

Scientific/Technology Challenges for the Nanotechnology Community

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Committee on Technology
National Science and Technology Council



Challenges for Moving Nanotechnology Forward

- Exploring the vast “nanomaterials” space
- Developing and implementing highly controlled, cost-effective processes for nanomanufacturing
- Advancing state-of-the-art for measurement and characterization of matter at the nanoscale

Los Alamos National Laboratory Chemistry Division

Periodic Table of the Elements

1A																	8A
1 H Hydrogen 1.008																	2 He Helium 4.003
3 Li Lithium 6.941	2A															10 Ne Neon 20.18	
4 Be Beryllium 9.012																	18 Ar Argon 39.95
11 Na Sodium 22.99	12 Mg Magnesium 24.31															36 Kr Krypton 83.80	
19 K Potassium 39.10	20 Ca Calcium 40.08	3B	4B	5B	6B	7B	8B		11B	12B	31 Ga Gallium 69.72	32 Ge Germanium 72.64	33 As Arsenic 74.92	34 Se Selenium 78.96	35 Br Bromine 79.90	54 Xe Xenon 131.3	
37 Rb Rubidium 85.47	38 Sr Strontium 87.62	39 Y Yttrium 88.91	40 Zr Zirconium 91.22	41 Nb Niobium 92.91	42 Mo Molybdenum 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.1	45 Rh Rhodium 102.9	46 Pd Palladium 106.4	47 Ag Silver 107.9	48 Cd Cadmium 112.4	49 In Indium 114.8	50 Sn Tin 118.7	51 Sb Antimony 121.8	52 Te Tellurium 127.6	53 I Iodine 126.9	86 Rn Radon 222
55 Cs Cesium 132.9	56 Ba Barium 137.3	57 La* Lanthanum 138.9	72 Hf Hafnium 178.5	73 Ta Tantalum 180.9	74 W Tungsten 183.8	75 Re Rhenium 186.2	76 Os Osmium 190.2	77 Ir Iridium 192.2	78 Pt Platinum 195.1	79 Au Gold 197.0	80 Hg Mercury 200.6	81 Tl Thallium 204.4	82 Pb Lead 207.2	83 Bi Bismuth 208.9	84 Po Polonium (209)	85 At Astatine (210)	118 Og Oganesson (?)
87 Fr Francium (223)	88 Ra Radium (226)	89 Ac~ Actinium (227)	104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (263)	107 Bh Bohrium (264)	108 Hs Hassium (265)	109 Mt Meitnerium (266)	110 Ds Darmstadtium (267)	111 Uu Ununium (268)	112 Uub Unbium (269)	114 Uuq Ununquadium (289)		116 Uuh Unhexium (288)			
Lanthanide Series*		58 Ce Cerium 140.1	59 Pr Praseodymium 140.9	60 Nd Neodymium 144.2	61 Pm Promethium (145)	62 Sm Samarium 150.4	63 Eu Europium 152.0	64 Gd Gadolinium 157.3	65 Tb Terbium 158.9	66 Dy Dysprosium 162.5	67 Ho Holmium 164.9	68 Er Erbium 167.3	69 Tm Thulium 168.9	70 Yb Ytterbium 173.0	71 Lu Lutetium 175.0		
Actinide Series~		90 Th Thorium 232.0	91 Pa Protactinium (231)	92 U Uranium (238)	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)		

element names in **blue** are liquids at room temperature
 element names in **red** are gases at room temperature
 element names in **black** are solids at room temperature

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Functional Properties

- High strength, toughness
- Corrosion resistance
- Superhardness and wear resistance
- Catalytic
- Conducting
- Semiconducting
- Superconducting
- Magnetic
- Photovoltaic
- Fluorescent
- Piezoelectric
- Thermoelectric

X-rays and Neutrons: Essential Tools for Nanoscience Research June 16, 2005

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Various Size Effects in Gold

