Green Chemistry: Molecular Design-Build

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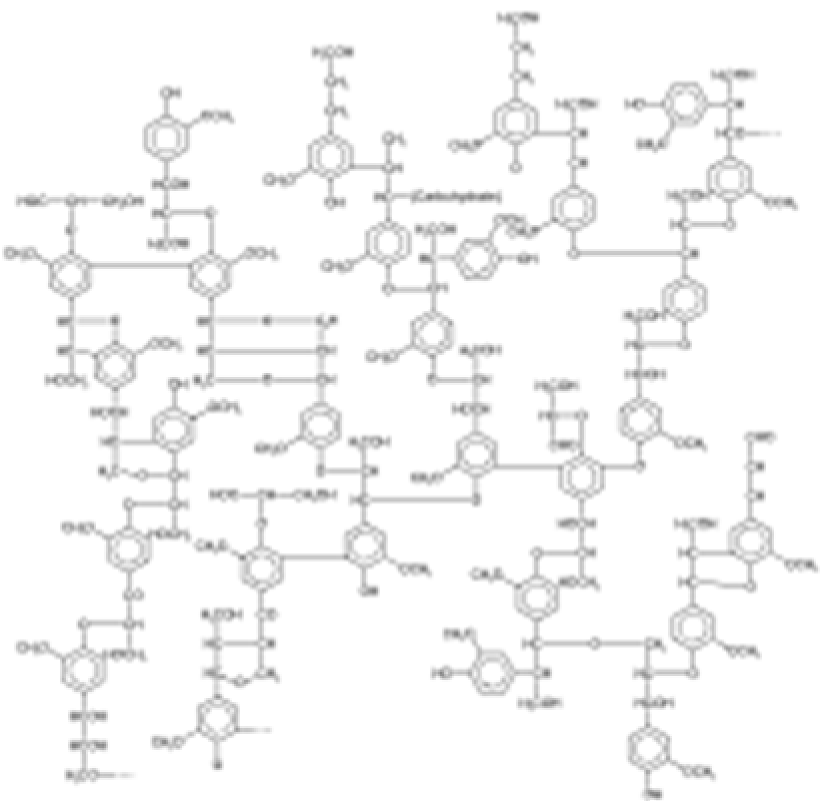
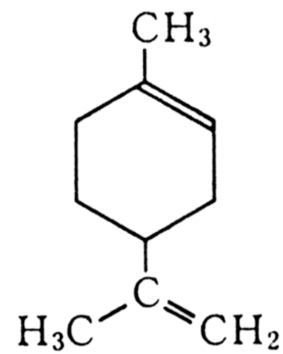
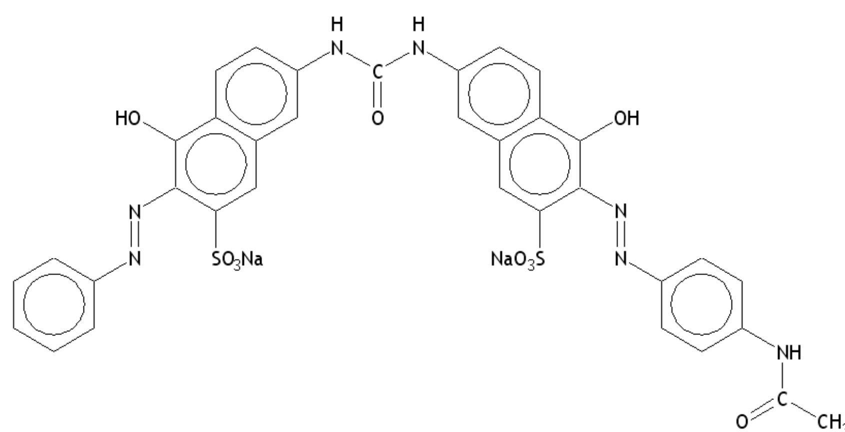
Why am I here talking about chemistry?

- Everything is a chemical.







Green Chemistry Joins College Curriculum

By MARK PRATT
The Associated Press
Tuesday, October 9, 2007;

"When you think about chemistry, most people think about the hazards," said Paul Anastas, who coined the term green chemistry in 1991 while working at the U.S. Environmental Protection Agency. He is now director of Yale University's Center for Green Chemistry and Green Engineering.

The Washington Post

Green chemistry: Voluntary restraint is the target

FINANCIAL TIMES

By Sarah Murray
Published: September 18 2007
…Known as "green chemistry" the idea is to redesign materials and products in ways that cut or eliminate hazardous and toxic elements.

THE WALL STREET JOURNAL

"Green Chemistry Wins Converts"

CNN

October 9, 2007

Environmental awareness fuels green chemistry

- Story Highlights
- Green chemistry: The development of products that won't hurt the environment
- Only about a dozen colleges teach green chemistry
- Yale chemistry director: Green chemistry is useless unless it is profitable
- Businesses are seeking graduates with backgrounds in green chemistry

The bottom line on green design

"People who originally thought green chemistry was just about environmental concerns are now seeing that it also increases process efficiencies," says Paul Anastas, professor of green chemistry at the Center for Green Chemistry and Green Engineering at Yale University in the US, who is seen by many as the father of green chemistry. "This is an engine for the innovation side of the business and an ability to distinguish yourself in the market with new products with new capabilities."

The Economist

Definition of the Field

- ***GREEN CHEMISTRY:***

  The design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances.

Twelve Principles of Green Chemistry

1. It is better to prevent waste that to treat or clean up waste after it is formed.
2. Synthetic methods should be designed to maximize the incorporation of all materials used in the process into the final product.
3. Wherever practicable, synthetic methodologies should be designed to use and generate substances that possess little or no toxicity to human health and the environment.
4. Chemical products should be designed to preserve efficacy of function while reducing toxicity.
5. The use of auxiliary substances (e.g. solvents, separation agents, etc.) Should be made unnecessary wherever possible and, innocuous when used.
6. Energy requirements should be recognized for their environmental and economic impacts and should be minimized. Synthetic methods should be conducted at ambient temperature and pressure.
7. A raw material of feedstock should be renewable rather than depleting wherever technically and economically practicable.
8. Reduce derivatives - Unnecessary derivatization (blocking group, protection/ deprotection, temporary modification) should be avoided whenever possible.
9. Catalytic reagents (as selective as possible) are superior to stoichiometric reagents.
10. Chemical products should be designed so that at the end of their function they do not persist in the environment and break down into innocuous degradation products.
11. Analytical methodologies need to be further developed to allow for real-time, in-process monitoring and control prior to the formation of hazardous substances.
12. Substances and the form of a substance used in a chemical process should be

Twelve Principles? Isn’t that how it is done now?

- Entire industries are geared toward cleaning up after wasteful chemical syntheses.
- Industrial chemicals do not have minimal hazard as a performance criterion
- Persistence of chemicals in the biosphere and in our bodies is a major global health issue. (CDC >150 chemicals since 1945)
- The vast majority of organic chemicals are made by depleting (non-renewable) feedstocks
- Our chemical industry deals with safety through engineering and security through barricades.

The Change in Thinking

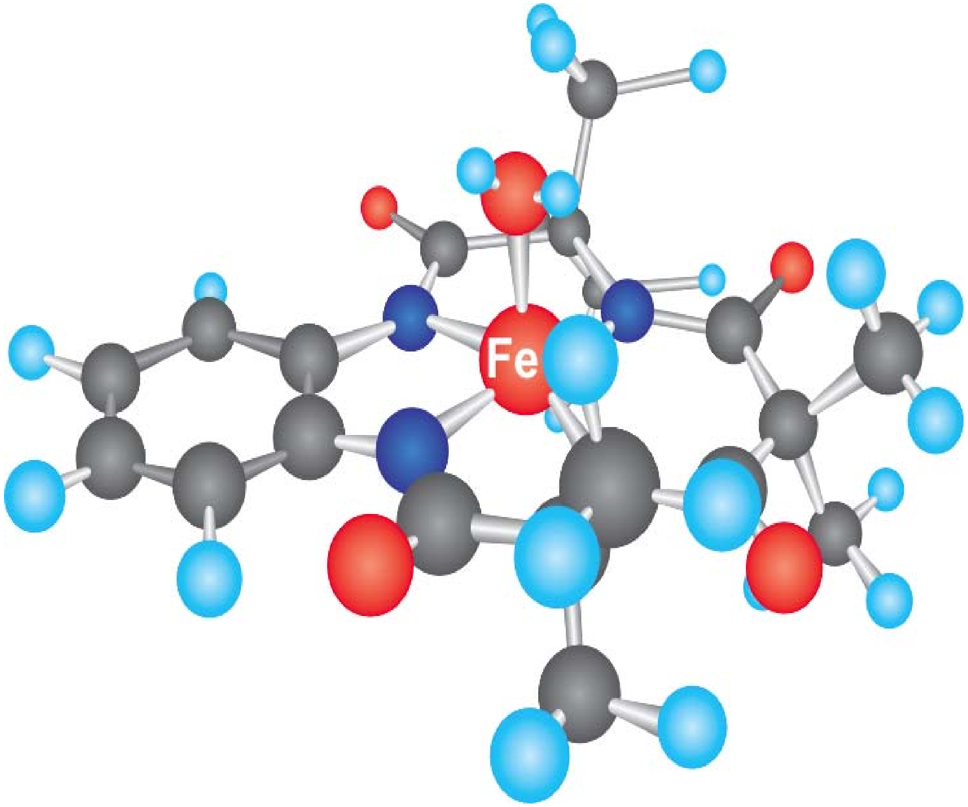
- Hazard must be recognized as a ***design flaw***

- Green Chemistry moves our consideration of how to deal with environmental problems from the ***circumstantial*** to the ***intrinsic.***

Circumstantial

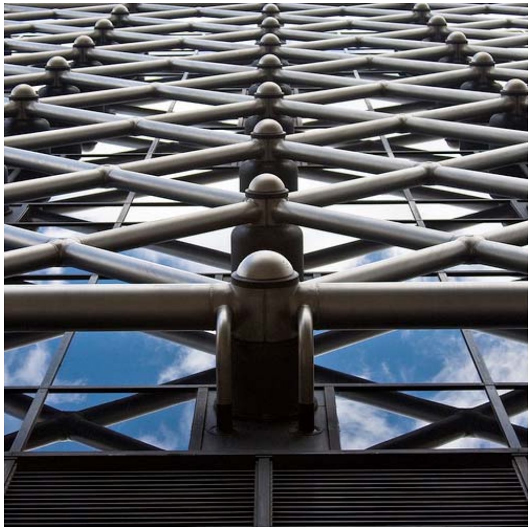
- Circumstantial
  - Use
  - Exposure
  - Handling
  - Treatment
  - Protection
  - Recycling
  - Costly

Intrinsic



- Intrinsic
  - Molecular design for reduced toxicity
  - Reduced ability to manifest hazard
  - Inherent safety from accidents or terrorism
  - Increased potential profitability

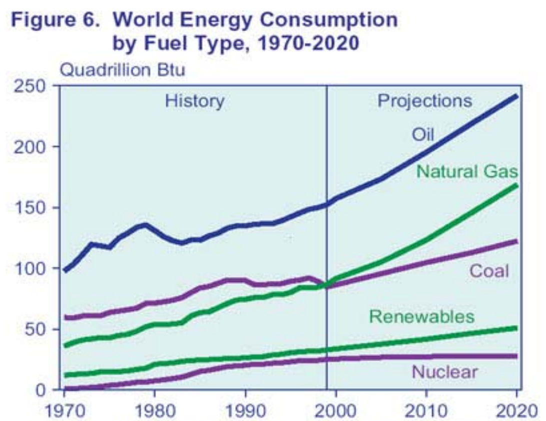
Everything in a building is made of is a chemicals



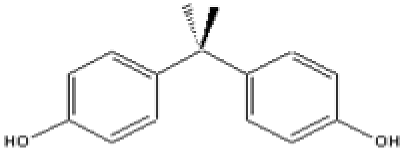
- Its exoskelton
- Its framework
- Its utility systems
- Its grouts, adhesives, paints, coatings, carpets, etc.

