Breakout Report on Catalysis

Identification of Grand Challenges

Catalysis Breakout

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Catalysis is the enabling technology for energy, chemicals, pharmaceuticals…

Improved catalysis for small molecules (Ammonia, methanol…) critical to reducing energy consumption and CO_2 emissions on a significant scale.

Catalysts are reactive materials – the active site is critical!

Selectivity is an overarching issue.

Grand Challenge Themes

- **Catalysts by Design** – structure and function
  - ○ Discovery and lead generation, improvement targets
  - ○ Model and measure
  - ○ Make materials, from model to industrial scale , that incorporate multiple functions defined at the molecular level
  - ○ Cross –cutting need for significantly advanced tools: computational, experimental, spectroscopic, etc.

- **Translation to technology**
  - ○ Realization of design – new synthesis strategies , scale up, aging, etc
  - ○ Realize benefits from the same tools for better understanding and scientific design

- **Modeling and characterization tools** that advance the entire continuum from discovery, design and translation to practice
  - ○ Reaching longer length and time scales with higher accuracy, representing complex environments, complex reaction networks, better uncertainty quantification
  - ○ Build better science, experimental and computational definition of active sites and their function while accelerating application
  - ○ Go significantly beyond what conventional DFT can do today

- **Database development and implementation as a key enabler** of all of the above

“If materials scientists could ________, then new pathways of ________ materials discovery would be possible.”

If materials scientists could ________	Then new pathways of _____materials discovery (by experimental and computational means) would be possible
Identify reactive sites by computation and experiment	catalytic
Accurately calculate/predict key parameters (stable structure, energetics, active sites, intermediates)	catalytic
Identify reliable, key descriptors, and knowing the limitations (e.g. certain materials classes) of their applications	catalytic
Determine minimum accuracy requirements and improve the accuracy of computational methods	catalytic
Seamlessly integrate multi-scale computational tools	catalytic
Bridge the knowledge gap from small molecule catalysis to that of more complex chemistries	catalytic
Establish best practices for developing and maintaining local AND national databases	catalytic
Make better use of information science, Adapt data mining tools (e.g. machine learning & massively parallel computing) from other fields to identify leading candidates for catalytic materials.	catalytic

“If materials scientists could ________, materials/product engineers would be able to ________.

If materials scientists could ________	Materials/product engineers would be able to ______
Design more tunable catalysts with wider operating conditions	Realize significant downstream gains (energy use in reactors, separations,)and enable the use of alternative materials and reactor/process designs.
Integrate and develop computational and experimental tools that transcend all relevant length and time scales	Scale up processes faster and with more confidence (shorter time to market) Translation to technology
Create and continue to grow databases containing the properties and performance of catalytic materials, especially well-defined model systems	1. Develop more accurate models and computational screening techniques. 2. Narrow parameter space and more accurately inform experimental high throughput and combinatorial screening efforts. Databases
Develop the ability to predict catalytic properties of materials to the levels of accuracy commonly achieved by modeling tools available for more basic physical properties	-Embrace the inherent complexity of catalytic systems and the inherent need for a more interdisciplinary approach to modeling catalytic materials Design
More accurately predict the influences of the catalyst’s operating environment (pressure, temperature, liquid phase) on performance (conversion, selectivity, stability).	Rationally select appropriate environmental conditions for globally optimized catalytic process Translation
Better understand the influence of catalyst/ support interaction on electronic, physical, and chemical properties of the catalytic material	Rationally select support materials for optimal performance Design
Develop synthesis techniques and HT methods for atomic level structural control of catalysts	Translate promising lab scale leads to commercially relevant scales Translation

"Materials/product engineers need to be able to ________, which materials scientists could enable by __________."

Materials/product engineers need to be able to _______	**Which materials scientists could enable by _______**
Synthesize catalysts whose performance and critical properties meet or exceed requirements dictated by systems-level objectives	1. Computational screening of catalytic materials by filtering out those materials whose predicted critical properties/ performance metrics are below a threshold value Translation 2. Developing tools based on thermodynamic/phase diagram information and/or data mining of literature to suggest appropriate synthesis techniques, conditions, and precursor materials .
know how an expected contaminant can affect catalyst performance	Understanding deactivation mechanisms and designing poison-tolerant catalysts Translation
Develop, optimize, and incorporate new/alternative catalytic materials into a process on a time scale that is less than those associated with the expected market value.	1. More accurate, stream-lined, multi-scale modeling making use of extensive data bases 2. Many other factors.
Know the expected stability and associated lifetime of new candidate catalytic materials under expected operating conditions	1. More accurate, high throughput accelerated testing with clear correlation to real-time testing 2. The development of multi-time scale computational methods to predict the evolution of structure and composition under operating conditions
Develop catalytic materials with high selectivity	Design

Grand Challenges ideas that were not significantly incorporated into the 3 framework questions on the previous slides

- Establishing materials and testing standards for i.) evaluating and reporting catalytic performance (e.g. TOF) , ii) characterization protocols (e.g. BET measurements), and iii.) verifying identification of materials . This could include the possible creation of an ASTM-type organization for the maintenance of a catalytic materials library.
- Accounting for the strong temporal dependence of material structure/properties and the inherent difficulties that this imparts on developing standards and reliable data for databases.
- Computational modeling of amorphous materials
- Open access & data bases (industrial contribution, export laws, who maintains?)
- In-situ surface characterization in HTR studies
- Using statistics to reconcile/correlate findings from characterization techniques at the local level with those at the macro-level
- Local versus national databases.
- Electrocatalysis: influence of applied electrochemical potential, electric double layer
- Synthesis techniques with better size selectivity
- “let’s not forget the importance/usefulness of simple/model surfaces”.
- Significant need for advanced/new in-situ spectroscopic, microscopic techniques for evaluating catalyst structure/properties under real operating conditions (White, Federica)
- Changing research culture so that experiment and modeling are intimately integrated into the development of catalytic materials