THE FUTURE OF CHEMISTRY

Gopalan Endowment Lecture, Madras Christian College, Chennai

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DR. S. SIVARAM

A 201, Polymers & Advanced Materials Laboratory,
National Chemical Laboratory,
Pune, 411 008, INDIA

Tel : 0091 98607 99954
Fax : 0091 20 2590 2615
Email : s.sivaram@ncl.res.in
www.swaminathansivaram.in

My tributes to an outstanding teacher who dedicated his life to educate and inspire many generations of young men and women at Madras Christian College, Department of Chemistry and in the process continued the distinguished traditions of this Department

Dr. R. Gopalan Endowment Fund

Three and a half decades (1966 - 2002)
of devoted teaching and quality
research in chemistry at
Madras Christian College
Tambaram, Chennai, India.

FOUR DECADES IN CHEMISTRY : THE JOURNEY FROM MCC AND BEYOND

(A reflection on my personal and professional journey)

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

Tel : 0091 20 2590 2600
Fax : 0091 20 2590 2601
Email : s.sivaram@ncl.res.in
Visit us at : http://www.ncl-india.org

Frontiers in Chemistry
A Conference to Commemorate the Birth Centenary of Professor S.V. Anantakrishnan
Madras Christian College, Chennai
October 2, 2008

MCC Chennai 021008

EDUCATION AT MCC

- **Committed teachers who were genuinely interested in the student**
- **An ambience of research and scholarship**
- **Liberal education; apart from English and Hindi (prose and poetry) I had an opportunity to learn philosophy and economics; a class in moral instruction introduced me to the Old Testament ; led to a life long love affair with books**
- **No early specialization**
- **A small class of just twenty !**
- **A compelling urge to excel !**

Lesson 8 : Teachers who are committed and show genuine interest in their pupil make good institutions great

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

WHAT IS CHEMISTRY ?

- Chemistry is primarily a qualitative and intuitive science. Many of the discoveries are characterized by a sheer audacity of imagination rather than evidence based reductionism
- Advances in chemistry has been propelled by human needs and wants, in peace and war (eg, Indigo, Bakelite, Ammonia, Penicillin)
- Chemistry is uniquely utilitarian; Many famous chemists have been preoccupied with concerns of the society
- The utilitarian aspect of chemistry ahs probably contributed to it being less romantic than other branches of natural science. Human mind is often more fascinated by the unreachable- exploding stars, contracting universe, cure for cancer or understanding human cognition

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

Marcellin Bertholet, 1860

(1827- 1907)

CHEMISTRY AND CHEMICAL INDUSTRY

- **Chemical science and industry have been closely intertwined throughout its history**
- **Creation of wealth has always been the underlying motivation for many of the epoch making discoveries**
- **More than any other breed of scientists, chemists have always exhibited a heightened awareness of society's problems and an altruistic desire to solve them**
- **For over a century and a half, academic and industrial chemistry have enjoyed a healthy and symbiotic relationship. Every major landmark in applications of chemistry can be traced back to the fundamental insights gained through painstaking and sustained research in academia**

HISTORY OF CHEMISTRY : 20TH CENTURY

- Nineteenth century marked the end of vitalism and beginning of reductionism in science (Bertholet)
- The belief became prevalent that all problems can be solved by breaking them into parts
- Evolution of quantum mechanics and its applications to chemistry gave rise to the belief that one can understand chemical and physical states of matter *ab initio,* based on electronic theory
- This led Paul Dirac to state that " all problems in chemistry are problems in applied mathematics "

TIMELINES IN THE HISTORY OF CHEMISTRY

- 1900 : Ernest Rutherford/ J J Thompson : Nothing left to discover in Physics
- 1915 : Niels Bohr : Chemistry is solved
- 1916 : G. N. Lewis : The concept of a bond – ionic, covalent and coordinate- electron sharing and pairing
- 1930 : P. M. Dirac : All problems in science are problems in applied mathematics
- 1930 : Quantum chemistry, the first book written; valence bond and molecular orbital concepts

TIMELINES IN THE HISTORY OF CHEMISTRY

- 1920-50 : Mark, Staudinger, Carrothers , Flory, Ziegler, Natta: The concept of macromolecules, tacticity in polymers
- 1933: Linus Pauling : H Bond, van der Walls forces, Resonance, hybridization of orbitals, The nature of the chemical bond
- 1930-40 : Hammet, Whitmore, Lowry, Ingold : Physical organic chemistry
- 1950-60 : R.B Woodward : The beginning of the art of organic synthesis
- 1970 : The grammar of chemistry: The orbital rules (Woodward- Hoffman)
- 1990 : Allotropes of carbon; three and two dimensional solids

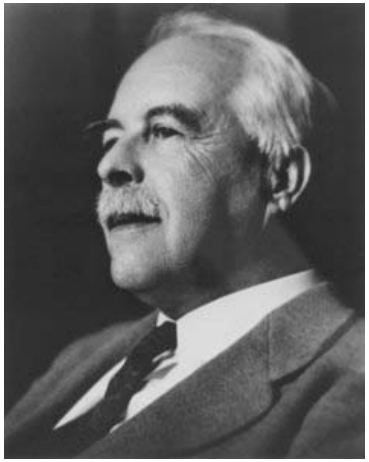
[CONTRIBUTION FROM THE CHEMICAL LABORATORY OF THE UNIVERSITY OF CALIFORNIA]

THE ATOM AND THE MOLECULE.

BY GILBERT N. LEWIS.

