



# *Research Needs for Nanotechnology Commercialization*

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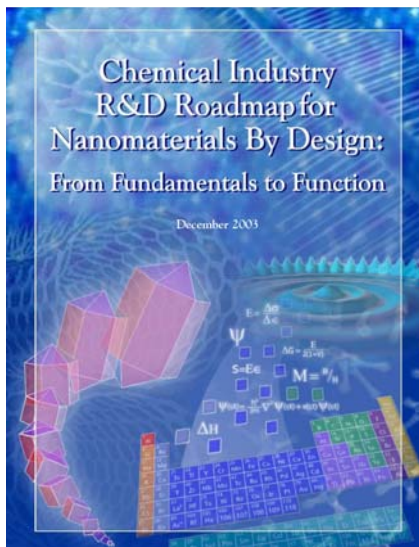
*Oak Ridge National Laboratory*

*AIChE 2005 Annual Meeting*

*November 3, 2005*

# 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:

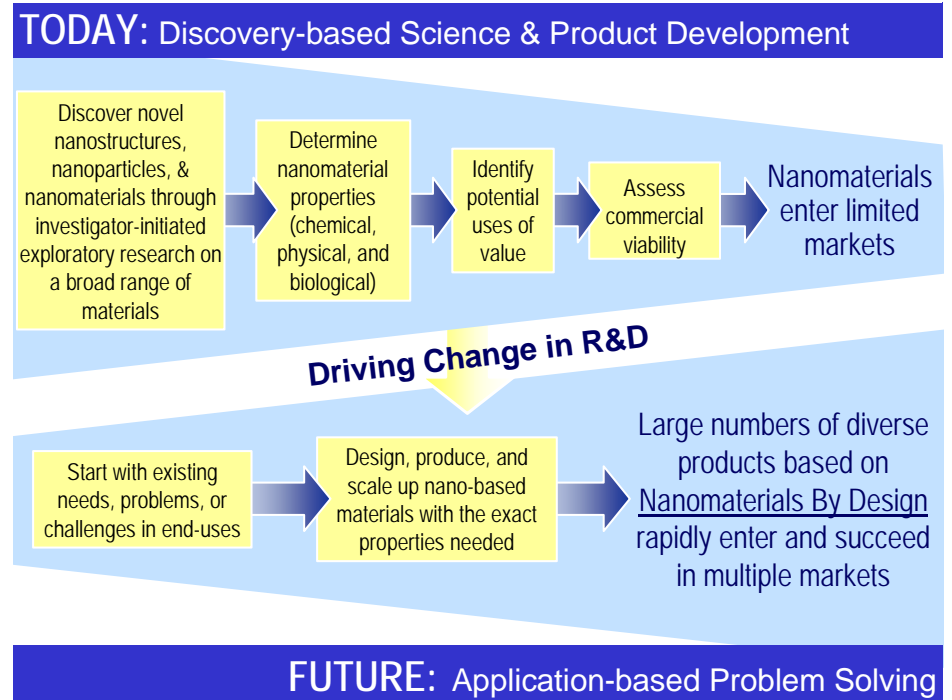
- NNI in development of Strategic Plan
- NSF, DOE, and DOD program managers in developing FY05 solicitations
- Interagency Working Group on Manufacturing R&D to develop white papers

