Chemical Industry VISION2020 Technology Partnership

Estimation of the Economic Effect of Nanomaterials in the Chemical Industry

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Los Alamos

There is significant investment in nanotechnology R&D

- NNI budget ca. $1B/yr
- Questions:
  - what will come out of it?
  - where should spending be concentrated to maximize benefit?

Nanotechnology holds promise in diverse fields

- Potential major advances in
  - Energy conversion and storage
  - Pharmaceuticals and diagnostics
  - Catalysis
  - Separations
  - High-performance materials
  - Coatings
  - Electronics
  - Sensors

Nanotechnology in the Chemical Industry

- The chemical industry represents a major prospect for substantial, near-term adoption of nanoscale technologies with sustained benefits.
  - generates more than 70,000 diverse products
  - everyday items to materials used in high-technology industries
  - products are essential to key industries, including health care, communications, food, clothing, housing, energy, electronics, and transportation.
- **Importantly, the chemical industry employs materials and processes particularly suited to improvement through application of nanoscale technologies**.

Projections for the chemical industry

- The production of nanomaterials by the chemical industry is projected to surpass $1B by 2007 and to reach $35B by 2020*.
- Because of the widespread use of nanomaterials, this economic impact will not be confined to the chemical industry, but will be felt throughout numerous other industries.

*Study #1677, The Freedonia Group, Inc

Nanotechnology Benefits Analysis Project

Scope: **Analyze potential impact of materials by design using nanotechnology on energy efficiency, waste reduction & economic competitiveness for the chemical industry**

Nanotechnology Chemicals Plus Project

Approach

- Use *Nanomaterials by Design*, industrial steering team, and industrial market analysis reports to scope study
- LANL to determine economic, energy, and waste impacts
  - Analyze top 50 chemical process flow sheets for implementation of nanotechnologies for existing products
  - Use information from market analysis reports for new processes and products

Nanotechnology Chemicals Plus Project

- Industrial team prioritized scope of work
  - Top Market Opportunities:
    - energy
    - transportation
    - construction
    - Electronics
  - Top Target Materials:
    - catalysts
    - coatings
    - high-strength materials

These materials represent about $4B, or roughly 10%, of the $35B projected 2020 market for nanomaterials

Economic Benefits to the Chemical Industry from Nanomaterials by Design

- **Method**
  - **Identify applications of nanomaterials and use economic models to estimate value created**
  - **Consider four specific benefits**
    - **Increased selectivity and activity of catalysts by controlling pore size and particle characteristics**
    - **Replace precious metal catalysts by catalysts tailored at the nanoscale**
    - **More resistant hard coatings which improve manufacturing and eliminate the need for chromium electroplating**
    - **Membranes by design that can remove unwanted molecules from gases or liquids by controlling pore size and membrane characteristics**

Example Applications

- Chemical Industry
  - Reduce feedstock and energy usage through catalyst selectivity
  - Reduce precious metal usage
- Petroleum Refining
  - Reduce alkylation temperature by improved catalysts
  - Increased gasoline yield
  - Reduce precious metal usage
- Automotive Industry
  - Improved tools and dies – hard coatings
  - Reduced precious metal usage in auto catalysts
- Maritime Industry
  - Reduce ship fouling with coatings
  - Longer wear surfaces with coatings
- Manufacturing
  - Improved tools and dies-hard coatings
- Natural Gas
  - Membranes for removing N_2 and CO_2

Estimating impact of nanotechnology on catalysis

- **Consider flowsheets for top 50 chemicals**
- **Catalysis expert defined**
  - **18 processes where catalysts tailored at nanoscale could improve selectivity**
  - **13 processes with no benefit from nanotechnology**
  - **19 processes without catalysis**
- **For 18 processes, assume 50% selectivity increase through nanoscale tailoring**
- **Calculate cost and energy savings through program from PNNL report PNL-10684 (1995)**
- **Extrapolate to all chemicals production**

