

Enhancing Innovation and Competitiveness Through Investments in Fundamental Research

Arlington, Virginia
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Challenges for Chemists

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NRC COMMITTEE ON BENCHMARKING THE RESEARCH COMPETITIVENESS OF THE U.S. IN CHEMISTRY

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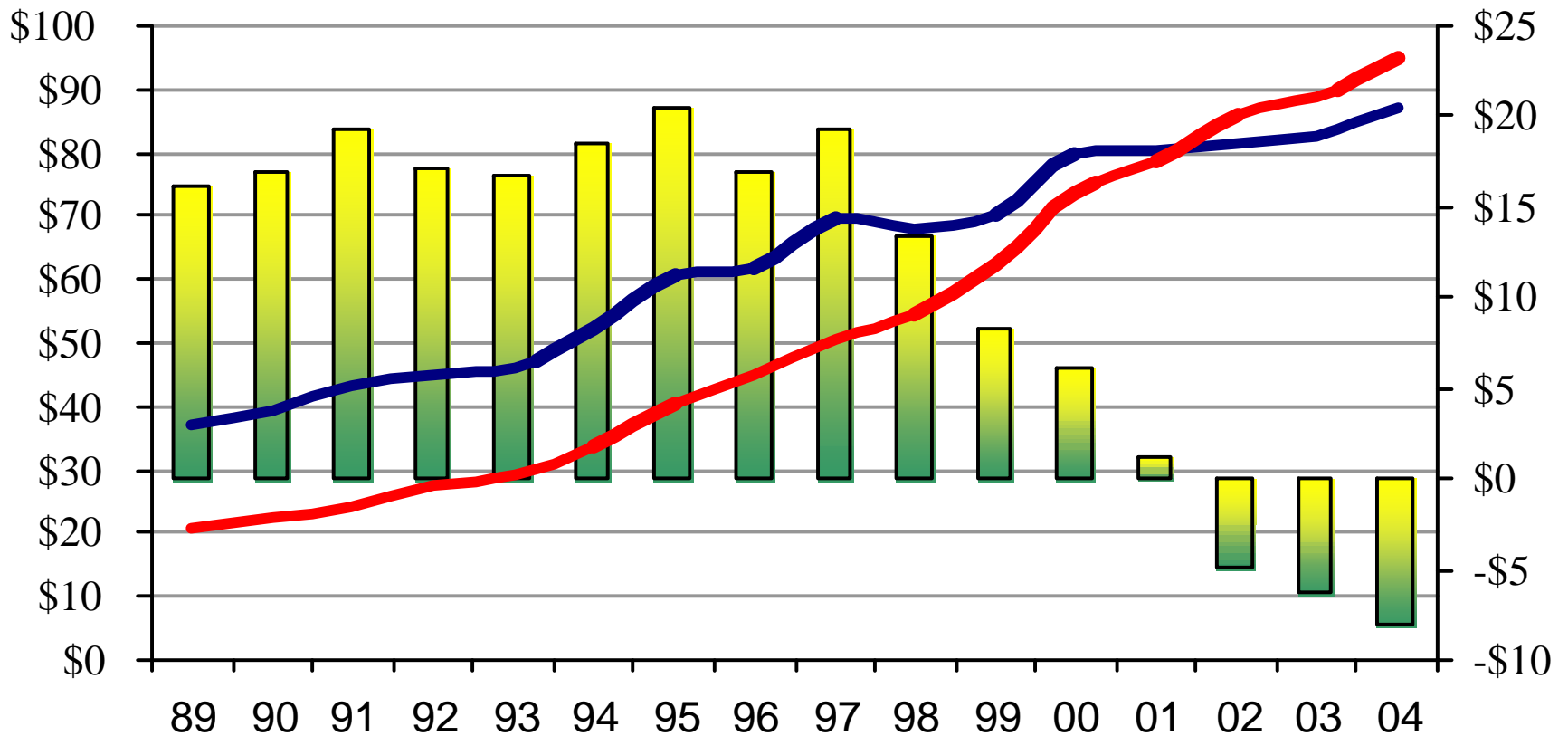
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Chemical Production Migration

