# *Combinatorial Methodologies for Advanced Materials: An ATP Technology Cluster*

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*SPIE Optoelectronics 2000* *San Jose, CA* *January 26, 2000*

# Agenda

- ➔The NIST Advanced Technology Program
- ATP and Combinatorial Methods
- The FY1999 Combinatorial Methods Cluster
- Plan Forward: FY ’00 Open Competition
- The ATP Selection Criteria





# *NIST is…..*


**Measurements and Standards Laboratory**

**Advanced Technology Program**

**Manufacturing Extension Partnership**

**National Quality Program**

# What ATP Looks For

- **Path-breaking** technology
  - Opens up new possibilities
  - Revolutionary in nature
- **Infrastructural** technology
  - Supports R&D, production and business of an entire industry
- **Multi-use** technology
  - Many distinct applications`

**ATP Ground Rules:**

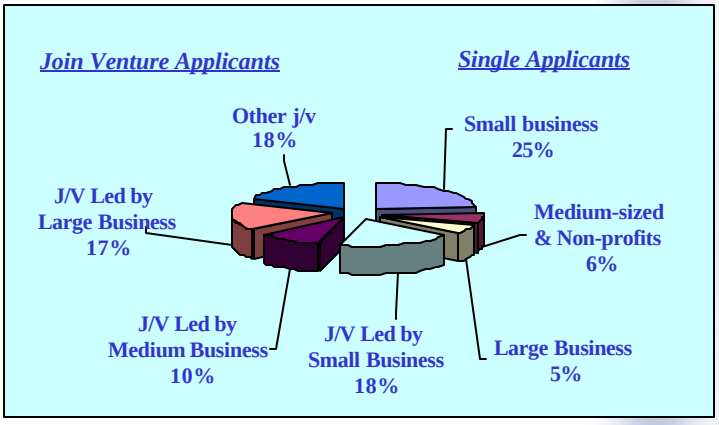
- Not subject to Freedom of Information Act (FOIA)
- Confidential reviews by Federal employees
- Companies retain patent rights*





# *$1,496 M to 468 ATP Awardees*

## *1990 - 1999*




*Substantial University Participation*
*More than 125 Universities have participated*

# Total ATP Investment

**Electronics and Photonics ($329M)**

- Microelectronics
- Optoelectronics
- Optics Technologies
- Power Technologies
- Wireless Electronics
- Organic Electronics

**Information Technology ($389M)**

- Advanced Learning Systems
- Component-Based Software
- Digital Video
- Information Infrastructure for Healthcare
- Electronic Commerce
- Dependable Computing Systems
- Integration of Manufacturing Applications

**Biotechnology ($254M)**

- DNA Technologies
- Tissue Engineering
- Drug Discovery Methods
- Proteomics
- Medical Devices & Imaging

**Chemistry and Materials ($344M)**

- **Catalysis & Biocatalysis**
- **Combinatorial Methods**
- **Separations/Membranes**
- **Nano-technology**
- **Engineered Surfaces**
- **Sensors**
- **Composites**





# *ATP Technology Cluster*

## *Catalysis and Biocatalysis Technologies*

| Awardees | Technology Challenges |
|---|---|
| **The Dow Chemical Co.** | Breakthrough Process….Propylene to Propylene Oxide |
| **Genencor International, Inc.** | Continuous Biocatalytic Systems…. Renewable Resources |
| **Phillips Petroleum Co.** | Computational Methods for Catalyst Design |
| **General Electric Company** | Biosynthesis of Monomers |
| **ABB Lummus Global*** | Thin-Film Solid Acid Catalyst for Refinery Alkylation |
| **B.F. Goodrich/3M Co.** | Tailored Optical Polymers Through a Novel Catalyst System |
| **Sun Company, Inc.** | Breakthrough Process for Oxidation of Alkanes |
| **BP Amoco** | Elastomeric Polypropylene and Elastic Non-wovens Venture |
| **W.R. Grace/Cryovac*** | Polar-Tolerant Organometallic Catalytic Technology... |
| **Maxygen, Inc.** | Whole Genome Shuffling…. |
| **Henkel/GE** | Biosynthesis of Chemical Intermediates |
| **Dyax Corp.** | A Phage-Display-Based Platform Technology.. |