J. Amer. Chem Soc., 38, 762-785 (1916)
cited 1038 times

Received January *26, 1916.*



October 23, 1875
- March 23, 1946

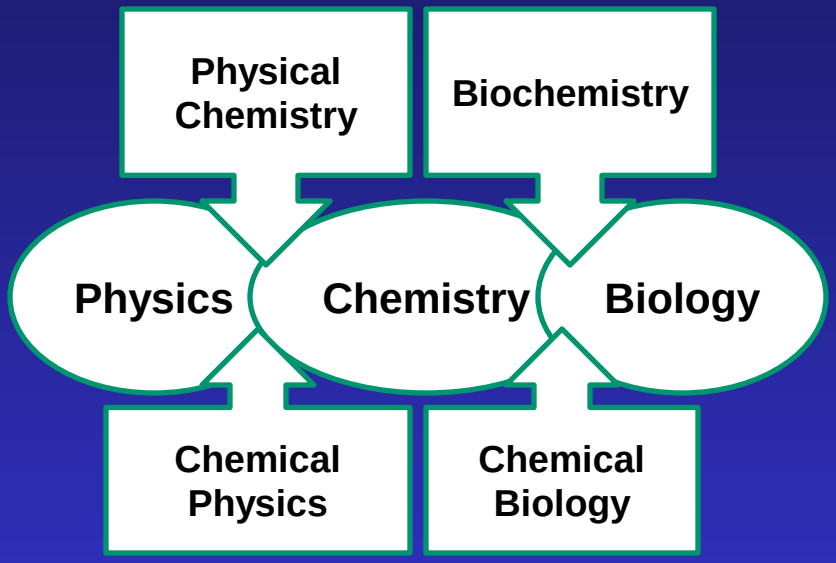
In a paper entitled “Valence and Tautomerism” I took occasion to point out the great importance of substituting for the conventional classification of chemical substances, as inorganic or organic, the more general classification which distinguishes between polar and nonpolar substances. The two classifications roughly coincide, since most inorganic substances are distinctly polar, while the majority of organic substances belong to the nonpolar class; thus potassium chloride represents the extreme polar type and methane the nonpolar. Nevertheless, there are many inorganic substances which, under ordinary circumstances, are predominantly nonpolar, and many organic substances which, at least in a certain part of the molecule, are strongly polar.

This article was apparently unknown to Sir. J. J. Thomson when he wrote, in 1914, an extremely interesting paper on the “Forces between Atoms and Chemical Affinity” in which he reached conclusions in striking accord with my own, and discussed in considerable detail the theories of atomic and molecular structure which led him to these conclusions.

To enable us to appreciate the importance and the usefulness of a distinction between the polar and nonpolar types of chemical molecules no hypotheses are necessary, but in a more minute examination of the nature of such a distinction some theory of structure is indispensable. Such a theory I have employed for a number of years in the interpretation of chemical phenomena, but it has not hitherto been published.

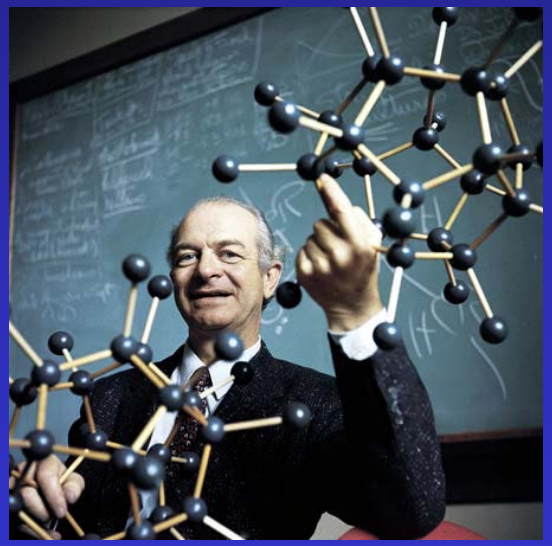
LINUS PAULING AND THE NATURE OF THE CHEMICAL BOND

- **Established chemistry as an overarching science that bridges physics on one side and biology on the other**



Created a new discipline called Quantum Chemistry

Retrieved chemistry which was slipping into the hands of the early twentieth century physicists



1901- 1994
Nobel Laureate, 1954

UNDERSTANDING CHEMISTRY : CHEMISTRY IS ESSENTIALLY A QUALITIATIVE SCIENCE !

1. Electrophilic	Nucleophilic
2. Acidic	Basic
3. Lewis Acid	Lewis Base
4. Electron accepting	Electron donating
5. Hard acids and bases	Soft acids and bases
6. Covalent bonds	Coordinate or ionic bonds
7. Strong bonds	Weak bonds
8. Hydrophilic	Hydrophobic
9. Electronegative	Electropositive
10. Polar	Non polar

UNDERSTANDING CHEMISTRY : CHEMISTRY IS ESSENTIALLY A QUALITIATIVE SCIENCE !

11. Electronic	Steric
12. Inductive effect	Resonance effect
13. Exothermic	Endothermic
14. Oxidation	Reduction
15. Kinetic (Enthalpy)	Thermodynamic (Entropy)
16. Chiral	Achiral
17. Linear	Branched
18. Self organization	Self assembly
19.Molecular	Supramolecular

CHALLENGE TO CHEMISTRY

- Chemistry is an old subject . Its practice has been known for over three centuries
- The ancient heritage is both a strength and a burden
- Difficult to change mindsets, often frozen under the weight of tradition
- It is always difficult to teach an old dog new tricks
- Its transformation to a new order poses innumerable challenges
  - *Structure and organization of teaching departments in universities*
  - *Teaching pedagogy and learning resources*
  - *Integration of research with teaching and learning with practice*
  - *Regulatory frameworks, health, safety and liabilities*
  - *Resource constrained science : sustainability issues*
  - *Models for converting knowledge to wealth*

