IS THERE A NEED TO REINVENT CHEMISTRY ?

Dr. S. Sivaram,
National Chemical Laboratory,
Pune-411 008, INDIA

Tel : 0091 20 2590 2614
Fax : 0091 20 2590 2615
Email : s.sivaram@ncl.res.in
Visit us at : http://www.ncl-india.org

National Institute for Interdisciplinary Science and Technology, Thiruvananthapuram

February 10, 2011

INTERNATIONAL YEAR OF CHEMISTRY

International Year of CHEMISTRY 2011

- Celebrate the achievements of chemistry
- Improve public understanding of chemistry
- Champion the role of chemistry in addressing the critical challenges of our society
  - Food and nutrition
  - Clean water
  - Sustainable energy
  - Climate change
- Broader outreach and engagement
- Get younger people more interested in chemistry

Madam Curie, Nobel Prize in Chemistry , 1911

What is Chemistry?

It is about making forms of matter that never existed before eg. plastics, detergents, drugs, Insecticides etc.

Design & make

Analysis

Why and how reactions occur

Quality control
Environment
Health care
Crime detection

Chemistry has extraordinary impact on society

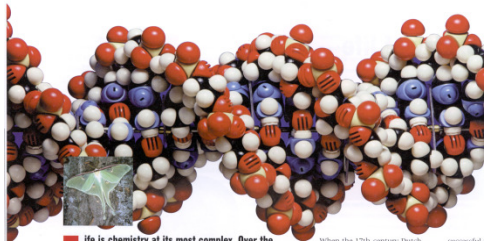
Good and bad !

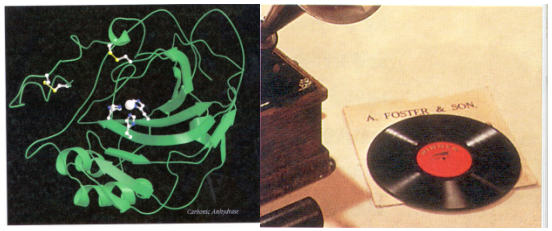
Chemistry is the central, useful and creative science - Ronald Breslow

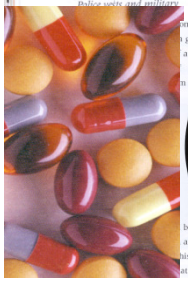
Central

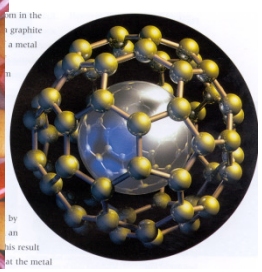
Underpins many other scientific disciplines

Biology, geology, material science



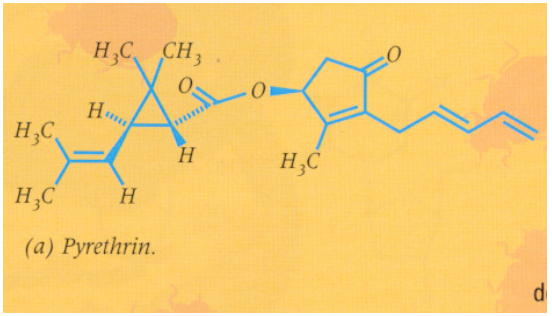


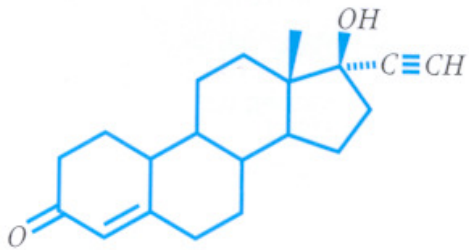




Creative

Designs structures with new and unique properties





Norethindrone (Norlutin)

Figure 14. Norlutin, the first contraceptive pil

Useful

Provides many materials essential to everyday life,

Knowledge to better human, veterinary and plant care, better food, environment

Chemistry creates its own object. This creative power, similar to that of arts distinguishes it fundamentally from the other natural and historical sciences

Bertholet, 1860

The ESSENCE of CHEMISTRY
is not just to discover
but to
CREATE

CHEMISTRY has the ability to

CREATE NOVEL EXPRESSIONS of MATTER

CHEMISTRY
is the ART of MATTER !

CHEMISTRY is the science of the structure and transformation of non living and living matter

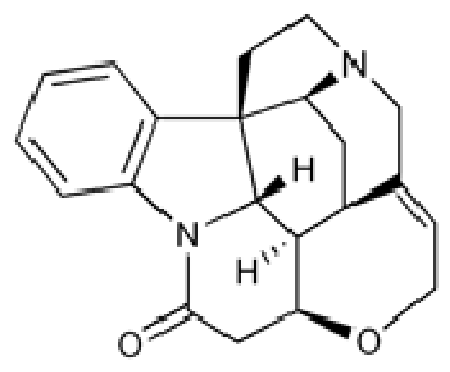
Jean Marie Lehn

CHEMISTRY VERSUS CHEMICALS

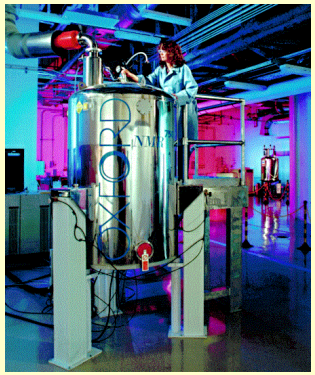
- **Chemistry in popular language has a positive connotation. It is used to describe the somewhat intangible forces that result in successful relationships between two or more individuals**

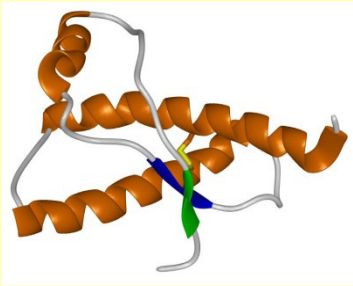

DOPAMIN, ENDORPHINS, OXYTOCIN, FENYL-ETHYLAMIN...
IF YOU BELIEVE THIS STUFF, LOVE IS NOTHING MORE THAN AN ORDINARY CHEMICAL PROCESS... HOW CYNICAL!
DON'T WORRY
I'LL PROVE THEM WRONG! IT ALSO SAYS THIS CHEMICAL PROCESS FADES OUT AFTER 2 OR 3 YEARS, RIGHT?
YES. SO?
I REST MY CASE
2006
©jeroen - www.kartoen.be
JEROEN

