Nano4EARTH Roundtable Discussion Summary: Catalysts

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Overview

The National Nanotechnology Initiative (NNI) launched the National Nanotechnology Challenge on climate change (Nano4EARTH) to convene and mobilize the broad nanotechnology community to accelerate solutions for climate change. The NNI, with support from the National Nanotechnology Coordination Office (NNCO), has organized a series of roundtable discussions on particularly promising areas that could have near-term impacts (four years or less) on climate change. These promising areas were identified at the Nano4EARTH kick-off workshop. Among them was *catalysts,* which was the focus of the fourth and final roundtable discussion.

Global industrial CO_2 emissions account for 9 Gt CO_2 per year[1]; reimagining industrial processes using nanocatalysts offers a potential avenue to mitigate emissions and reach the 2030 decarbonization goals. Nanocatalysts made with some earth-abundant elements have been shown to improve the energy efficiency and sustainability of major industrial processes and reduce their overall greenhouse gas (GHG) emissions. On that account, NNCO assembled 10 subject-matter experts from different sectors – including academia, national laboratories, small and large businesses, and technology development organizations – to discuss and identify the most pressing near-term needs, opportunities, and challenges to expand the use and adoption of nanocatalysts for climate solutions. The agenda and list of invited participants for the roundtable can be found here.

Industrial process optimization through nanocatalysts

Through a brainstorming session that was divided into production lifecycle stages, participants identified process inputs and products that they believe should be optimized to mitigate climate impact. Table 1 lists those deemed by participants as most pressing, and asterisks denote those that could have the biggest impact in GHG emissions and energy savings.

Table 1. Industrial process optimization through nanocatalysts

Lifecycle stage	*Process inputs and products*	*Description*	*Opportunity area*
Feedstock (inputs needed for creation of industrial products at scale)	*Green/blue hydrogen	Green/low carbon intensity energy feedstock and precursor for industries that currently rely on fossil fuels as feedstock materials.	Green/blue hydrogen at scale, through the use of nanocatalysts, could provide feedstock for many energy- and GHG-intensive industries, such as the production of ammonia, lower-emission fuels, and benzene, toluene, ethylbenzene, and xylenes

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[1] https://www.iea.org/energy-system/industry

			(BTEX) chemicals. Green/blue hydrogen also facilitates the sustainable use and conversion of captured CO_2.Nanotechnology would also play a role in new infrastructure needs (e.g., advanced materials for pipelines and other containers).
	Biomass waste	Utilization of abundant biomass waste, such as wood waste lignin, agricultural residues, or algae biomass.	Biomass waste can be used to create bio-oils, such as biodiesel and sustainable aviation fuel, providing a renewable source of hydrocarbons. Biomass waste can also be used to create polymers (e.g., nanocellulose).
	Hydrocarbons from alternative sources	Hydrocarbons sourced from different processes (e.g., biomethane vs. fossil methane).	Replacing or supplementing the use of fossil hydrocarbons. There are different challenges, based on the source of the feedstock (e.g., renewable vs. fossil hydrocarbons or biomethane vs. fossil methane), which can affect purity of the feedstocks and processing requirements.
Production (specific product generation process at scale)	*Utilization of captured CO_2	Production of value-added products using captured CO_2.	Provide low or net-zero GHG methods to produce methanol, lower-emission fuels, C_2 products, sustainable aviation fuel, among others.
	Production of carbon products from renewable sources	Utilizing renewable energy and feedstocks to create new carbon-based products.	Producing carbon products from feedstocks that are considered waste (e.g., lignin, food waste) to avoid the extraction of new fossil hydrocarbons.
	Increased production through optimized physicochemical characteristics of nanocatalysts	Augmenting catalyst activity and selectivity through design and engineering improvements.	Developing novel characterization techniques for nanocatalyst rational design, tunability, and precision engineering can optimize catalytic processes and facilitate scale-up.
End-of-life (product life/utilization	*Waste plastic recycling	Collection, recycling, and repurposing of plastic waste for a	Currently, the limitations of plastic and mixture recycling leave a lot of potential feedstock materials in

after intended use)		circular economy.	the landfill, representing potential value and energy that could be harnessed.
	*Recycling waste mixtures	Devising a scalable, sustainable, and economic method to recycle waste mixture.	
	Design materials for recyclability	Incorporate circularity and life-cycle considerations in product and catalyst design.	Designing future waste as feedstock, such as designing products and catalysts for easy extraction of valuable materials (e.g., lithium from electronic wastes and critical materials/components from catalysts).

Nanotechnology for catalyst optimization

Participants discussed promising nanocatalyst design that could be used to optimize industrial processes and voted for the biggest opportunity areas (Table 2).

Table 2. Advance nanocatalyst design	
Opportunity areas	*Description and example nanocatalysts and processes to target*
Nanocatalysts made of Earth-abundant materials	Replacing cost-prohibitive and unsustainable precious metal catalysts. Examples: Earth-abundant transition metals available in the United States, nickel, cobalt to replace platinum, nanoscale carbon structures as catalysts, anything that reduces use of critical materials, and catalysts produced from waste (e.g., mine tailings)
Novel metal-based nanocatalysts	New materials with increased efficiency and stability. Examples: bi- and trimetallic nanoparticles (synergistic effect), mixed metal oxides (e.g., perovskites), single-atom catalysts, aerosolized metal nanoparticles (1–10 nm), and process-specific catalysts (catalysts for electrochemical CO_2 reduction reaction, Fischer-Tropsch catalysts for syngas processing, reforming catalysts for hydrogen production)
Structural substrates	Nanoscale substrates and binders that increase surface area, number of active sites, and stability of the catalyst. Examples: zeolites, metal-organic frameworks (MOFs), covalent organic framework (COFs), perovskites, and active/optimized binders for catalysts
Active surface area and facets	Increasing efficacy of nanocatalysts by exploring different shapes and configurations to increase active surface area and facet-effect enhancing the mass transfer in chemical reactions/production. Examples: physical modifications in nanocatalysts (e.g., zeolites), such as pore size, topology, and morphology.