Chemistry Trade Balance

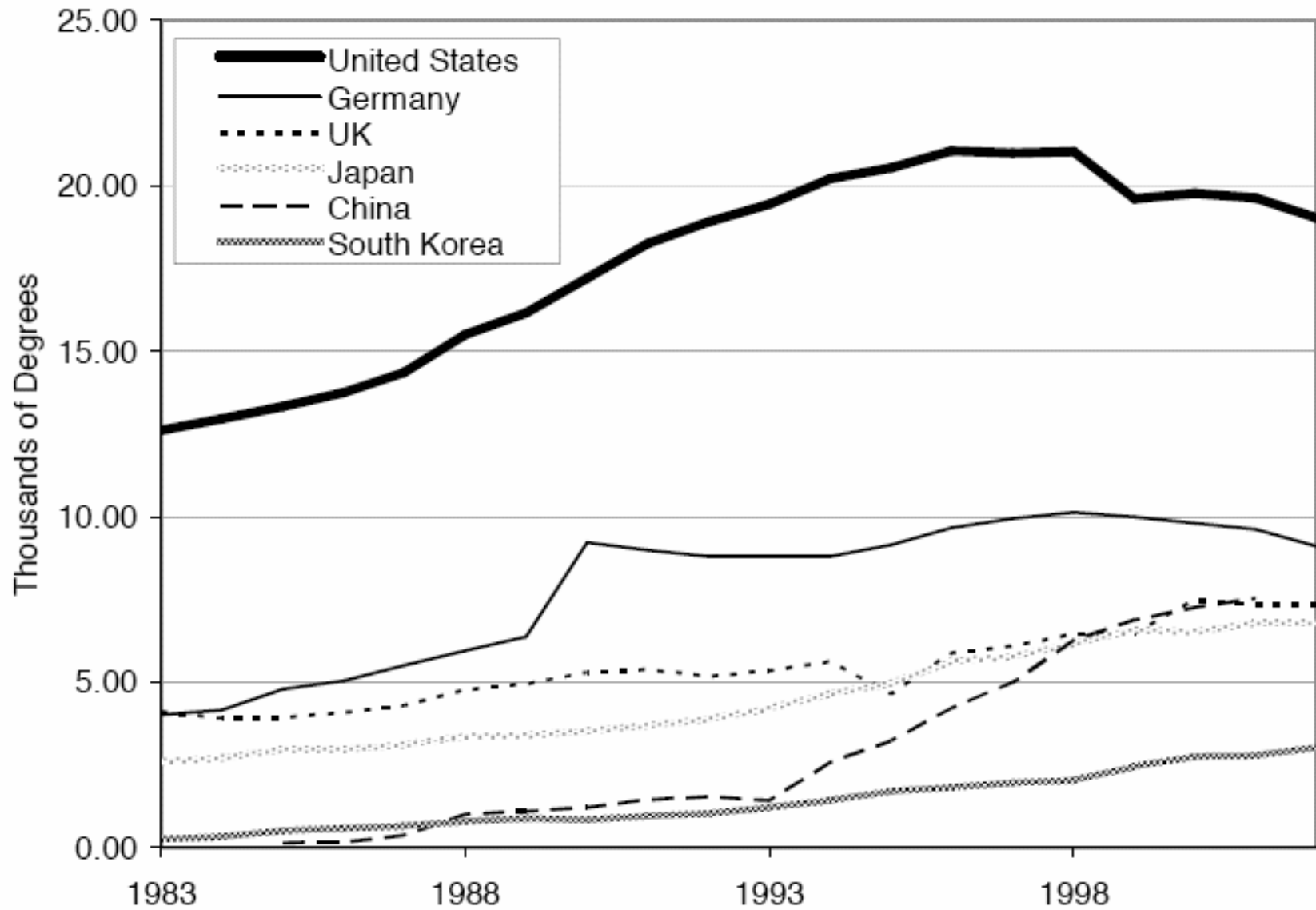


Trade Balance (right axis)

Exports (left axis)

Imports (left axis)

