NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## An ATP Project Area for 1999

John D. Hewes, Ph.D.

Chemistry and Life Sciences Office
Advanced Technology Program
National Institute of Standards and Technology
Gaithersburg, MD
**http://www.atp.nist.gov/www/ccmr/ccmr_off.htm**
**1-800-ATP -FUND**

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

atp™ ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## Outline

- Introduction
- University opportunities
- Economic benefits to the US
- The Opportunity for ATP
- Conclusions

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## What is the ATP?

- Unique government/industry partnership
- Different from other government programs
  - *Intellectual Property retained by awardees*
  - *~50% cost-share*
  - *Mix of small-, med.-, large companies*
- Opens new opportunities for U.S. industry in global markets

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

atp™ ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## Universities and the ATP

- Universities = U.S. research excellence
- Universities/Labs/non-profits can participate
  - *Can initiate project with a non-profit*
  - *As a subcontractor to a single company or a j/v, or*
  - *As a j/v partner with at least two for-profit companies*
    - *Both for-profits substantially involved in the R&D*
    - *Both for-profits contributing toward the matching-fund requirement.*

*Over 300 individual instances of university participation in ATP projects*

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

atp™ ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## Project Proposals

- Single Company Proposals
  - *Limited to 3 years and $2M total NIST funds*
  - *NIST pays only direct costs*
  - *Large companies cost share at least 60%*
- Joint Venture Proposals
  - *Less than 5 years with no limit on award amount*
  - *Must involve two or more for-profit companies*
    - *Both doing research + contribute to cost share*

## Potential Economic Benefit

- Effects of the ATP
  - *Would it happen without ATP?*
  - *Accelerates R&D and commercialization?*
  - *Increases/broadens opportunities for new products and processes?*
  - *Collaboration and synergies likely?*

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

atp™ ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## High Technical Risk

- Technical challenges which display ***significant recognized*** uncertainty of success
- Success will ***dramatically change*** the future direction of technology and its market impact
- Risk may be high in developing single innovations and/or integrating technologies

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

atp™ ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## ATP reacted to U.S. industry needs

- February ‘98: Industry starts input to ATP
- March ‘98: Working Group Discussion
- June - August ‘98: ATP program development
- Oct. ‘98: Budget approved
- Nov. 18, ‘98: Atlanta Workshop
- Winter ‘98: Program announcements
- Spring ‘99: Competition begins
- Fall ‘99: Projects awarded

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

atp™ ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## Chemicals and advanced materials mfr.'s want to use methods for discovery

***BUT……*** Large entry barriers exist:

- Expensive *vs.* R&D budgets, ROI
- Investment in non-core technologies or businesses
- Integration of new base technologies
- Current manufacturing assets--comfort levels attained

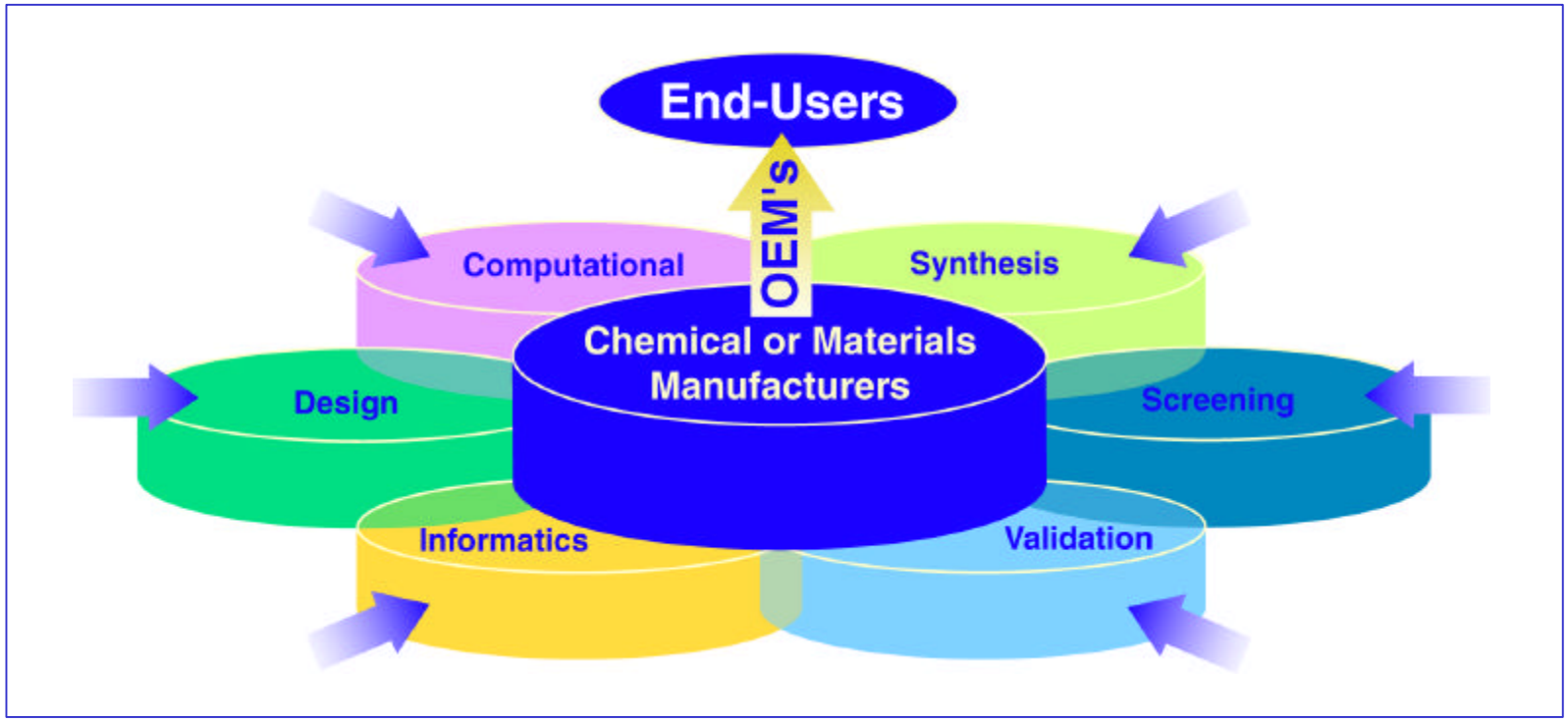
***Risk/reward ratio is too high for many sectors***