Low dimensional materials (optimizing surface area and facet)	2D nanomaterial catalysts. Examples: MXene, transition metal dichalcogenide (TMDC) monolayers, graphene oxide, and reduced graphene oxide

Nanocatalyst optimization through design and production changes is a way to use less catalyst while increasing the overall yield of the reaction. However, nanocatalyst design is not trivial. Participants discussed that nanoengineering is critical for catalyst optimization – impactful properties could arise from a single atom change. Active sites can be designed to maximize mass transfer and overall diffusivity through an enhanced surface-to-volume ratio. For example, tuning the 2D material design can modify the electronic properties of the material, providing new functionalities and improving performance. Multi-application and dynamic nanocatalysts are also of interest.

Participants emphasized that active sites of nanocatalysts are dynamic and significant restructuring happens during a chemical reaction; harnessing these changes into application areas is of interest. For example, by better understanding and harnessing catalysts' restructuring, engineers can incorporate end-of-life considerations for nanocatalysts, such as self-healing and self-separating properties, to ease recyclability and circularity. However, the dynamic nature of catalysts and the complexity of nanocatalyst synthesis/manufacture may also pose a challenge for achieving catalyst stability and economical viability under industrial conditions at scale.

Identifying key hurdles to applying nanocatalysts to industrial processes

Participants paired industrial processes for optimization (Table 1) with promising nanocatalyst design (Table 2), which revealed key hurdles and potential solutions.

Table 3. Key hurdles and solutions

Process + nanocatalysts	**Hurdles**	**Potential solutions**
Waste plastic conversion + metal-based nanocatalysts	• Catalyst deactivation (sintering + coke formation) • Precious metals' deactivation by impurities • Mixing catalysts, gas, and materials • A single catalyst cannot handle a mixture of materials • Poor mass transfer on catalysts due to crosslinked network of waste plastic	• Strong catalyst - support interaction via epitaxy • Selective C-C bond cleavage • Bio-inspired processive catalysts • Convert to mixtures and use without product separation • Use "waste" heat
CO_2 to product +	• Earth-abundant materials	• Rational

Earth-abundant/metal based nanocatalysts	easily accessible in the United States ● Earth-abundant elements are less reactive	nanocatalyst design and optimization
Hydrogen production + carbon nanomaterials + carbon nanotubes (CNT)	● End uses for carbon produced (if not high-quality CNT) ● Cost of production for high-quality CNT ● Coupling of catalysis and transport in CNT reactor ● Control of nanoparticle size distribution via nucleation and growth ● Detachment of CNT from catalysts' support ● Relationship of catalysts and CNT product	● Correctly designed nanocatalyst for high temperature reaction ● Experimental studies of catalyst formation and CNT growth in flow reactors
Lignin feedstock utilization + metal-based nanocatalysts	● Product selectivity ● Separation cost	● Develop optimal hydrogenolysis catalysts (mono-metal and bimetallic with high surface area stable support) with high conversion and yield of monomers and low coke formation

The discussion highlighted the need for broad awareness and access to existing federally-funded infrastructure, that includes an expansion of tools (e.g., dynamic NMR) and possible study conditions (e.g., catalyst formation in the gas phase). Participants also discussed the need for wider accessibility to *in-situ and operando* measurements capable of multi-modal (e.g., multiple techniques at once) characterization to understand structural formation of active catalytic sites. These tools are critical to get a complete picture of the reactions being studied. National labs and some Universities have *in-situ and operando* capabilities as part of their shared infrastructure. Data gathered using these tools will help expand domain knowledge that can be paired with artificial intelligence and machine learning (AI/ML) tools to accelerate rational design of nanocatalysts.

AI/ML could help expedite nanocatalyst discovery, but standardized data and curated databases are essential to take advantage of these tools. Participants suggested that a single catalyst application could be chosen as a use case to prove that AI/ML are useful for this task. Zeolites have emerged as a good first case, but data is not available for other catalysts. Data should include structural/topology formation, surface characteristics, and other atomic-scale interactions. These data are needed to accelerate rational design of nanocatalysts. Participants stated that databases and initiatives inspired by the Materials Genome Initiative could be beneficial to accelerate catalyst discovery through high-throughput screening and targeted validation experiments.

Participants discussed broad hurdles that apply to many processes in which nanocatalysts are needed. Overall, redesigning processes and retrofitting plants is cost-prohibitive – new solutions need to be drop-in replacements to be adopted in the short-term. Life-cycle assessments can help identify and prioritize industrial processes’ components that need to be replaced or optimized first, as current catalyst design is slow and expensive. For example, ammonia production through the Haber-Bosch process is very energy and GHG intensive. One of the biggest offenders in the Haber-Bosch process is the feedstock to get hydrogen. Currently, most of the hydrogen used to produce ammonia comes from fossil hydrocarbons. If green hydrogen – produced by electrolysis using an effective nanocatalyst – is used, the overall process could be sustainably and economically scaled.

In summary, roundtable participants highlighted the advantage of nanocatalysts’ enhanced reactivity and precise tunability over traditional catalysts. It is clear that nanocatalyst reimagination and optimization can have a large impact on achieving climate change goals if the hurdles to their design, scale-up, and adoption are met. These challenges present a collaborative opportunity for public and private capital, industry, start-ups, and basic and applied researchers. Novel reimagination of nanocatalyst with circularity and environmental, health, and safety concerns at the forefront of their design, represent a needed paradigm shift in a new generation of sustainable industrial processes.