THE PAST 50 YEARS: GREAT SUCCESSES

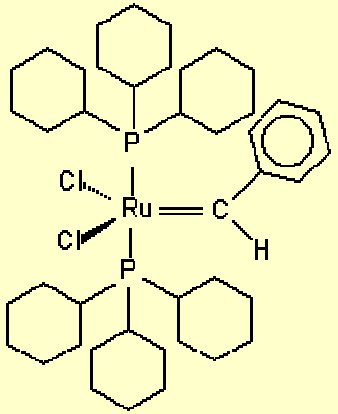


strychnine

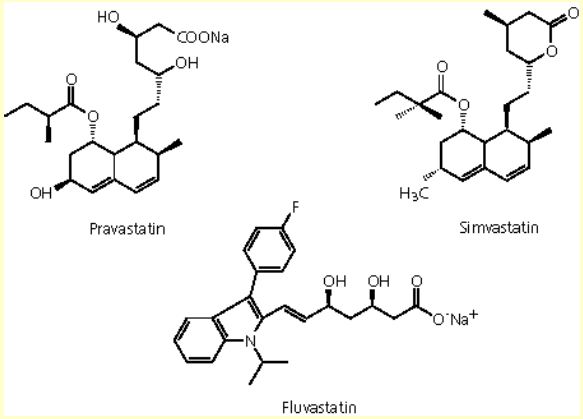




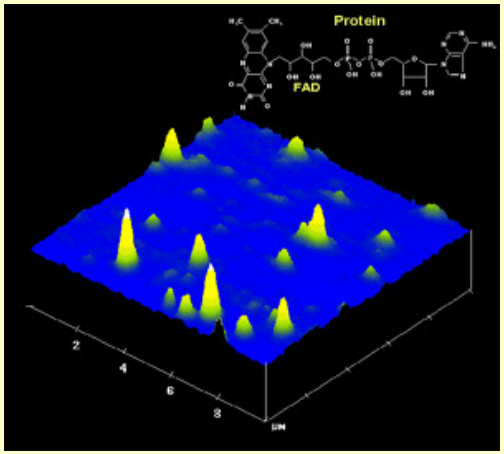
protein NMR



ROMP catalyst



statins



single-molecule spectroscopy

CH_y, NO_x ⟶ CO_2 + N_2

CHEMISTRY'S HOARY PAST

- **Aspirin, Indigo, ammonia, Antibiotics, Lipitor, Nylon, Teflon, Polyethylene, rayon, synthetic rubber, fuels**

- **Nylon stockings, Hula Hoop, Packaged Foods, Bullet Proof Vests**

Is Chemistry today capable of capturing the public imagination ?

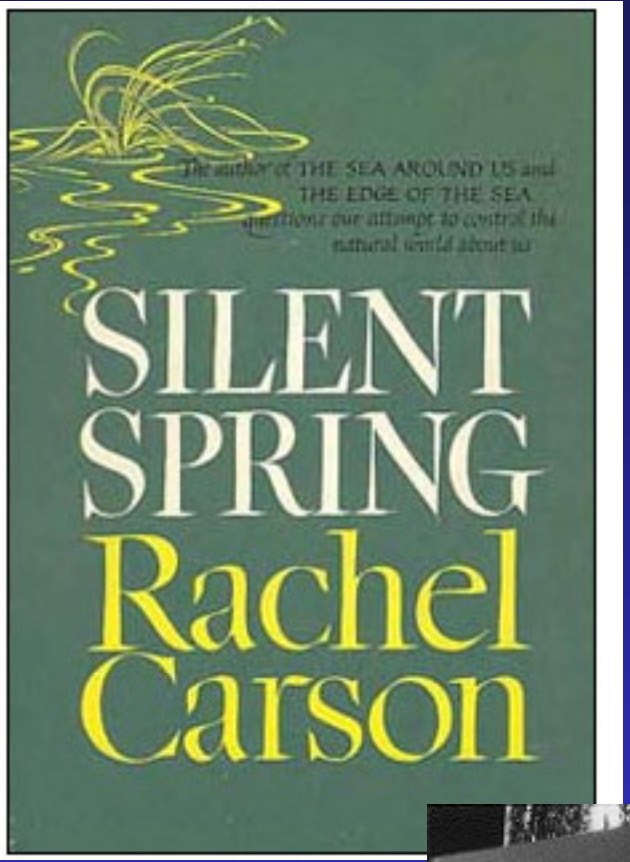
Can you recollect the last major impact making discovery in chemistry ?

C 60 and Graphene ?

Element carbon was once the monopoly of the chemist; it is no more !

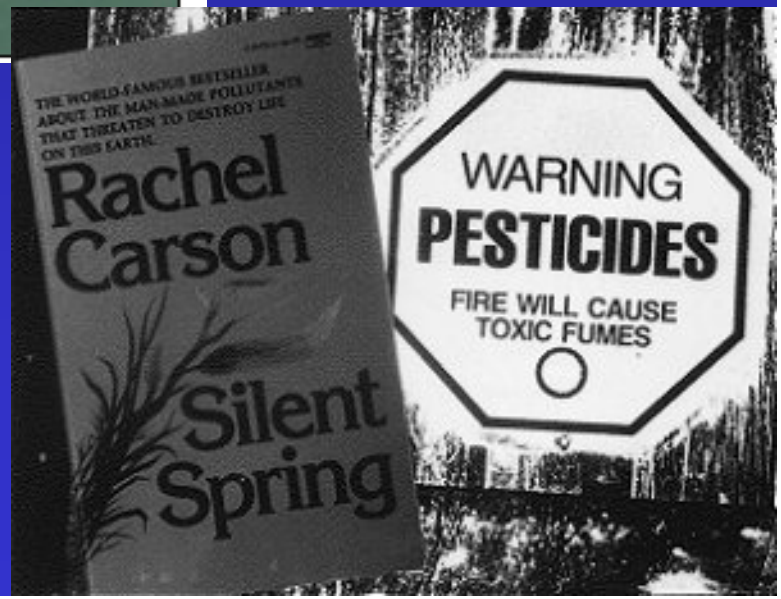
CHEMISTRY VERSUS CHEMICALS

- Chemicals, on the other hand, usually gets bad press. They leak, spill, leach, poison and pollute. They are used as weapons of mass destruction