Example results for catalysis

TOP 50 CHEMICALS CATALYST IMPROVEMENT CALCULATIONS

Processes that do not use catalysts (yellow)
Processes where nanotechnology would not improve catalyst performance (green)

Chemical	Produced Using Catalyst?	Nanotechnology Increases Selectivity?	Annual Production (B Lbs/yr)	Feedstock Price ($/Lb)	Feedstock Cost (B$/yr)	Old Selectivity	New Selectivity	Old Feedstock Losses (B lbs/yr)	New Feedstock Losses (B lbs/y)	Feedstock Cost ($/lb)	Cost Savings ($/yr)	Base Energy Loss (Q/yr)	Energy Loss w New Selectivity (Q/yr)	Net Energy Savings (Q/yr)
Sulfuric acid	Yes	Yes	88.8	0.04	3.552	99.5	99.75	0.476	0.32	0.115	0.01794	0.0008	0.0006	0.0002
Nitrogen	No	-	58.7		0.000									0
Oxygen	No	-	42.38		0.000									0
Ethylene	No	-	40.41	0.315	12.729									0
Ammonia	Yes	Yes	35.95	0.14	5.033	99	99.5	0.625	0.601	0	0	0.2944	0.2919	0.0025
Lime	No	-	34.72	0.03	1.042									0
Phosphoric acid	No	-	25.36	0.34	8.622									0
Sodium hydroxide	No	-	24.02		0.000									0
Propylene	Yes	Yes	22.6	0.315	7.119	95	97.5	0	0	0	0	0.143	0.126	0.017
Chlorine	No	-	22.28	0.13	2.896									0
Sodium carbonate	No	-	20.89	0.06	1.253									0
Urea	No	-	16.84	0.09	1.516									0
Nitric acid	Yes	No	16.08	0.11	1.769	95								0
Ethylene dichloric	Yes	Yes	15.94	0.16	2.550	99	99.5	0.261	0.237	0.315	0.00756	0.0203	0.0188	0.0015
Ammonium nitrat	No	-	15.33	0.08	1.226									0
Vinyl chloride	yes	No	13.23	0.265	3.506	98								0
Benzene	Yes	Yes	12.01	0.143	1.717	N/A								0
Ethylbenzene	Yes	Yes	10.99	0.32	3.517	99	99.5	0.029	0.015	0.315	0.00441	0.0042	0.0032	0.001
MTBE	Yes	Yes	10.86	0.21	2.281	100	100							0
Carbon dioxide	No	-	10.79		0.000									0
Styrene	Yes	Yes	8.94	0.55	4.917	90	95	0.693	0.16	0.33	0.17589	0.02	0.0173	0.0027
Methanol	Yes	Yes	8.73	0.13	1.135	99	99.5	0.155	0.116	0	0	0.0367	0.0362	0.0005
Formaldehyde	Yes	Yes	6.98	0.21	1.466	91	95.5	0.736	0.351	0.068	0.02618	0.0061	0.0029	0.0032
Xylene	Yes	Yes	6.38	0.31	1.978	N/A								0
Toluene	Yes	Yes	6.03	0.36	2.171	N/A								0
Hydrochloric acid	No	-	5.75	0.03	0.173									0
p-Xylene	yes	Yes	5.66	0.35	1.981	70	85	0.841	0	0.33	0.27753	0.0936	0.0648	0.0288
Terephthalic acid	Yes	Yes	5.64	0.275	1.551	90	95	0.66	0.66	0.35	0	0.0078	0.0061	0.0017
Ethylene oxide	Yes	No	5.56	0.35	1.946	80								0
Ethylene glycol	Yes	No	5.12	0.47	2.406	99								0
Ammonium sulfat	No	-	4.72	0.07	0.330									0
Cumene	Yes	No	4.57	0.435	1.988	99								0
Potash	No	-	3.76		0.000									0
Phenol	Yes	No	3.71	0.55	2.041	97								0
Acetic acid	Yes	No	3.6	0.455	1.638	99								0
Butadiene	Yes	Yes	3.18	0.32	1.018	90	95	1.588	1.331	0.34	0.08738	0.0806	0.0704	0.0102
Carbon black	No	-	3.02	0.4	1.208									0
Acrylonitrile	Yes	Yes	2.83	0.46	1.302	66.5	83.25	0.654	0.071	0.3	0.1749	0.0235	0.0096	0.0139
Propylene oxide	Yes	No	2.7	0.72	1.944	90								0
Vinyl acetate	Yes	No	2.66	0.48	1.277	90								0
Titanium dioxide	No	-	2.53	0.85	2.151									0
Acetone	Yes	Yes	2.39	0.285	0.681	90	95	N/A				0.0081	0.0075	0.0006
Cyclohexane	Yes	Yes	2.21	0.3	0.663	100	100	0.004	0.004	0.143	0			0
Aluminum sulfate	No	-	2.18	0.08	0.174									0
Sodium silicate	No	-	1.8	0.34	0.612									0
Adipic acid	Yes	No	1.75	0.625	1.094	90								0
Calcium chloride	No	-	1.39	0.1	0.139									0
Caprolactam	Yes	No	1.38	0.77	1.063	95								0
Sodium sulfate	No	-	1.34	0.06	0.080									0
Isobutylene	Yes	No	1.29	0.32	0.413	99								0
Total					**99.867**						**0.7718**			**0.0838**