REDEFINING CHEMISTRY

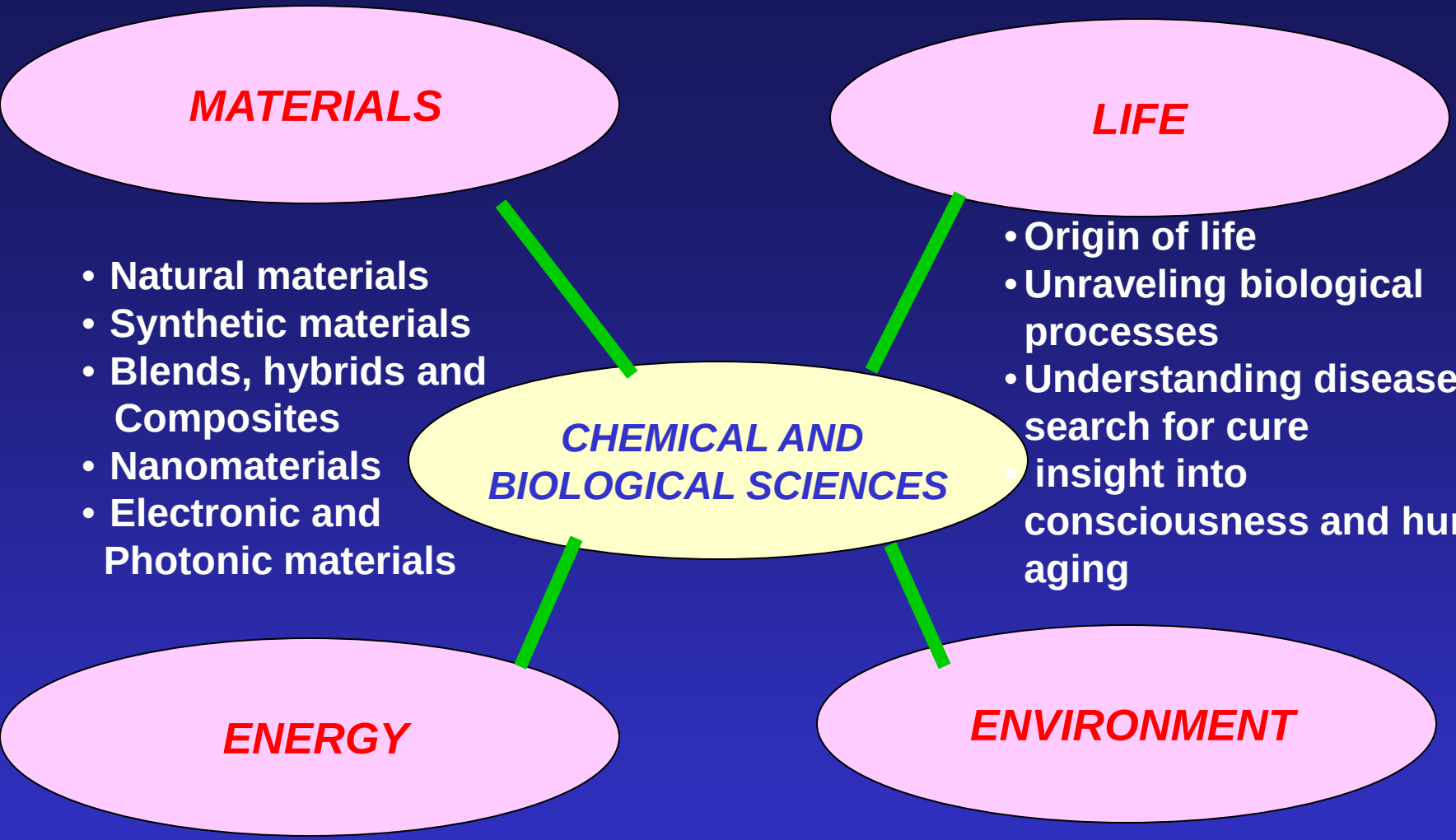
- **Chemistry will continue to be a body of knowledge essential for science to function**
- **But chemistry as a discipline is noticeably in trouble**
- **Changing nature of chemistry is an evolution, not a paradigm shift**
- **Science began centuries ago as a unitary discipline and included mathematics, astronomy, anatomy and alchemy**
- **During the 1700's, in the Age of reason, scientific disciplines as we broadly understand today took shape**
- **Now science is evolving again, back into a multidisciplinary endeavor with key focal points as the interface between chemistry and physics, chemistry and biology and biology and physics.**
- **From a study of elements to molecules to the current time to the study of molecular interactions and functions , leading to the creation of many sub disciplines, seemingly away from the core discipline of chemistry and into increasingly multidisciplinary space that has made chemistry vulnerable.**