# 3M/BFGoodrich: Project TOPCAT

**OBJECTIVES:**

- ***Develop Novel Catalysis Systems***
- ***Tailor New High Performance Optical Materials***
- ***Implement New Designs and Components to Construct High Performance Optical Communication Links***
  - ***< 0.1 dB/cm attenuation at 850 nm***
  - ***$\Delta n > 0.02$***
  - ***$\Delta n$ constant over temperature range***
  - ***Solder Reflow Compatible***
  - ***> 2,000 hours at 125 C in air***


**PROGRAM STATUS:**

- ***Completed 4th Year Review of this 5 Year Program***
- ***Demonstrated Bench Scale Working Wave-Guides***
- ***Demonstrated Key Elements of Continuous Fabrication***
- ***Program Meeting Milestones***
- ***1 US Patent and 7 Applications***
- ***Major Spin-Off Opportunities Defined***





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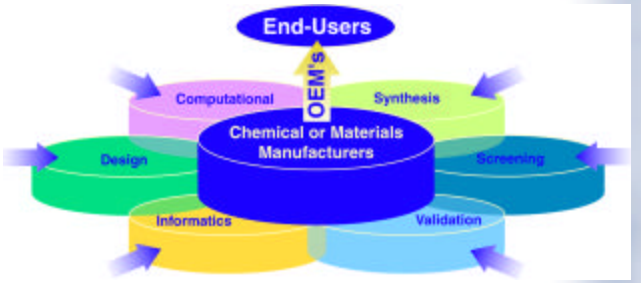
# ATP and Combinatorial Methods

ATP is funding the development of a *methodology*

- End-use application areas open
- Systems integration is a key risk factor




*Infrastructure focused on specific applications*





# Target Applications

| | |
|---|---|
| **Adhesives** | |
| **Catalysts** | |
| **Electronic Materials** | Polymers/Chemicals<br>Phosphors<br>Magnetic Materials<br>Ceramics<br>Semiconductors |
| **Polymers** | Membranes<br>Encapsulants/packaging |
| **Biomaterials** | Bio-sourced polymers<br>Bio-compatible materials<br>Bio-degradable polymers |
| **Optical materials** | Coatings<br>Photo-refractives<br>Opto-electronics<br>Non-Linear Optical materials |
| **Structural materials** | Metals and alloys<br>Composites<br>Ceramics/metal oxides |
| **Coatings** | |
| **Glasses** | Fibers<br>Electronic<br>Magnetic<br>Optical |
| **Smart Materials** | Fluids<br>Solids |
| **Advanced Ceramics** | Specialty<br>Optical & Electronic<br>Super-conducting<br>Structural |

*Profit Margin, Cost/Benefit Define Combi Entry*

# *Opportunities and Issues*

**Polymers: $38B industry with $1.5B in R&D**

- *Engineering, commodity, blends and alloys, bio-compatibles*
- *Sensors for mechanical properties and bio-compatibilty*

? *Scalability: bulk- and processing-dependent properties*

**Electronic/Photonic Materials: $HUGE**

- *Phosphors, display materials, dielectrics, semi-conductors*
- *Lowered energy consumption, environmental impact*

? *Sample purity, spectral analyses, substrate interactions (scalability)*

**Catalysts: $10B catalyst industry, $12B R&D (incl. chemicals) feeding a $350B + chemicals industry**

- *Polymers, fine & specialty chemicals, commodity chemicals, fuel cells*
- *Cycle time to new products, lower cost/higher performance*