Natural Science & Engineering Doctoral Degrees



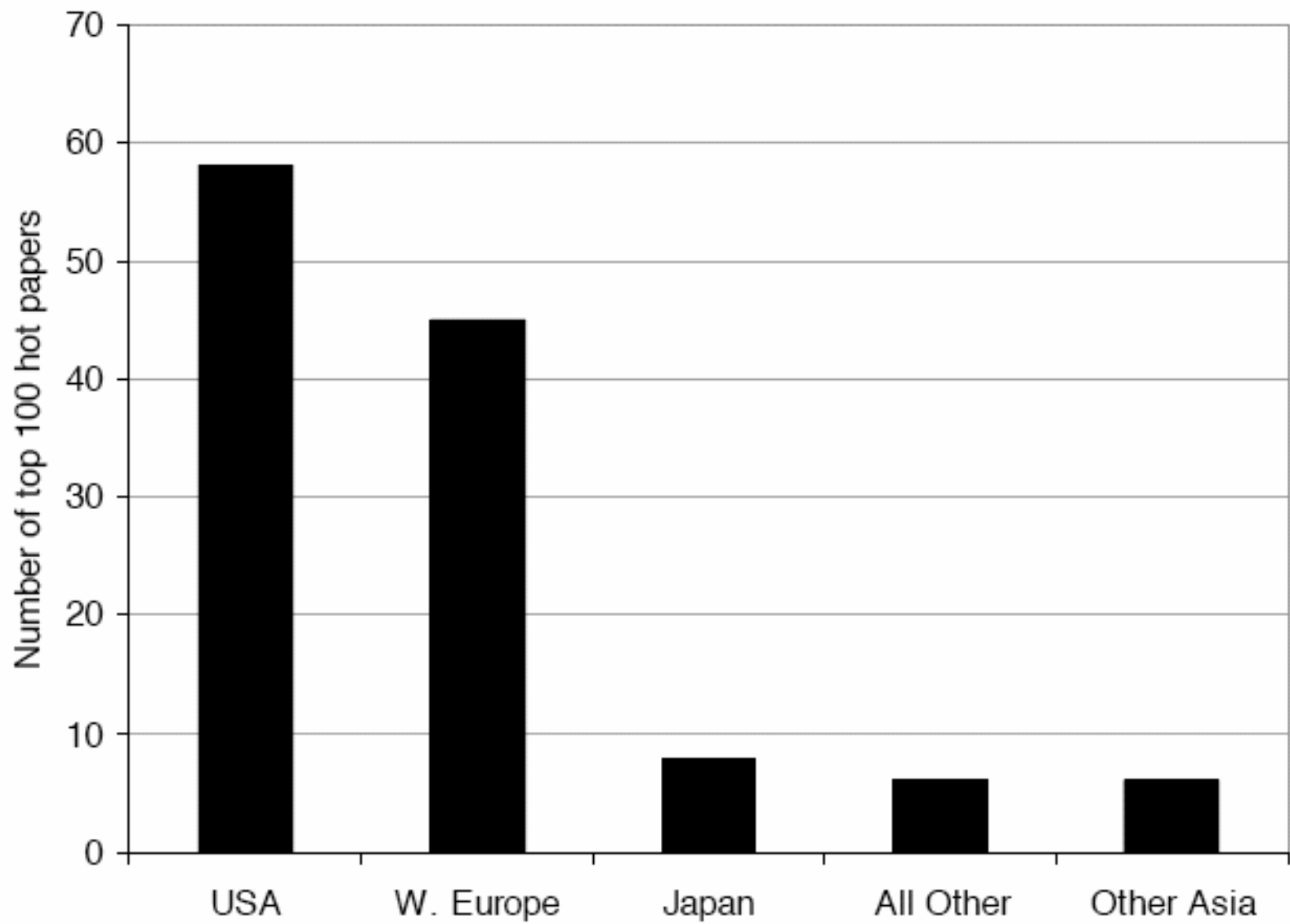
COMMITTEE ON BENCHMARKING THE RESEARCH COMPETITIVENESS OF THE U.S. IN CHEMISTRY

- What is the current position of U.S. chemical research relative to that of other regions or countries?
- What key factors influence US performance in chemistry?
- On the basis of current trends in the United States and abroad, what will be the relative U.S. position in the near term and in the longer term?

COMMITTEE ON BENCHMARKING THE RESEARCH COMPETITIVENESS OF THE U.S. IN CHEMISTRY

- What is the current position of U.S. chemical research relative to that of other regions or countries?
 - Publications **19% of All Chemistry Papers**
 - Citations **28% of Chemistry Citations**
 - Citations per paper
 - Most Highly Cited Papers and Authors
 - Virtual Congresses
 - Awards

Top 100 Hot Papers in Chemistry from 2004-06



ISI Data

Publications in American Chemical Society (ACS) Journals

Dramatic Increase in Papers from Other Countries

1988 36% non-US Papers

2001 57% non-US Papers

2005 62% non-US Papers

COMMITTEE ON BENCHMARKING THE RESEARCH COMPETITIVENESS OF THE U.S. IN CHEMISTRY

- What key factors influence US performance in chemistry?
 - U.S. Scientific Culture **Early Independence, Mobility**
 - Centers and Infrastructure
 - Graduate Students **Quality and Sources**
 - Research Funding

