Chemical Industry VISION2020 Technology Partnership

Research Needs for Nanotechnology Commercialization

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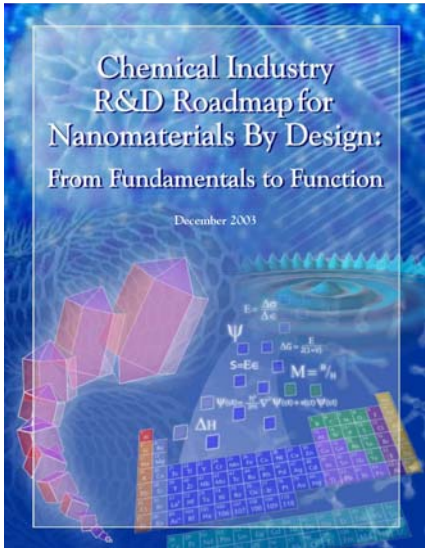
Vision2020 developed "Nanomaterials by Design" Roadmap (2003)

- Initiated by request from National Nanotechnology Coordination Office
- Involved input of over 90 participants from 16 companies, government, academia
- R&D areas identified:
  - Fundamental Understanding & Synthesis
  - Manufacturing & Processing
  - Characterization Tools
  - Modeling & Simulation
  - Environment, Safety, and Health



Roadmap used by:

- NNI in development of Strategic Plan
- NSF, DOE, and DOD program managers in developing FY05 solicitations
- Interagency Working Group on Manufacturing R&D to develop white papers

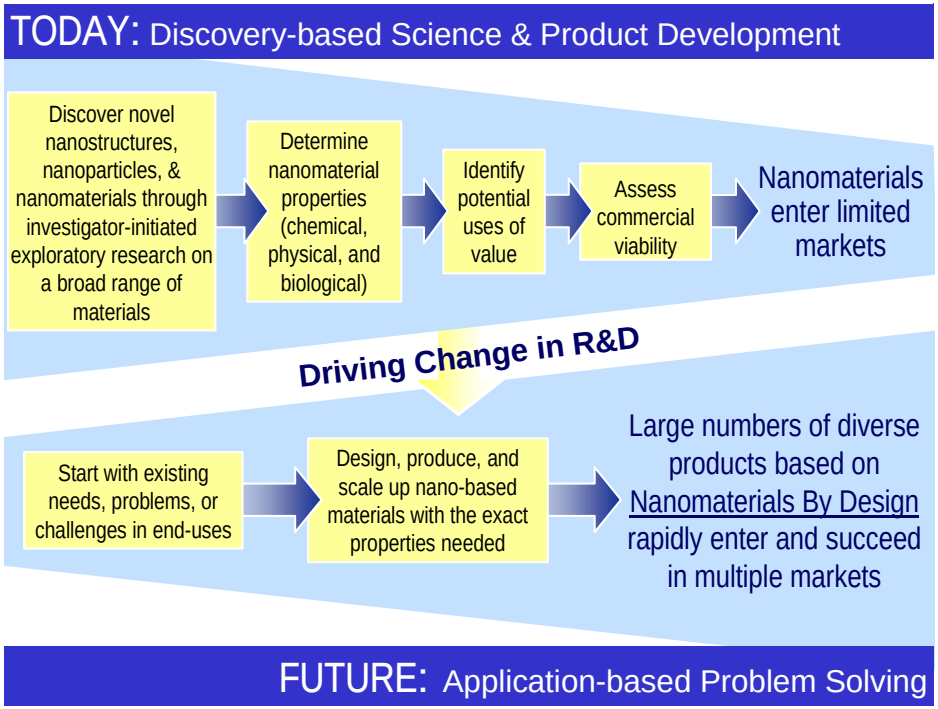
http://www.chemicalvision2020.org/nanotechnology.html

Implementing the Roadmap: First Industry Workshop (Feb. 2005)