Dickson, et. al.; Ga. Tech

Goodman; Texas A & M

Halas and West; Rice

Scanning Tunneling Micrograph of Au Clusters on Titania

Catalytic Activity

Cluster Morphology vs. Size

Plasmon Resonances on Nanoshells of varying thickness at $\sim 120\text{nm}$ diameter

Electron Quantum Size Effect at $\leq 1\text{nm}$

Enhanced Surface Sites for Catalysis at $\sim 3\text{nm}$

8 9 10 11

55 147 309

Photo by C. Radloff

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Nanostructures All made of ZnO

Courtesy ZL Wang; Georgia Tech

100%

5%

100%

100%

100%

100%

100%

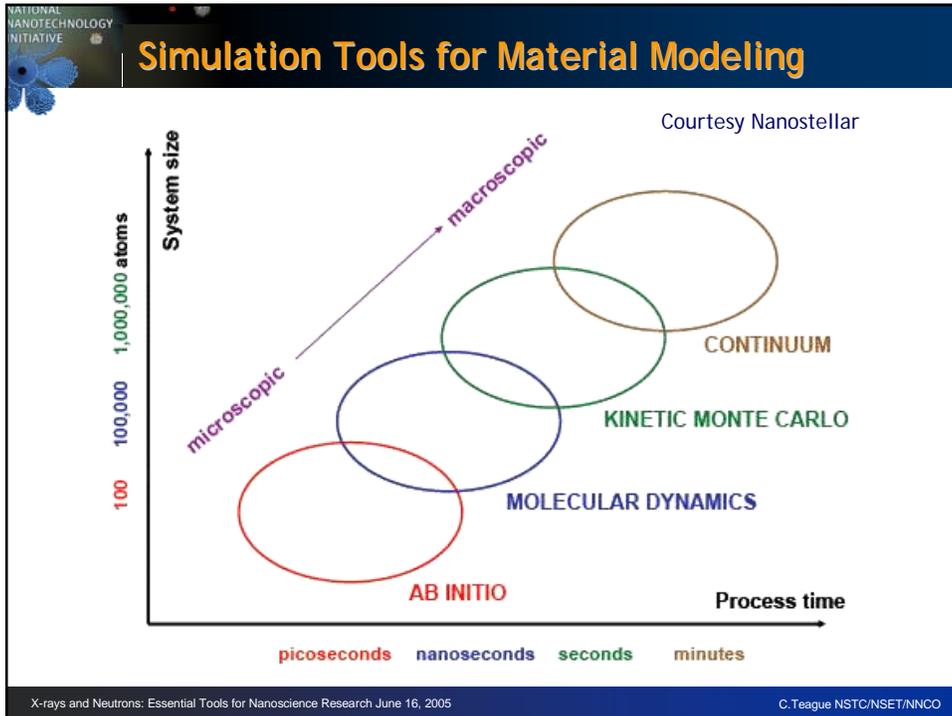
100%

100%

10%

20%

5%



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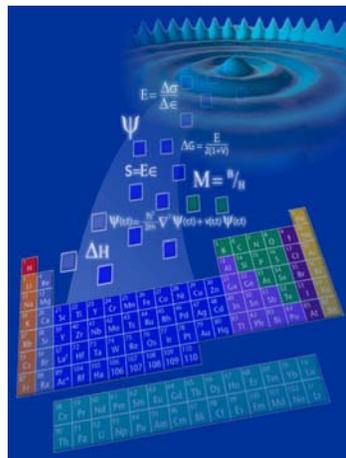
High-throughput Screening w/ *ab initio* Methods

- *Ab initio* methods defined as those that accurately solve the fundamental quantum mechanical equations for states of the electrons of a system
- Enabled by major advances in algorithm development and in computing power
- Examples:
 - Predicted band gaps in semiconductors and simulated annealing methods to find phase of largest band gap of $\text{Al}_{0.25}\text{Ga}_{0.75}\text{As}$ (Franceschetti and Zunger -1999)
 - Calculated formation energies of 200 transition metal hydrides (Smithson -2002)
 - Formation energies and structural parameters for 80 binary alloys in 176 different structures - 14,000 alloy structures (Morgan, et.al. 2004)

