U.S. DEPARTMENT OF ENERGY

Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

Dynamic Catalyst Science and Data Analytics R&D

Dr. G. Jeremy Leong, Technology Manager– Advanced Manufacturing Office R&D Projects

University of Houston

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Outline

Overviews

- About DOE/EERE/AMO
- Programmatic Interests in Chemical Manufacturing: Challenges and Opportunities
- Congressional Direction
- Dynamic Catalyst Science
- Meeting Questions
- Anticipated Meeting Outcomes

Acknowledgements and many thanks to:

Presenters:

- David West – SABIC
- Lars Grabow – University of Houston
- Rebecca Fushimi – Idaho National Laboratory
- A.J. Medford – Georgia Institute of Technology
- Jeff Weissman – Precision Combustion

Participants:

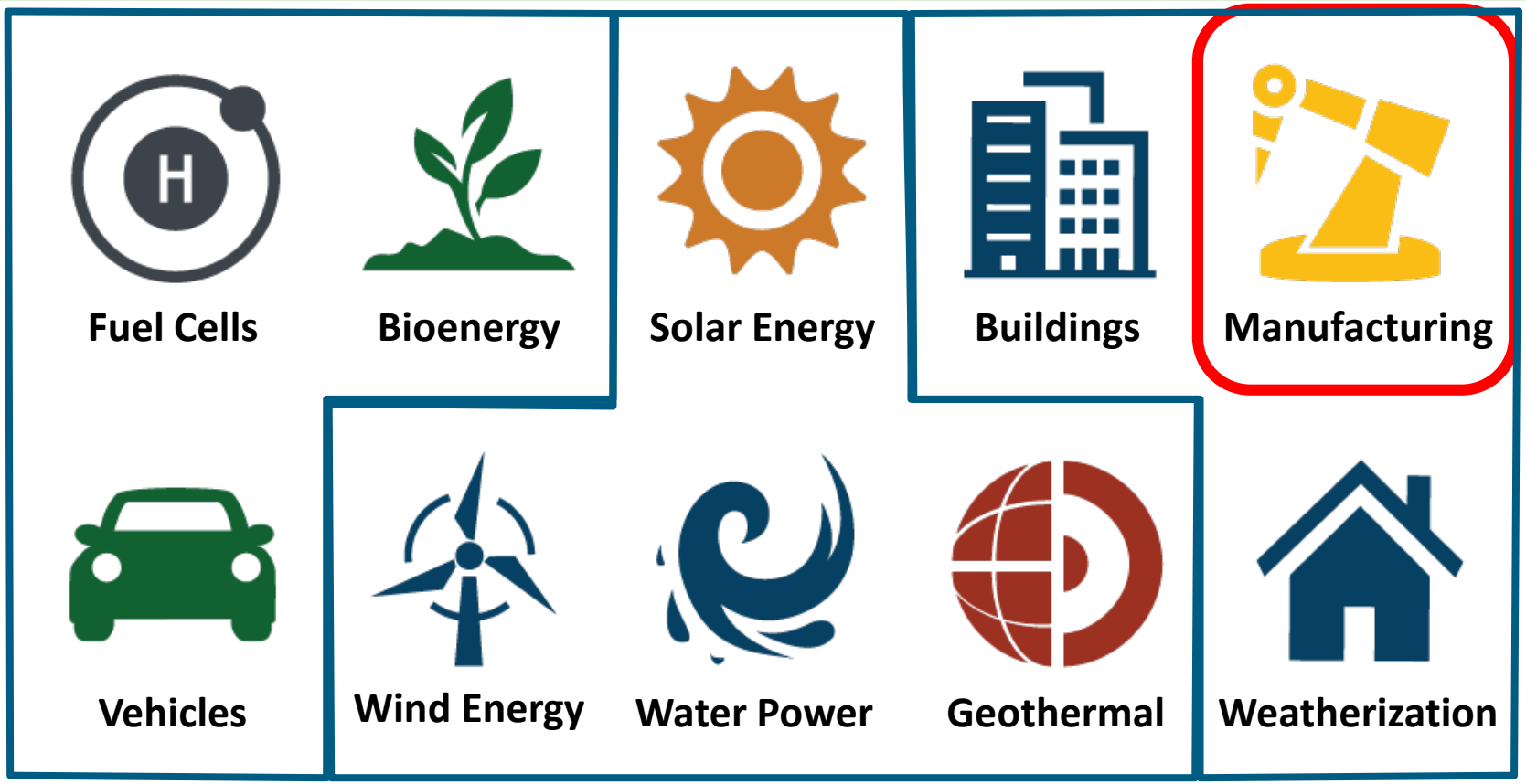
Office of Energy Efficiency and Renewable Energy