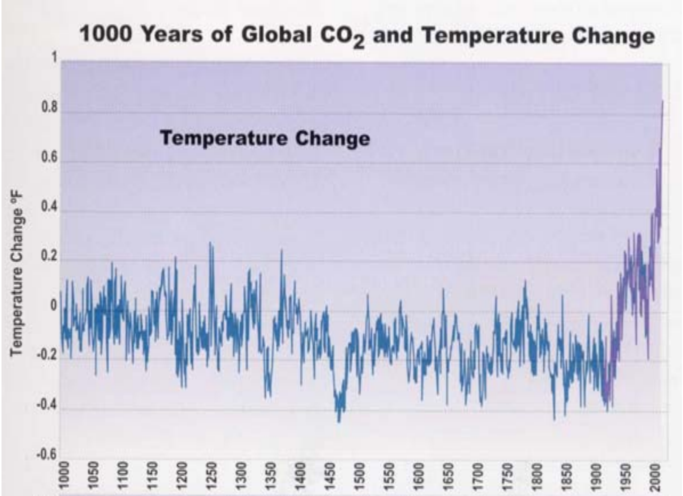
Sustainability Challenges

- Energy
- Water
- Climate
- Health
- Food production
- Toxics



Sources: **History:** Energy Information Administration (EIA), Office of Energy Markets and End Use, International Statistics Database and *International Energy Annual 1999*, DOE/EIA-0219(99) (Washington, DC, February 2001). **Projections:** EIA, World Energy Projection System (2002).



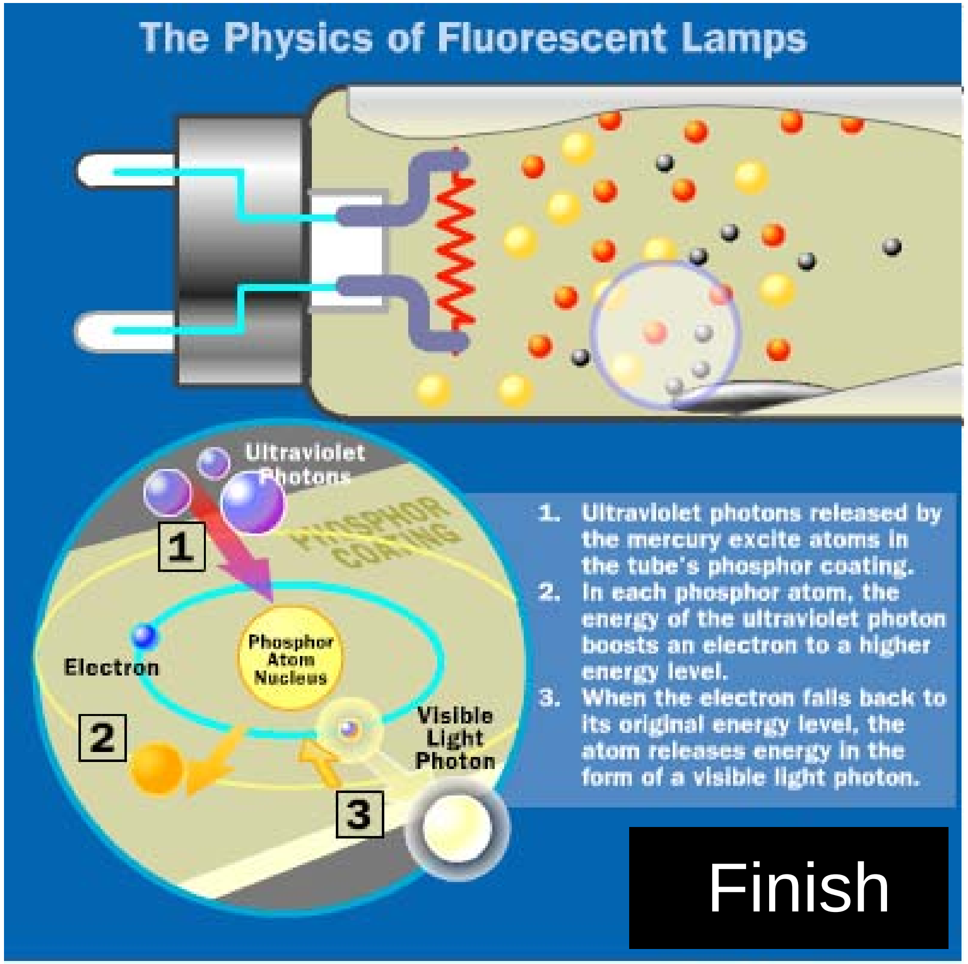


Doing the right things wrong

- Biofuels that compete with crops
- Purifying water with acutely lethal substances
- Energy-saving compact fluorescent light bulbs based on mercury
- Precious, rare, toxic metals in photovoltaics
- Agricultural crop efficiency from persistent pesticides
- Health care - Pharmaceutical manufacture that generates 100s to 1000s of times more waste than product




An example of doing the right things wrong in the built environment


The Physics of Fluorescent Lamps
Ultraviolet Photons
PHOSPHOR COATING
1
Phosphor Atom Nucleus
Electron
2
3
Visible Light Photon
1. Ultraviolet photons released by the mercury excite atoms in the tube's phosphor coating.
2. In each phosphor atom, the energy of the ultraviolet photon boosts an electron to a higher energy level.
3. When the electron falls back to its original energy level, the atom releases energy in the form of a visible light photon.
Finish

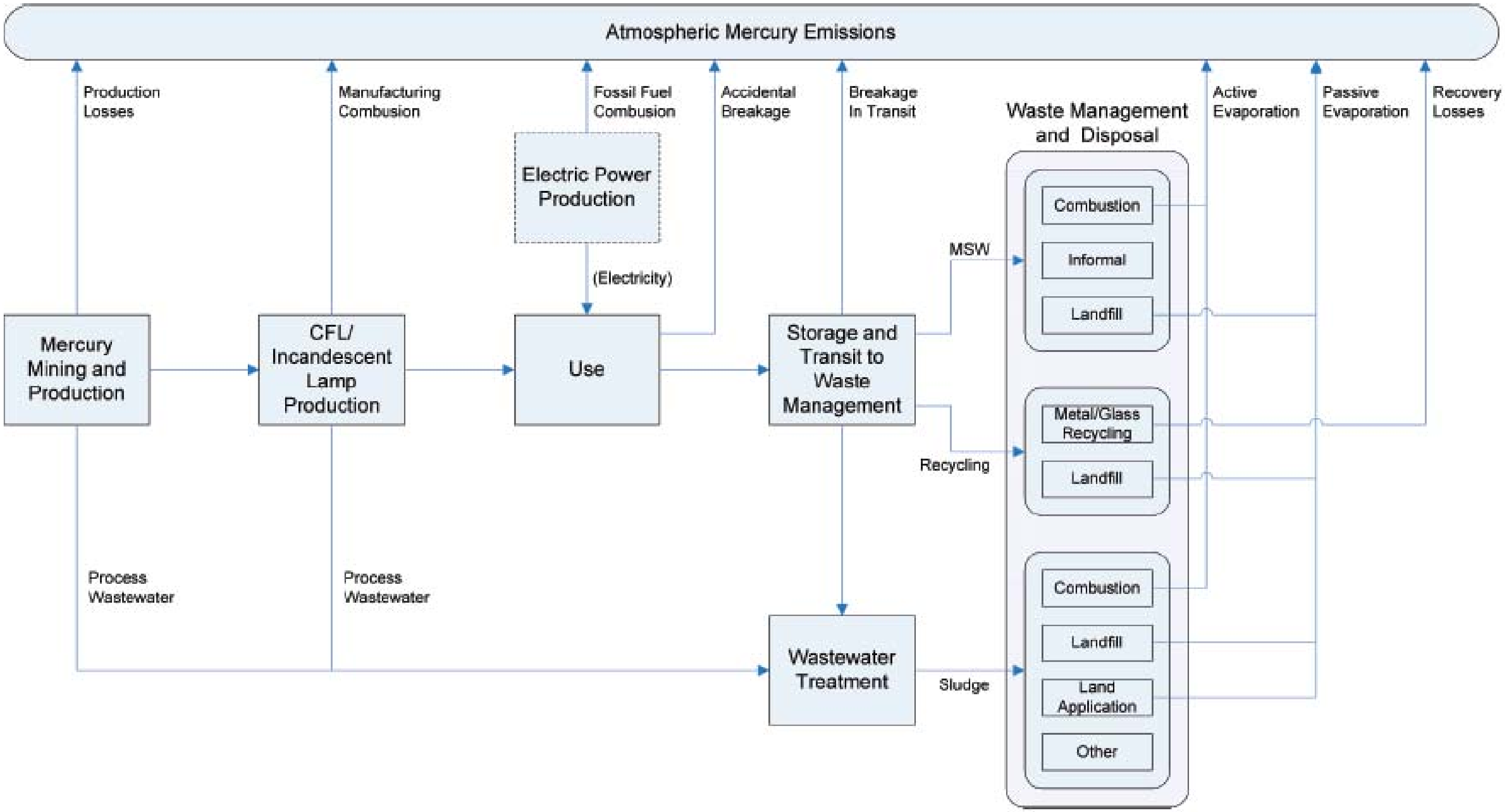


FIGURE 1. Mercury and the life cycle of the CFL. Note: adapted from ref *18*.