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Nanomaterials By Design

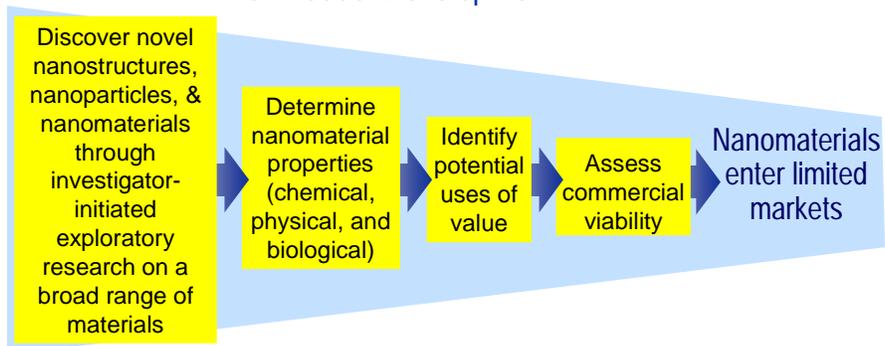
The ability to employ scientific principles in deliberately creating structures with nano-scale features (e.g., size, architecture) that deliver unique functionality and utility for target applications



Based on Chemical Industry R&D Roadmap for Nanomaterials By Design: From Fundamentals to Function

Nanomaterial Development: Today

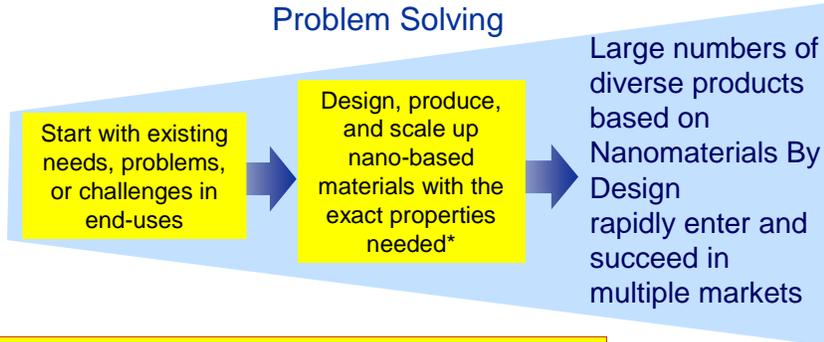
TODAY: Discovery-based Science & Product Development



Based on Chemical Industry R&D Roadmap for Nanomaterials By Design: From Fundamentals to Function

Nanomaterial Development: Future

FUTURE: Application-based Problem Solving



* Based on established understanding and methods

Based on Chemical Industry R&D Roadmap for Nanomaterials By Design:
From Fundamentals to Function

Developing and Implementing Nanomanufacturing Processes

Nanomanufacturing includes:

- All means that have the capability to reproducibly transform matter – from a bulk form or from individual atoms, molecules, and supramolecular structures – into nanoscale or nanostructured materials, devices, or systems with desired properties and performance characteristics typically in large quantities
- Design, simulation, and implementation that enable cost-effective synthesis and production of nanomaterials - nanostructures
- Assembly methods and technologies

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Nanomanufacturing: Building Blocks

BaHg₁₁ MoPt₂
Al₂Cu Fe₃W₃C

55 147 309 561 711 atoms

NRL Center for Computational Materials Science

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Forms of Nanostructures - Size Dependent

Example - Single Crystal Pt Particles

Courtesy B Lee and KJ Cho

Tetrahedron Cube

2 4 6 8 10 12 nm or higher

Truncated Octahedron (TO)

2 nm 0.196 nm

Z.L. Wang et al., Science 272, 5270 (1996); Surf. Sci. 380, 302 (1997); J. Phys. Chem B 102, 3316 (1998); J. Phys. Chem B 102, 6145 (1998)

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Possible Nanomanufacturing Steps Based on Directed Self-Assembly

Attach oligomeric, polymeric, or biomolecular tethers

Form nanospheres, nanorods, ...

