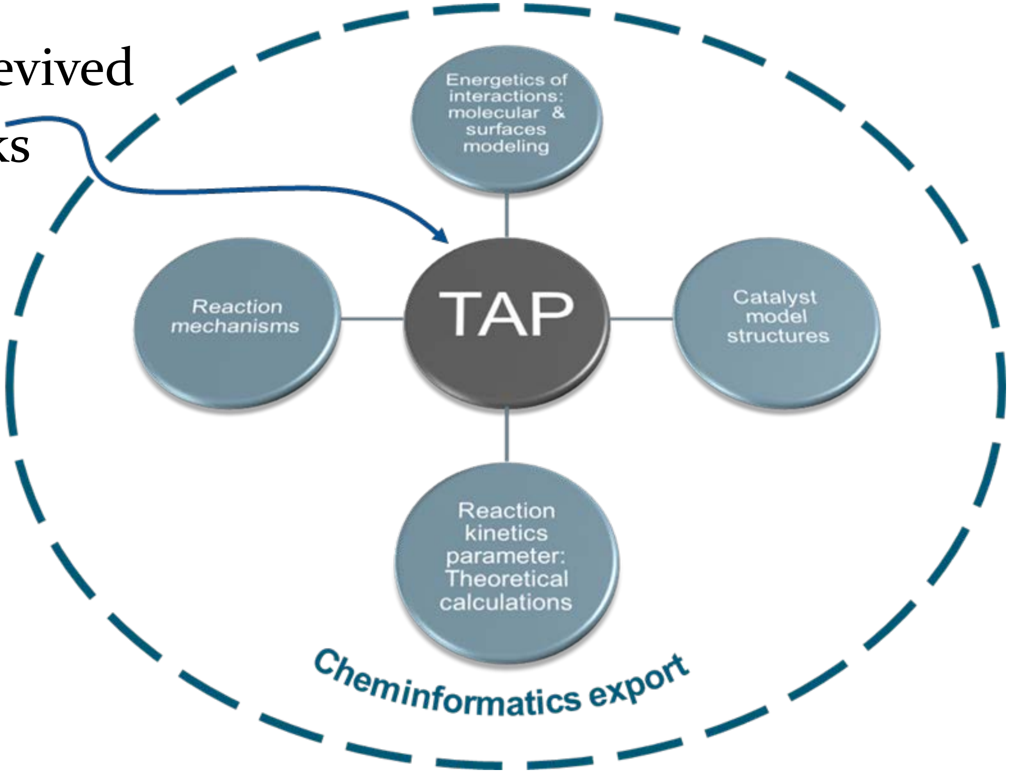
Leveraging knowledge and capabilities to facilitate technology development