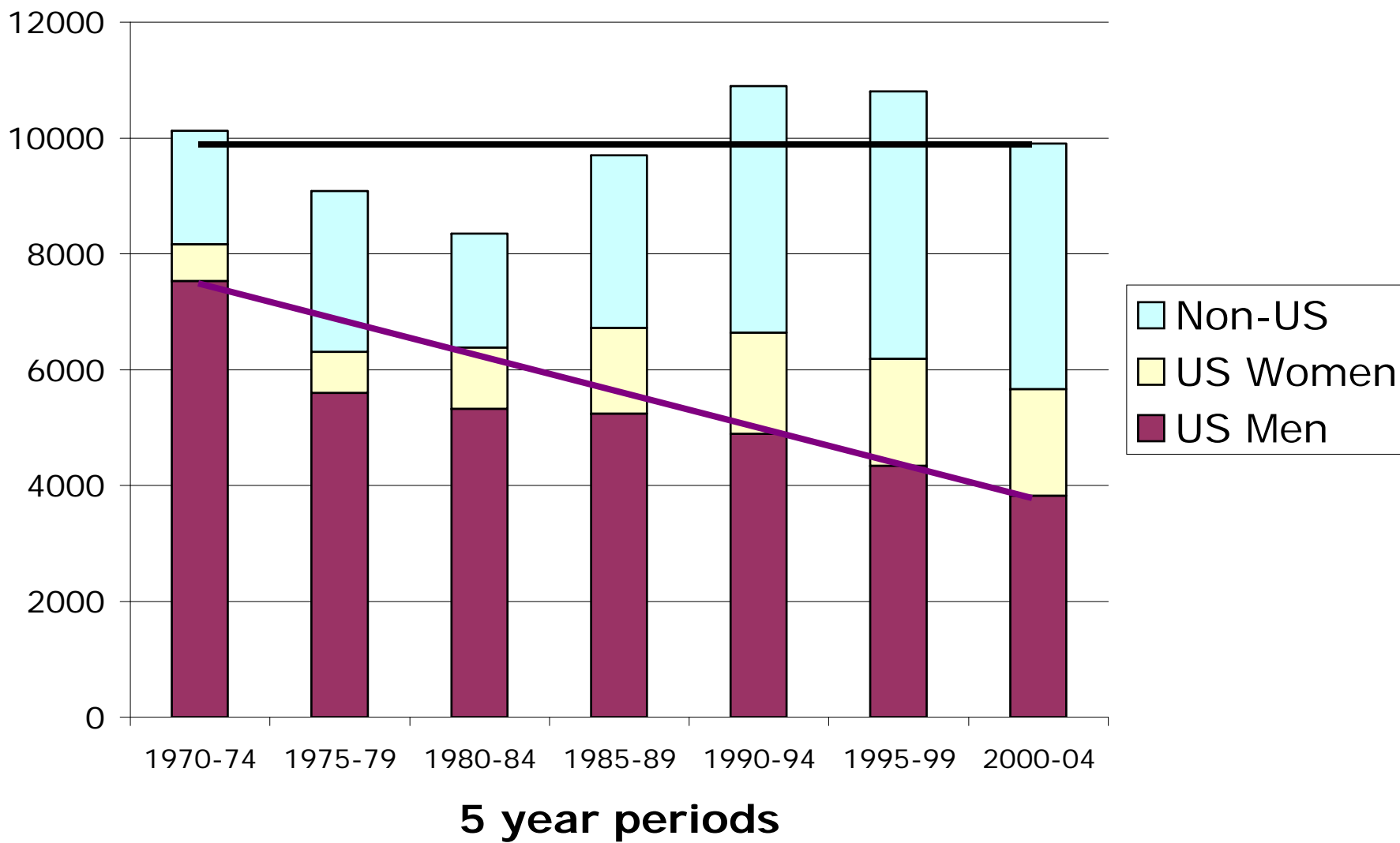
U. S. Scientific Culture

Physicist Serge Feneuille,
Chair of France's new
High Council for Science and Technology:

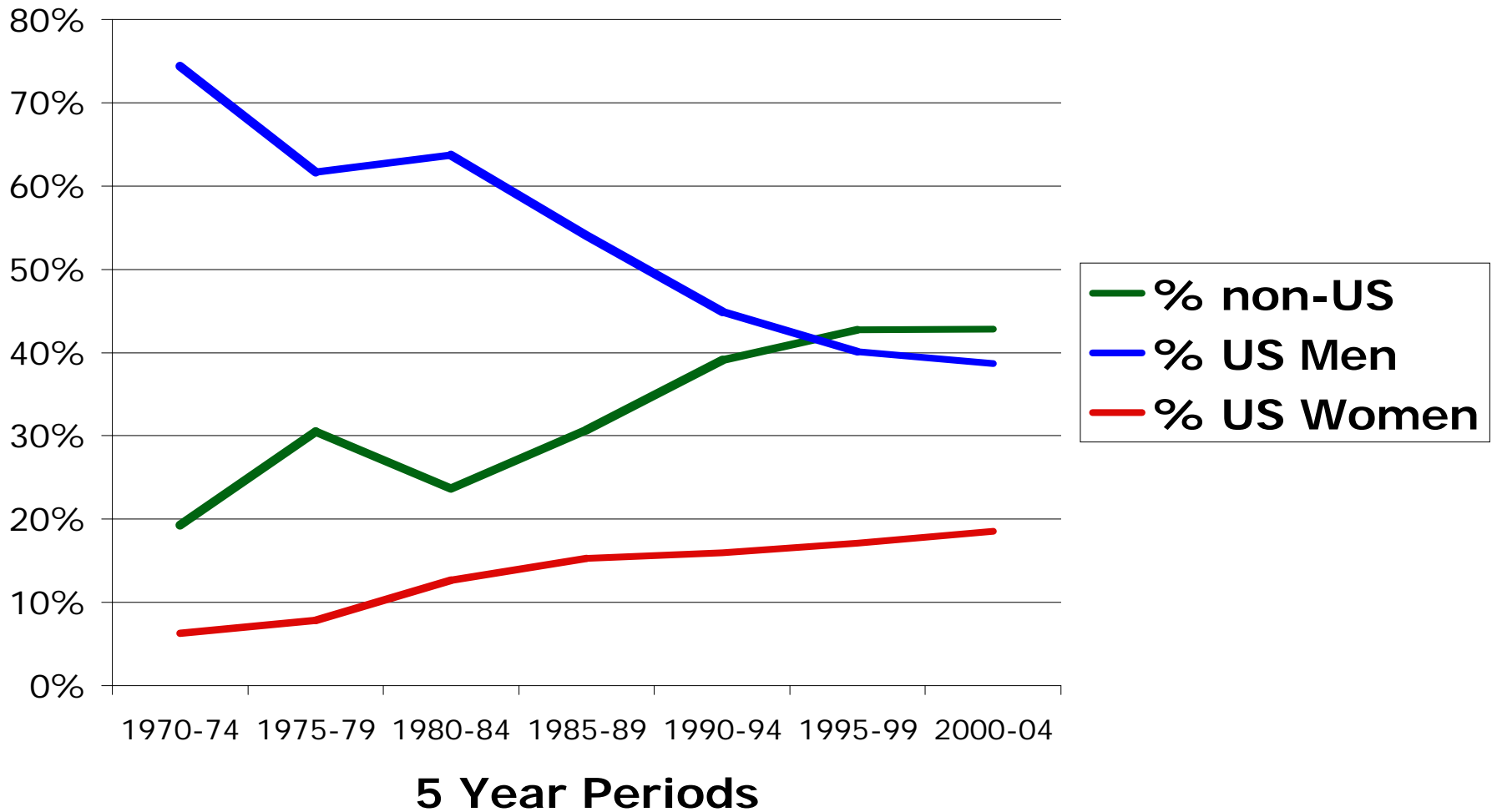
“The American system of research funding has led to autonomy for research groups, competition, and dynamism, three things that we don't have enough of in France.”