Published 1964
Drew public attention to the indiscriminate use of chemical pesticides

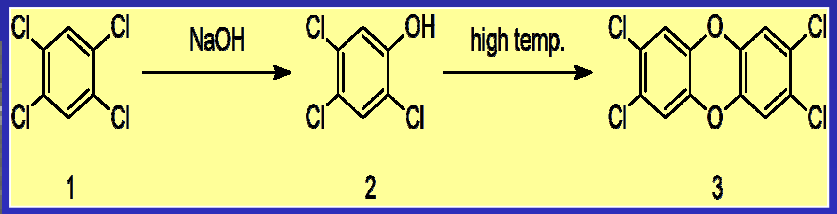
- ***Watershed event in the history of chemistry***
- ***Public perception of chemistry changed for ever***
- ***Industry first reacted with retribution and vindictiveness***
- ***However. wisdom prevailed and a period of deep introspection began***



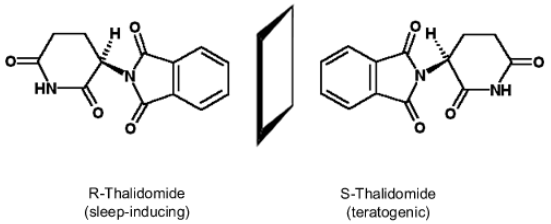
THE UGLY SIDE OF CHEMISTRY

A child victim of the Bhopal gas disaster.

- Minamata
- Love Canal
- Seveso
- Bhopal
- Thalidomide
- DDT



$$H_3C-Hg^{+}\ X^{-}$$



PUBLIC AND GOVERNMENT PERCEPTION OF CHEMISTRY

- **Chemistry is invisible to the public**
- **Chemistry is considered "mature" economically**
- **Chemistry is associated with pollution/global warming**
- **"Good" and "Bad" are not balanced in perceptions of chemistry**

Only the chemistry prize has preserved the traditional aura of obscurity. It goes to Gerhard Ertl for his studies on the role of surfaces in catalyzing chemical reactions. Since an awful lot of industrial chemistry is catalyzed and the chemical industry lies at the base of most manufacturing, there is good argument this is the most important prize. But glamorous? Sadly not .

The Economist , October 13, 2007

Bill Bryson, "A Short History of Nearly Everything", Random House, 2003 p. 137:

When the wife of the great Austrian physicist Wolfgang Pauli left him for a chemist, he was staggered with disbelief. "Had she taken a bullfighter I would have understood," he remarked in wonder to a friend. "But a *chemist*. . ."

Better Things for Better Living
(1985)

Better Things for Better Living through Chemistry
(1935)

Few Names with Chemistry !

American Chemical Society

National Chemical Laboratory

Feeble attempts to rejuvenate chemistry

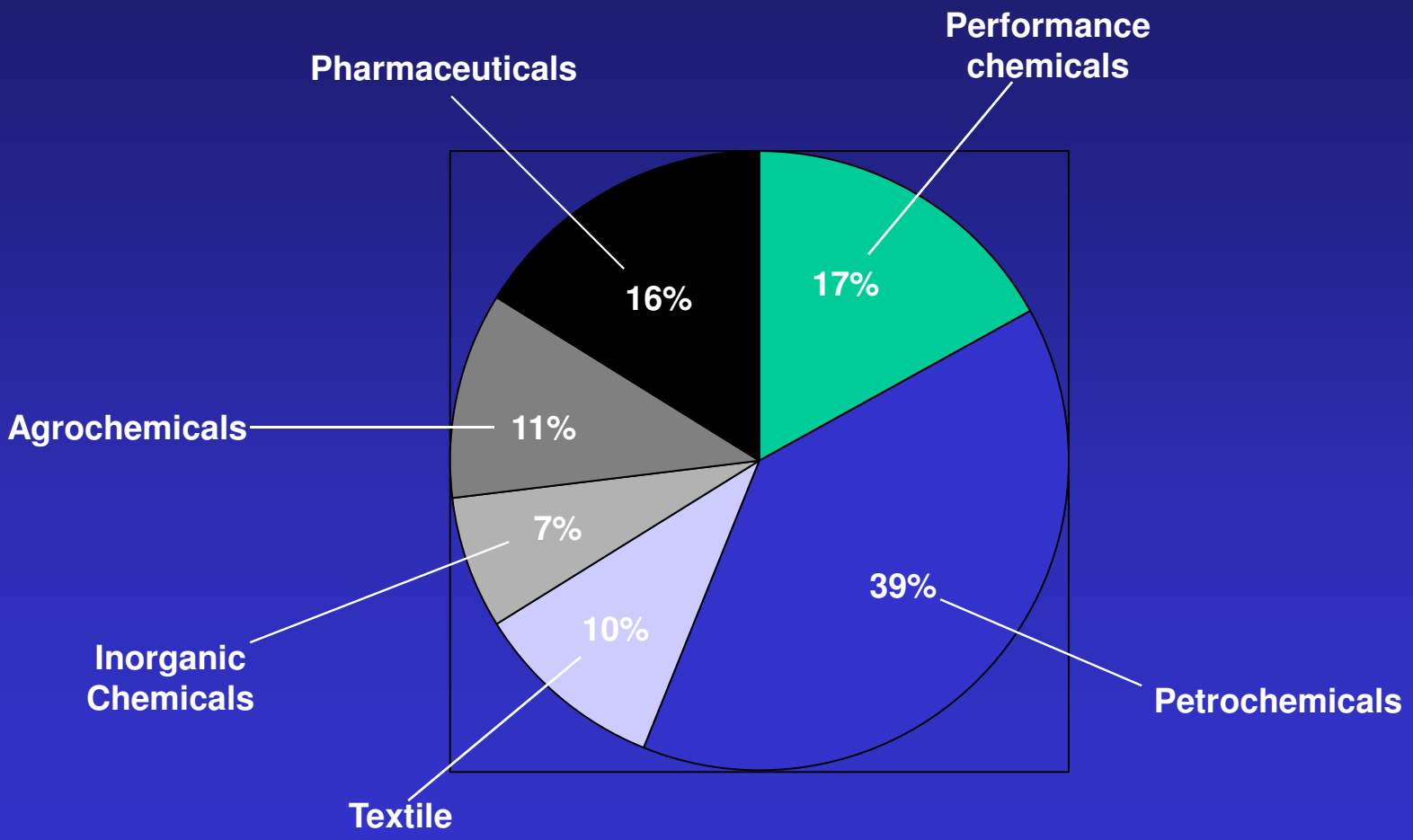
- Green Chemistry
- Combinatorial Chemistry