Directed self-assembly of building blocks

Scaffolds and structures for:

- Catalysis
- Hydrogen storage
- Fuel cells
- Tissue engineering
- Drug delivery
- Electronics

Increasing scale of self-assembly of building blocks directed by:

- Electric fields
- Structured light
- Templated substrates
- Free-energy minimization

H. O. Jacobs, A. R. Tao, A. Schwartz, D. H. Gracias, G. M. Whitesides

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A Sampling of Carbon Nanotube Forms

(a) Armchair nanotube

(b) Zigzag nanotube

"Arbitrary" nanotube

S. Iijima in Nature 1991

Observation by TEM of multi-wall coaxial nanotubes with various inner and outer diameters, d_i and d_o , and numbers of cylindrical shells N : (a) $N = 5$, $d_o = 6.7$ nm, (b) $N = 2$, $d_o = 5.5$ nm, and (c) $N = 7$, $d_i = 2.3$ nm, $d_o = 6.5$ nm

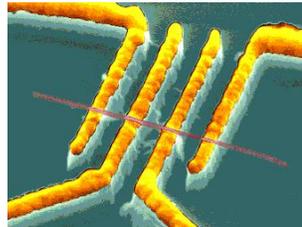
From Dresselhaus, Dresselhaus, and Sato Carbon 1995

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Electronic Applications of Nanotubes



"It takes about 0.1 g of CNTs per TV"



"For nanotubes to be useful in nanoelectronics, one would need 10^8 to 10^9 nearly identical nanotube segments"

Potential Commodity Markets for CNTs



Worldwide annual production of automobiles is about 50 million
5 kg of CNT per automobile
=> 250 million kg market

The challenge:
MWCNT in ton qtys. => \$250 - \$1250/kg
To be considered for light weighting automobiles, need \$5/kg



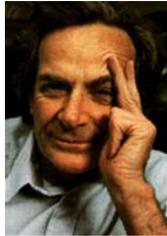
1 billion kg of copper produced annually in U.S. for home wiring
Cost of copper is ~\$3.30 per kg

Need to reduce cost of commodity levels of production by factor of ~ 50 - 250

Feynman's Measurement Challenge

*"It would be very easy to make an analysis of any complicated chemical substance; all one would have to do would be to look at it and see where the atoms are. The only trouble is that the electron microscope is one hundred times too poor ... I put this out as a challenge: **Is there no way to make ~~the electron microscope~~ more powerful?"***

*X-ray and Neutron Scattering
and Spectroscopies*



- Richard P. Feynman, 1959,
"There's Plenty of Room at the
Bottom"

Imaging and Chemical Information

- Atomic scale imaging

- Approaches:

- Field Ion Microscope (Atom Probe)
 - Scanned Probes (STM, AFM)
 - High Resolution Transmission Electron Microscopy

- Takes advantage of broad spectrum "interaction"

- Lacks specificity or requires specific sample

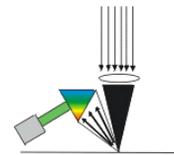
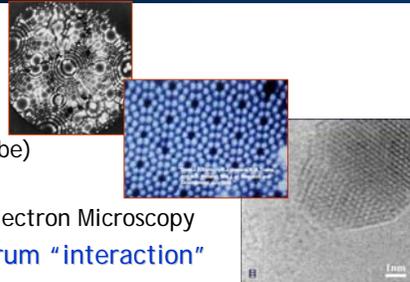
- Chemical Information