S. Ritter, C&EN, November 29, 2004, p.31

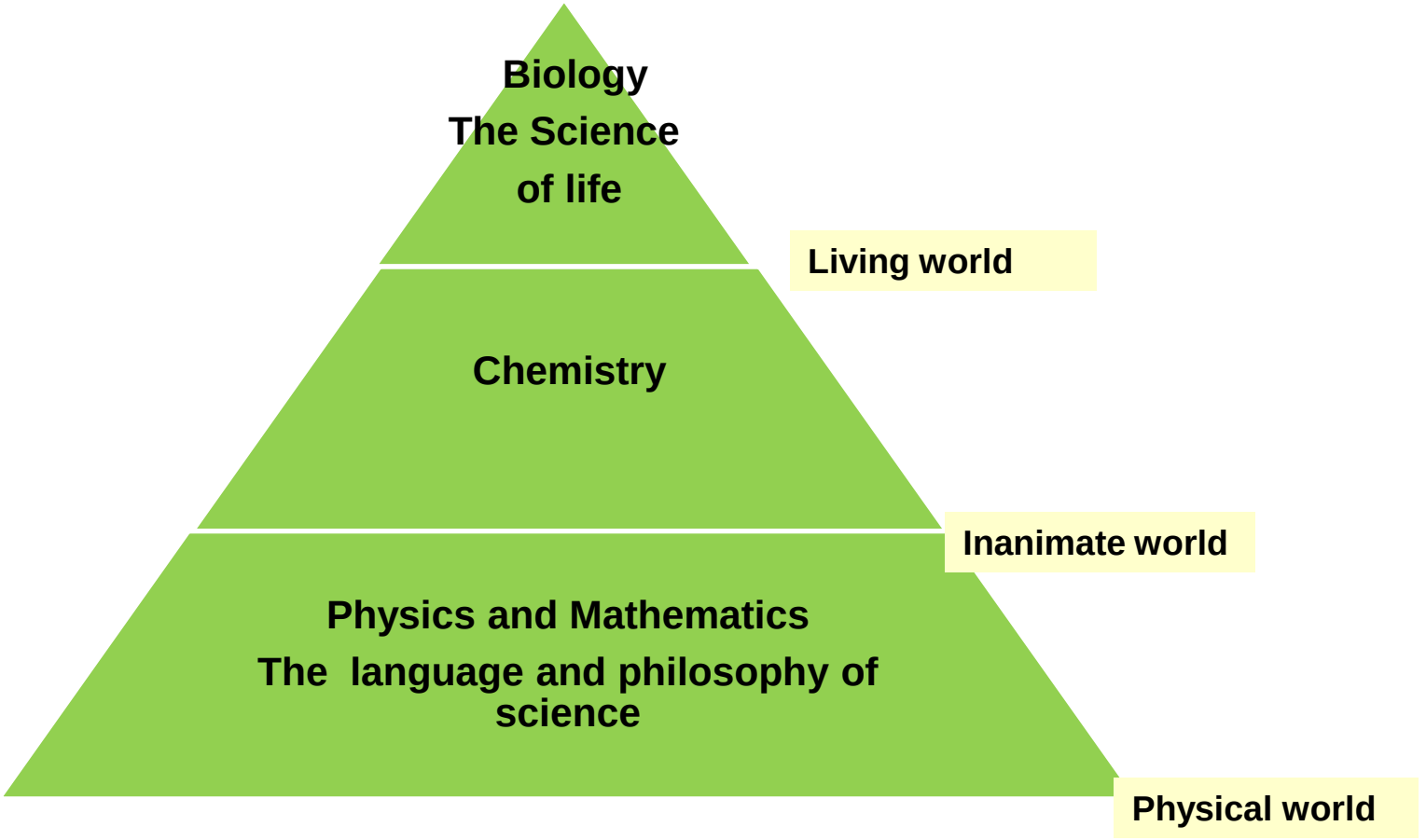
THE CURRENT ARCHITECTURE OF CHEMISTRY

- Chemical synthesis
- Chemical structure, dynamics and mechanisms
- Chemical measurements and imaging
- Theory, models and computational methods
- Environmental chemical sciences
- Chemistry of life processes
- Chemical catalysis
- Macromolecular, supramolecular and nanochemistry

www.CEN-ONLINE.Org, March 30, 2009


MATERIALS
• Natural materials
• Synthetic materials
• Blends, hybrids and Composites
• Nanomaterials
• Electronic and Photonic materials
LIFE
• Origin of life
• Unraveling biological processes
• Understanding diseases/ search for cure
• insight into consciousness and human aging
CHEMICAL AND BIOLOGICAL SCIENCES
ENERGY
• Newer forms of energy & their storage
• Interconversion of energy
• Efficient use of energy
ENVIRONMENT
• Global climatic changes
• Stratosphere ozone depletion
• Conservation of biosphere
• Quality of air / water
• Adverse consequence of excessive consumption

HEIRARCHY OF SCIENCE



P. Oppenheim and H. Putnam, Unit of science as a working hypothesis, H. Feigl, M. Scriven, G. Maxwell (eds.), Concepts, Theories and the Mind – Body Problem, Vol.2, University of Minnesota Press, 1958

PHYSICS, CHEMISTRY AND BIOLOGY: STYLE AND APPROACH

Physics	Search for “simple” systems to test “theory” based hypothesis on the structure of matter
Chemistry	Understand molecular and structural diversity in the organization of matter, mostly “non-living”
Biology	Understand molecular and structural diversity in the organization of matter, mostly living

Chemistry and Biology are two distinctive cultures and the rift between them is serious, generally unappreciated and counter productive.

Arthur Kornberg, 1987

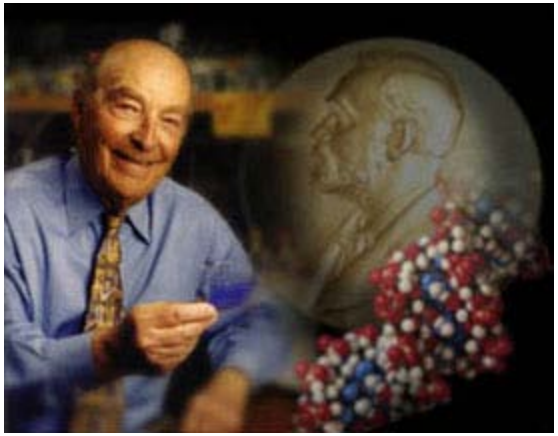
LANGUAGE OF CHEMISTRY

Language of Chemistry

Physical World

Biological World

The Two Cultures: Chemistry and Biology,
A. Kornberg, Biochemistry, 26, 68888 (1987)



Arthur Kornberg 1918-2007 Nobel, 1959

THE EMERGENCE OF REDUCTIONISM AND THE BEGINNING OF THE CHEMISTRY - BIOLOGY DIVIDE

- Nineteenth century marked the end of vitalism and beginning of the reductionism as a philosophical thought in science
- Vitalism was the dominant philosophical thought up to that time
- The reductionists believed that all complex systems can be understood as a sum of its parts
- Evolution of quantum mechanics and their applications to chemistry gave rise to the belief that one can understand chemical and physical states of matter *ab initio,* based on atomic and electronic theory
- The chemists and physicists of the period focused attention on problems that can be solved by the reductionist approach
- Biology proved too complex for this approach; hence was abandoned by most chemists and physicists

COMPLEX MATTER via SUPRAMOLECULAR SELF ASSEMBLY

Supramolecular Chemistry

Molecular Recognition and Self Organization

Physical World

Biological World

Jean-Marie Lehn, Science, 295, 29 March 2002

J-M Lehn
1939
Nobel, 1987

COMPLEXITY IN CHEMISTRY AND BIOLOGY

- The recognition that chemistry can extend beyond molecules is marked by the award of Nobel to Pederson, Cram and Lehn in 1987 for their contributions to the area of supramolecular chemistry
- Chemistry had reached the limits in terms of construction of molecules, from Wohler`s urea to Wilsttatter`s cyclooctatetrene to Woodward`s vitamin B12 and ultimately to Kishi`s Palytoxin,. Synthesis posed no further challenges.
- The beginning of the concept of *Emergent Properties : when whole becomes larger than the sum of the parts*
- Biology is characterized by emergent properties, systems more important than molecule or assembly of molecules; shape or form is more important than chemical composition or structure

COMPLEXITY IN CHEMISTRY AND BIOLOGY

- Emergent properties are characteristic of complex systems – Ant colonies, flight of birds, behaviour of crowds, droplets of water and ice, behaviour of cells, neural networks, cognitive science, musical notes, traffic on a road, climate and atmospheric science etc . These systems are characterized by high level of collective or cooperative behaviour.
- Does reductionist approach limit our ability to understand emergent properties?
- Is there need for a new stream of thought to connect the simple molecular understanding of matter provided by chemistry with the complex emergent behavior of biological system ?