BASF
The Chemical Company

The only company that dares to call Itself a chemical company

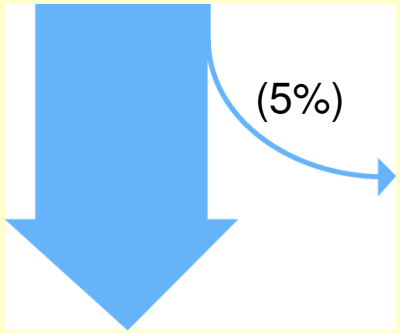
WORLD CHEMICALS MARKET

A THREE TRILLION $ INDUSTRY



THE CHEMICAL INDUSTRY

crude oil



fuel
(energy)

transportation,
heating

petrochemicals
(materials)

commodities

specialties

biological
sources

(synthesis)

pharma

The chemical industry no longer includes invention (innovation) in its business model.

I am absolutely certain that synergy between research, education and industry is one of the great aspects of modern chemical science and one of the best investments a society can make in future. Unfortunately this happy relationship is still not widely appreciated nor practiced

Elias J. Corey
Priestley Medal Address
Anaheim, CA, 2004

STRUCTURE OF CHEMISTRY

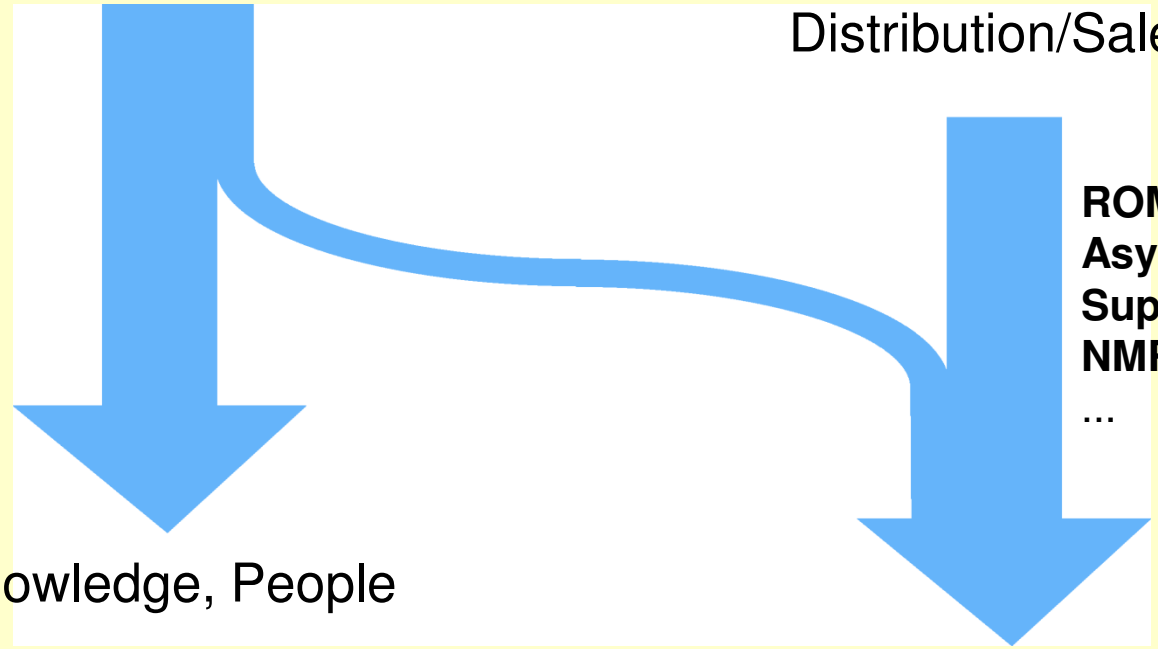
Money

University ← **Government** → Laws, Regulation

Industry

("Liebig" Model:
Professor/Student/Problem/Thesis)

(Development, Manufacturing,
Distribution/Sales)



Knowledge, People

Products/Solutions for Problems

CHEMISTRY AT CROSSROADS

- **Chemistry is at the end of one wave of development and struggling to begin another; perceptible shift in the centre of gravity of the discipline**
- **There are still many important opportunities in both fundamental and applied science**
- **Chemistry offers fewer puzzles to solve; What confronts are number of problems**
- **Longer term curiosity driven research is more important than in the past, but harder to justify**

In the future, functions will be more important than molecules. Molecules are no longer enough (they never really were)

IDENTITY CRISIS : DOES CHEMISTRY HAVE GRAND CHALLENGES ?