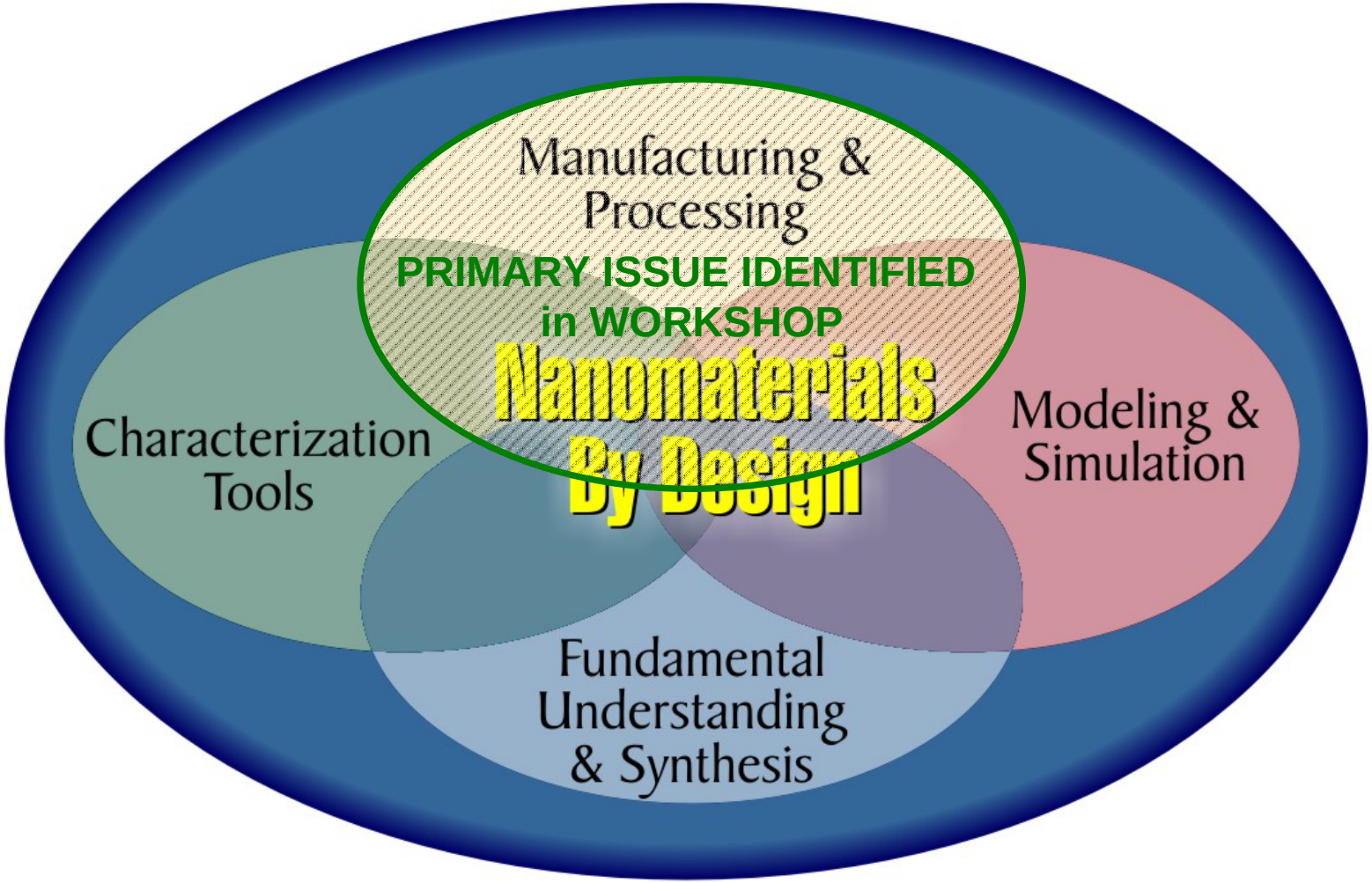
Workshop identified…

- High-priority R&D needs for nanotech commercialization
  - R&D needs are relevant to chemicals but apply across multiple industries
  - Chemical industry applications focus on near-term wins with significant impact on energy savings & economy
- Focused research needs for existing NNI programs
- Gaps to be filled by applied programs in nanotechnology

Pursuing the Roadmap Vision



Issues for Commercialization:
The Chemical Industry View



Strong intersection of needs in manufacturing & processing!

