

## Dynamic Catalyst Science Roundtable

*Initiated by the DOE/EERE Advanced Manufacturing Office*

University of Houston  
Student Center South | Heights Room 224 | 4455 University Drive  
Houston TX | 10 AM – 4:15 PM, February 26, 2020

### AGENDA

Time	Activity
9:30 AM – 10:00 AM	<b>Check in and Networking</b>
10:00 AM – 10:20 AM	<b>Welcome, EERE AMO – Introduction and Objectives</b> <ul style="list-style-type: none"> <li>Meeting Host: Mike Harold and Lars Grabow, University of Houston</li> <li>Jeremy Leong, Technology Manager, Advanced Manufacturing Office</li> </ul>
10:20 AM – 10:40 AM	<b>Industry Perspective, R&amp;D Challenges, Opportunities</b> <ul style="list-style-type: none"> <li>David West, SABIC</li> </ul>
10:40 AM – 11:00 AM	<b>Connecting Atomistic Modeling, Laboratory and Industrial Scales</b> <ul style="list-style-type: none"> <li>Lars Grabow, University of Houston</li> </ul>
11:00 AM – 11:20 AM	<b>Structure/Kinetics of Complex, Industrial Catalysts</b> <ul style="list-style-type: none"> <li>Rebecca Fushimi, Idaho National Laboratory</li> </ul>
11:00 AM – 11:20 AM	<b>Extracting Knowledge for Industrial Catalysis through Machine Learning</b> <ul style="list-style-type: none"> <li>A.J. Medford, Georgia Institute of Technology</li> </ul>
11:20 AM – 11:40 AM	<b>Industry Perspective, R&amp;D Challenges, Opportunities</b> <ul style="list-style-type: none"> <li>Jeff Weissman, Precision Combustion, Inc.</li> </ul>
12:00 PM – 1:00 PM	<b>Light Lunch and Refreshments (Provided by University of Houston)</b>
1:00 PM – 2:30 PM	<b>Overview of Chemical Manufacturing Industry Stakeholder Research Priorities</b> <ul style="list-style-type: none"> <li><b>Chemical Manufacturing Representatives</b>, To start the discussion, industry representatives are invited to share a 10 minute overview of their perspective on the R&amp;D needs for dynamic catalyst science to accelerate catalyst development and enable efficient chemical manufacturing.</li> </ul>

<p><b>2:30 PM – 3:30 PM</b></p>	<p><b>R&amp;D Gaps and Opportunities</b> <i>Facilitated Discussion, Sabine Brueske, Energetics</i> <i>Suggested Topics</i></p> <ul style="list-style-type: none"> <li>• What are the critical knowledge gaps in catalyst science needed to advance chemical manufacturing at present? <ul style="list-style-type: none"> <li>▪ What are the most impactful tools that are being used now, their advantages and limitations?</li> <li>▪ What advanced capabilities are essential for the future, e.g. high-performance computing (HPC), data analytics, structural/kinetic characterization <i>in operando</i>, multiscale modeling/simulation?</li> <li>▪ What opportunities can be uniquely addressed using dynamic catalyst science?</li> <li>▪ What are the current limitations in the integration of catalyst science, reaction engineering and process development?</li> </ul> </li> <li>• What are the key research opportunities in catalyst science that can impact productivity in chemical manufacturing in the future? <ul style="list-style-type: none"> <li>▪ What are the driving forces for energy efficiency in chemical manufacturing? How can advanced catalyst help meet these goals?</li> <li>▪ What chemical manufacturing opportunities (e.g. feedstocks, products, processes) are on the horizon for the next 5, 20 years and what catalysis R&amp;D is needed to realize these opportunities?</li> <li>▪ To what extent will chemical manufacturing shift to distributed processes and how will advanced catalysts be needed?</li> </ul> </li> <li>• What is the role of industry, academia and government in the development of new tools? <ul style="list-style-type: none"> <li>▪ Are there research themes and topics that industry prefers to pursue collaboratively versus internally?</li> <li>▪ What are the current impediments to collaboration across industry, academia and government and how can they be addressed?</li> </ul> </li> </ul>
<p><b>3:30 PM – 3:45 PM</b></p>	<p><b>Break</b></p>
<p><b>3:45 PM – 4:00 PM</b></p>	<p><b>General Consensus of Top R&amp;D Priorities</b> <i>Facilitated Discussion, Sabine Brueske, Energetics</i></p>
<p><b>4:00 PM – 4:15 PM</b></p>	<p><b>Next Steps and Adjourn</b></p> <ul style="list-style-type: none"> <li>• Jeremy Leong, Technology Manager, Advanced Manufacturing Office</li> </ul>

*A summary report will be issued to all participants following the meeting. Meeting attendance will be included but specific comments will not be made identifiable.*