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

WHICH COMPANY IN THE WORLD PRODUCES ……

- Biodegradable fibers stronger than steel
- Biodegradable photo-detectors more sensitive than the most advanced photonics technology
- Biodegradable super-hydrophobic surfaces
- Toughest ceramic biodegradable nano-composites
- Biodegradable data storage media that carry one bit of information for every three molecules

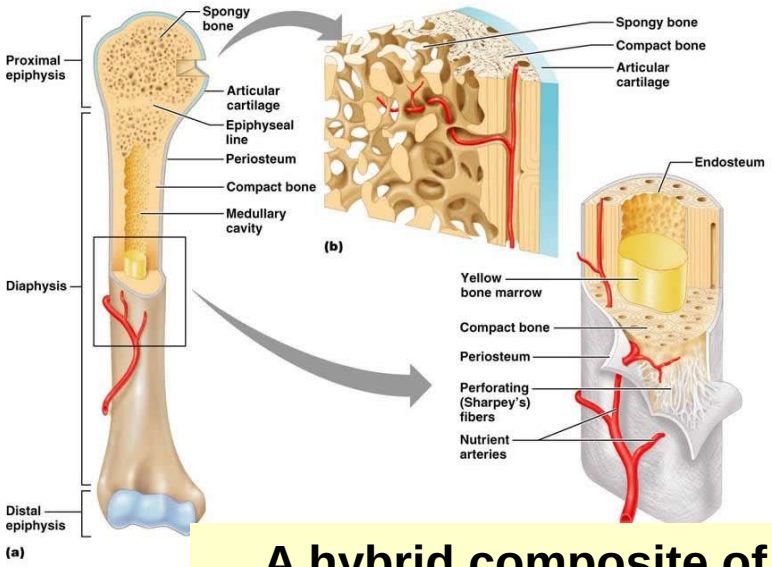
Superhydrophobic surface

Abalone shell

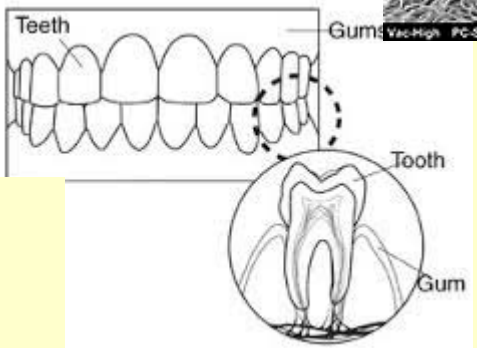
Surface Photonic Gratings

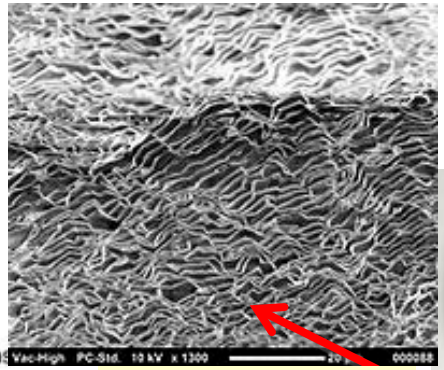
This company is called Life Inc.,

Its materials are the most advanced on this planet



A hybrid composite of Hydroxyapatite and Collagen Type II

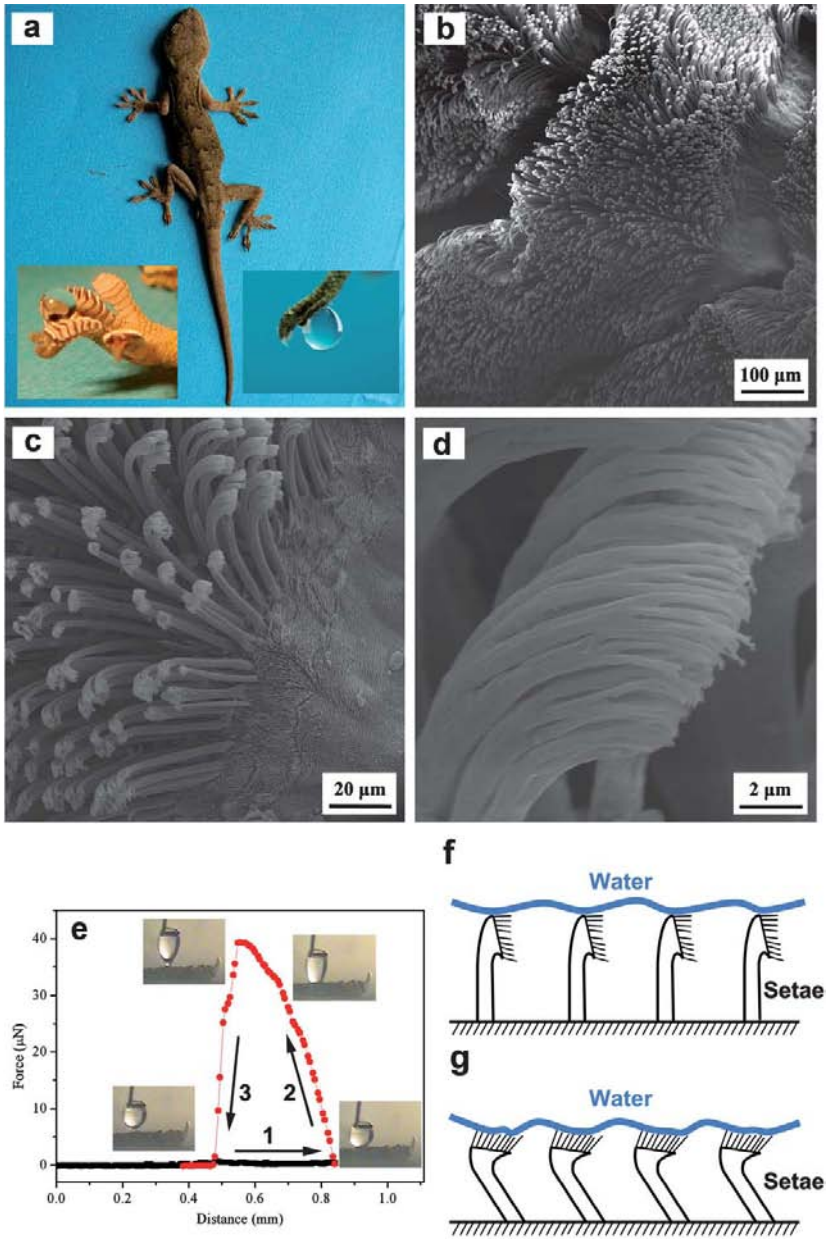




Aragonite layers in the nacre of a blue mussel

SUPER HYDROPHOBIC GECKO FEET WITH HIGH ADHESIVE FORCE TOWARDS WATER

An illustration of functional integration of multiscale structures in biological materials