Priority R&D Needs for Nanotechnology Commercialization

Nanoscience

Synthesis and Assembly

Develop new paradigms to create nanoscale building blocks

Develop approaches for controlled assembly of nano-composites and nanostructures

Characterization tools

Develop analytical tools for measuring and characterizing nanomaterials

Modeling and Simulation

Develop models of nanomaterials processing and predict bulk properties of materials that contain nanomaterials

Bridge models between scales, from atoms to self-assembly to devices

Nanotechnology

Manufacturing & Processing

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

- Synthesis
- Separation
- Purification
- Stabilization
- Assembly

Characterization tools

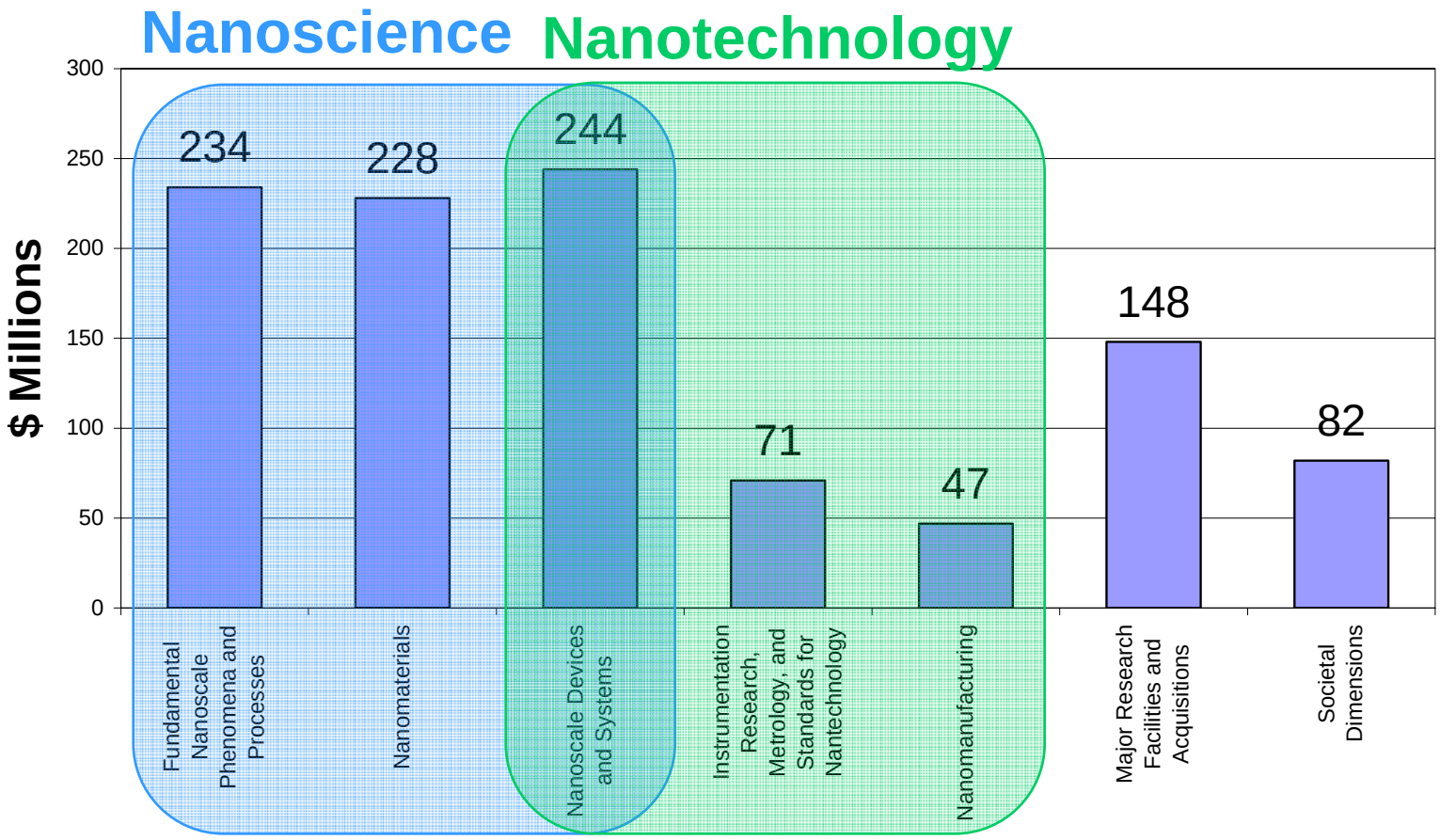
Develop real-time tools for measuring and characterizing nanomaterials, particularly online and in-process