Mercury and the life cycle of the CFL

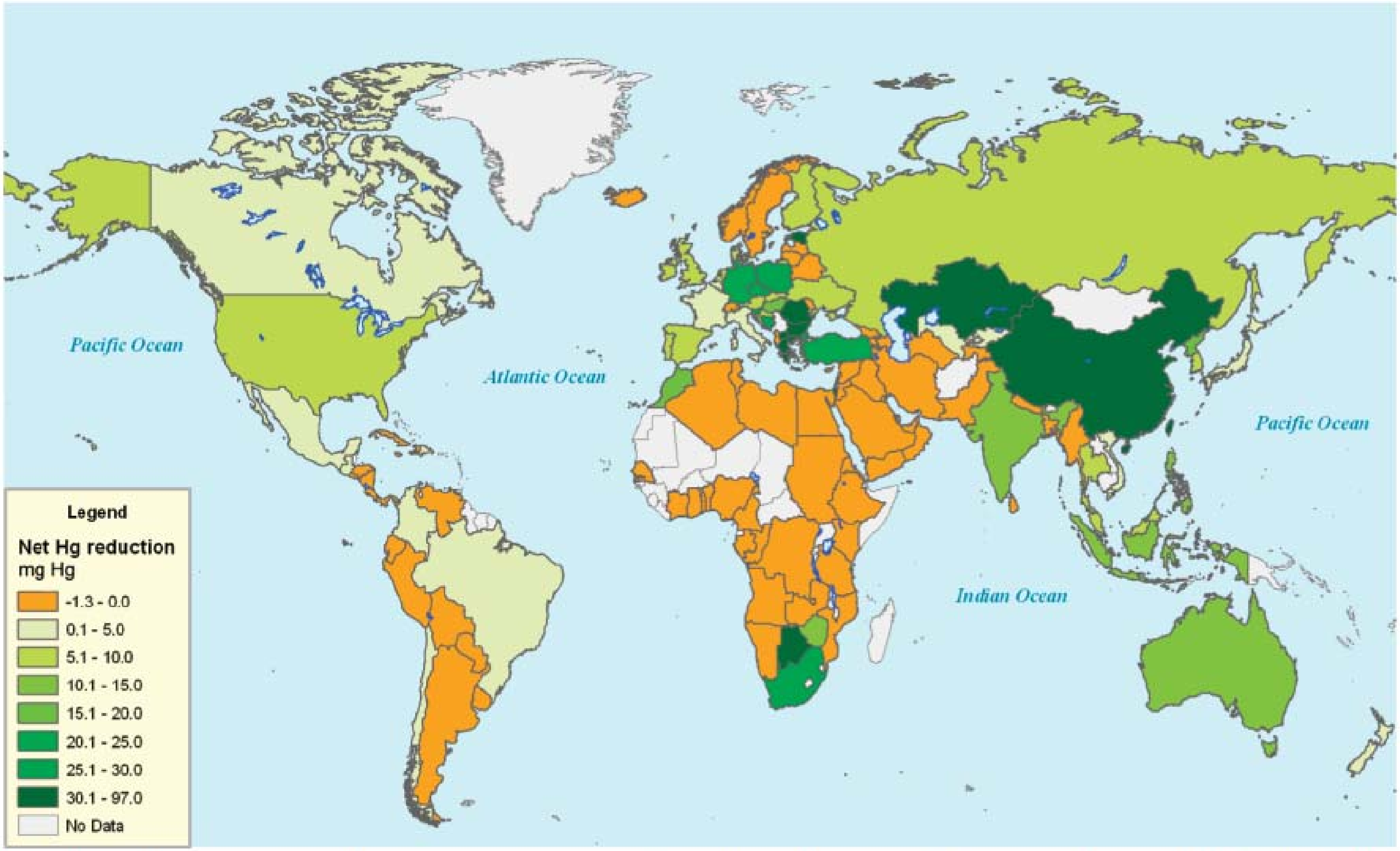
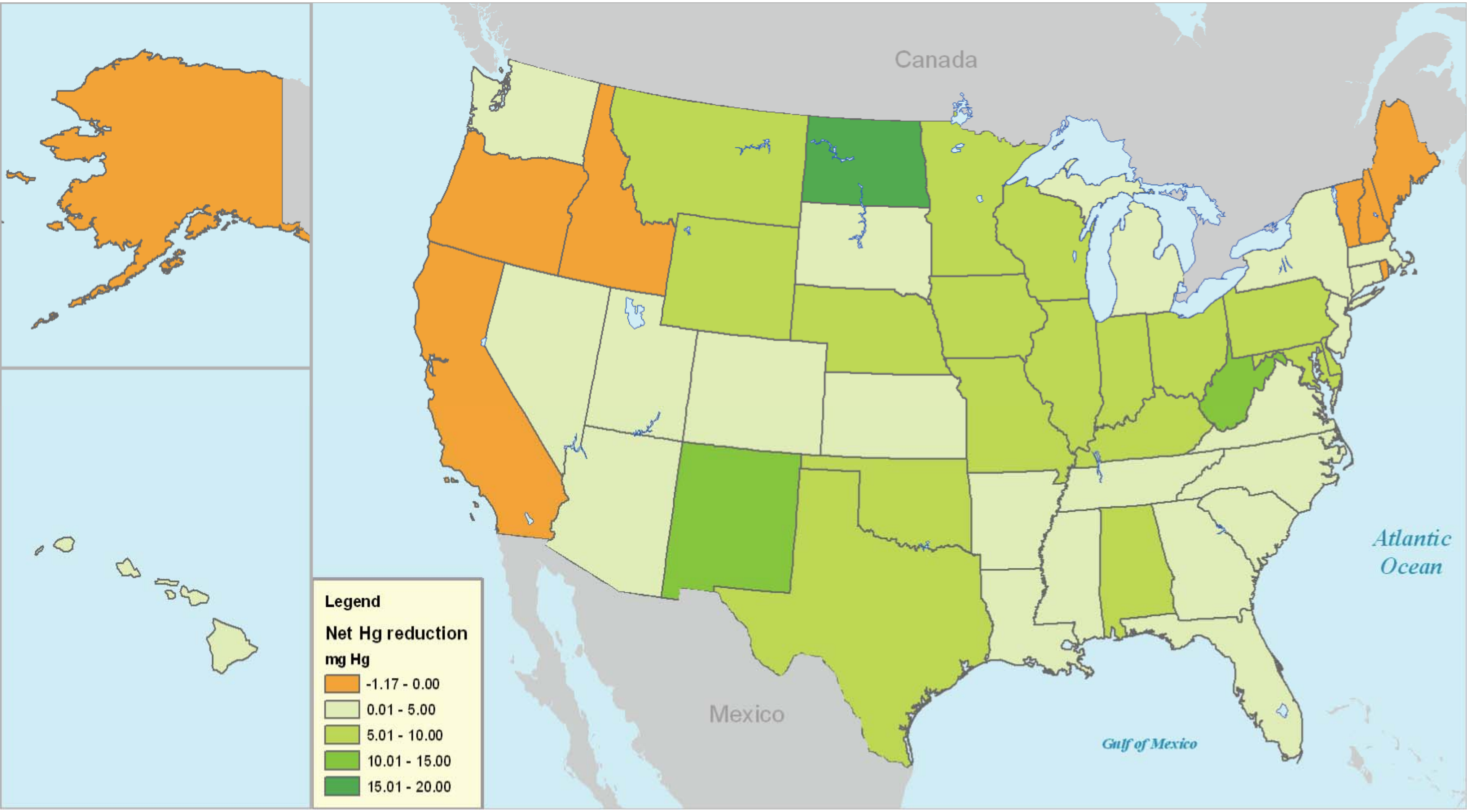
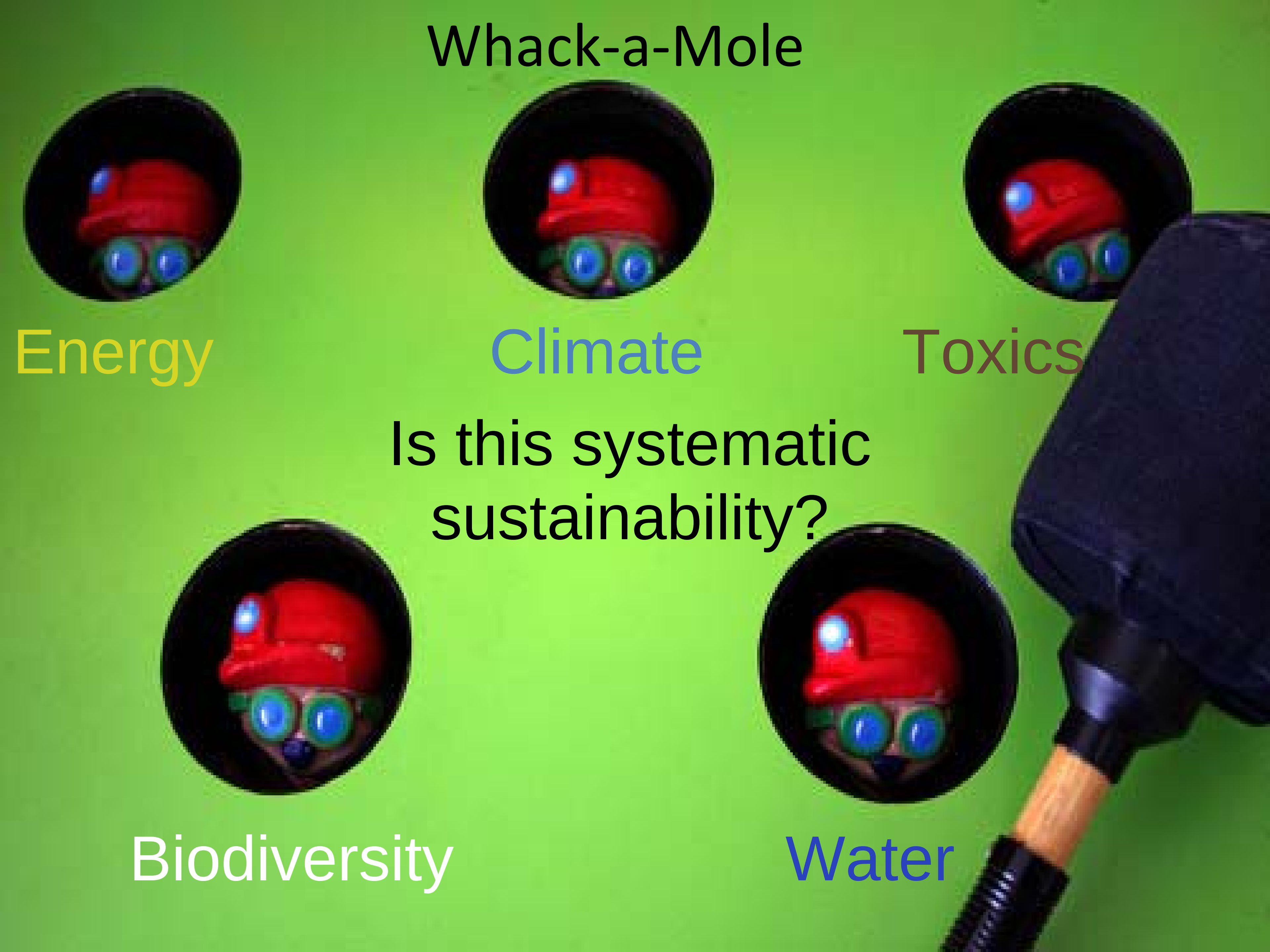


FIGURE 3. Net reduction in atmospheric mercury emissions from the replacement of one incandescent bulb with a CFL in 130 countries.



Net reduction in atmospheric mercury emissions from the replacement of one incandescent bulb with a CFL in the United States.