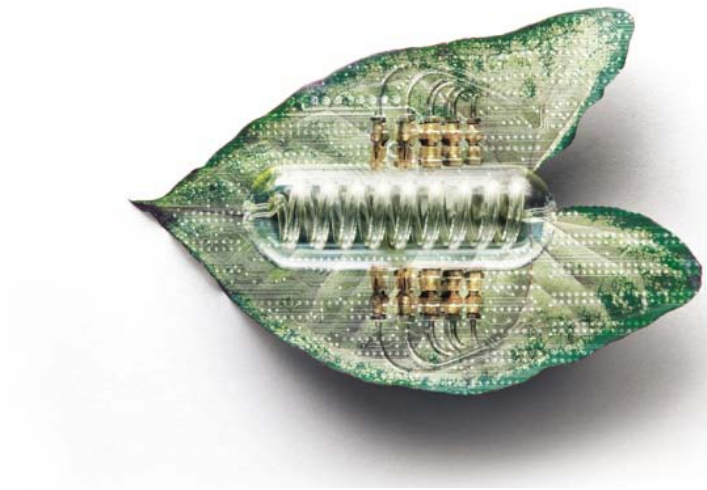
K. Liu et al.,Nanoscale, 4, 768 (2012)

BIO-INSPIRED MATERIALS CHEMISTRY

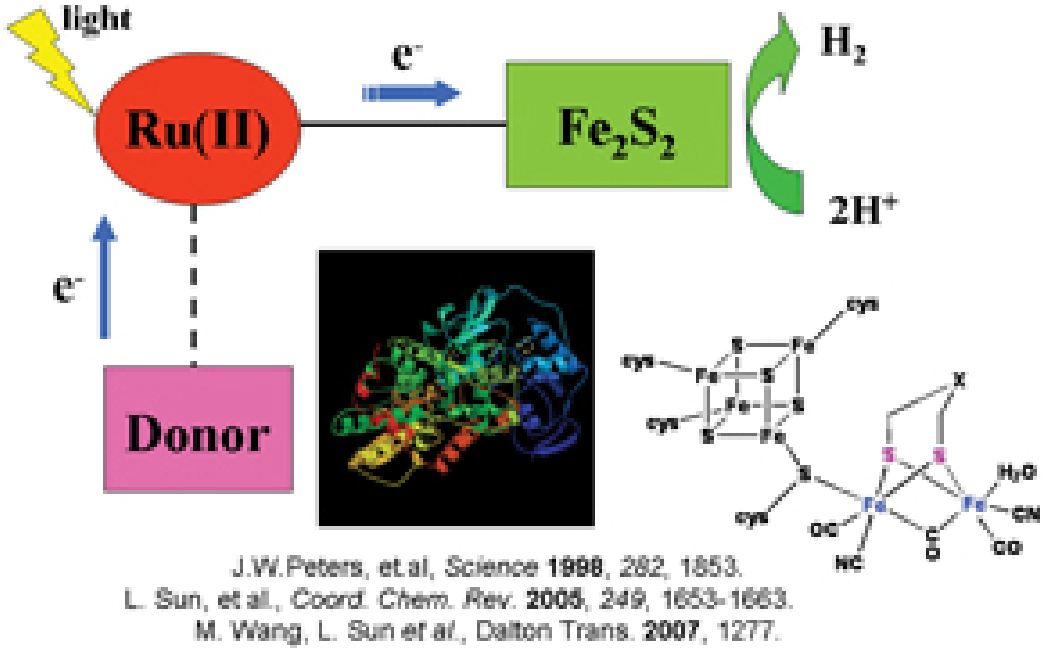
- Bio-smart Surfaces
- Bio-mineralization
- Bio-glass and Bio-ceramics
- DNA nanomaterials via conjugation
- Bio-nanomaterials
- Bio-composites

E.Dujardin and S. Mann, Adv. Mater.,14, 1 (2002)

AN ARTIFICIAL LEAF



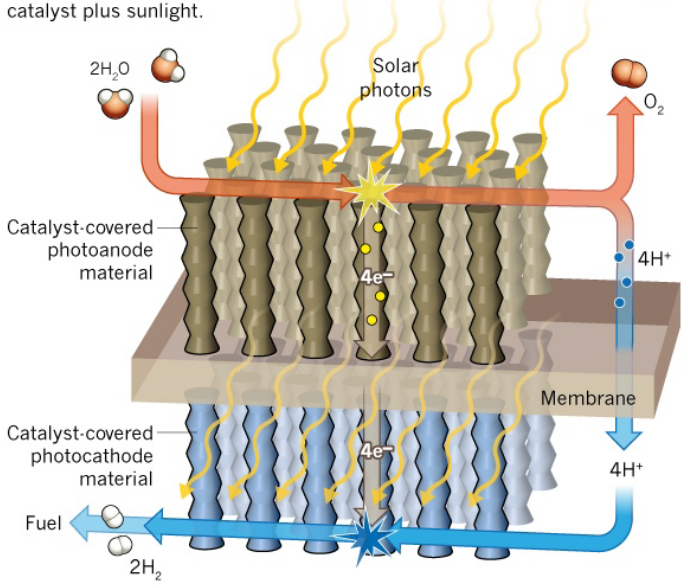
To mimic the function of FeFe-hydrogenase active site



J.W.Peters, et al, *Science* **1998**, 282, 1853.
L. Sun, et al., *Coord. Chem. Rev.* **2005**, 249, 1653-1663.
M. Wang, L. Sun *et al.*, Dalton Trans. **2007**, 1277.