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

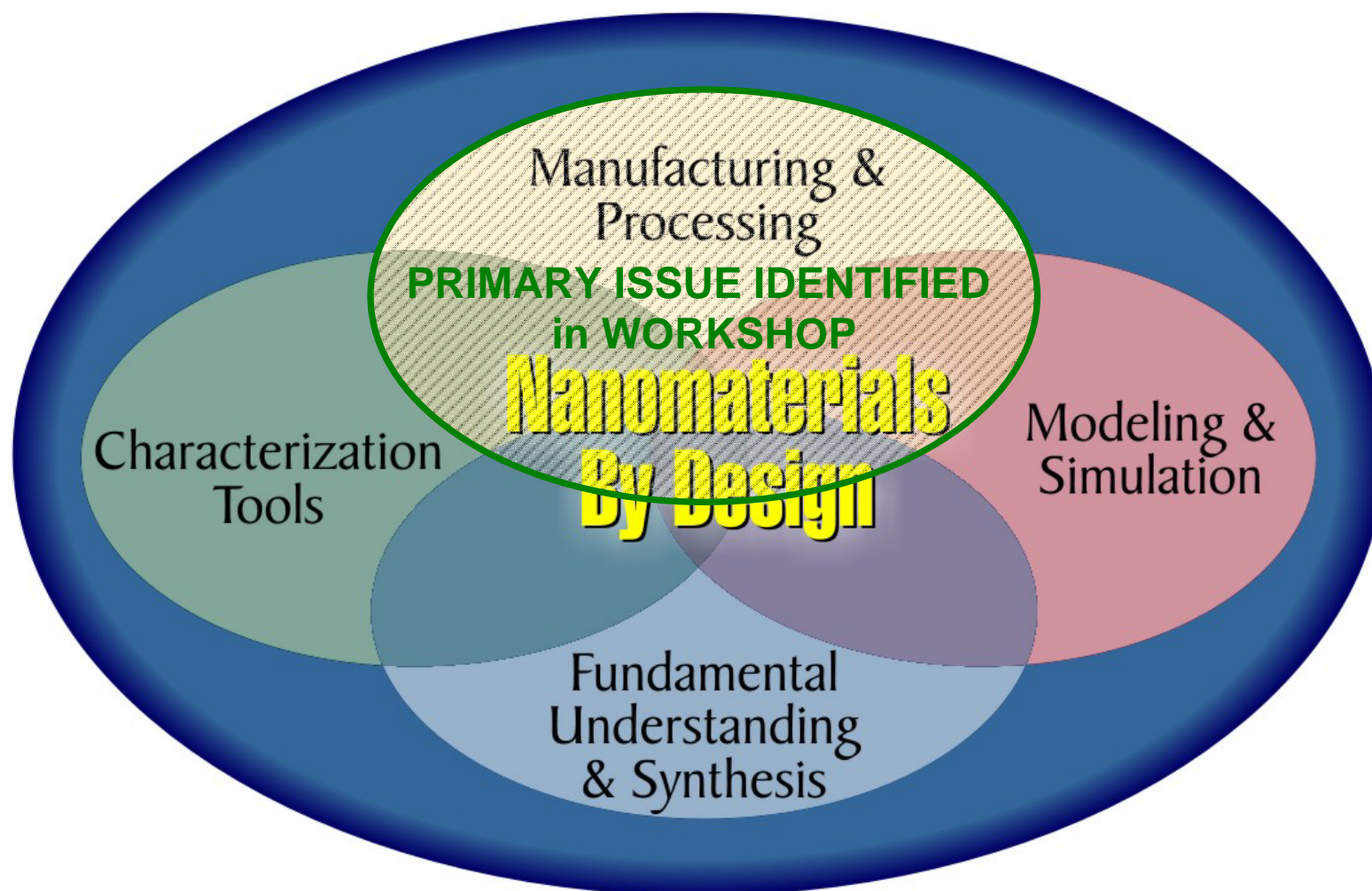
Workshop identified...

- 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 nanocomposites 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