- **Biology : Understands life processes, cures for Cancer and Alzheimer, Human genome, synthetic biology, …..**

- **Physics / Astrophysics : Exploding stars, Black holes, quarks, energy, matter, Grand unified theory, Hubble telescope, Supercollider, Geo-engineering, computers, semiconductor chips, internet …….**

- **Chemistry : ?**

Some Answers : Nature 2 August 2006 , p 500 by Philip Ball

Chemistry has not lost its identity; it has instead gained important footholds within the domains of other sciences – albeit rarely at the initiative of chemists

D. Seebach

THE STRUCTURE OF SCIENTIFIC REVOLUTIONS

- **New experimental techniques enable new science (Dyson)**

eg : X Ray, NMR, PCR, STM

- **Scientific revolutions ensues when current theories are no longer able to explain experimental evidences (Kuhn)**

eg : Discovery of oxygen or quantum mechanics

TWO FORMS OF SCIENTIFIC EVOLUTION

Normal Science : Develops and existing or accepted idea
Discovery science: Fundamental changes in thought

PUZZLE AND PROBLEM

Puzzle :

"Though the outcome can be anticipated, often in detail so great that what remains to be know itself uninteresting, that the way to achieve that outcome remains very much in doubt"

Answer is not important; the elegance of solution is

Problem :

"The really pressing problems, e.g. a cure for cancer or creation of an inexhaustible source of clean energy, are often not puzzles at all, largely because they may not have any solution"

Answers are important; Strategy to arrive at a solution unknown

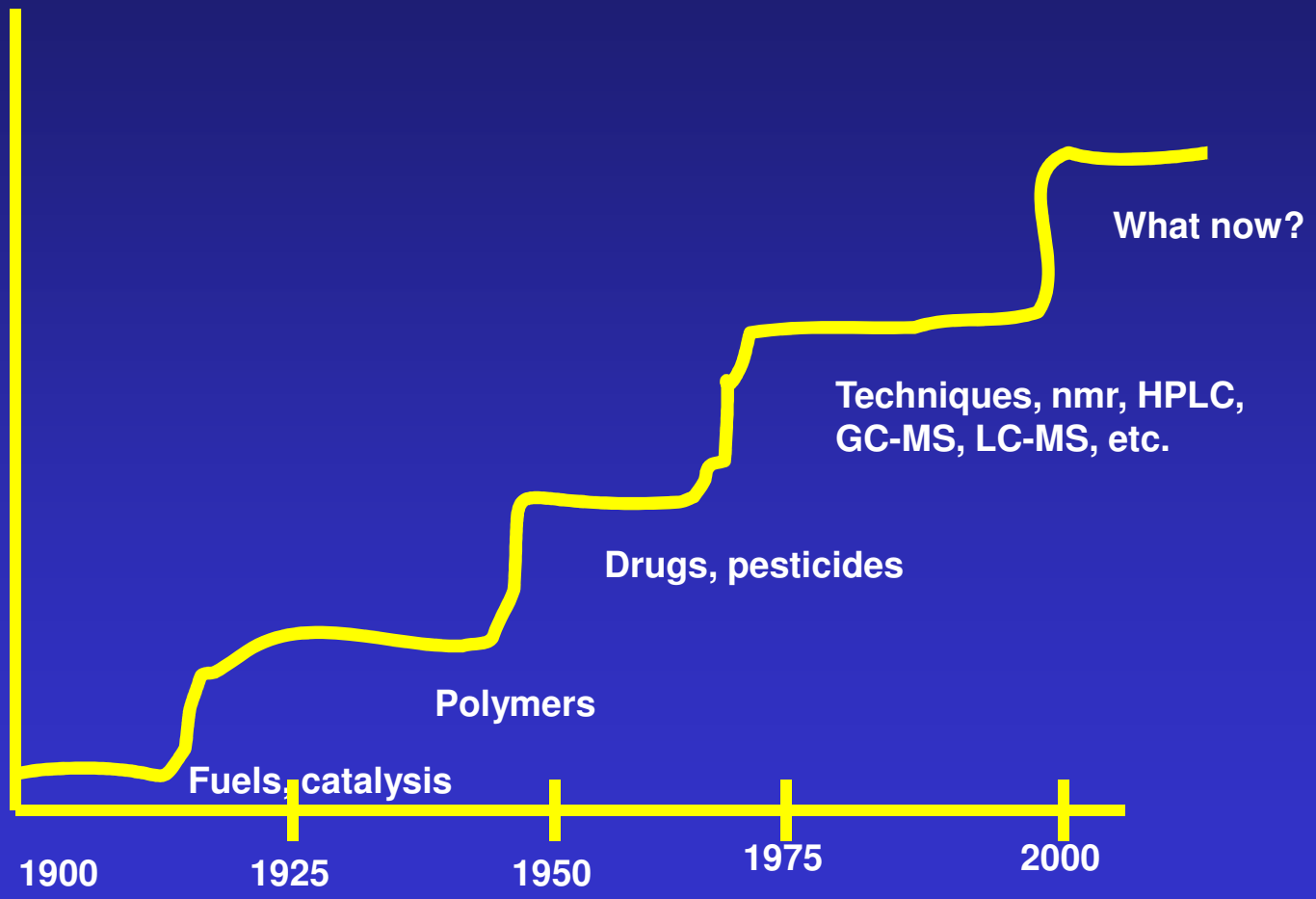
Thomas Kuhn
The Structure of Scientific Revolutions

CHEMISTRY : CENTRAL SCIENCE

- **Central to the sustenance of civilization on earth**
- **Key to management of resources on this planet**
- **Key to understanding the mysteries of life**

Chemistry is the science of the real world; the world today is searching for innovative solutions for many of its vexing problems. Chemistry must become part of this solution and dispel the image that it is the cause of the problem

CHEMISTRY : THE NEXT FRONTIER ?



IS CHEMISTRY SCIENTIFICALLY MATURE? CAN WE...

… *really* understand molecules / reactions?

… engineer function?

… design drugs?

… make materials by design?

… rationalize the origin of life?

… understand life / thought?

… build a cell?

Chemistry is still in its infancy!