Sustainable
TRANSPORTATION

Renewable
ELECTRICITY GENERATION

Energy Saving
HOMES, BUILDINGS, & MANUFACTURING

EERE Technologies Offices



AMO works collaboratively with other EERE Technology Offices, providing expertise to address manufacturing challenges and issues. Including:

- Vehicles program - Energy storage, materials
- Bioenergy program - DOE plastics
- Fuel Cells - H2@Scale initiative to increase production and use of hydrogen
- Fuel Cells, Vehicles, and Wind programs - carbon fiber and composite materials

AMO Vision and Mission

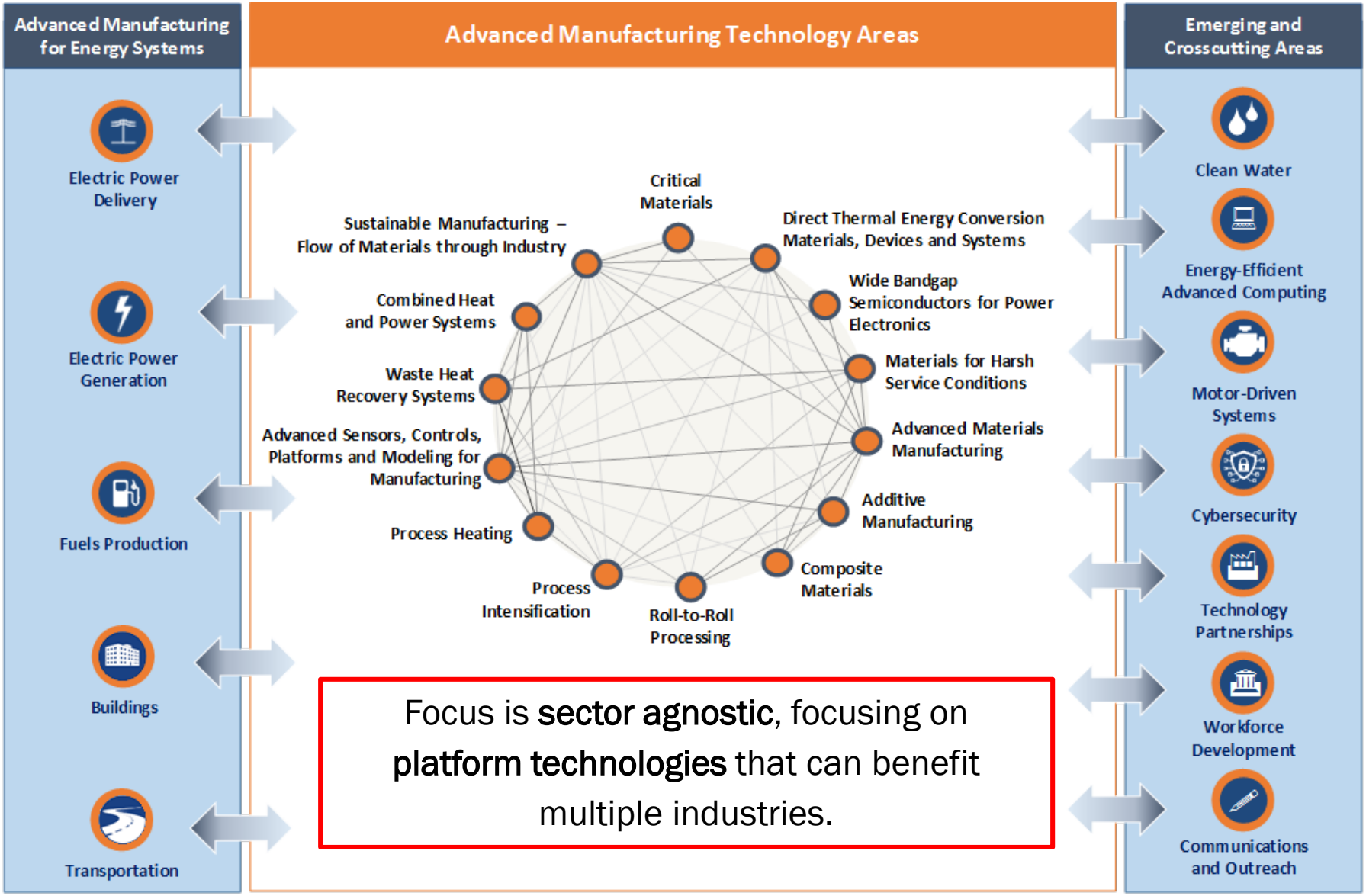
VISION: U.S. global leadership in sustainable and efficient manufacturing for a growing and competitive economy.