Chemical Industry Application Areas

Catalysts, coatings, ceramics, sorbents, membranes

NNI Investment Favors Nanoscience

FY 2006 Requested Funding by Program Component Area



Where are the funding gaps?

- **Fundamentals & Synthesis**
  - Significant activity in this area
  - *Industry perceptions*:
    - much of this work is not relevant
    - work does not focus on important issues (e.g., scalability of synthesis) for industrial implementation
  - Industrial input/review of fundamental research programs may provide improve relevance of work
- **Metrology & Characterization**
  - Most NNI efforts in Instrumentation Research target development of new tools for research
  - Limited focus on developing needed instruments for rapid characterization and in-process monitoring in nanomanufacturing

Where are the funding gaps?

- **Modeling & Simulation**
  - Multiscale modeling is an important, long-term effort
  - Generating academic work relevant to industrial needs is challenging
  - Stronger connection of computational user centers to industry or industrially relevant problems is needed
- **Unit Operations for Manufacturing & Processing**
  - Few programs are dedicated to issues of nanomanufacturing (those that do may not fully address scale-up issues)
  - Research center or virtual center dedicated to process development may improve focus for progress in this area

Needs Mapped to NNI PCAs and Agency Activities

Priority R&D Needs Relevant to the Chemicals Industry

Primary / Secondary	Fundamental nanoscale phenomena, processes and behavior	Nanomaterials	Nanoscale devices and systems	Instrumentation research, metrology, and standards for nanotechnology	Nano-manufacturing
Manufacturing and Processing	**A**	**B**	**C**	**D**	**E**
1-Combined Manufacturing and Processing			NSF		1-NSF 2-DOE 3-DOD 4-NIST 5-EPA
Characterization tools					
2-Develop analytical tools for measuring and characterizing nanomaterials	NIST		NIST	1-NIST 2-NSF 3-DOE 4-DOD	
3-Develop real-time, on-line and in-process tools for measuring and characterizing nanomaterials,			1-NSF 2-NIST	NIST	
Fundamental Understanding and Synthesis					
4-Develop new paradigms for creating nanoscale building blocks based on understanding of physics and chemistry at the nanoscale	DOE	1-NASA, 2-NSF 3-DOD	1-NSF 2-NASA		
5-Develop new paradigms for controlled assembly of nanocomposites and spatially resolved nanostructures with long-range order			NASA		
Modeling and Simulation					
6-Develop models of nanomaterials processing and computational tools to predict bulk properties of materials that contain nanomaterials	1-NSF 2-DOE 3-NIST	1-DOE 2-NASA			
7-Develop methods for bridging models between scales, from atoms to self-assembly to devices.	NIST	1-DOE 2-NASA	NSF		

Note: Agency activities identified in NNI Supplement to President's FY06 Budget Request

Semiconductor/Chemical Industries Jointly Define R&D Needs

Teams develop specific needs in common R&D areas (July 2005):

Fundamentals & Synthesis – New strategies, scalable assembly

- Jun Liu, SNL/PNL
- Azar Alizadeh, GE
- Miki Oljaca, Cabot
- Don Anthony, Council for Chemical Research

Metrology & Characterization – Real-time methods & tools

- Mike Garner, Intel
- David Wollman and David Seiler, NIST
- Ji Ung Lee, GE
- Bill Grieco, Rohm and Haas
- Emory Ford, Vision2020/MTI

Modeling & Simulation - Multiscale modeling methods & tools

- Joey Storer and Robert Haley, Dow
- Sadasivan Shankar and Mike Garner, Intel
- Francois Leonard and Eliot Fang, Sandia National Laboratory