SPLITTING WATER

Artificial photosynthesis uses photons from sunlight to split water molecules into oxygen and hydrogen, which can be used to make fuel. Every two molecules of water yield one oxygen molecule (O_2), as well as four pairs of protons (H^+) and electrons (e^-). The protons and electrons migrate across a membrane, where a photocathode recombines them into hydrogen using a catalyst plus sunlight.



T. Norin, U. Pandit, Chemistry Int.,p.4 (2008)
J. Marshall, Nature, p.22, 5 June 2014

BIOLOGY TOOLS THAT ARE SHAPING THE FUTURE OF CHEMISTRY

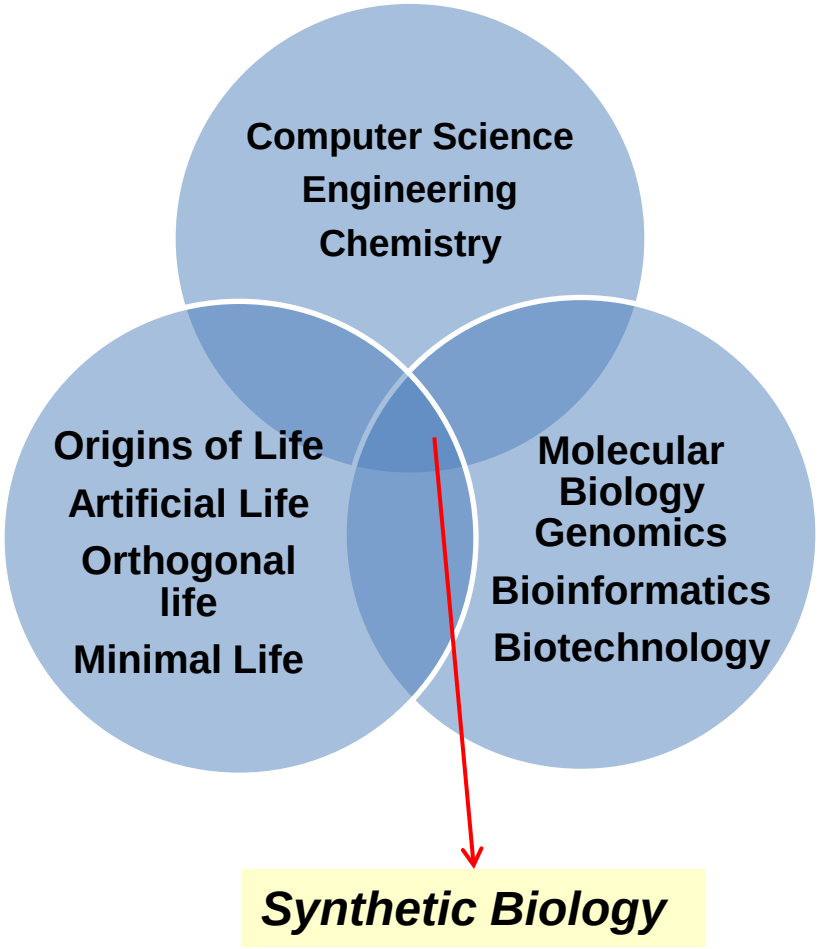
- Plant molecular biology
- Genetic engineering
- Protein engineering
- Genomics and metabolomics
- Industrial microbiology
- Catalytic thermo-philic enzymes
- Bioreactor engineering and fermentation
- Directed evolution to create adaptive organisms
- Metabolic pathway engineering
- ***Synthetic biology***

SYNTHETIC BIOLOGY: APPLYING ENGINEERING TO BIOLOGY

Synthetic biology is the engineering of biology; the synthesis of complex, biologically based (or inspired) systems which do not exist in nature. The engineering perspective may be applied to all levels of the hierarchy of biological structures- from individual molecules to whole cells, tissues and organisms