Whack-a-Mole
Energy
Climate
Toxics
Is this systematic sustainability?
Biodiversity
Water

Principles of Green Engineering

1. Inherent rather than circumstantial
2. Prevention rather than treatment.
3. Design for separation.
4. Maximize mass, energy, space, and time efficiency.
5. “Out-pulled” rather than “input-pushed”.
6. View complexity as an investment.
7. Durability rather than immortality.
8. Need rather than excess.
9. Minimize material diversity.
10. Integrate local material and energy flows.
11. Design for commercial “afterlife”.
12. Renewable and readily available.

Anastas and Zimmerman, Environmental Science and Technology, March 1, 2003

What does this mean for the built environment?

- It means doing the right things right.
- You can’t build a green building from toxic and unsustainable components.
- You can’t bake a delicious cake from rotten eggs and spoiled milk.

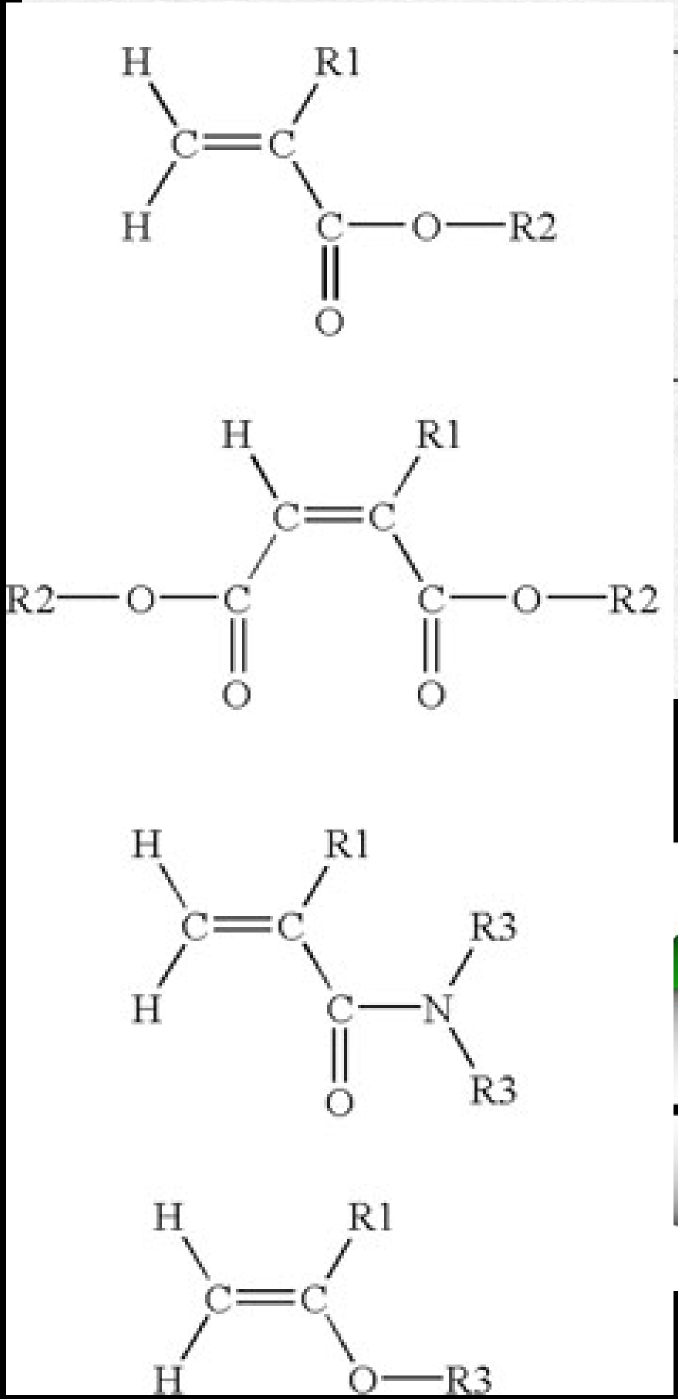
How to do the right things right? Molecular Design-Build

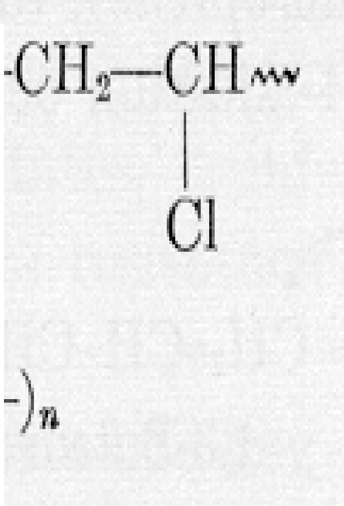
- Know that the real foundation of any building or any structure is the molecules you make it from.
- Understanding the intrinsic nature of the materials.
- Reducing the adverse consequences of materials – the global, physical and environmental hazards

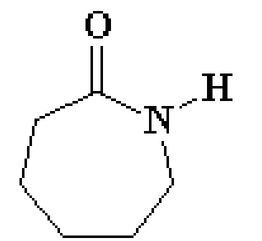
Established Examples of Green Chemistry and Molecular Design-Build

CARPET TILE

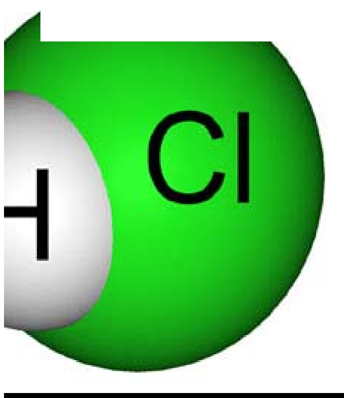
- OUT: PVC backing
- IN: polyolefin resins
- 50% lighter, more durable
- low VOCs, no phthalates
- “infinitely” recyclable



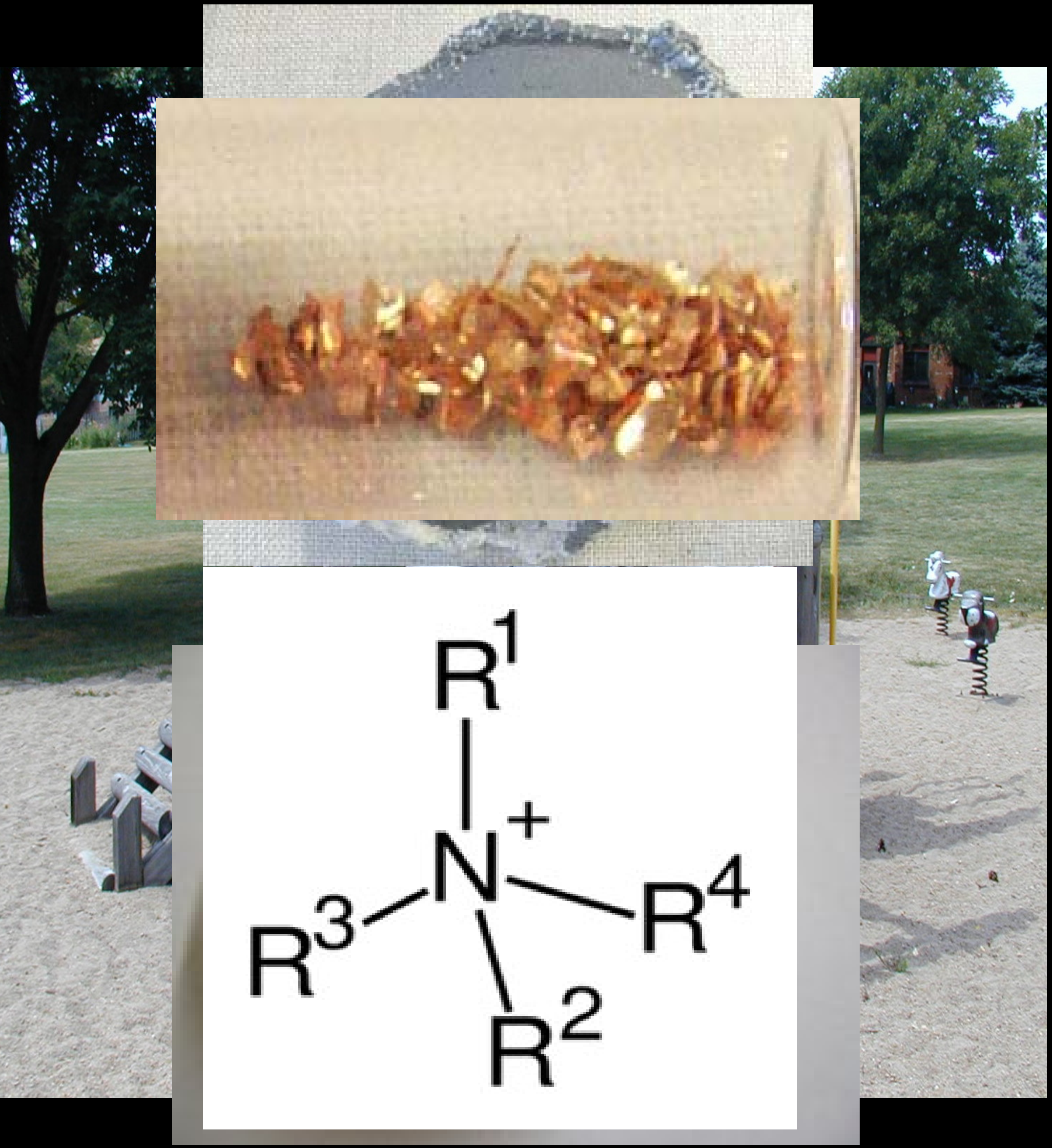




ε-caprolactam



WOOD PRESERVATIVE



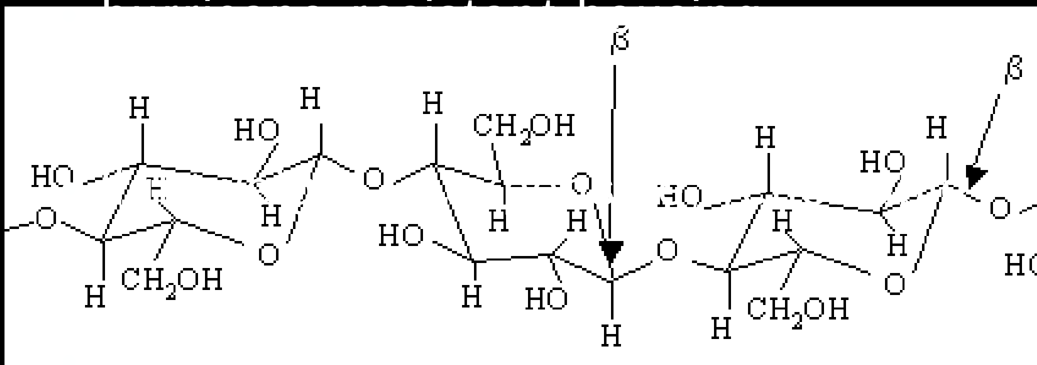
- OUT: chromium(VI) & arsenic
- IN: alkaline copper quaternary
- eliminated 90% of U.S. arsenic use
- no hazardous waste

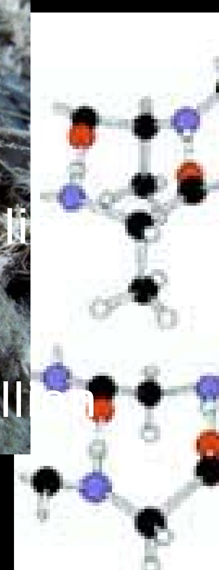
LIGHTING

- OUT: wasted watts, mercury, premature burnout
- IN: LEDs & digital intelligence

- readily replaces existing fixtures
- low energy use
- extremely durable

COMPOSITE STRUCTURES





- non-toxic
- est. energy savings of 100 trilli... Btu by 2020
- est. CO2 reductions of one milli... metric tons per year

ON THE HORIZON

“In situ carbonation of peridotite for CO_2 storage” – Proceedings of the National Academy of Science, Sept. 22, 2008

Peter B. Kelemen and Jürg Matter

- Natural CO_2 sequestration in rock formations in Oman
- Adding 1 wt% CO_2 to the peridotite would consume ¼ of all atmospheric CO_2, an amount approximately equivalent to the increase since the industrial revolution.