Nanotechnology Benefits Analysis Summary Table

Example	Cost Savings ($B per Year)	GNP Increase after 3 years (Billions of $)	Employment Increase after 3 years (000's of Jobs)	Personal Income Increase after 3 years (Billions of $)	Energy Savings (Quads per Year)	Waste Reduction per Year
Chemical Catalysts Selectivity Increase	2.5 to 4.0	10 to 15.	150 to 240	9 to 14.	0.2 to 0.4	
Chemical Catalysts Precious Metal Reductions	0.02				--	
Chemical Use of Membranes for Separations	0.07				0.03	
Refinery Catalysts Precious Metal Reductions	0. 01 to 0.05	0.8 to 2	10 to 30	0.9 to 2	--	100 to 300 M Gal. Of Waste water 1 to 2 M Tons Toxic Emissions
Refinery Process Temperature Reductions	0.2 to 0.7				0.02 to 0.08	
Refinery Catalysts Selectivity Increases	0.12 to 0.25				0.06 to 0.12	
Refinery Use of Membranes for Gas Separation	0.08				0.001	
Automobile Catalysts Precious Metal Reductions	0.3 to 1	1.3 to 5	20 to 80	1.2 to 5	--	
Trucking Industry Fuel Combustion Catalysts	0.4 to 2	1.5 to 8	25 to 130	1.3 to 7	0.06 to 0.3	
US Navy Antifouling Coating Fuel & Pollution Abatement savings	0.7				0.07	$46 M in pollution abatement costs
US Navy Nanomaterial Hard-Coating Savings	0.35				--	
US Shipping Industry Antifouling Coating Fuel & Pollution Abatement Savings	0.8	4 to 7	70 to 110	5 to 7	0.08	Up to $460 M in pollution abatement costs
US Shipping Industry Nanomaterial Hard-Coating Savings	1 to 2				--	6,000 to 12,000 tons of chromic acid
Manufacturing Industry Hard-Coating Savings	2 to 3.5	10 to 20	150 to 300	14 to 20		
Natural Gas N_2 and CO_2 Removal by Membranes	1 to 3	2 to 6	30 to 85	2 to 6	--	