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## Implementation Strategy




*Infrastructure focused on specific applications*

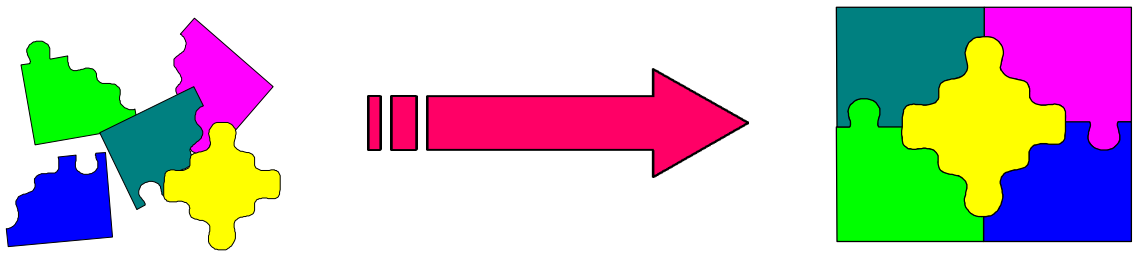
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

atp™ ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## Integration of technologies is the key

- Design of experiments (statistics tools)
- Validation (computational/molecular modeling)
- Synthesis and processing (deposition, robotics)
- Screening (sensors, robotics, etc.)
- Informatics (database hardware/software)