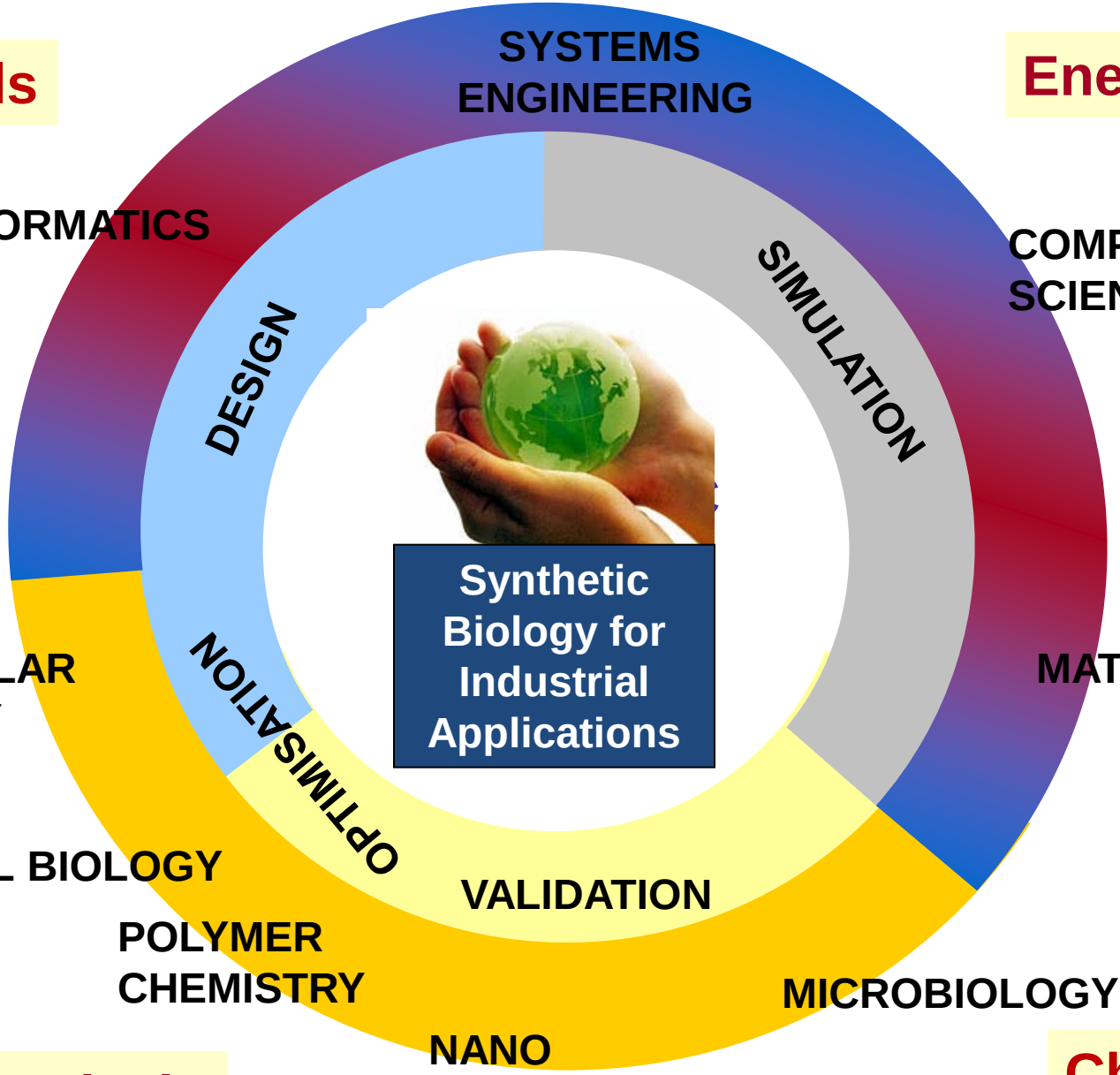
European Union , 2005

Objective
Engineering new biological pathways
Creating, de novo, new organisms



D. Endy, Nature, 438, 449 (2005)
D. Endy and I.Deese, Adventures in Synthetic Biology, Issue 1, 2005

SYNTHETIC BIOLOGY: AN INTEGRATIVE SCIENCE



Materials

Energy

BIOINFORMATICS

COMPUTER SCIENCE

MOLECULAR BIOLOGY

MATHEMATICS

CHEMICAL BIOLOGY

POLYMER CHEMISTRY

MICROBIOLOGY

NANO TECHNOLOGY

Pharmaceuticals

Chemicals

CHANGING FACE OF BIOLOGY AND CHEMISTRY

- **Chemistry and biology are becoming more and more an interdisciplinary pursuit**
- **However, students usually learn chemistry and biology 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 and vice versa ?**
- **Structure, function and dynamics constitute the central theme of chemistry. All chemistry must be taught in the context of this theme**

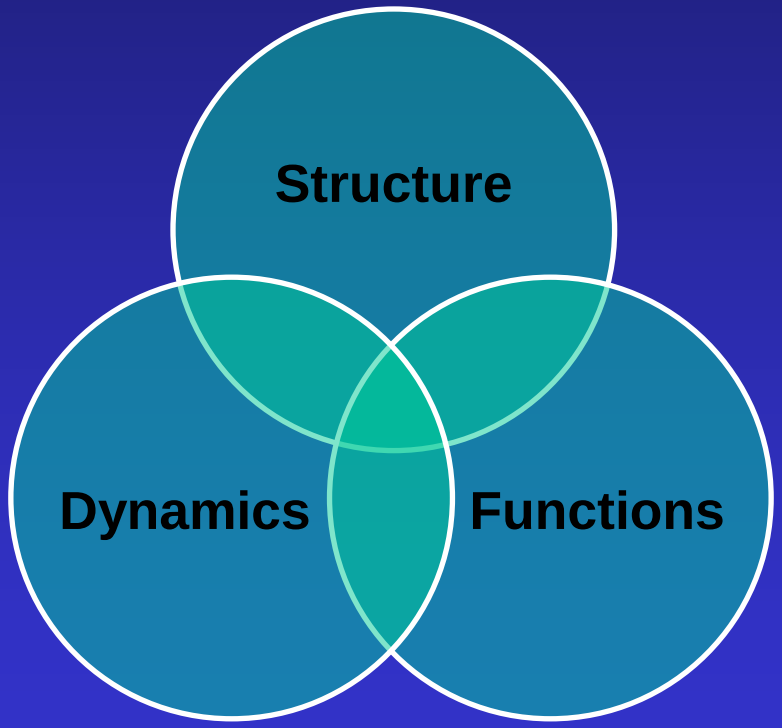
Why don't we teach chemistry and biology the way it is practiced today ?

INTEGRATION OF CHEMISTRY AND BIOLOGY

Molecules can be organic, inorganic or biologically derived, small or big, single or assemblies and involving a range of inter and intra -molecular forces

CHEMISTRY

Progression from atoms to molecules to larger molecular assemblies



BIOLOGY

Progression from whole organisms to molecular structure

J. Chemical Education, 88, 1257 (2011)

IS CHEMISTRY SCIENTIFICALLY MATURE? CAN WE...

… *really* understand molecules / reactions?

… selectively insert oxygen, nitrogen and carbon into C-H bonds?

… engineer functions?

… design drugs?

… make materials by design?

… rationalize the origin of life?

… understand life / thought?

… build a cell?

Chemistry is still in its infancy!

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

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

THE FUTURE OF CHEMISTRY

“ Chemistry, by its very culture has been blindly reductionist. I am often reminded that chemists work on molecules, but they must also work on problems where molecules may be only part of a solution. We think of ourselves as experts in quarrying blocks from granite; we have not thought it our job to build cathedrals from them ”

George M. Whitesides, Angew. Chem. Intl. Ed., 2004

For chemistry to become sustainable, we have to move from a reductionist thinking to a system based thinking; from “bottoms up” design to” top down” understanding

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

- **Reinventing Chemistry, Angew. Chem.Int.Ed., 54, 3196 (2015)**
- **Assumptions Taking Chemistry in New Directions, Angew Chem. Int. Ed., 43, 3632 (2004)**
- **What will Chemistry do in the Next Twenty Years? Angew Chem. Int. Ed., 29, 1209 (1990)**

1950 - 2010

Celebrating Sixty Years of Science

THANK YOU