- Requires spectroscopy

- Inherently poorer signal to noise

- Selective interaction with very low cross section

- Chemical Imaging is MOST challenging



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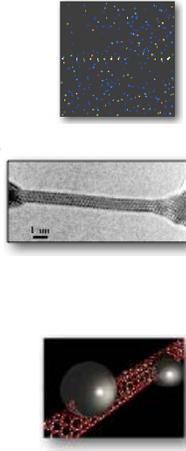
Extraordinary Scientific Opportunities

by direct observation of individual nanostructures

Key challenges identified in several TEAM workshops

- three-dimensional atomic-scale structure, shape, and defect distribution
- spectroscopic identification and location of individual dopant atoms
- direct imaging of the atomic-scale structure of glasses
- electronic structure of individual point defects
- non-spherical charge density and valence electron distribution
- in-situ observation of properties and response to external variables
 - temperature, stress, chemical activity, and applied electric and magnetic fields...

... all with unprecedented spatial, spectral & temporal resolution



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Courtesy U. Dahmen, DOE

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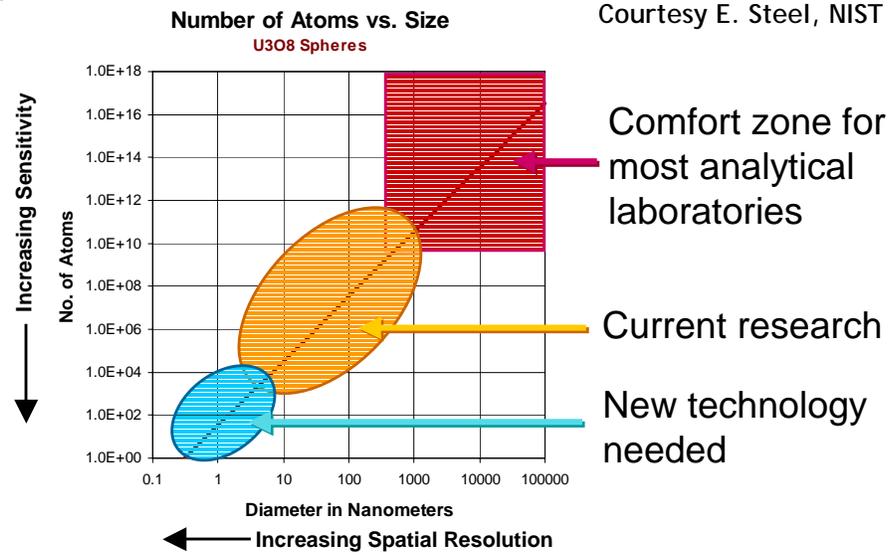
Where to go in the future of characterization?

Still need dramatically improved sensitivity

Courtesy E. Steel, NIST

Number of Atoms vs. Size

U3O8 Spheres



Increasing Sensitivity

No. of Atoms

Diameter in Nanometers

Increasing Spatial Resolution

Comfort zone for most analytical laboratories

Current research

New technology needed

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Nanoscale Material Characterization

Improve Sensitivity \longleftrightarrow Increase Spatial Resolution

These two needs are often incompatible

- Improve probe
 - Increase Intensity
- Improve detectors
 - Change detector efficiency
- Increase interaction with specimen
- Improve Probe
 - Reduce size
- Reduce interaction volume
 - Change probe physics

New technology is needed to break through this incompatibility



Chemical Characterization

- Higher Speed -
 - At nm sized pixels a 1 X 1 mm area would take 1000 pixels x 1000 pixels x ~1 sec = 12 days
- Higher Sensitivity
 - From 100's of atoms to single atom
 - Zeptogram analysis
- Move from 1D and 2D to 3D
 - Spectroscopic tomography
 - Know each atom and relationship to all others



Summary

- Three major challenges for moving nanotechnology forward
 - Exploring the vast “nanomaterials” space
 - Developing and implementing highly controlled, cost-effective processes for nanomanufacturing
 - Advancing state-of-the-art for measurement and characterization of matter at the nanoscale