MISSION: Catalyze research, development and adoption of energy-related advanced manufacturing technologies and practices to drive U.S. economic competitiveness and energy productivity.

MULTI-YEAR PROGRAM PLAN:

- Describes the Office mission, vision, and goals
- Identifies the technology, outreach, and crosscutting activities the Office plans to focus on over the next five years.

AMO: A Broad R&D Portfolio



AMO: Three complementary strategies

R&D Projects: Bridging the innovation gap

Research and Development Projects to support innovative manufacturing processes and next-generation materials

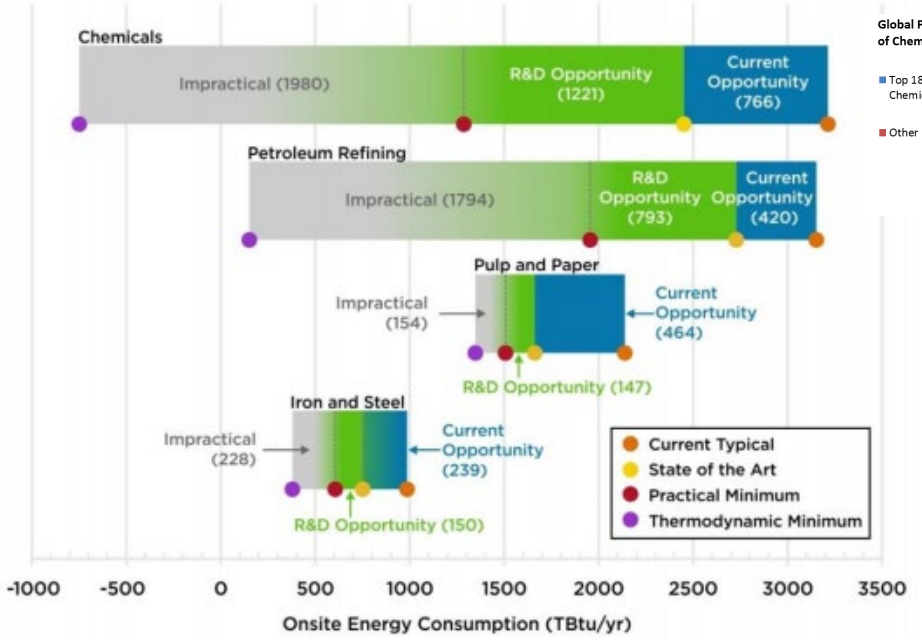
R&D Consortia: Public-Private consortia model

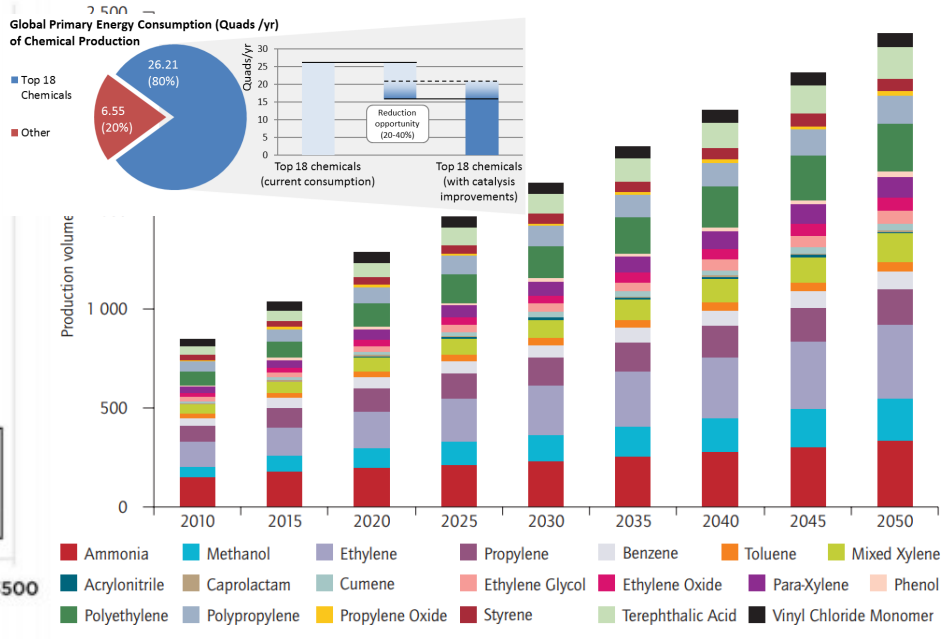
R&D Consortia offer affordable access to physical and virtual tools, and expertise, to foster innovation and adoption of promising technologies