SOME PROBLEMS OF CHEMISTRY

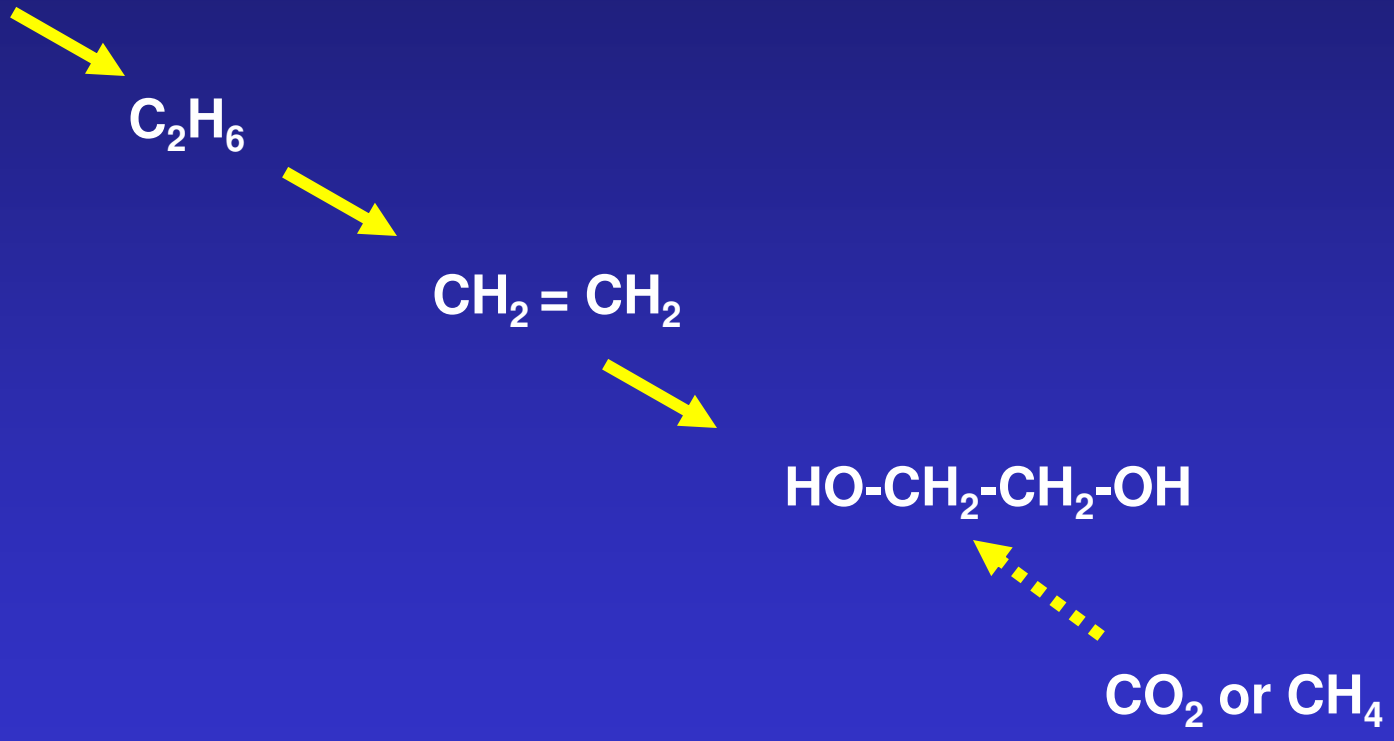
- **Simple molecule chemistry**

  CO_2, H_2, H_2O, CH_4, NO_x, O_2
- **Energy production**
- **Understanding earth : Global stewardship**
- **Impossible materials**

  GMR, Negative index of refraction, High Tc, self healing materials, etc.
- **Complex systems : Systems biology, environmental modeling, the cell**
- **Origin of life**
- **Chemical basis of consciousness**

REINVENTING THE HYDROCARBON CHAIN

Petroleum (complex hydrocarbon)



REINVENTING THE CHAIN: THE CHEMICAL ECONOMY

petroleum

- fuel
  - transportation, heating
- petrochemicals
  - commodities
    - specialties
      - pharmaceuticals
        - fermentation
        - natural products

nuclear

- heat
  - electricity
    - H_2

? H_2 thermal cycles

? Electrocatalysis

? "Hydrogenochemicals"

? Fuel cells

? Materials

Similarly, what are the chemical economies for: *CH_4*, *coal*, and *biomass*?

ALIGNING CORE AREAS TO LARGER SOCIETAL NEEDS

Core areas

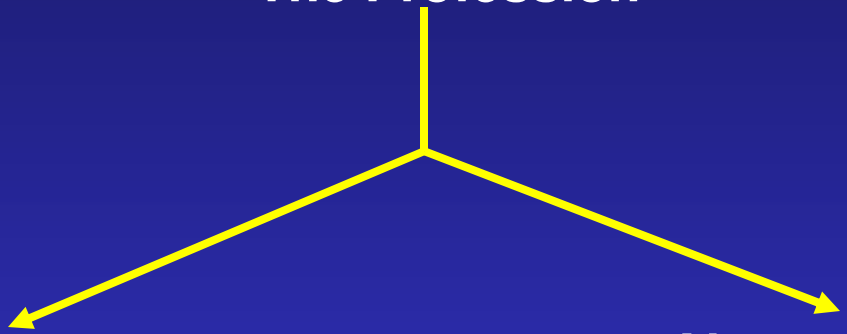
- Catalysis
- Physical Chemistry
- Analytical chemistry
- Organic Chemistry
- Theoretical chemistry
- Polymer Science
- Chemical Engineering
- Biology
- Materials chemistry

Areas of coalescence

- Energy
- Environment
- Functional materials
- Information Technology
- Computational science
- Health and human wellness
- Sustainable processes

CHEMISTRY WILL AND MUST CHANGE

Chemistry
The Profession



Reinvention

New problems

Absorption or evaporation into

Biology
Materials
Energy
Environment

- ***Has Chemistry been a little arrogant about its relationships with other disciplines?***

- ***Does Chemistry care about what other disciplines need from it pedagogically, intellectually, or methodologically ?***

FUTURE OF CHEMISTRY

- **Systems, not molecules**
- **Functions, not molecular structure**
- **Problems, not puzzles**

No longer "What is it?" but "What does it do?
Chemistry must move beyond molecules and learn to solve the entire problem. Only then the flow of ideas, problems and solutions between chemistry and society will become more animate and visible

IS CHEMISTRY ON THE THRESHOLD OF A NEW REVOLUTION ?