? *Scalability, reproducibility, high temp/pressure, kinetics*



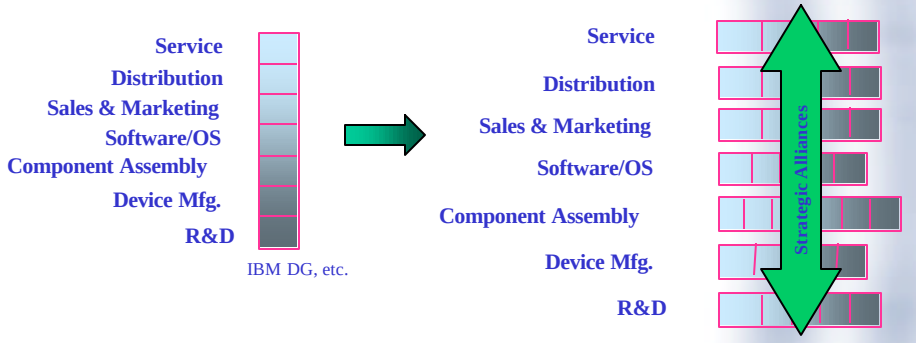


# *Enabling Technologies & Needs*

| | |
|---|---|
| **Design** | • Literature/Patent Data mining as input<br>• Statistics, modeling, design of experiments<br>• Diversity analysis/clustering analysis<br>• Computational: Molecular Modeling, QSAR, QSPR |
| **Fabrication** | • Chemical/Physical/Plasma Deposition<br>• Ink jet<br>• Thermally-driven transport (e-beam, LEED, laser, etc.)<br>• Laser ablation |
| **Characterization** | • Lab-on-chip, integrated and scalable designs<br>• Sample size --understanding interfacial properties, diffusion, mass transport at micro-scale<br>• Mechanical and physical properties<br>• on-line Error Identification and Validation |
| **Informatics** | • Data Mining, inter-connectivity, parallelism, registration, … |

*Systems Integration is a Significant Challenge*

# "Horizontalization" of industry sectors




Computers & Electronics
<1980's

Computers & Electronics
>1980's





# "Horizontalization" of Industry


Chemicals & Materials
<1990's

Chemicals & Materials
>1990's

*The ATP Encourages Strategic Alliances*

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# Combi for Materials : Drivers

- **Reduced innovation cycle times <u>across organization</u>**
  - *Discovery*
  - *Process and product development*
  - *Customer service and manufacturing*
- **More efficient use of capital for R&D and manufacturing**
  - *Time-to-market and ROI of R&D $'s*
- **New products/new technologies = new markets**
- **Allows for "out-of-box" discovery**
  - *Broadens spectrum of materials in development*



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# *Why ATP?*

<u>Chemicals and materials sectors have unique drivers...</u>

- *Low investment in non-core technologies or businesses*
- *Long pay-back of R&D capital investment (R&D ROI)*
- *Difficult displacement of installed R&D or mfg. assets (ROA)*
- *Leverage of commodity/specialty materials profits (6-7%)*

<u>especially with respect to combinatorial methodologies</u>

- *Integration of new base technologies and systems*
- *Validation of technology and business model*
- *Significant technological hurdles in materials discovery and process/product development with current technology*

# The ATP Opportunity

- **Focus base technology innovation toward applications**
- **Bring leading-edge, generic technologies to more industries**
  - *Spur discontinuous innovation in industrial R&D*
  - *Help develop lower-cost hardware and software tools*
  - *Facilitate systems integration: Hardware and software*
- **Improve competitive stance in portfolio industries**
  - *Challenge threats to intellectual property*
  - *Reduced commercialization cycle times*
  - *Permit discovery with "out-of-box" ingredients*





# Combinatorial Methods

## Vision

Facilitate development of new research tools and methodologies within U.S. chemical and advanced materials industries that will significantly impact the breadth and speed of innovation.

# ATP Technology Cluster

## *Combinatorial Methods for Advanced Materials R&D*

## *Results of the FY 1999 Open Competition*

| | | |
|---|---|---|
| **Nonlinear Dynamics/UOP LLP** | **"Combinatorial Tools and Advanced Data Analysis Methods for Heterogeneous Catalysts"** | **$14,715K (ATP) + $15,186 (j/v) (5 yrs.)** |
| **GE/Avery-Dennison** | **"Combinatorial Methodology for Coatings Development"** | **$3,127K (ATP) + $3,200K (j/v) (3 yrs.)** |
| **Catalytica/Combi Chem/Exxon** | **"A Strategy for Reclaiming U.S. Leadership in High-Value Polymers (Polyolefins)"** | **$4,861K (ATP) + $6,049K (j/v) (3 yrs.)** |