Technical Partnerships: Direct engagement with Industry

Driving a culture of continuous improvement and wide scale adoption of proven technologies, such as CHP, to reduce energy use in the manufacturing sector

Opportunities in Advanced Chemical Manufacturing R&D; Energy Bandwidth Study and Technology Roadmaps





Why is this important now?

- Significant growth in production volume is expected within the chemical sector
- Energy bandwidth studies show potential for significant energy savings in chemical sector
- Advances in chemical industry has direct impacts toward U.S. global leadership, economic competitiveness, and energy dominance

What gaps or opportunities remain in AMO mission space?

- Bridging the gap between fundamental and applied catalysis research relies on stewarding greater level of enduring interagency/office and industry engagement

https://www.energy.gov/sites/prod/files/2015/08/f26/chemical_bandwidth_report.pdf

https://www.americanchemistry.com/Catalysis-Roadmap/

Catalytic Process and Chemical Manufacturing R&D

Programmatic priority:

Lower energy intensity/increase productivity for chemical manufacturing

- Target large volume, highest energy consuming chemicals including plastics/polymers and their precursors
- Develop alternative chemical pathways/innovative technologies

Key focus areas

- Innovative conversion technologies (anticipated workshop Spring 2020)
- **Dynamic catalyst science**

Congressional Direction

- Energy and Water Development and Related Agencies Appropriation Act, 2020
  - Energy Programs
    - Energy Efficiency and Renewable Energy
      - Advanced Manufacturing
        - » $5,000,000 for dynamic catalyst science coupled with data analytics.

Opportunities in this space to define, foster, and expand R&D efforts in this area

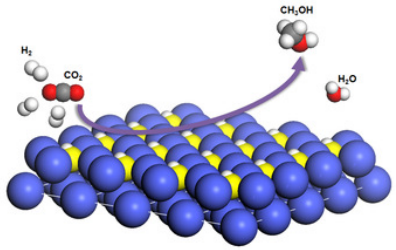
Dynamic Phenomena in Chemical Manufacturing

- Manufacturing processes today:
  - Centralized, large scale, designed for **steady-state**
  - *but change is inevitable*…
    - Feedstocks and market demands
    - Startup, shutdown, servicing interruptions
    - Degradation, deactivation and regeneration
    - Accidents, failures, upsets

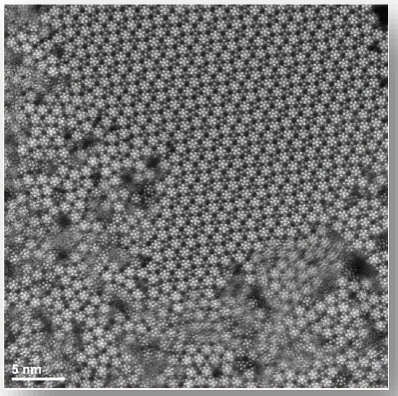
- Manufacturing processes in the future could be:
  - Distributed, smaller scale, robust, flexible to changing operating conditions
    - Coupled with or driven by renewable energy systems
  - *Forced dynamic operation*…
    - Improved efficiency, productivity, economics

Challenges to Address for Industrial Catalysis

- Model Catalyst
  - Well-defined structure
  - ***Detailed*** kinetics



- Industrial Catalyst
  - Complex multicomponent systems
  - Ill-defined surface, amorphous phases
  - **Coarse,** global kinetics