- **Responsibility for solving some of the most interesting problems in science and technology**
- **Exceptionally wide range of tools**
- **Chemistry offers a balance of skills; synthetic, computational, ability to handle complexity**
- **Existing body of knowledge insufficient**

CHALLENGE OR CRISIS OF CHEMISTRY

- **Inadequacies of theory ; eg: Complex and coupled networks, protein- ligand binding, catalysis, non-equilibrium systems, non-covalent interactions**

- **Peer Review Systems: Encourages safe science at the cost of risky science**

- **Demise of industrial R&D Centres : No longer great source of innovation and discovery as well as providers of jobs (DuPont Central R&D, GE Corporate Research, BASF etc)**

- **Teaching Pedagogy , departmental structure and textbooks**

- **Academic Social Systems : Diversity is rejected, conformity is rewarded**

" It is hard to understand the tightly compartmentalized minds of the chemists of that day. An extreme example at the chemistry library at Cambridge University, an imaginary line divided the room into two parts, one for physical chemists and the one for organic. The library had two sets of the Journal of the Chemical Society, since an organic chemist was not supposed to cross the imaginary line to use the volumes on the physical side of the library, and vice versa "

Frank Westheimer
J. Biological Chemistry, 278,11729 (2003)

TEACHING AND EDUCATION

- **Archaic**
- **Non-demanding**
- **Not very relevant**

CHANGING FACE OF CHEMISTRY

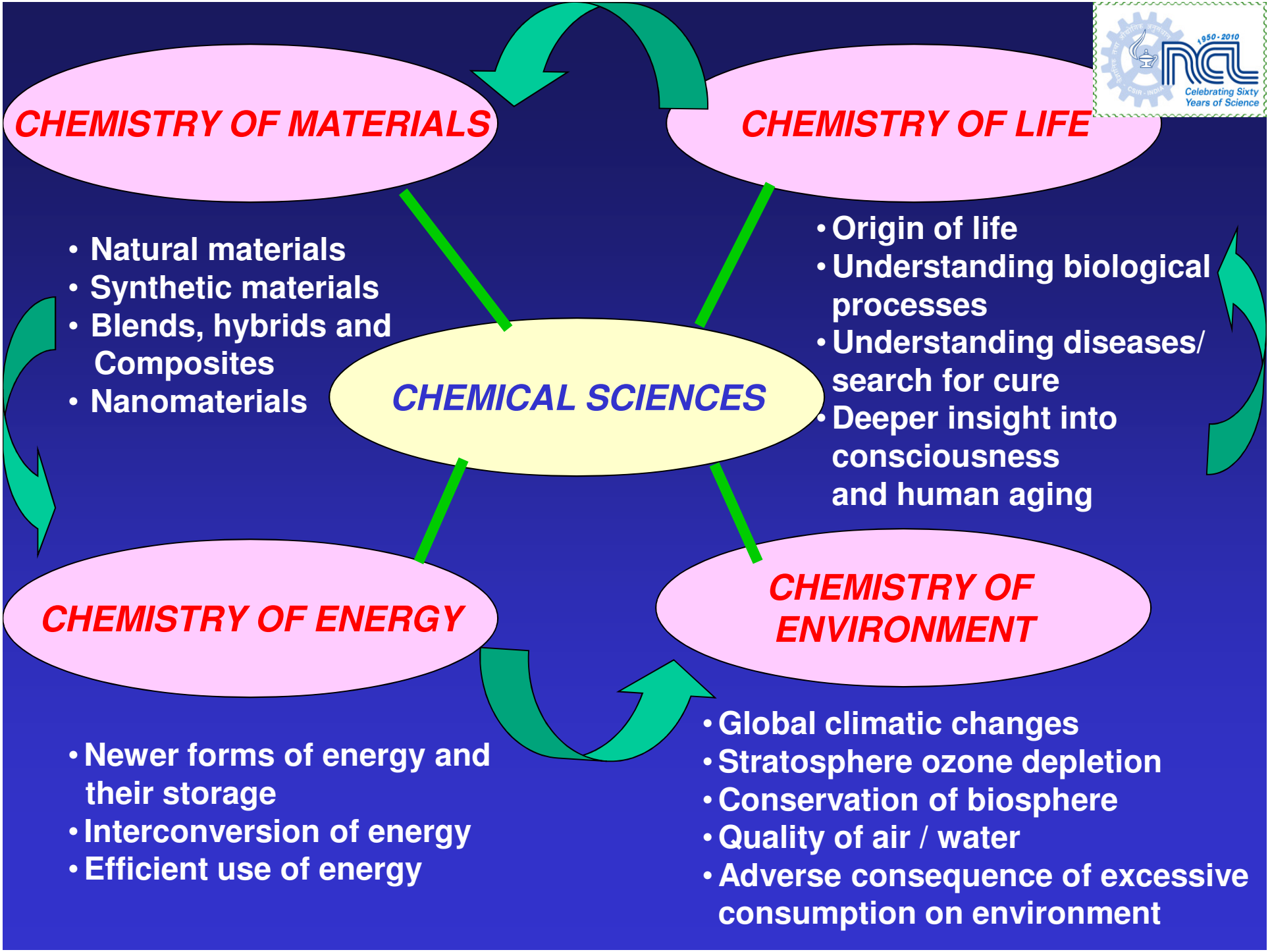
- **Chemistry is becoming more and more interdisciplinary pursuit**
- **However, students usually learn chemistry in isolation**
- **Is there a case for teaching science in an integrative fashion ?**
- **Can principles of chemistry be illustrated using familiar biological phenomena or ecosystem behavior or semiconductor physics ?**
- **Structure and function constitute the central theme of chemistry. All chemistry must be taught in the context of this theme**
- **We tend to teach chemistry in the chronological order of its evolution. This is unnecessary**
- **We should teach chemistry in the context of contemporary knowledge. The origins of chemistry must be covered in a module called "History of Science"**

In the world of research traditional disciplines are not relevant; Why don't we teach chemistry the way it is practiced ?