Cement and CO2

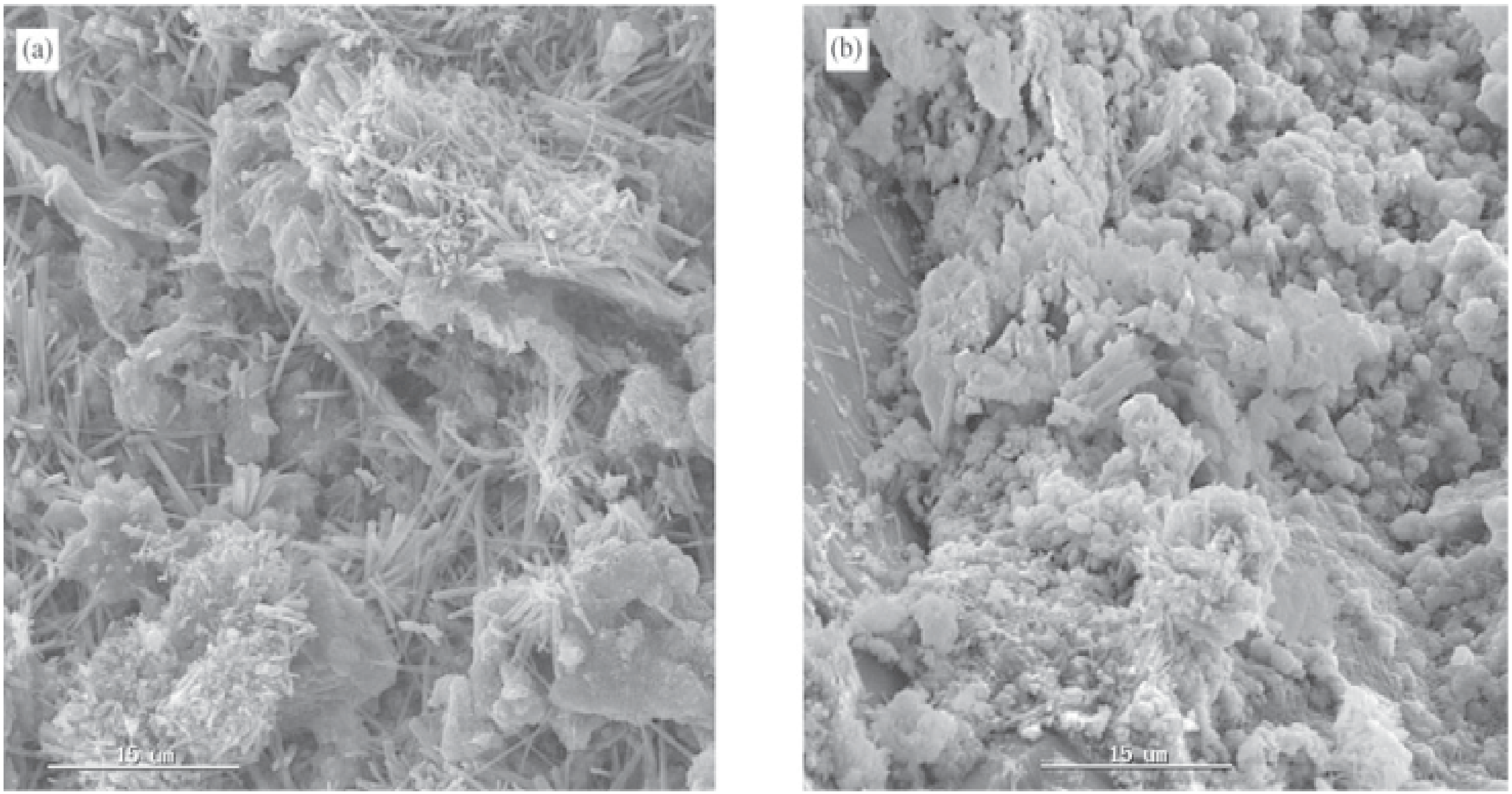
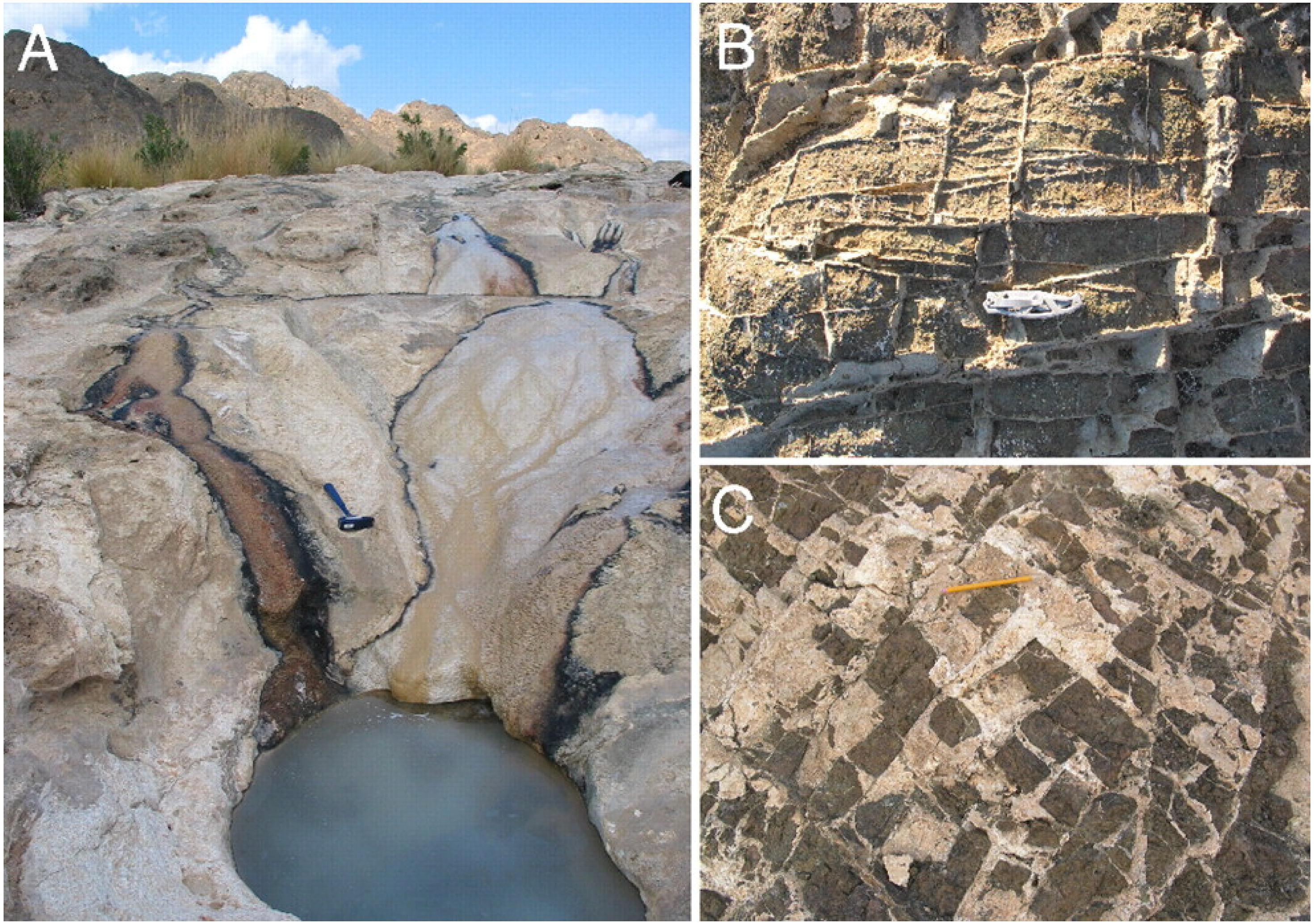


Figure 3. Photomicrographs of Concrete: a) region of formation of ettringite; b) portlandite and calcium silicates.

Silva, et al., Met. Res., 2002

Photographs of travertine and carbonate veins in Oman



Kelemen P. B., Matter J. PNAS 2008;105:17295-17300


We must think of trees as more than just dumb lumber…

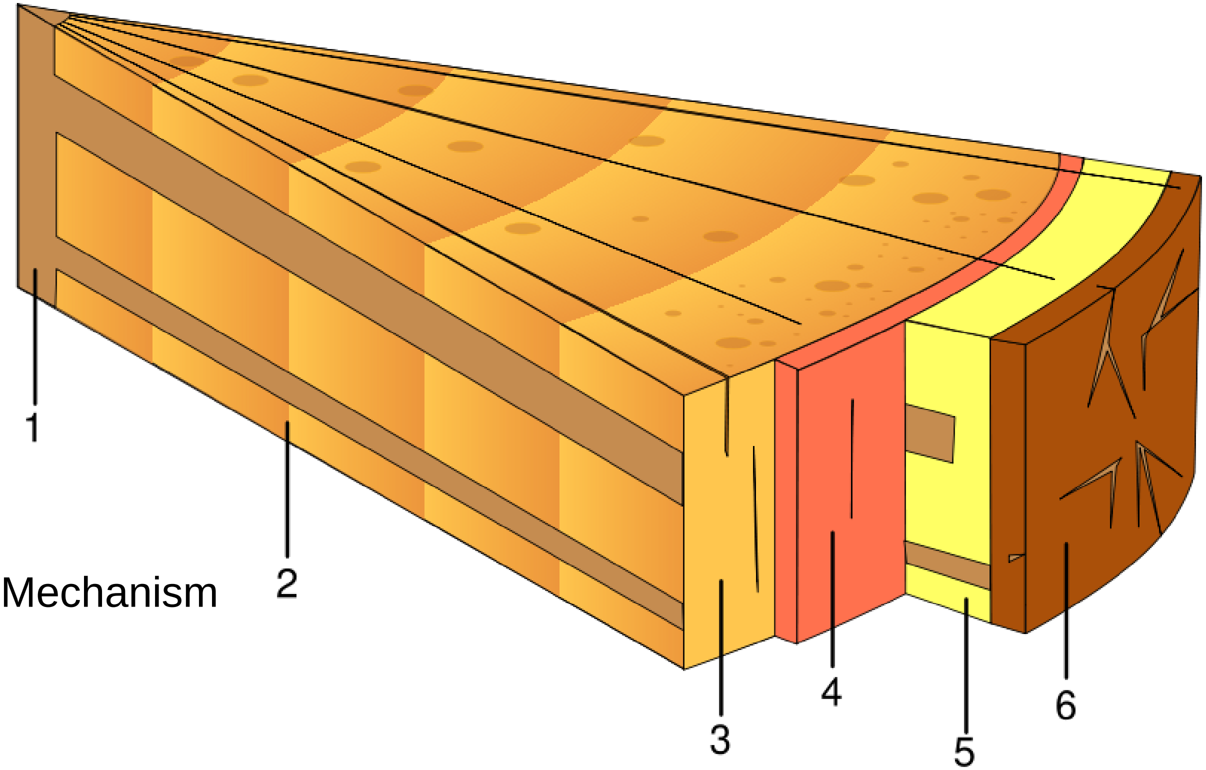
It's not that it doesn't work as a computer,
It just works better as a paperweight.

