Research Needs for Nanotechnology Commercialization

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Using the priority research and development needs outlined in the *Chemical Industry R&D Roadmap for Nanomaterials by Design: From Fundamentals to Function* (Chemical Industry Vision202 Technology Partnership [www.ChemicalVision2020.org], December 2003), a group of industrial, academic, and government lab partners defined the following key R&D needs that will be critical to the successful commercialization of nanotechnology. These recommended R&D needs are being communicated to the key members of the National Nanotechnology Initiative (NNI) as part of the NNI-Chemical Industry Consultative Board for Advancing Nanotechnology (NNI-ChI CBAN).

1. Fundamental Understanding and Synthesis:

A. Develop new paradigms for creating nanoscale building blocks based on understanding of physics and chemistry at the nanoscale.

Continued research aimed at developing new, more efficient ways of synthesizing high-quality nanomaterials is encouraged. In addition to current wet chemistry, gas phase, and self-assembly technologies, new concepts involving new solvents and processes are sought. Efforts should emphasize the need to develop methodologies for synthesis based on scientific understanding, rather than synthesis based purely on scouting and discovery methods. Research should focus on materials of relevance to specific applications, such as catalysts, sorbents, coatings, adhesives, resins, and nanofibers and on materials that exhibit properties of commercial interest, including mechanical, electrical, magnetic, optical, thermodynamic, transport, surface, and absorption/adsorption properties. R&D goals should include the need for scalability, reproducibility, and controllability.

B. Develop new paradigms for controlled assembly of nanocomposites and spatially-resolved nanostructures with long-range order.

Revolutionary improvements in methods for assembly of nanoscale building blocks are needed to develop commercial-scale approaches for fabrication of products/devices incorporating newly discovered nanomaterials and nano-derived functionalities. High-rate nanomanufacturing processes should target traditional applications of interest to the chemical industry, including catalysts, sorbents, coatings, adhesives, resins, and membranes, as well as emerging applications needs in electronics and medical.

2. Metrology and Characterization:

Develop real-time analytical tools for measuring and characterizing nanomaterials, with specific attention to on-line and in-process tools for process and quality control in manufacturing.

In addition to ongoing efforts in development of characterization tools for R&D, there is a need to develop deployable process monitoring tools that can be used to ensure nanomaterial and nanoscale product consistency on a manufacturing scale. Such instruments would include real-time, on-line characterization tools and rapid quality control tests for samples. Nanomaterial characterization capabilities needs include:

- In-situ particle size and shape
- In-situ analysis of composition or function (including charge; surface energy; functionalization; magnetic, electrical, or optical properties, etc.)
- Characterization of surface chemistry at the nanoscale, including fractional coverage and thickness of coatings on nanoparticles
- Characterization of the quality of particle dispersions in a liquid or solid matrix

3. <u>Modeling and Simulation:</u>

A. Develop computational tools to predict bulk properties of materials that contain nanomaterials.

Computational tools are needed to predict the properties of materials that contain nanomaterials. These tools may provide the most rapid benefit to industry by providing a means to screen options for nanomaterials design

B. Develop methods for bridging models between scales, from atoms to self-assembly to devices.

The development of models that bridge multiple scales – from atoms to molecules and mesoscale structures to devices and processes – is seen as a valuable, long-term effort.

In both cases, university and/or national laboratory efforts utilizing supercomputers will be necessary, and ongoing efforts in these venues should be expanded. Industry involvement would likely focus on guidance in model development, with some limited validation of models. To accelerate application of these tools, computational tools should target industrially interesting materials, and be focused on problems of intermediate complexity, for example ones that could be solved in a near-to-mid-term timeframe but not so small as to be of only trivial interest.

4. <u>Manufacturing and Processing:</u>

Develop unit operations and robust scale-up and scale-down methodologies for manufacturing.

Because of the unique physics and chemistry at the nanoscale, new approaches beyond classical chemical engineering unit operations will be necessary in many cases to commercialize nanoscale technology. Five classes of unit operations for processing of nanoscale materials were identified:

i. **Synthesis** – form desired nanoscale building blocks from precursors in commercial quantities with consistent quality.
ii. **Separation** – separate nanoscale materials from precursors, reaction media, etc.
iii. **Purification** – tailor the isolation of nanoscale materials by function (separate by desired property, such as size, composition, charge, magnetic, electrical, optical, functionalization, etc.).
iv. **Stabilization** – use processes such as surface modification, dispersion, etc. that allow a consistent nanomaterial product to be utilized while retaining desired nanomaterial functionality.
v. **Assembly** – integration of nanoscale materials into devices/products through a variety of top-down and bottom-up processes, including self-assembly, directed assembly, etc.

Not all processes will require all unit operations, and some processes will combine unit operations. Multidisciplinary teams will be needed, working at the laboratory and pilot scale, to translate the discoveries of nanoscience into new processes for effective nanomaterial production. Progress will require fundamental R&D to develop a general understanding of the basic principles that allow processing that retains the nano-derived functionality.

Research and development is also needed to develop unit operations applicable across a range of nanomaterials of commercial interest, such as inorganic oxides, clays, and carbon nanomaterials, and in a variety of matrices, such as polymers, pure liquids, solutions, sol gels, and metals. Catalysts, coatings, ceramics, sorbents, and membranes are priority materials for application in the chemical industry. Further, development of manufacturing processes is needed to accelerate the controlled, high-rate synthesis of functional nanoscale materials for these applications and the integration of the engineered materials into devices. Government support, in the form of test beds at research centers, may be useful to overcome the barriers presented by the risk of capital investment in unproven technology.

Ultimately, R&D in the area of manufacturing and processing will integrate developments in each of the other key areas, building on the fundamentals of synthesizing namomaterials, using on-line characterization tools for efficient and consistent process control, and employing computational tools to design both nanomaterials and manufacturing schemes.