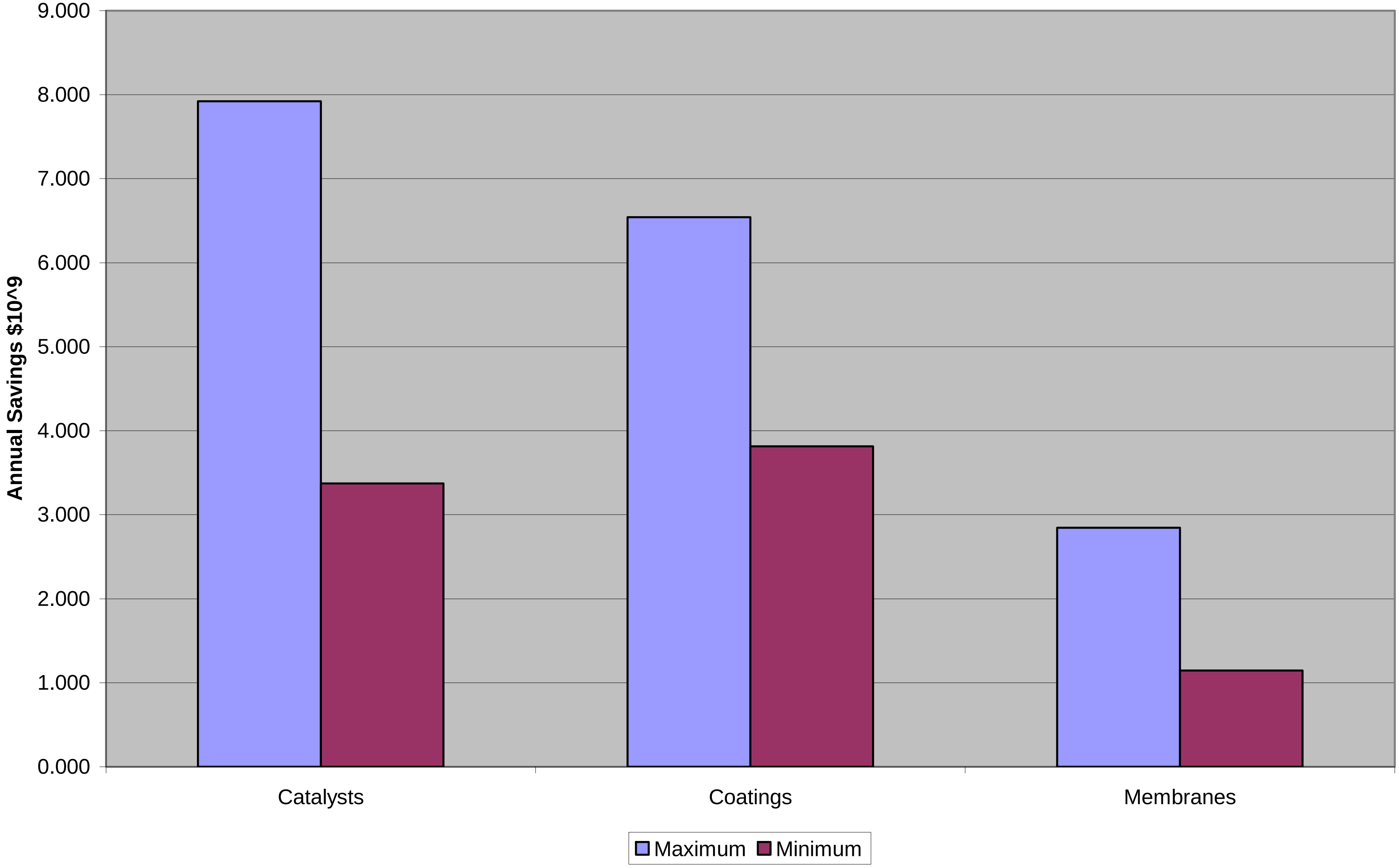
Estimated Impact of Nanomaterials by Design to Chemical Industry Examples

	Cost Savings $billion/year	**Energy Savings** Trillion BTU/year	**Nanomaterial Application**
Chemical	2.5 – 4	200 – 400	catalysts
Petroleum	1–1.7	80 – 200	catalysts
Automobile	0.3 – 1		catalysts
Shipping	1.7 – 2.7	80	coatings
Manufacturing	1.7 – 3.5		coatings
Natural Gas	1 – 2.7		membranes