1 : Pith
Vertical Nutrient Transport

2 : Ray
Horizontal Nutrient Transport

3 : Heartwood/Sapwood
Structural Support / Self Healing Mechanism

4 : Vascular Cambium
Growth Mechanism

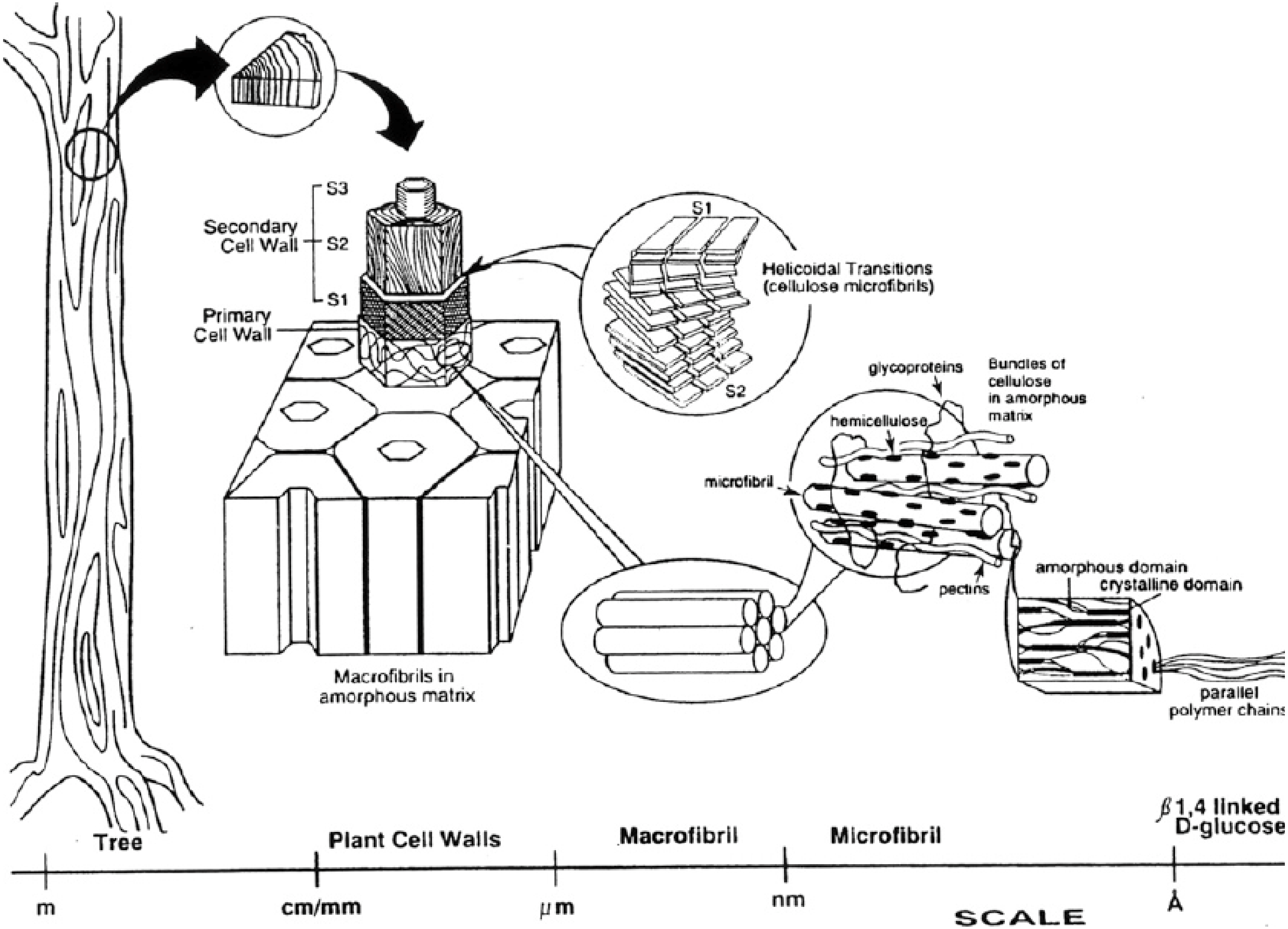


Structural Components of Wood

5 : Living Phloem/Cork Cambium
Secondary Integument Layer

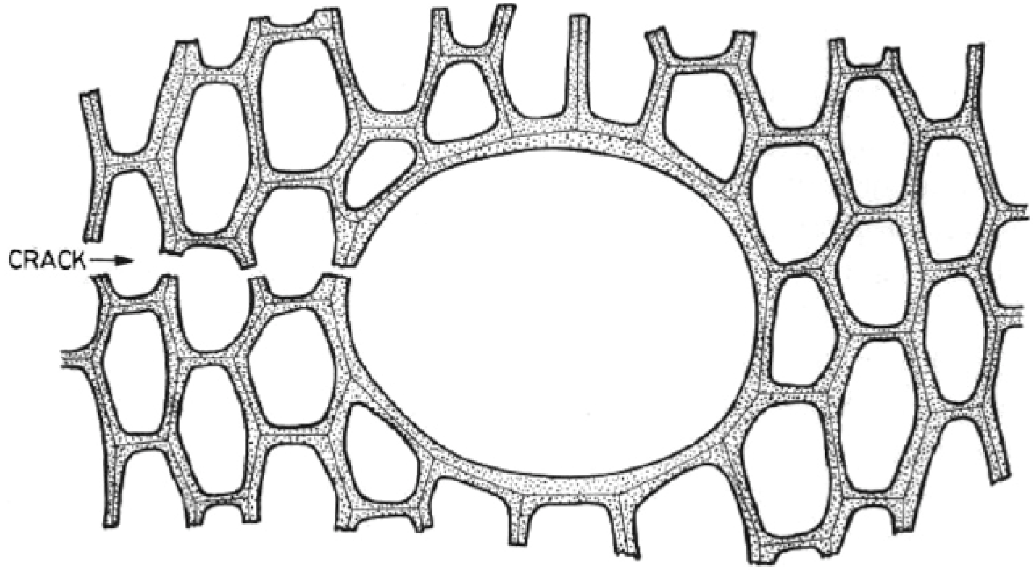
6 : Cork
Primary Integument Layer

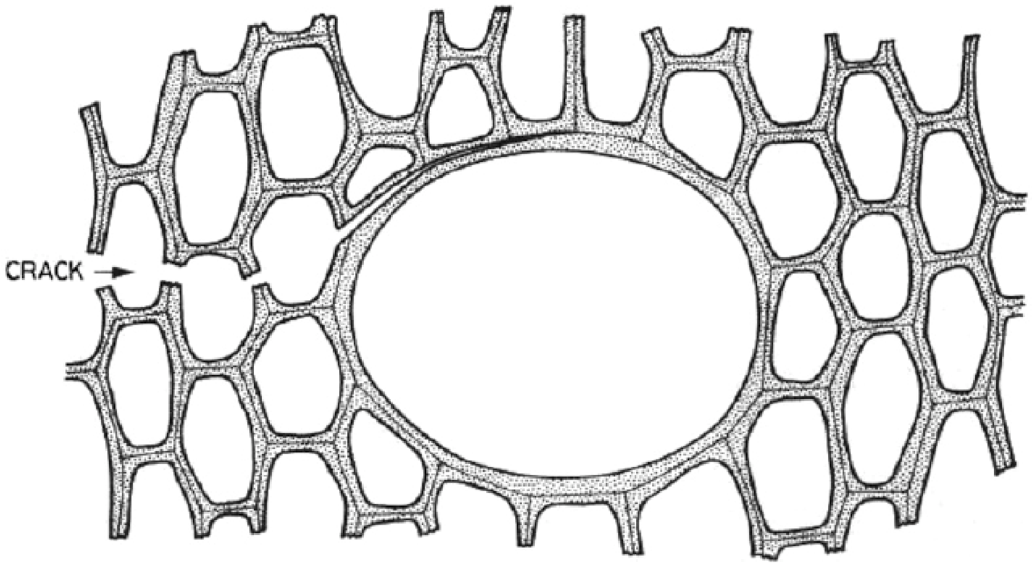
Bark



Hierarchical structure of cellulose in wood.