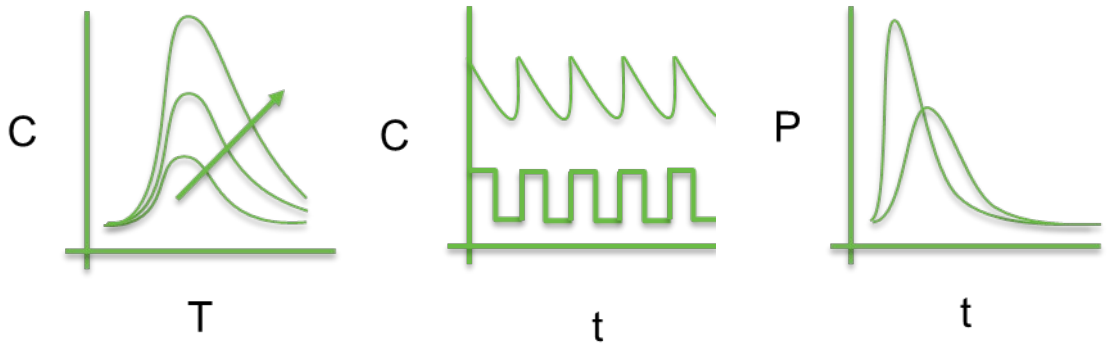


STEM image of [001] zone for M1 phase of MoVNbTe Oxide

Dynamic Catalyst Science

Advanced tools to understand complex industrial catalysts.

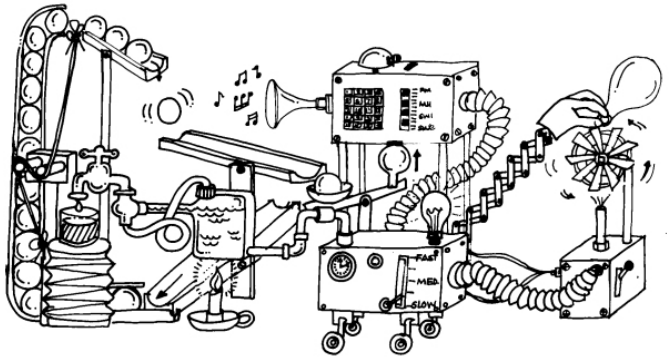
The use of ***temperature***, ***concentration*** or ***pressure*** transients to perturb the state of a chemical system.

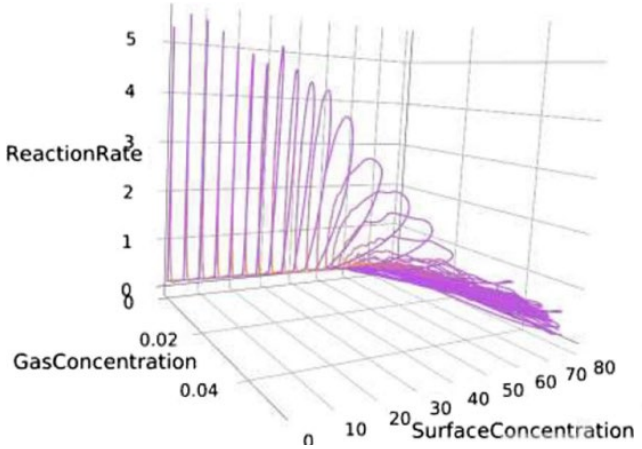


Response or relaxation indicates how the system works.

Challenges of Dynamic Catalyst Science

- Complex experimental design, maintenance and research execution
- Complex physical models, $\frac{\partial C}{\partial t}$
- Data science, data analytics
  - For time-dependent systems
  - Data → Information and Knowledge
  - Multiscale phenomena
    - Molecular event
    - Industrial process





Dynamic Data

New catalyst formulations, guidance for process conditions

Questions to consider during the meeting

- Critical knowledge gaps in catalyst science to advance chemical manufacturing?
  - Today's most impactful tools, advantages and limitations?
  - Advanced capabilities essential for the future
    - high-performance computing (HPC), data analytics, structural/kinetic characterization *in operando*, multiscale modeling/simulation?
  - Unique opportunities for dynamic catalyst science?
  - Current limitations to integrate catalyst science, reaction engineering and process development?
- Key research opportunities in catalyst science that can impact *productivity* and *energy efficiency* in chemical manufacturing?
  - Chemical manufacturing opportunities on the horizon for the next 5, 20 years? What catalysis R&D is needed?

Anticipated outcomes of this roundtable

1.) Bringing together academia, industry, and NLs in this space

2.) Roundtable References:

- Presentations and Summary report will be available on the DOE AMO website – estimated end of April 2020
- Link will be distributed to attendees by email

3.) Next Steps:

- Summary report will be used to inform programmatic direction based on industry priorities
- Engage in follow-on discussions regarding collaborative opportunities

Thank You

G. Jeremy Leong, Ph.D.
R&D Projects Technology Manager
Advanced Manufacturing Office
Jeremy.Leong@ee.doe.gov

For additional information:

energy.gov/eere/amo/advanced-manufacturing-office