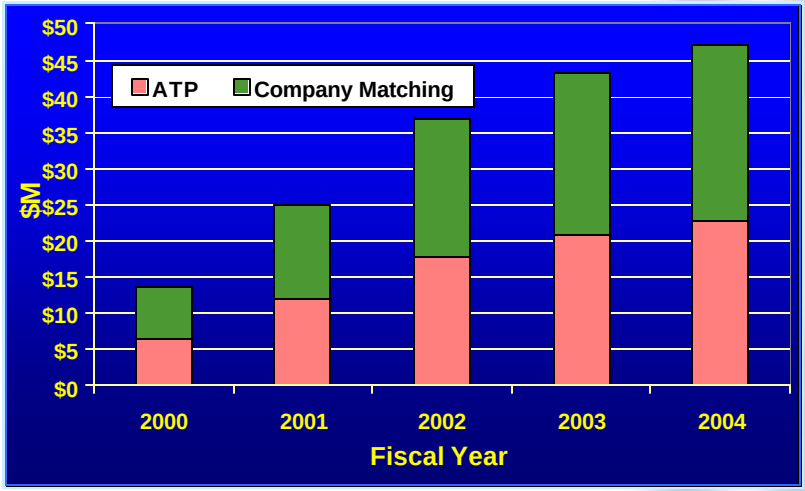
Find out more on: http://www.atp.nist.gov





# ATP Combi Methods Cluster

## Cumulative Project Expenditures, 1999 - 2004



# *ATP Combi Methods Cluster*

## *Technical Challenges and Outcomes*

| | |
|---|---|
| ➲Discovery | • Sample scalability; Structure-property prediction<br>• Systems integration<br>• Informatics |
| ➲Optimization | • Scalability of reaction<br>• Pressure-Temperature control |
| ➲Processing | Scalability of reactor designs |
| ➲Process Control | Information connectivity |





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# Technical Challenges



| Organic Molecules Discovery | vs. | Solid State Materials |
|---|---|---|
| • Discrete molecules of C, H, F, N, O, P | | • Extended structures of many elements potentially in metastable states |
| • Finite number of active sites, can be characterized and modeled computationally | | • Ill-defined distribution of active sites and structures |
| • Synthesis usually leads to substances of >85% purity; parallel purification techniques employed before characterization | | • "Pure" solids are meaningless especially with small samples having interfacial effects with the library substrate |
| • Structures reproducible (*a priori*) | | • Reproducible structures hard, if not impossible, to create *a priori* |
| • Chemical characterization, biological activity well developed for rapid or parallel, methods | | • Characterization of properties and composition not straightforward |
| • Descriptors for diversity | | • No ideas exist about how to do it |
| • Registration of library samples straightforward | | • No ideas exist about how to do it |
| • Synthetic building blocks available | | • A few building blocks available |



# Plan Forward—FY '00



## Challenges for High Throughput Catalyst RD&E

### *Informatics*

**Design of the Library**
- ✓ *Computational/Modeling: QSPR*
- ✓ *Statistics and control of error*
- ✓ *Design of Experiments*

**Informatics**
- ✓ *Increasing Information/Bandwidth*
- ✓ *Experimental complexity*
- ✓ *Data integration/analysis*
- ✓ *Hardware control*
- ✓ *Expert systems for data analysis*

### *Micro-Characterization*

**Screening**
- ✓ *MEMS: Lab-on-chip, Sensors*
- ✓ *Deposition/library fabrication*
- ✓ *Process control*
  - ▪ *Temperature/pressure*
- ✓ *Scalability Predictions*
  - ▪ *Interfacial properties*

**Synthesis and Processing**
- ✓ *Automation: $10^3$ -$10^4$ samples*
- ✓ *Reproducibility*
- ✓ *Validation*

# Issues--Informatics

- Assembly of a high-performance data mining toolbox that extends a database management system with additional operators;
- Acceleration of the design process from atomic level chemistry to engineering design by developing relationships:
  - Properties = f (chemistry, processing, microstructure…)
  - Processing: phase changes, high temp. & pressure, etc.;
- Integration of diverse databases to functionally specific data bases;
- Development of Quantitative Structure Property Relationships for materials (QSPR);
- Development of a query language linking different methods for querying the data with appropriate optimization methods.





# Micro-reactor Technology Characterization Issues

Miniaturization of reaction, processing, and testing apparatus
Integration of "reactor", sensor, logic on chip
Clear understanding of "scalability"
    Validation of micro- vs. bulk properties
    Structure-property prediction tied to library design and characterization
Deposition of samples of known composition
    ink jet, PVD, CVD, etc…..