Manufacturing & Processing – Chemical industry focused

- Bill Grieco, Rohm and Haas
- Dan Coy, Nanophase
- Charlie Gause, Luna nanoWorks

Fundamentals & Synthesis:
Experimentally Verified Understanding

- Gas-Phase Synthesis of Carbon Nanotubes and Nanowires
  - Fundamental relationship between catalyst nanostructure, growth conditions, and resulting nanotube/nanowire structure
    - Development of experimentally validated model
      - temperature, pressure, atmosphere, catalyst structure/composition, surface interaction
      - fundamental understanding of nucleation and growth
    - Determination of catalyst nanostructure
      - fundamental understanding of nucleation
      - mechanisms to predefine or self assemble catalyst
- Solution-Phase Synthesis of Nanoparticles, Nanowires, and Other Nanostructures
  - Fundamental understanding of the nucleation and growth
  - Ability to predict the final product and structures
  - Control of compositions and doping

Fundamentals & Synthesis:
Additional Experimental and Modeling Needs

- Self Assembly Processes (block copolymers, micelles, etc.)
  - Broad families of materials
    - nanostructured templates, CNT, nanocrystals, catalysts, nanoporous/low-k
  - Fundamental understanding of assembly processes
    - limits of size, separation, location, composition of self assembled structures
    - dynamics/kinetics of nucleation and growth
    - development of nonequilibrium structures
  - Models of self assembly processes
    - diffusion, shape, and size Interactions with surfaces and interfaces
    - nonequilibrium effects
  - Experimental understanding and models for interaction of self assembly with…
    - EM fields, optical inputs, thermal gradients
    - topology, edges, openings and non-uniformities
  - Functionalization of nanoparticles and macromolecules to enable polymers with unique complex properties
    - example: polymers with low CTE, low modulus and low moisture absorption
  - Integration of top-down patterning and bottom-up self assembly

Metrology & Characterization:
Key Needs for Manufacturing

- **Large volume nanotube characterization of electronic properties**
  - Bandgap distribution
  - Could be useful for characterizing other nanoparticles
  - On wafers or as grown
- **In line particle characterization (1-50 nm)**
  - Particle size distribution
  - Particle surface morphology distribution

Metrology & Characterization:

Large Volume Electronic Property Characterization

- No single tool to characterize bandgap distributions of large numbers of nanotubes
- Fluorescence is a likely characterization tool, but research is needed to understand:
  - fluorescence cross sections of CNT versus diameter, chirality, and bandgap in different chemical environments
  - interactions that can cause quenching (nanotube bundles, SiO_2, high k, chemicals/solvents)
  - conditions where fluorescence could be applicable

Metrology & Characterization:
In situ Nanoparticle (sub-50nm) Monitoring

- Current techniques are not compatible with *in situ* monitoring applications
  - Small angle x-ray scattering
    - measure particle size distribution and surface area
    - compatibility with flow cell demonstrated
  - Brownian motion techniques (light scattering)
    - sensitive to flow
  - TEM Holography (in development)
    - measure particle size and surface morphology
    - not compatible with flow systems
  - Particle mass spectrometry (proposal)
    - measure particle weight, composition, and surface chemistry
    - potential use in materials development, not in process
  - MEMs particle detectors (in development)
- Research is needed
  - Small angle x-ray scattering is most likely candidate
    - correlation of models to particle size and surface area distribution for different particles
    - smaller more compact x-ray source (commercial)

Modeling & Simulation

- Carbon Nanotube Synthesis and Electronic Properties
  - Atomic-level models of the growth kinetics of SWNT
    - function of catalyst design and processing conditions
    - mechanisms of control of tube diameter, chirality, branching, defect formation, and incorporation of impurities
  - Relationship between SWNT structure and transport properties
    - quantum mechanical treatment of electron transport taking into account the proper implications of symmetry and tube chirality
- Directed Self-Assembly for Sub-Lithographic Features
  - Develop modeling capabilities that predict nucleation and dynamics of self-assembly and structure formation at the nanoscale
    - advance the state-of-the-art in methods in self-consistent mean field theory
    - find simulations that bring process variables (shear/elongation, temperature, solvents) into play to help optimize self-organizing phenomena
- Nanomechanics and Interface Issues in Nanostructures
  - Model nanoscale devices from a purely mechanical perspective
  - Incorporate phemomena such as phonon transport self-consistently with electron transport and thermal diffusion
- Thermal Properties of Nanostructured Materials