Ref. 5

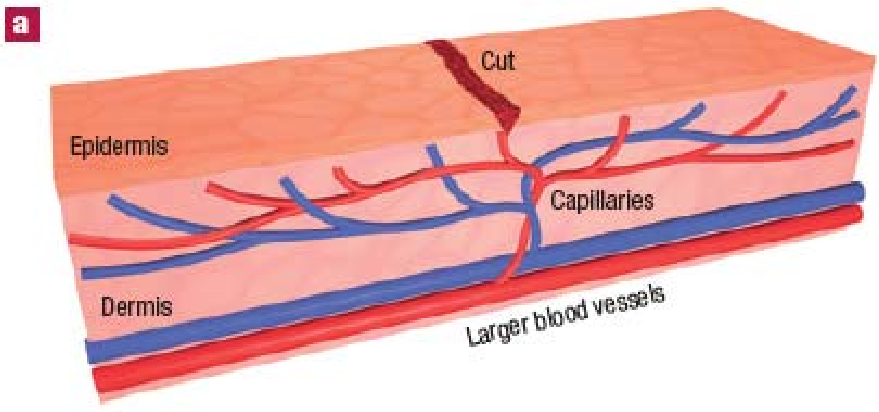




Natural systems are far more advanced: micro-vascular networks

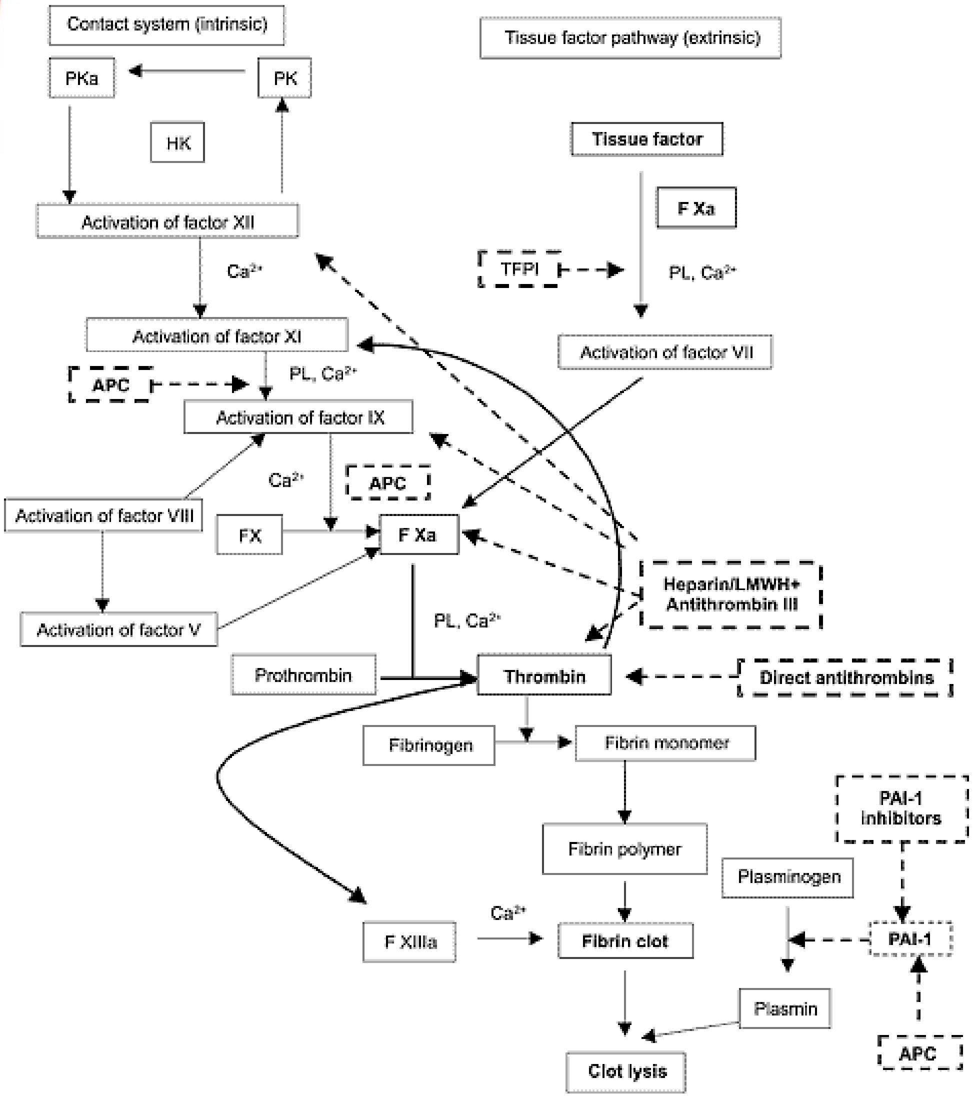
Cross section of woody species sap channel. (a) Schematic drawing of crack breaking into a sap channel, (b) a schematic drawing of crack splitting the wall of a sap channel.

Ref. 14



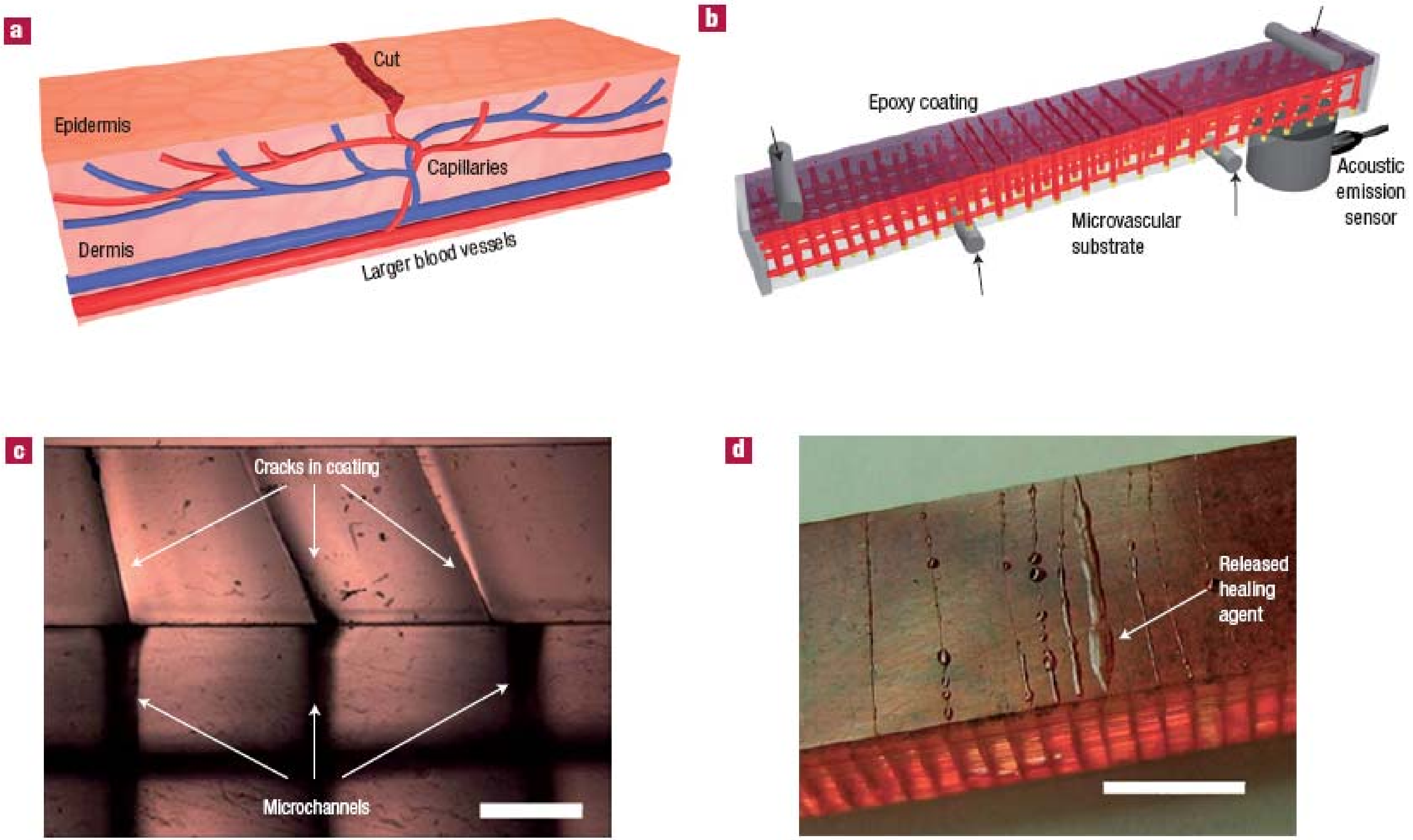
Our bodies have evolved very complex healing mechanisms.

When the skin is punctured and blood is exposed to air a complex oxidation pathway (right) is initiated which ultimately results in the closure of the wound.

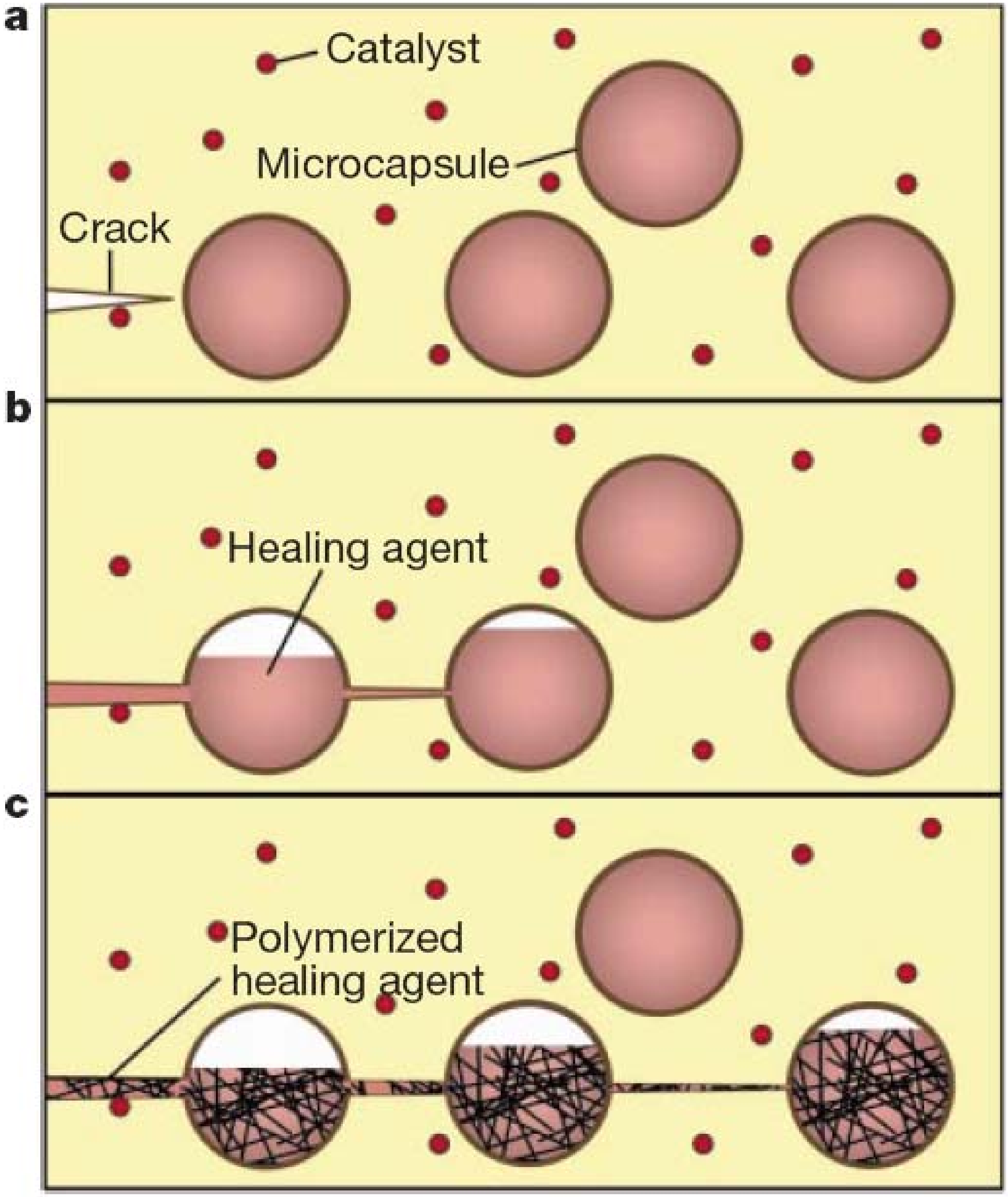


Ref. 15

Researchers have enjoyed great success in mimicking this process using synthetic materials.



Ref. 15



The autonomic healing concept

A microencapsulated healing agent is embedded in a structural composite matrix containing a catalyst capable of polymerizing the healing agent.

(a) Cracks form in the matrix wherever damage occurs;

(b) the crack ruptures the microcapsules, releasing the healing agent into the crack plane through capillary action;

(c) the healing agent contacts the catalyst, triggering polymerization that bonds the crack faces closed.