Science, November 2006

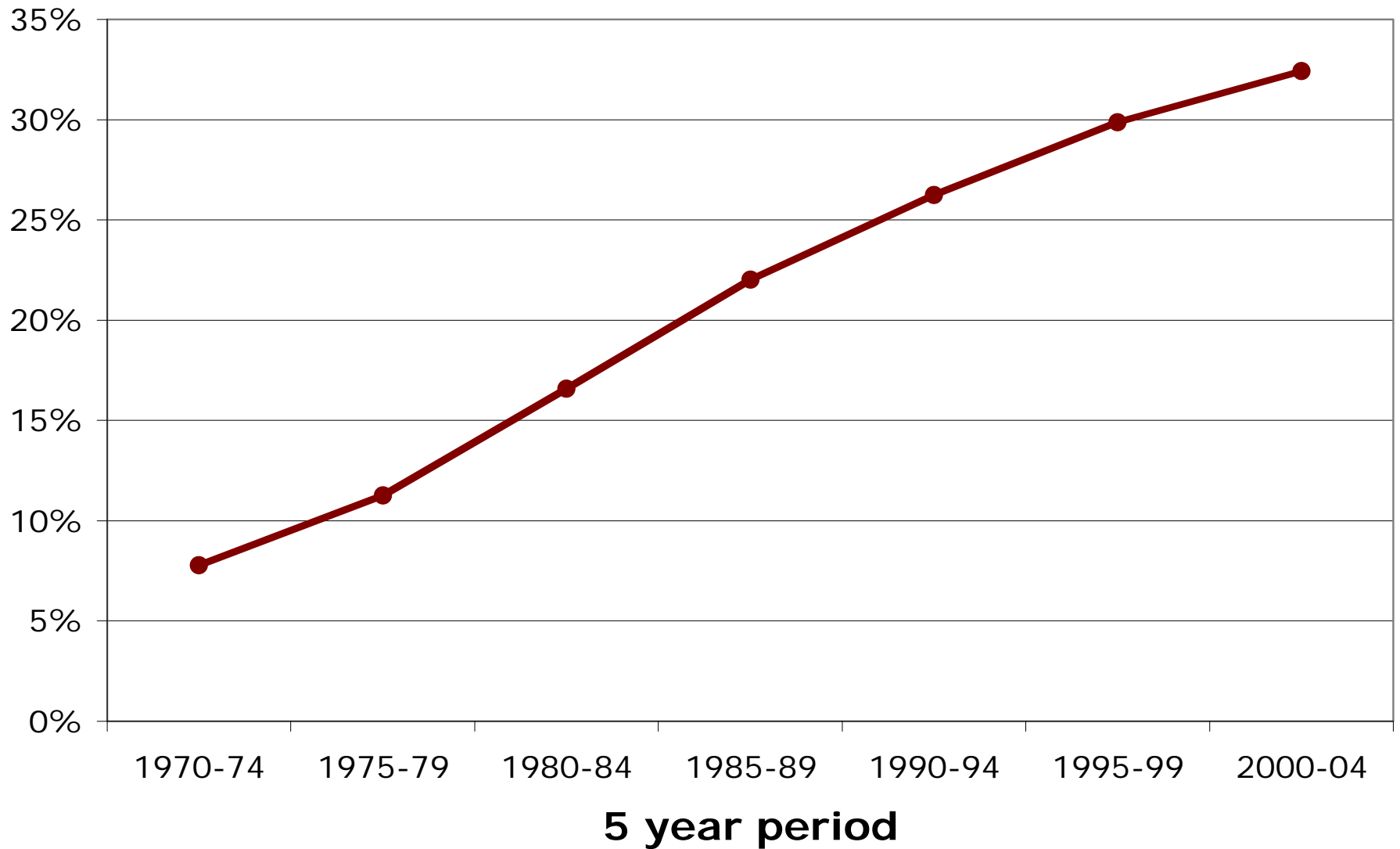
Chemistry PhD Demographics



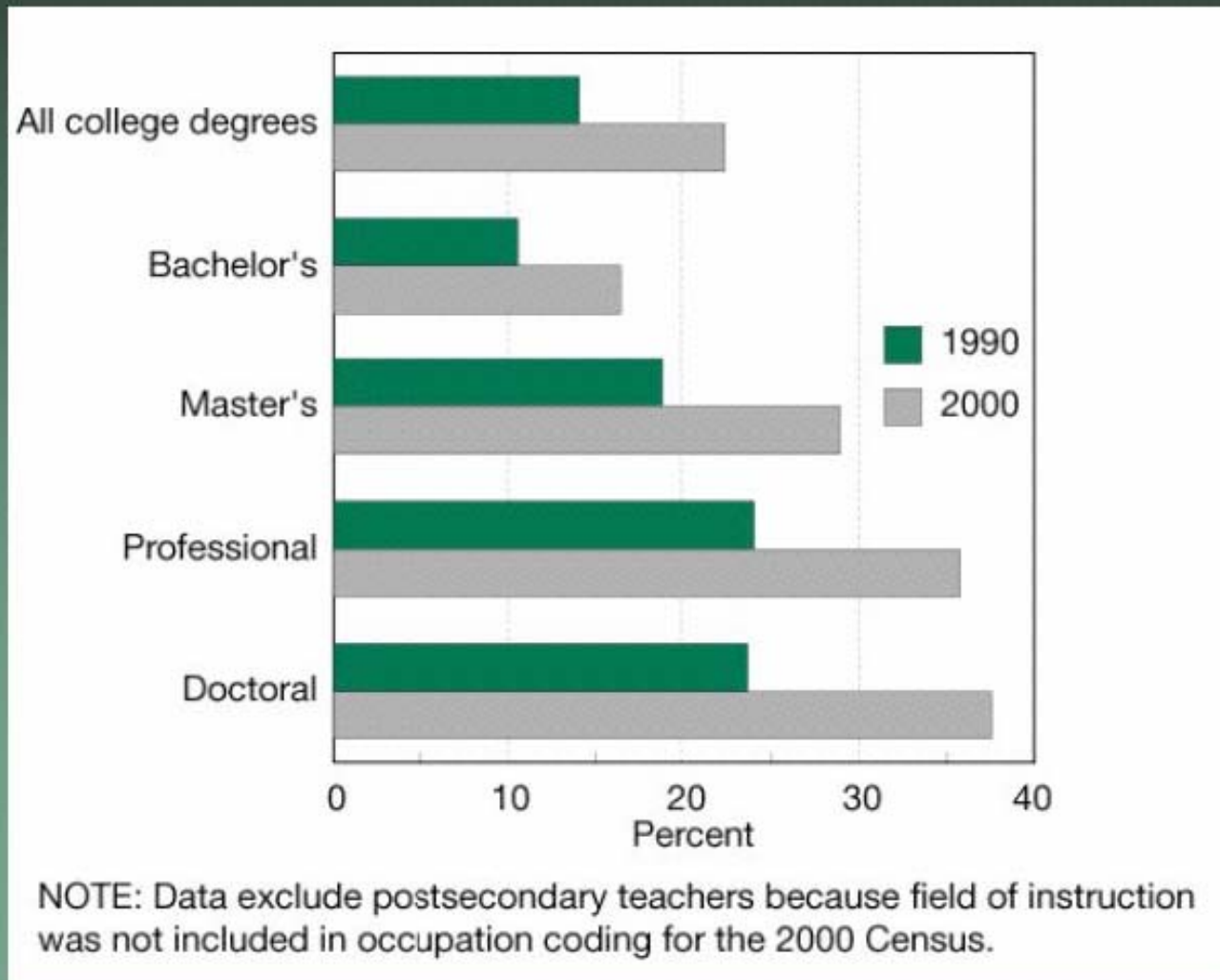
Increasing % of US Women and non-US PhD Chemists



Growing % of US PhD Chemists are Women



Foreign-born scientists and engineers in U.S. S&E occupations, by degree level: 1990 and 2000