Capabilities and Resources



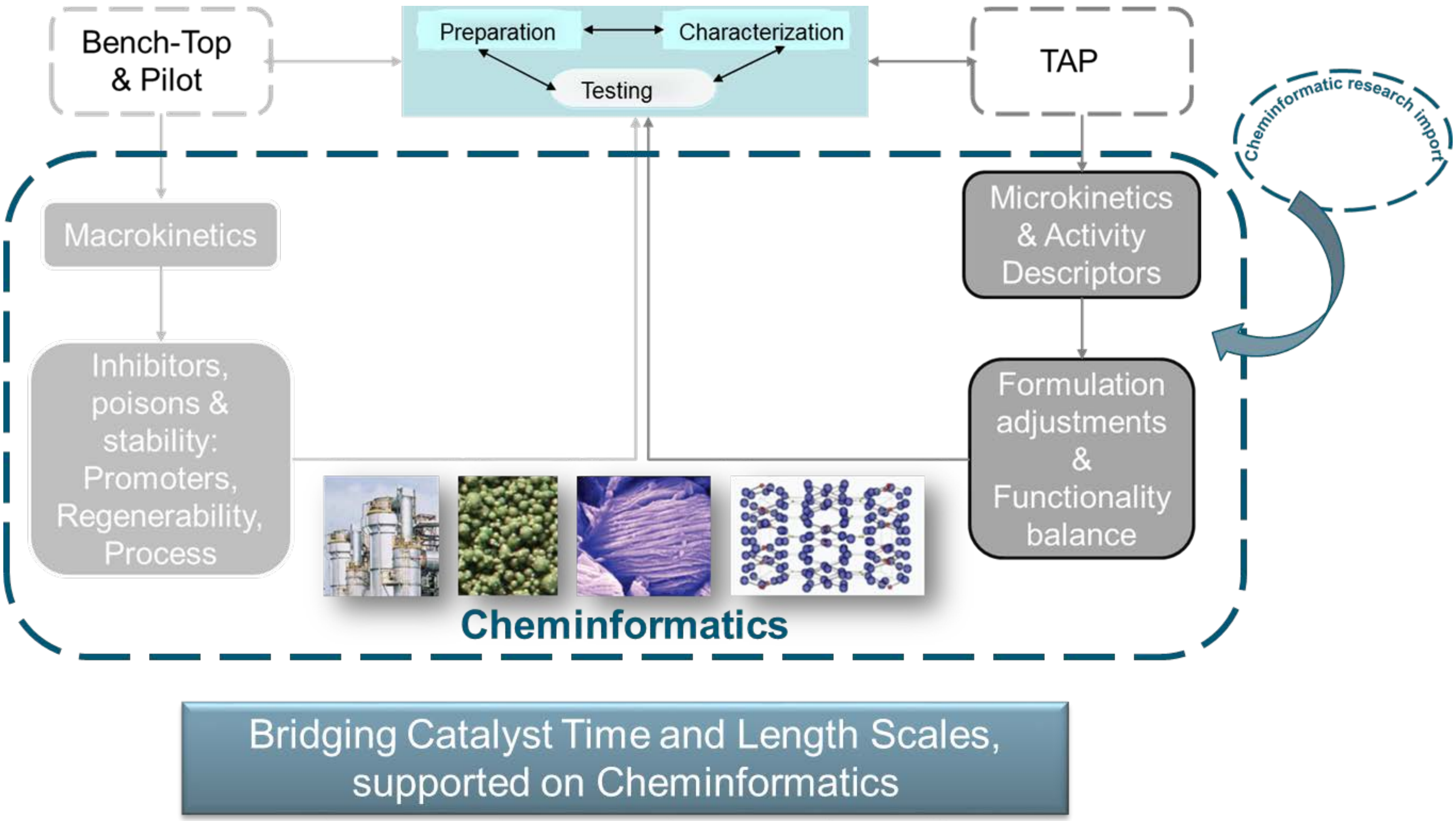
Unique resource: TAP

- Activity: How much it does
- Selectivity: Where it takes the feed
- Stability: How long it lasts
- Regenerability: Can it be revived
- Functionality: How it works