Manufacturing & Processing:
Research Needs

- Integrated manufacturing and separations processes for consistent, large scale manufacture of carbon nanotubes
  - High purity and low cost processes
  - Better catalysts for improved yield
  - Better control of tube chirality, diameter, length
  - Improved separations to ensure product purity

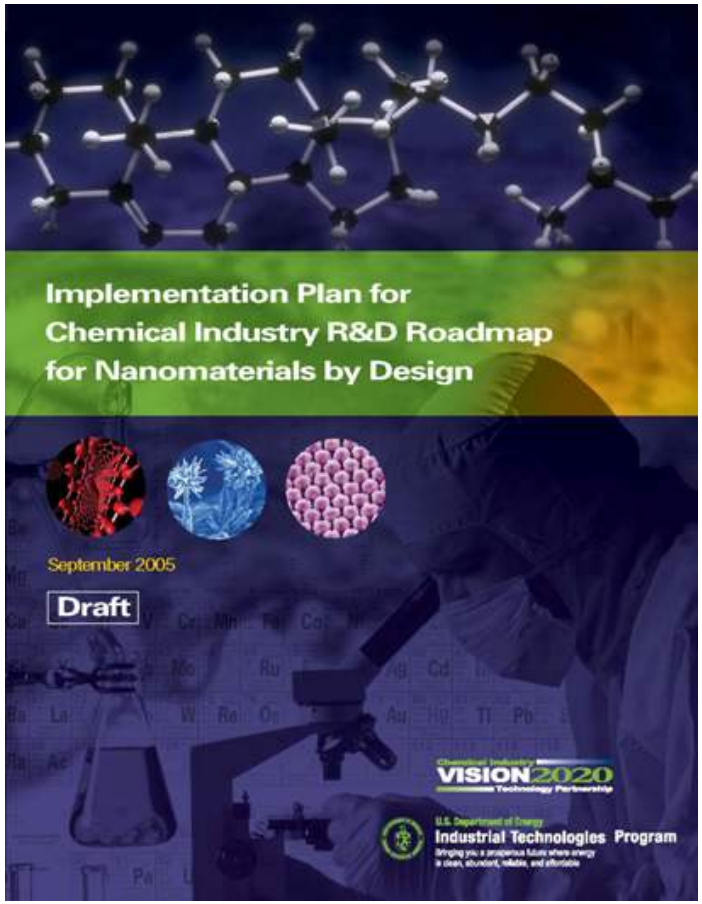
- Integrated manufacturing processes to deliver lower cost metal and metal-oxide nanoparticles at high purity
  - Improved control of particle morphology (size/shape)
  - Powder collection techniques that prevent particle agglomeration

Manufacturing & Processing:
Research Needs

- Integration of real-time characterization techniques for on-line process monitoring and process control
  - Optical and spectroscopic analyses for particle size distribution
- Scale-up of self-assembly processes for practical use commercial scale unit operations
  - Apply current lab/pilot scale techniques of molecular or biological self-assembly to larger scale processes
  - Develop appropriate *in situ* diagnostics and process control schemes to ensure consistent, low cost manufacture of nanostructures using these processes

Summary Report Planned

- Supported by DOE Industrial Technologies Program
- Expected completion in December 2005
- To be posted on Vision2020 web site:



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Actions in Progress

- Guiding research at NSF centers
  - Target list generated
  - Letter to center directors drafted
    - Identify ongoing research related to priority needs
- Advancing Metrology and Characterization
  - NIST interactions
  - Discussion towards Center of Excellence
- Advancing development of nanoscience to nanotechnology
  - Chemical industry Manufacturing & Processing team working to define a project appropriate for the DOE MPLUS Program
    - Target: In-process monitoring of nanomaterial synthesis