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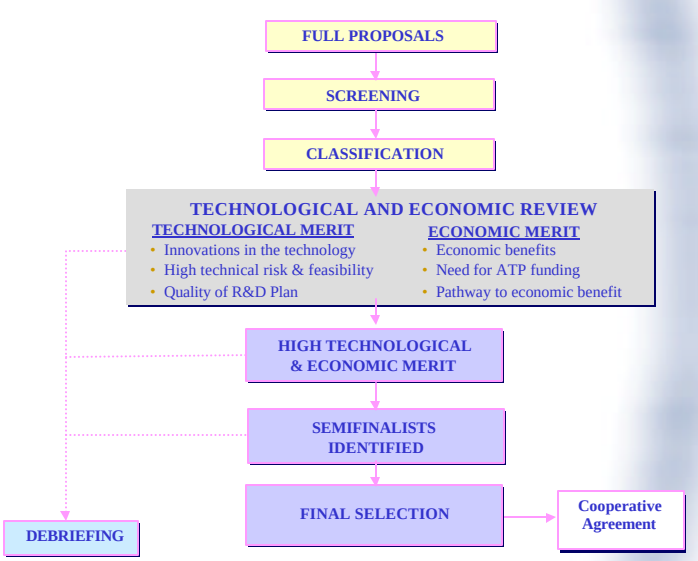
# FY '00 Open Competition

- Total of $50.7M in first year funding for FY 2000 for new awards. Proposal deadline is March 8, 2000 at 3:00 Eastern time.
  - The number of proposals funded depends on the quality of the proposals received and the amount of funding requested in the highest ranked proposals.
- **Proposers' Conference for potential proposers:**
  - Thursday, January 27, 2000, from 9:30 a.m. - 12:30 p.m. EST at the NIST Red Auditorium, 100 Bureau Drive, Gaithersburg
  - General information regarding the ATP;
    - Tips on preparing good proposals;
    - Opportunity for audience questions;
    - Attendance at this public meeting is not required;
    - No registration fee will be charged.

# Project Selection Process



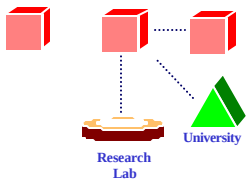





# ATP Eligibility

## SINGLE COMPANIES

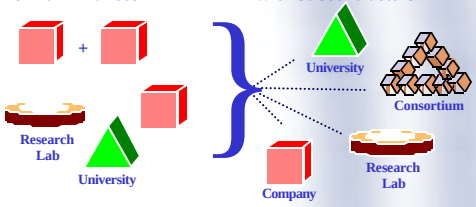
*Alone* *With Subcontractors*




- For-profit company
- 3-year time limit
- $2M award cap
- Company pays indirect costs
- Large companies cost share >60% of project cost

## JOINT VENTURES

*Formal Alliances* *With Subcontractors*




- At least 2 for-profit companies
- 5-year time limit
- No limit on award amount
- Industry share >50% total cost

- Intellectual property is owned by the for-profit companies
- ATP encourages teaming arrangements

# *Critical Elements of a Proposal*

- **Scientific and Technological Merit (50%)**
  - ✓ Innovations in the Technology
  - ✓ High Technical Risk & Feasibility
  - ✓ Quality of R&D Plan


ATP ranks proposals using six Selection Criteria

- **Broad-Based Economic Benefits (50%)**
  - ✓ Economic Benefits
  - ✓ Need for ATP Funding
  - ✓ Pathway to Economic Benefits





# *How to apply*

- Pre-proposals--Year-round submission
- Full Proposals—Annual Competition
  - *FY2000: due March 8, 2000 at 3:00 Eastern*
- Obtain and ***read*** the Preparation Kit
  - *Hardcopy or online or CD-ROM*
- Best Practice:
  *Multi-functional team assembles Proposal*
- Commercialization **and** Technical Plans are evaluated by our experts for feasibility