SOURCE: National Science Board, *Science and Engineering Indicators-2004*



Too Few US Students Study Science and Engineering

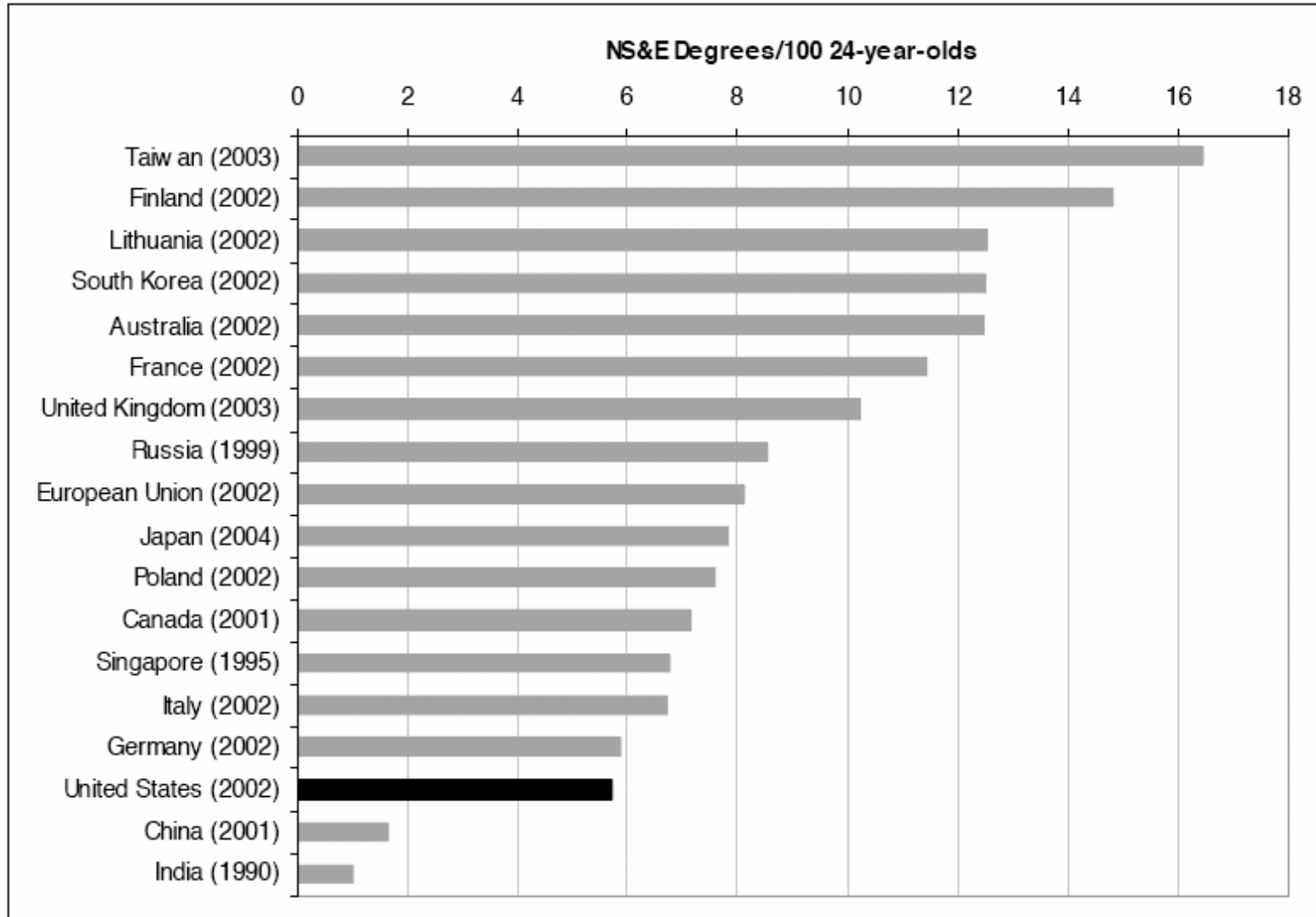


Figure 4.3 Natural science & engineering degrees (NS&E) per 100 24-year olds by country/economy.

Recruiting and Educating New Chemists

- Challenge students to find solutions to Chemistry's problems
- New chemists are **needed** to solve our problems
 - Environment
 - Energy
 - Materials
 - Catalysis
 - Drug Discovery and Synthesis
 - Nanoscience
- If we present these **needs and challenges** to the best and brightest students, we can attract them into the chemical sciences to meet critical human needs

What characteristics do we want our graduates to have?

- Expertise in a domain
- Breadth of scientific knowledge
- Ability to solve problems
- Find and define new problems
- Teamwork skills
- Oral, visual, and written communication skills
- Confidence and independence
- Creativity
- Expert learner

Expert Learners

- Learn important things in their field
- Learn to connect to other fields
- Challenge of continually being a beginner working along with experts in other areas
- Tenacity, courage, humility needed to work at the low end of the learning curve over and over again

Angelica Stacey “Training Future Leaders”

Can Creativity be Taught?

Choosing research areas and
designing research projects
is the most challenging task we face

How do we acquire skill in this area?

- Seminars, papers, making cross-connections
- Attitude of looking for new ideas everywhere
- Opportunities for writing proposals
and receiving feedback

Can Creativity be Taught?