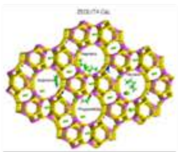


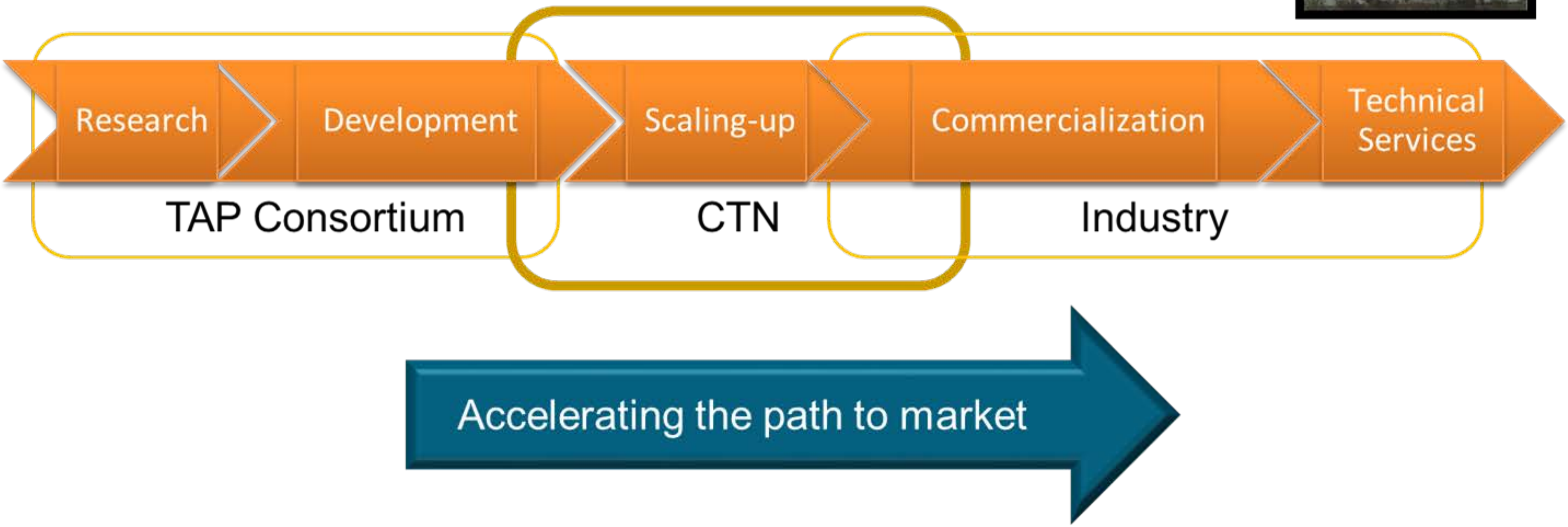
Basic Research Contributions to TAP R&D

CTN will link TAP outcomes to catalyst development



CTN within the Catalytic technologies supply chain





Program Focus and Deliverables

- Four major energy-intense processes:
  - Ammonia
  - Ethylene
  - Propylene
  - Methanol
- Three types of outputs:
  - Catalysts
  - Catalyst manufacturing methods
  - More energy efficient catalytic manufacturing processes

Program Success

- The identified scientific basis for a new catalyst synthesized using conventional methods allows its reproduction through manufacturing processes, as proved by an industrial partner.
- The identified scientific basis for a new synthetic method allows its reproduction through a newly designed manufacturing process that rises industrial interest.
- The potential process that uses a catalyst developed through CTN rises industrial interest

Program Application Process/Business Engagement

CTN Value Proposition

Academia

- An accelerated mechanism to connect research outputs with market
- Guidance and advice from industrial views, needs and problems
- A path to catalysts industrialization and commercialization
- A smooth mode of industry – academia liaison

Industry

- Direct translation of academia outputs to industry
- Access to and influencing mechanisms for world class R&D intellectual capital
- Access to potential results and early technologies
- Product slate diversification
- A smooth mode of industry – academia liaison

Program Application Process/Business Engagement

Case-by-case options through different R&D project types

- AOP collaborator / partner: subject to cycle schedule, approval by DOE and budget.
- FOA cost-sharing projects: limited to the announcement and call for projects, in the area of interest.
- Cooperative Research and Development Agreements. CRADAs are agreement between federal laboratories and nonfederal entities that allow the parties to collaborate.
- Strategic Partnership Projects (SPP). work for federal agencies and the private sector. Activities can include research and development or applied engineering.
- Agreement to Commercialize Technology (ACT agreement): The agreement allows a private sector to access our personnel and/or facilities under terms that are not as restrictive as a SPP.

Program Application Process/Business Engagement

- Industry engagement in two steps:
  - Socialization of the basics
  - Listening day workshop

- Funding needs include:
  - Strategic definition, planning and launching: ~ $300k
  - AOP for establishing the scientific basis of conventional manufacturing methods of new catalysts: ~ $2M/y
  - Tools growth: ~ $5M