***Most Common Error is Lack of Detail in Proposal***

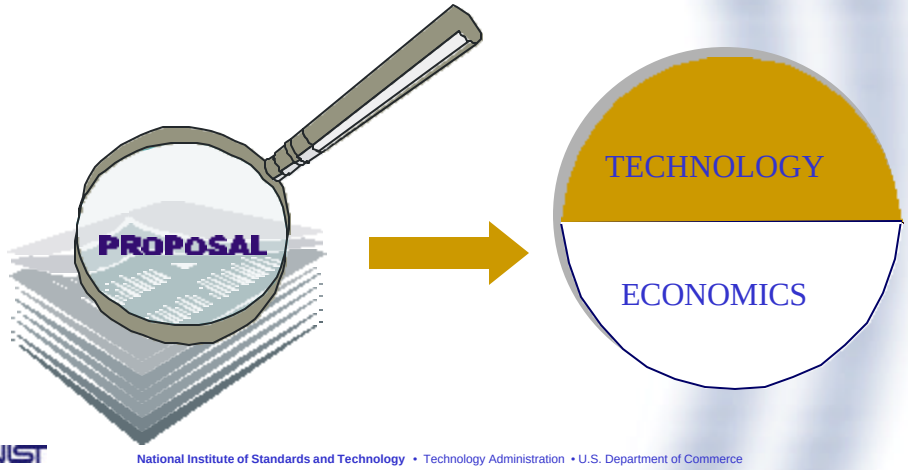
# *Intellectual Property*

- Companies incorporated in the U.S. keep intellectual property rights
- Universities and non-profit research organizations may receive share of return from royalties but cannot own title to intellectual property
- Companies can license
- Government reserves the right to royalty-free non-exclusive license for government use
  - Non-disclosure (trade secrets protected)
  - Government rights rarely invoked





# *ATP has only the written proposal to evaluate against the criteria to determine semifinalists*



# *Innovation*

- R&D Goals or Technical Approach
  - Comparison to state of the art
  - Unique with respect to current practice
  - Quantifiable objectives
  - Key technical barriers
  - Key innovations
- Technical leverage
  - Impact on knowledge base
  - Impact on other areas and applications

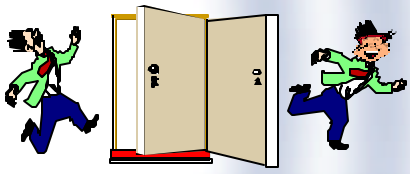


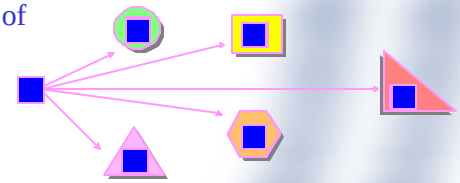


# *Economic Benefits*

## Relate Benefits to "Enabling" Nature of Technology

- **Pathbreaking** technologies - open up new possibilities
  - Revolutionary
  - Dramatic Improvements in
    - performance
    - cost
    - quality of life
- **Infrastructural** technologies - support R&D, production, and the business of entire industries
- **Multi-use** technologies - have many distinct applications





# Common Weaknesses

- Lack of sufficient detail for peer review
  - How you will reach technical objectives
  - What's innovative about the approach
  - Why a risky technical approach is needed
- Unsupported assertions that project meets ATP's criteria
- Misses ATP's niche
  - Low risk - product development, good engineering practice
  - Lacks demonstrated feasibility - Basic research





# Tips- Commercialization Plan

✓***What difference will ATP make?***
✓***Need for ATP Funding. Document your search for funding.***
✓Begin planning for commercialization at the outset
✓Understand that a fantastic technology may capture the imagination but not necessarily the market
✓Involve the marketing/product development/production people from the beginning.
✓Explain how the technology will impact the economy
✓Be specific, quantitative, and qualitative

# *Some helpful hints …*

- Proposals due at **3:00 p.m. (Eastern)** on March 8, 2000

  -- ***no fax or electronic transmittal***

- Late proposals rejected. ***NO EXCEPTIONS!***

- Overnight mail companies sometimes fail to deliver overnight

- Send your proposal in early

- **Read the Kit**

**What difference will ATP make -- is it really needed?**





# *Contact Information*

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

## To Get on the ATP Mailing List:

| | |
|---|---|
| Call toll-free: | 800-ATP-FUND<br>(800-287-3863) |
| Fax your name and address to: | (301) 926-9524 |
| Send an e-mail message to: | atp@nist.gov |