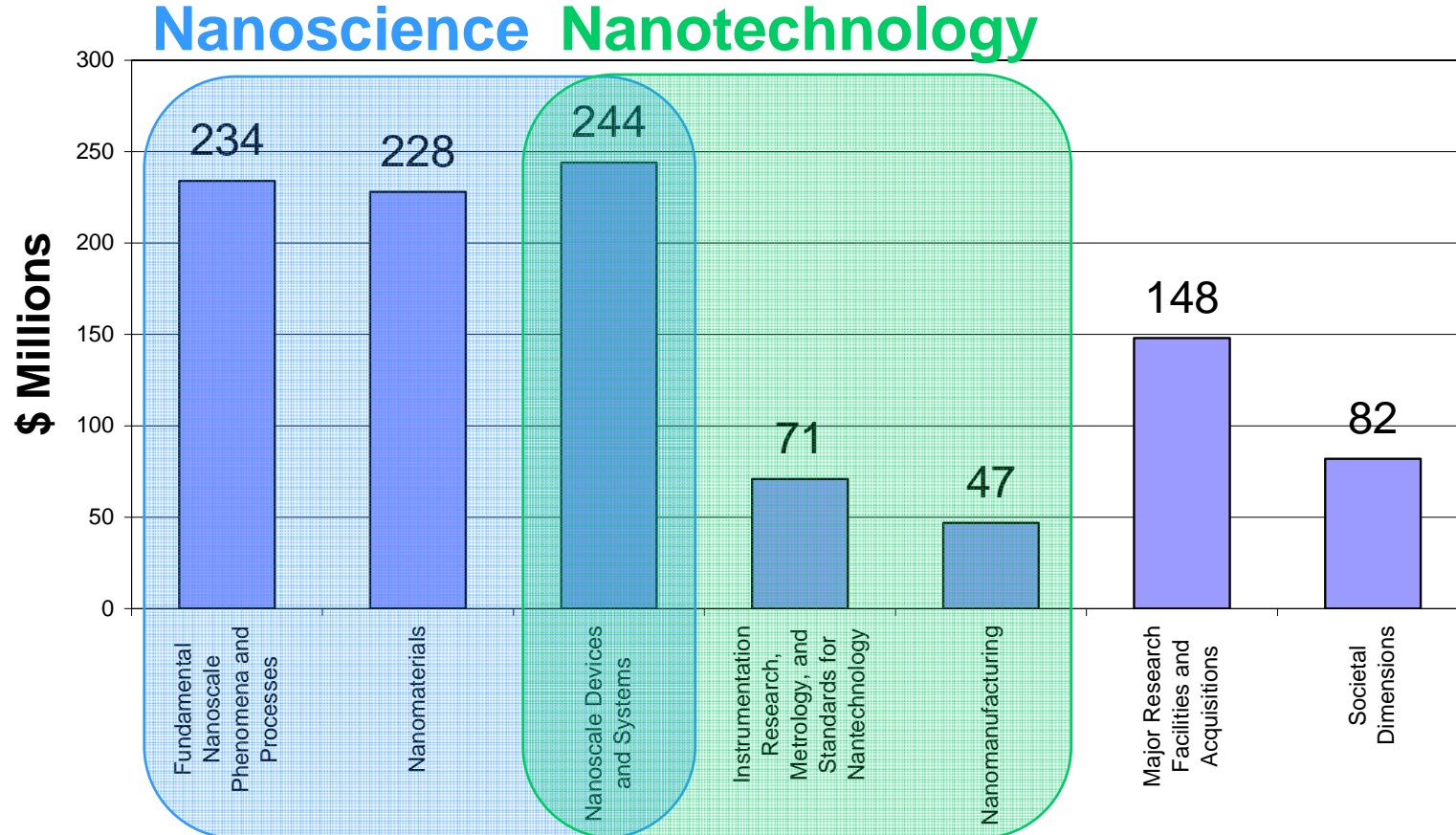
### Characterization tools

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 gaps?

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- **Fundamentals & Synthesis**

- Significant activity in this area
- *Industry perceptions*:
  - work is not directly applicable
  - 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 gaps?

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- **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 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

# 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/PNNL
- 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** – CPI-focused

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

# Fundamentals & Synthesis:

## Experimentally Verified Understanding

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- 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, etc.
  - 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

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- 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

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- **Characterization of nanotube electronic properties (bulk CNT samples)**
  - 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:

## Electronic Property Characterization

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- 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<sub>2</sub>, high k, chemicals/solvents)
  - conditions where fluorescence could be applicable

# Metrology & Characterization:

## *In situ* Monitoring of Nanoparticle (sub-50nm) Morphology

- 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 phenomena such as phonon transport self-consistently with electron transport and thermal diffusion
- Thermal Properties of Nanostructured Materials

# Manufacturing & Processing: Research Needs

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- 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

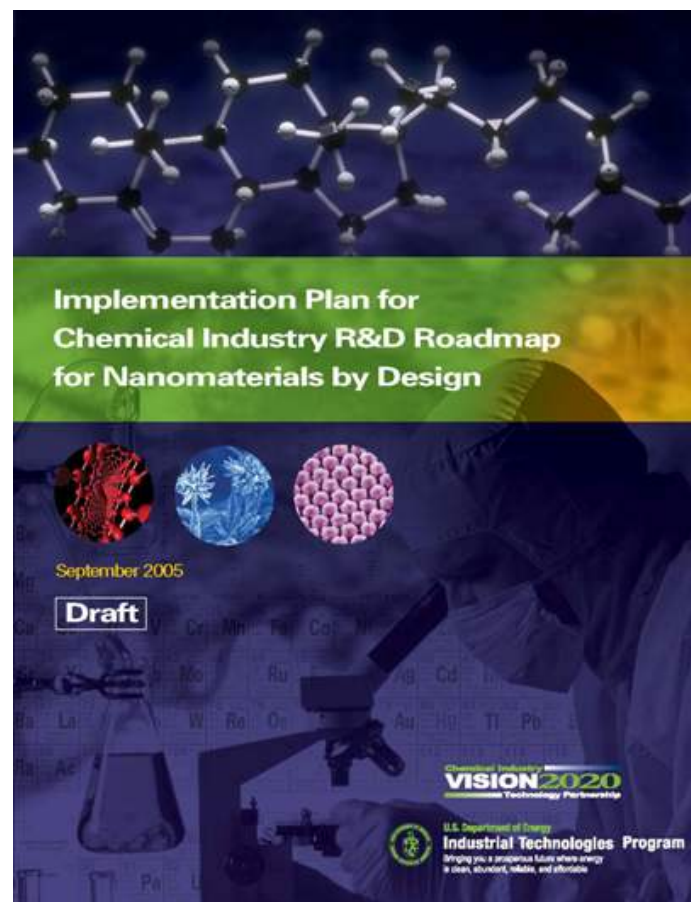
# Manufacturing & Processing: Research Needs

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- 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:



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

# Actions in Progress

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- 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

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**Thanks!**

# Needs Mapped to NNI PCAs and Agency Activities

Priority R&D Needs Relevant to the Chemicals Industry

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

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