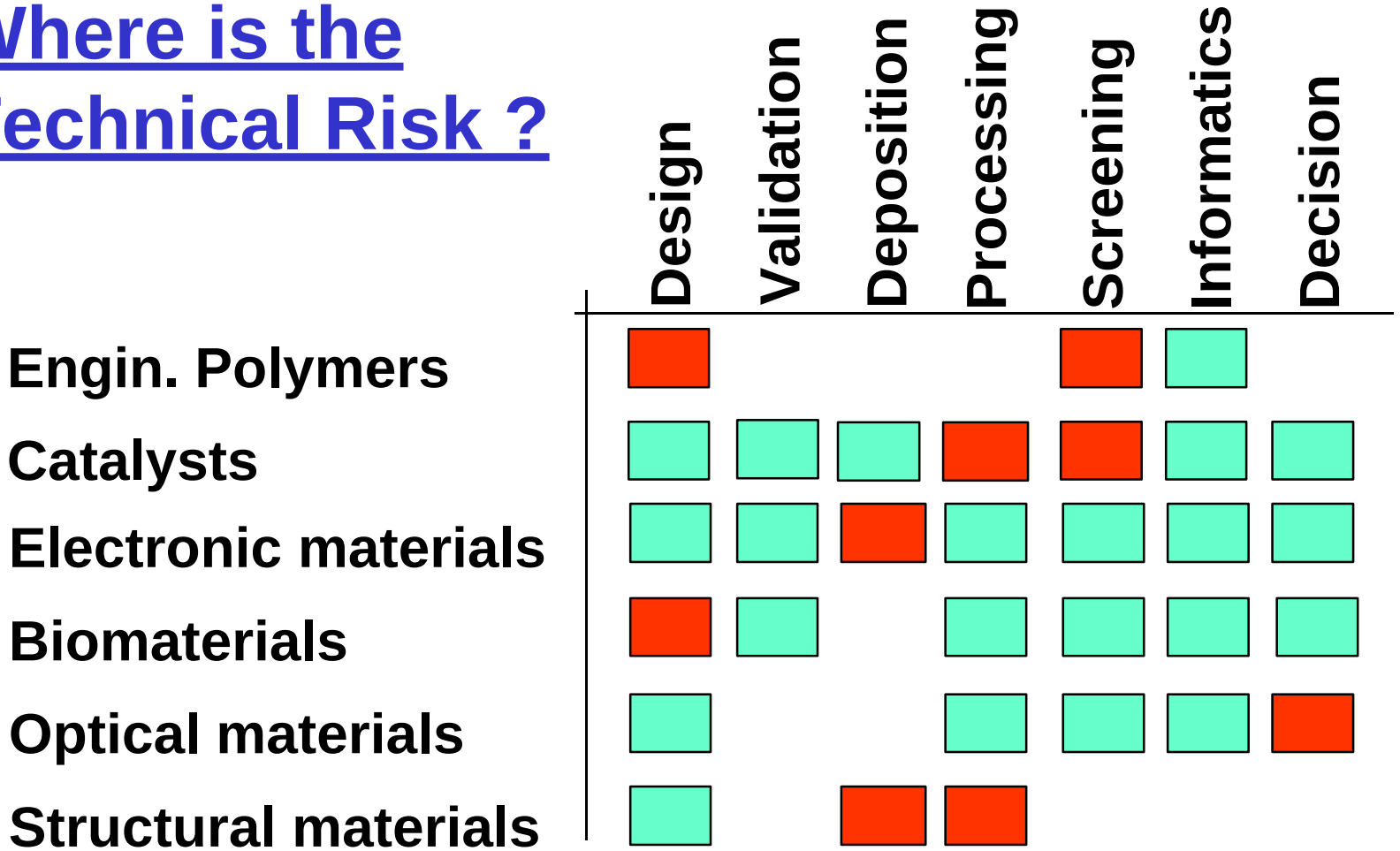


NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## Where is the Technical Risk ?



NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

atp™ ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## Technology Base Needs

**Synthesis and Processing**
- Automation
- Sensors

**Library Design**
- Statistics
- AI/expert systems

**Scalability**
- Interfacial vs. bulk properties

**Screening (HTS)**
- Sensors
- MEMS
- Robotics
- Massively parallel cpu's

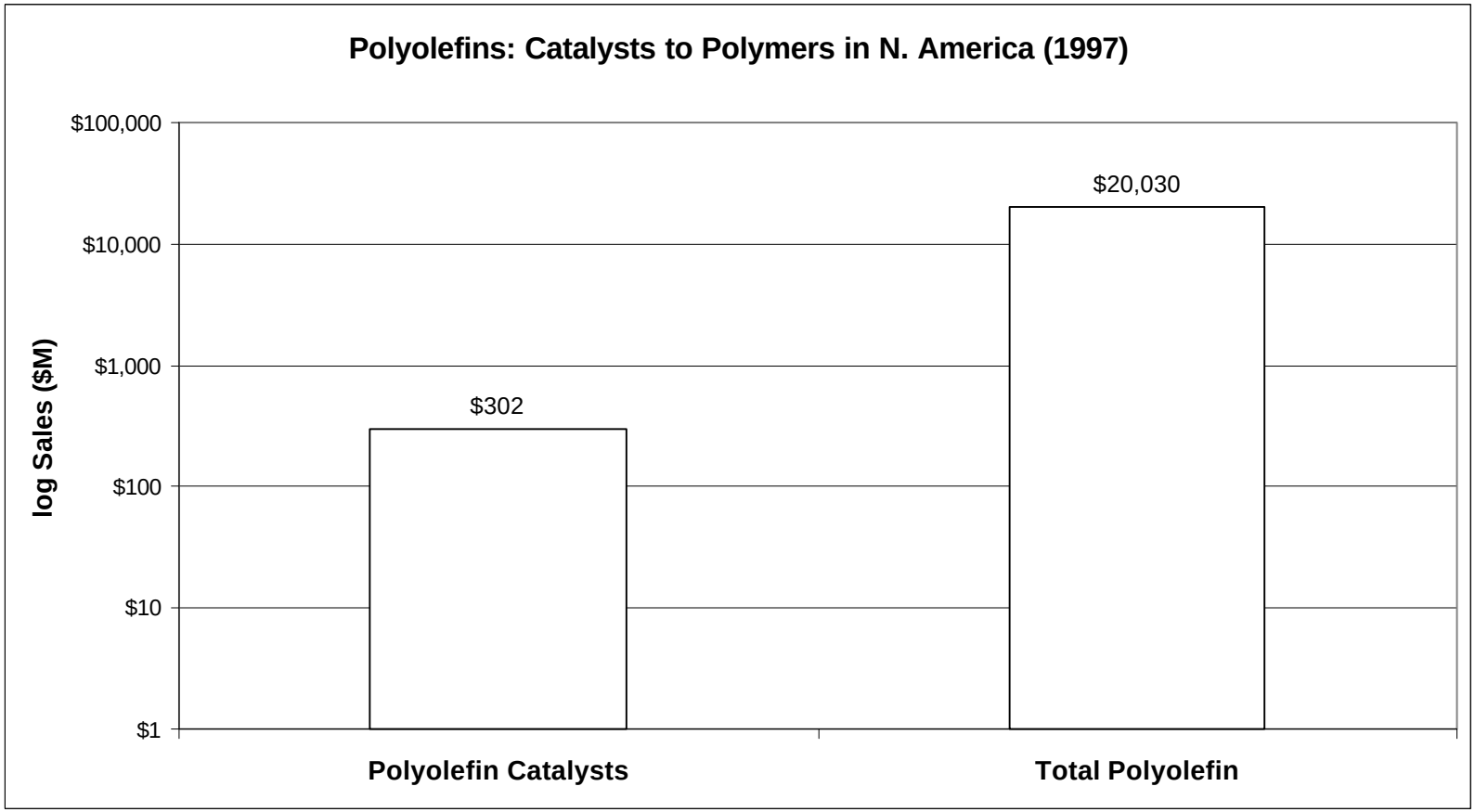
**Cheminformatics**
- Samples control
- Information flow
- Data integration
- Data analysis
- Hardware support