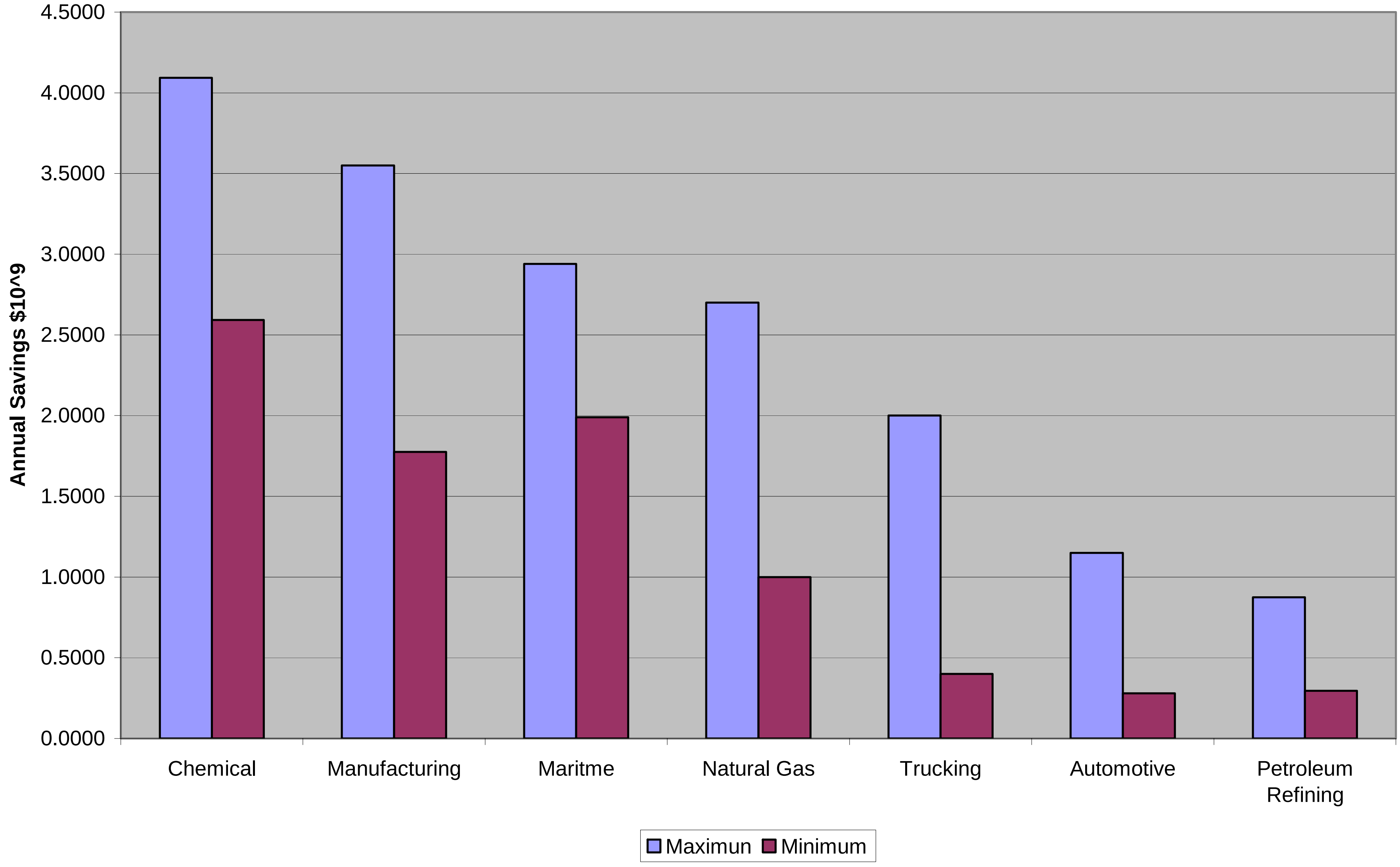
Overall, for this limited set of chemical industry applications:

- **Energy Savings = 0.5 to 1.1 quads/yr**
- **Value Creation = $10-20 B/yr**

Potential Cost Savings by Process Type



Potential Cost Savings by Industry



Summary

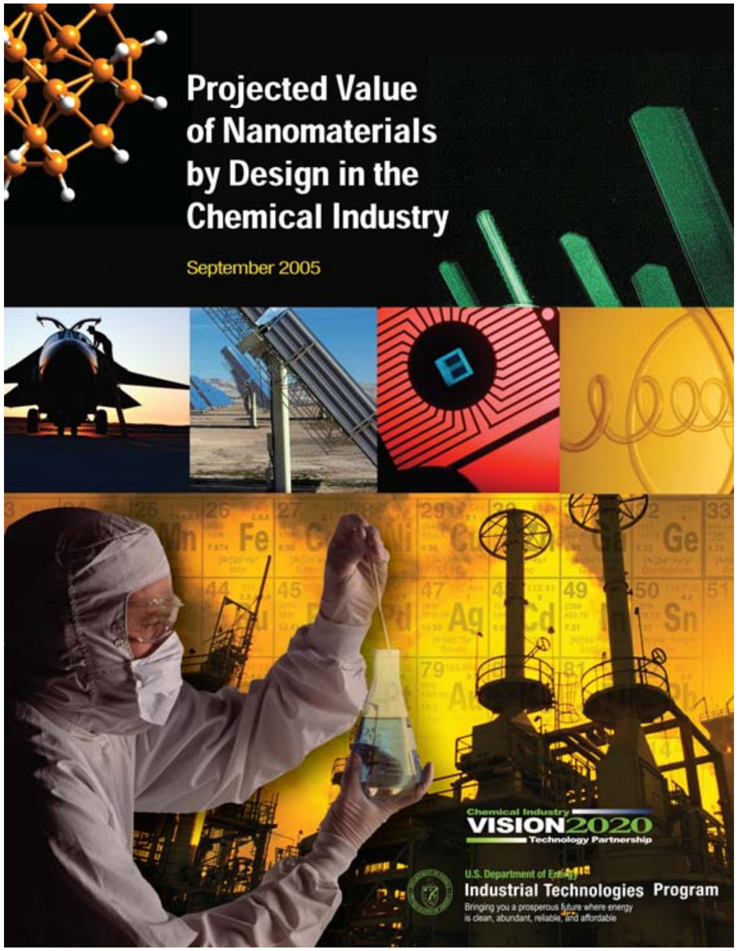
- **Nanotechnology is expected to provide a significant benefit to the chemical industry**

- **For a narrow set of materials**
    - **Catalysts, Coatings, Membranes**
- **In a limited set of applications**
    - **Chemical Industry**
    - **Petroleum Refining and Natural Gas production**
    - **Automotive Industry**
    - **Maritime Industry**
    - **Manufacturing**

- **Projected Impact:**
    - **Value Creation: $10-20 billion/year**
    - **Energy Savings: 0.5-1.1quadrillion BTU/year**
    - **GNP increase: $30 – 63B**
    - **Employment increase: 455,000 – 975,000 jobs**

Report available soon

- To be posted on Vision2020 web site:



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

Chemicals Plus

Overview

- Chemicals Industries of the Future Subprogram of DOE Industrial Technologies Program
- Support implementation of Vision2020 by allowing access to the unique capabilities of National Laboratories
- Fund studies that will lead to technology innovation and broad benefits for the chemical industry
- http://www.chemicalvision2020.org/chemicalsplus.html

FY04 Chemicals Plus Project: Nanotechnology Benefits Analysis

Investigators: Fred Roach & Gary Thayer, LANL

Implementation Mechanism: Chemicals Plus Project managed by David DePaoli & Sharon Robinson, ORNL

Technical Oversight: Industrial steering team

Funding Agency: Chemicals IOF of DOE ITP

Nanotechnology Chemicals Plus Team

Industrial Steering Team

- Jack Solomon, Praxair – Team Lead
- Steve Andrews, Ciba
- Margaret Blohm, GE
- Timothy Donnelly, Rohm & Haas
- Douglas Rundell, BP
- Guy Steinmetz, Eastman
- Hank Whalen, ACS
- Emory Ford, MTI
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