INTEGRATION OF TEACHING WITH PRACTICE

- **Students at a very early stage of their learning must experience the thrill of doing chemistry**
- **Chemistry, is in the ultimate, a sensual science. Its beauty lies not in the pages of drab textbooks, but in the perception of its colors, smell and even sound !**
- **Students must practice chemistry in all its dimensions**
- **Experiments must be open ended and must inculcate the discipline of inquiry based learning**
- **It is never too early to get students involved in research. Small research modules can completely replace traditional laboratory experiments**
- **Students must be given opportunity to do science so that they can discover whether "research is for me"**

If we have to infect young minds with the thrill of doing research, we should let student experience what goes on in the life of a scientist In a research laboratory


CHEMISTRY OF MATERIALS
• Natural materials
• Synthetic materials
• Blends, hybrids and Composites
• Nanomaterials
CHEMISTRY OF LIFE
• Origin of life
• Understanding biological processes
• Understanding diseases/ search for cure
• Deeper insight into consciousness and human aging
CHEMICAL SCIENCES
CHEMISTRY OF ENERGY
• Newer forms of energy and their storage
• Interconversion of energy
• Efficient use of energy
CHEMISTRY OF ENVIRONMENT
• Global climatic changes
• Stratosphere ozone depletion
• Conservation of biosphere
• Quality of air / water
• Adverse consequence of excessive consumption on environment
1950-2010
Celebrating Sixty Years of Science

CHEMISTRY OF MATERIALS

- Natural materials
- Synthetic materials
  - Organic
  - Inorganic
  - Hybrids
- Blend of natural and synthetic materials
- Nanomaterials
- Environmentally compatible materials

CHEMISTRY OF LIFE

- Synthesis using soft chemistry
  - Molecular recognition
  - Self assembly
  - Weak bonds
- Interaction of small molecules with large biomolecules
  - Chemical genetics
  - Structure function relationships
  - Target driven and diversity oriented molecular synthesis
- Chemistry of bio-macromolecules
  - Structure and conformation
  - Synthesis of natural / unnatural bio-macromolecules

CHEMISTRY OF ENERGY

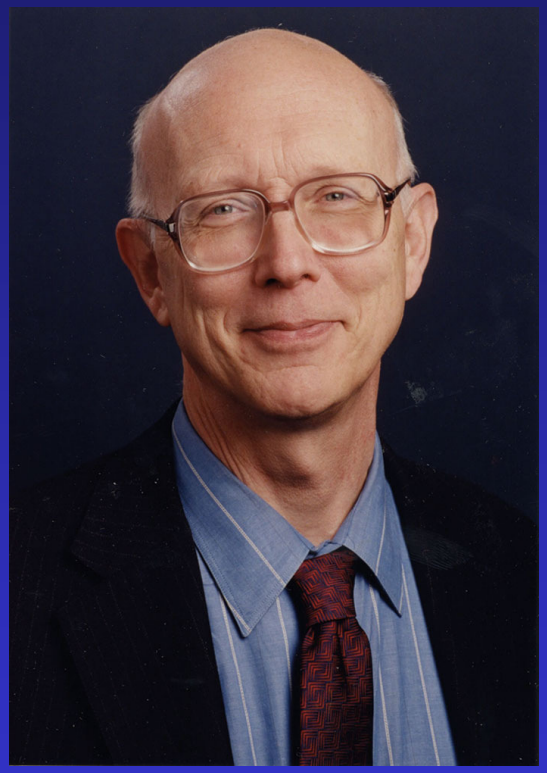
- **Minimize energy in intensity for chemical conversions**
  - **Chemical catalysts**
  - **Biological catalysts**
- **Minimize energy intensity in processing and fabrication**
  - **New materials**
- **Energy harvesting from renewable resources**
  - **Sunlight**
  - **Biomass**
  - **Hydrogen**

CHEMISTRY OF ENVIRONMENT

- Analytical chemistry / sensors
- Kinetics and chemical reaction modeling
- Computational chemistry
- Efficiency in use of materials
- Chemical / Biological fixation of CO_2
- Environmentally benign chemistry
  - Clean chemistry
  - Zero effluent / by product
  - Atom economy
  - Chemistry in aqueous medium
  - High yields / selectivities
  - Biological processes for chemical conversion
  - Economic use of by products / waste products
  - Recycling

REFERENCES

- Chemicals, Chemistry and Molecules
  Editorial, Current Science, 99(10), 1301 (2010)
- Where are the Champions?
  Nature Chemistry 2, 599 (2010)
- The Future of Chemistry
  Nature Chemistry 1, April 2009, 5-15
- The Future of Chemistry
  Angew Chem. Int. Ed., 43, 3618 (2004)
- International Journal of Philosophy of Chemistry, 12, 99 (2006)
  Special issue on " The Public Image of Chemistry"



I believe chemistry can be everywhere, if chemistry so chooses or that it can contract into an invisible part of the infrastructure of society

G. M. Whitesides

- **What will Chemistry do in the Next Twenty Years?**
  G.M. Whitesides, Angew Chem. Int. Ed., 29, 1209 (1990)
- **Assumptions Taking Chemistry in New Directions**
  G.M. Whitesides, Angew Chem. Int. Ed., 43, 3632 (2004)
- **Reflections in Chemistry – Priestley Medal Lecture**
  C&EN, March 26, 2007, p.12


1950 - 2010
CSIR - INDIA
Celebrating Sixty
Years of Science
THANK YOU