***Leveraging developments from pharmas***

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery




**Catalysts = $3.6 B**

**Commodity Polymers = $27 B**

Staff estimates, The Catalyst Group

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

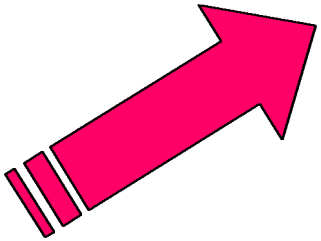
atp™ ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## Widespread potential benefits are possible

Estimated Markets for year 2001

| | |
|---|---|
| **Electronic Materials** | **$ 3.5 B** |
| **Specialty Polymers** | **$ 29 B** |
| **Optoelectronics** | **$ 29 B** |
| **Separations** | **$ 0.8 B** |



**SYSTEMS & COMPONENTS**

* Staff estimates, Freedonia, SRI, Frost & Sullivan

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

atp™ ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## Why Combinatorial @ ATP ?

- Applications mfr.'s have some combi. capabilities
  - ***May not develop others (non-core business assets)***
  - ***Awaiting one or more enabling technologies***
- Technology infrastructure can provide solutions
  - ***Need focus on specific applications***
  - ***Alliance development***
  - ***Systems integrations***

| ***Without ATP*** | ***With ATP*** |
| --- | --- |
| Resource-rich industries<br>Methodologies diffuse slowly | Resource-limited industries<br>Methodologies diffuse faster |

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

atp™ ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## ATP has an opportunity

- Bring leading-edge technologies to catalyst-based industries
  - *Lower-cost hardware and software tools*
- Integrate diverse technology base toward applications
  - *Hardware and software tools converge*
- Improve competitive stance in program industries
  - *Cycle time reductions impact market positions*

*Swift implementation of rapid through-put discovery could have a global impact*

# Combinatorial Discovery

## Conclusions

An ATP portfolio in combinatorial chemistry:

- Benefit society broadly with accelerated innovation
  - *Infrastructural technologies diffuse broadly to other industries*
  - *New materials and chemical products impact society*
  - *Reduced innovation cycle times*
  - *Basic research*
- Help establish U.S. competency in combinatorial methods
- Impact other industries via services, licenses of IP, etc.
- Promote research in basic sciences
  - *Build new capabilities and elucidate new phenomena*

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

ADVANCED TECHNOLOGY PROGRAM

# Combinatorial Discovery

## More Info:


**John D. Hewes, Ph.D.**

**Advanced Technology Program**

**National Institute of Standards and Technology**

**Gaithersburg, MD 20878**

**john.hewes@nist.gov**


**http://www.atp.nist.gov/www/ccmr/ccmr_off.htm**

**http://www.atp.nist.gov/fallmeeting/**

**Call (800) 287-3863**