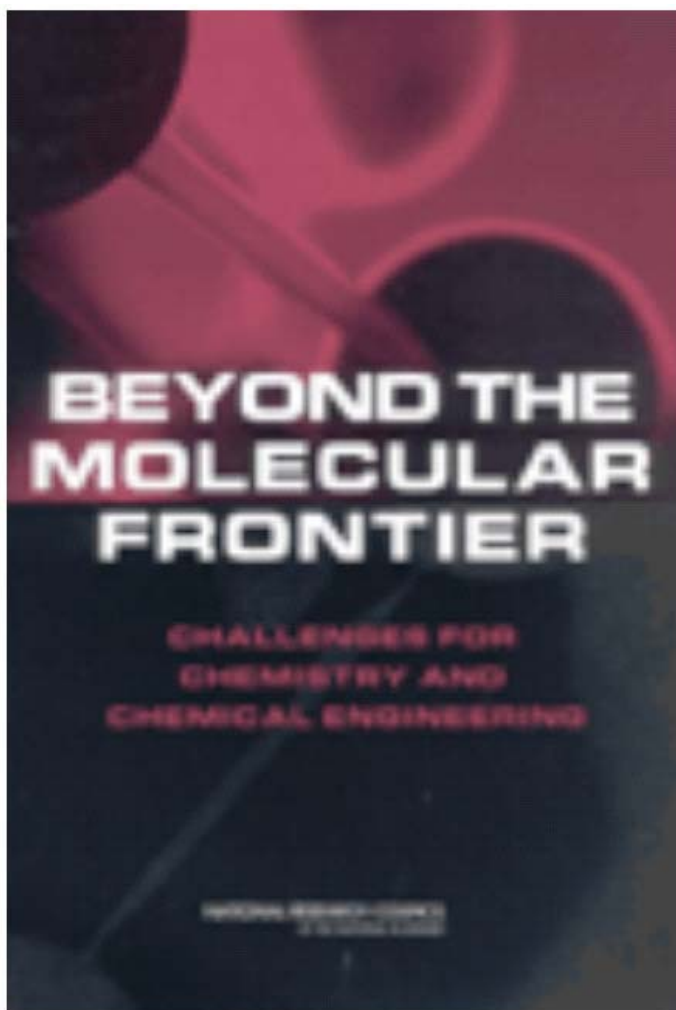
Original Proposal is a Requirement in Most Chemistry PhD Programs

– Demonstrates to the student that they can do it

– Standards for **significance** of problem are crucial
Faculty need to point out particularly creative work in seminars and courses
More open discussion of the crucial problems facing the chemical sciences



“Beyond the Molecular Frontier Challenges for Chemistry and Chemical Engineering”



National Research Council Report

of Committee Chaired by

Ronald Breslow

and

Matthew V. Tirrell

Five Major Societal Problems
That Will Require
Advances in Basic Chemistry

Five Advances in Basic Chemistry
That Will Enable New Opportunities

Five Major Societal Problems That Will Require Advances in Basic Chemistry

- Conquer Disease
 - Anti-viral drugs, Alzheimer's, malaria, tuberculosis
- Solve our Energy Problems
 - Sustainable Energy Sources: Solar, nuclear energy
 - Fuel Cells for Transportation (H_2 , CH_4 and CH_3OH)
- Clean the Environment
 - Materials from Renewable or Recycled Resources
 - Environmentally Benign Pesticides and Fertilizers
- Deter Terrorism
 - Sensors to Detect Biological and Chemical Warfare Agents
- Your Problem here

Five Advances in Basic Chemistry That Will Enable New Opportunities

- Catalysts for Direct Oxidation of Hydrocarbons by Molecular Oxygen for materials and power
- Computations accurate and powerful enough to predict non-covalent interactions
 - Protein folding, protein-protein interactions
- Nanoscience and Molecular Self Assembly
 - Multiproperty Nanoscale Materials
 - Molecular organization in complex systems
- Understanding electron transport
 - Photovoltaics and Fuel Cells
- **Your Advance Here**

Molecular Basis of Life Processes

NSF Workshop - 2004

- What are the essential molecular features of life?
- How do life processes emerge from networks of interacting chemical reactions?
- Can we view and direct molecular choreography in living systems?
- Can we find ways to bridge living and non-living systems?
- What are the molecular mechanisms responsible for development?
- What is the molecular basis of memory and learning?

Challenges in Homogeneous Catalysis and Organometallic Chemistry

2006 DOE Catalysis Meeting

New kinds of Catalysts

- Cheap first row metals - **Fe**
- Don't be afraid of paramagnetic systems - **Cr and Co**
- Invest in high throughput synthesis and screening
- New ligands
 - ***N*-heterocyclic carbenes**
 - **Resurgence of nitrogen ligands: amido and imido**
 - **Control of Regioselectivity and Enantioselectivity**

Challenges in Homogeneous Catalysis and Organometallic Chemistry

2006 DOE Catalysis Meeting

Chemicals from Coal: Renewed Interest in CO Chemistry

- Acetic Acid and Acetic Anhydride
- CO and ethylene oxide
- Fischer-Tropsch chemistry revisited?

Chemicals from Biomass

- Carbohydrates as source of commodity chemicals

Challenges in Homogeneous Catalysis and Organometallic Chemistry

2006 DOE Catalysis Meeting

Fine Chemicals from Hydrocarbons

- C-H Bond Activation and **Functionalization**
- New oxidation chemistry using molecular O₂



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