Ref. 13

Not enough to be inspired by nature's final products…

We must also be inspired by nature's processes…

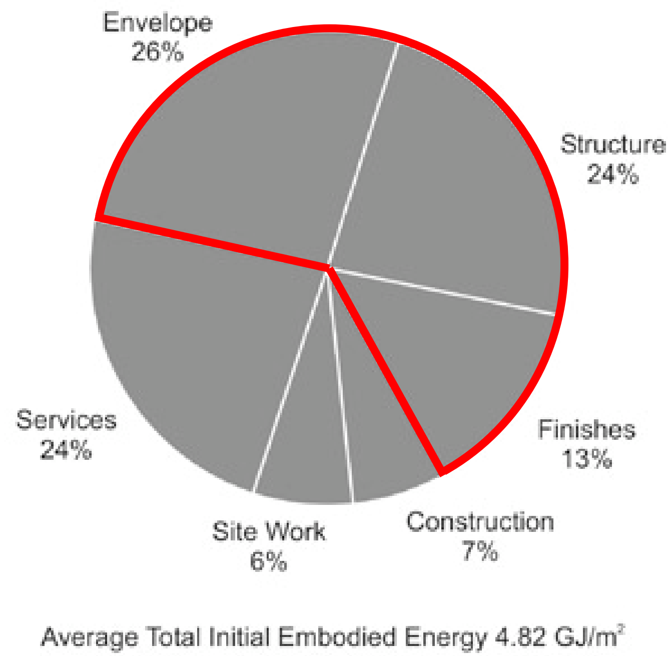
Local, renewable resources.

Ambient temperature and pressure.

Resilience.

	EMBODIED ENERGY	
MATERIAL	MJ/kg	MJ/m3
Aggregate	0.10	150
Straw bale	0.24	31
Soil-cement	0.42	819
Stone (local)	0.79	2030
Concrete block	0.94	2350
Concrete (30 Mpa)	1.3	3180
Concrete precast	2.0	2780
Lumber	2.5	1380
Brick	2.5	5170
Cellulose insulation	3.3	112
Gypsum wallboard	6.1	5890
Particle board	8.0	4400
Aluminum (recycled)	8.1	21870
Steel (recycled)	8.9	37210
Shingles (asphalt)	9.0	4930
Plywood	10.4	5720
Mineral wool insulation	14.6	139
Glass	15.9	37550
Fiberglass insulation	30.3	970
Steel	32.0	251200
Zinc	51.0	371280
Brass	62.0	519560
PVC	70.0	93620
Copper	70.6	631164
Paint	93.3	117500
Linoleum	116	150930
Polystyrene Insulation	117	3770
Carpet (synthetic)	148	84900
Aluminum	227	515700

NOTE: Embodied energy values based on several international sources - local values may vary.



Average embodied energy of buildings

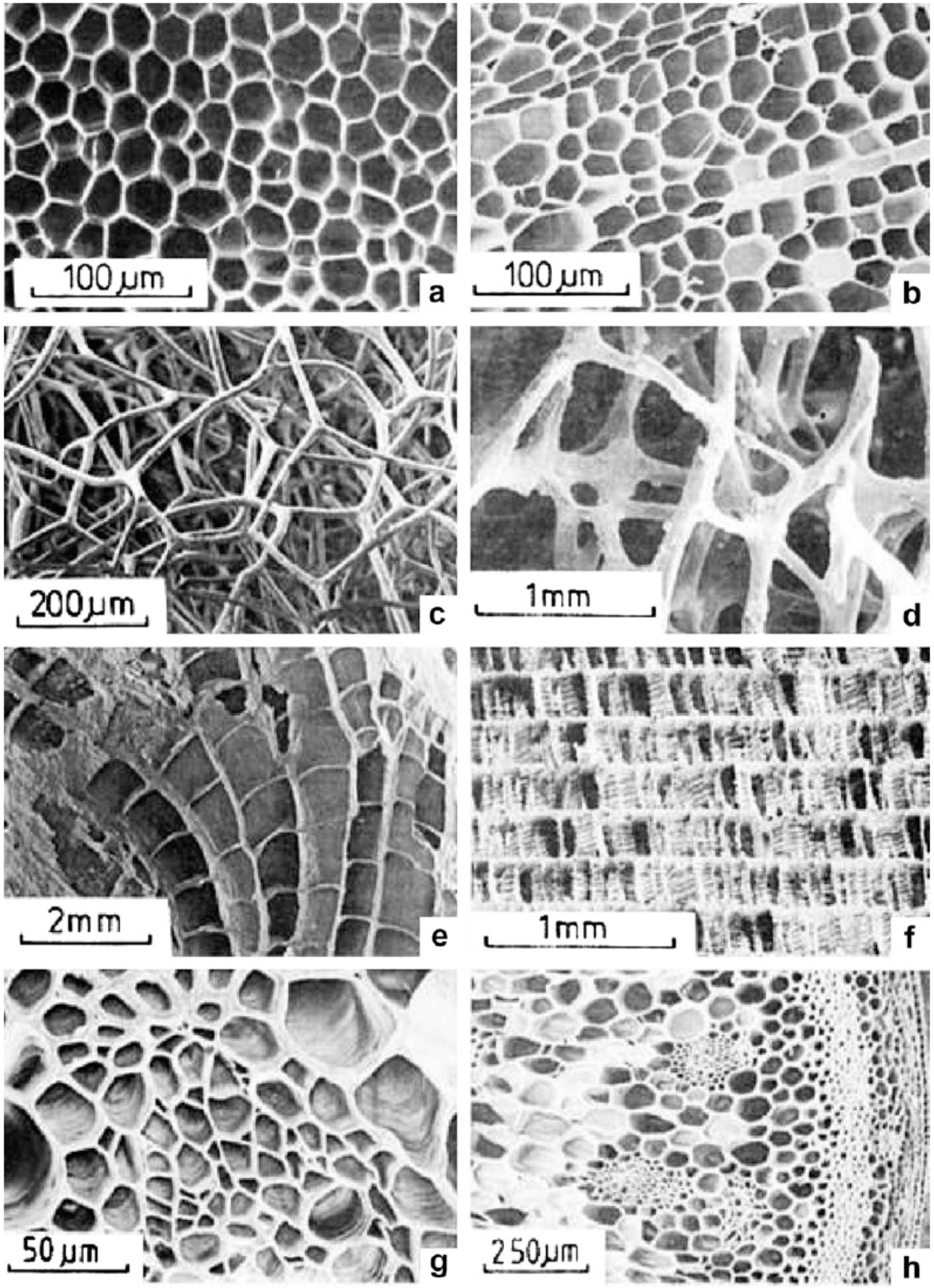
Average embodied energy of common building materials

1. Cole, R.J., Kernan, P.C. Build Environ 1996; 31:4:307-317.

Giants Causeway

Bushmills, Northern Ireland

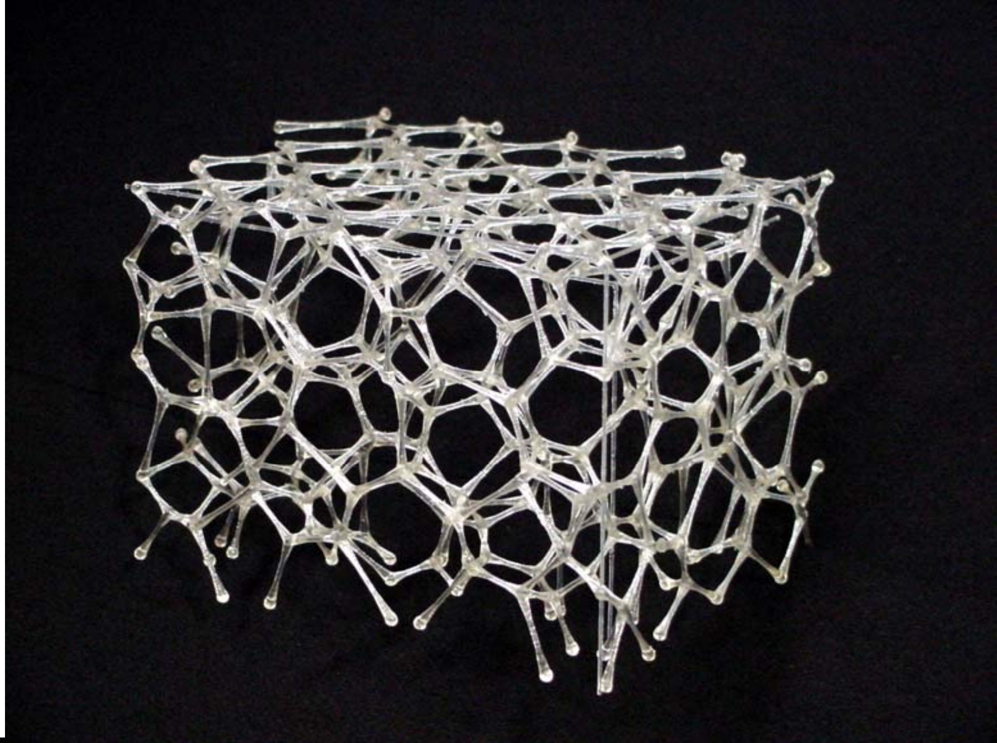
All throughout nature, regular structural forms emerge through basic processes of self assembly.

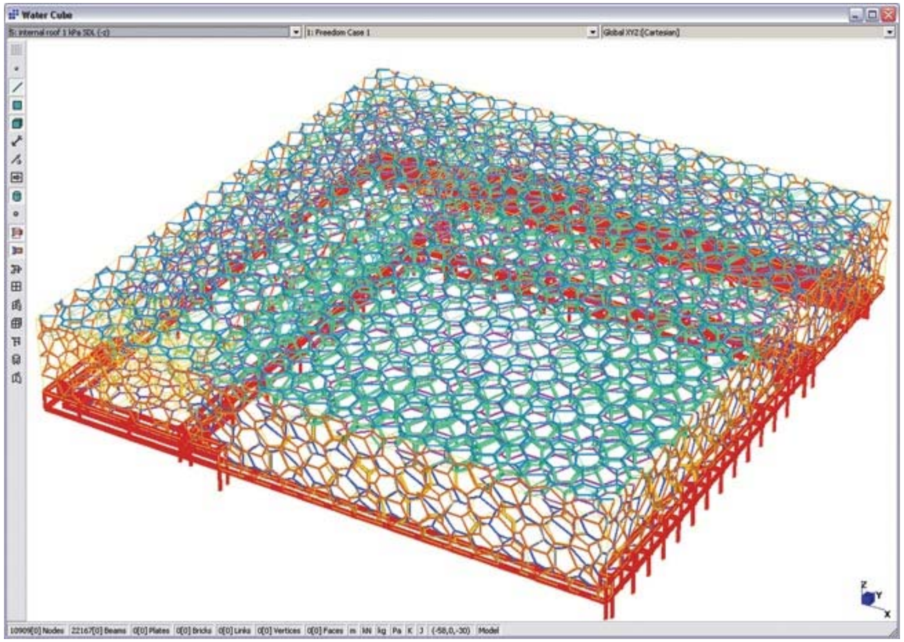


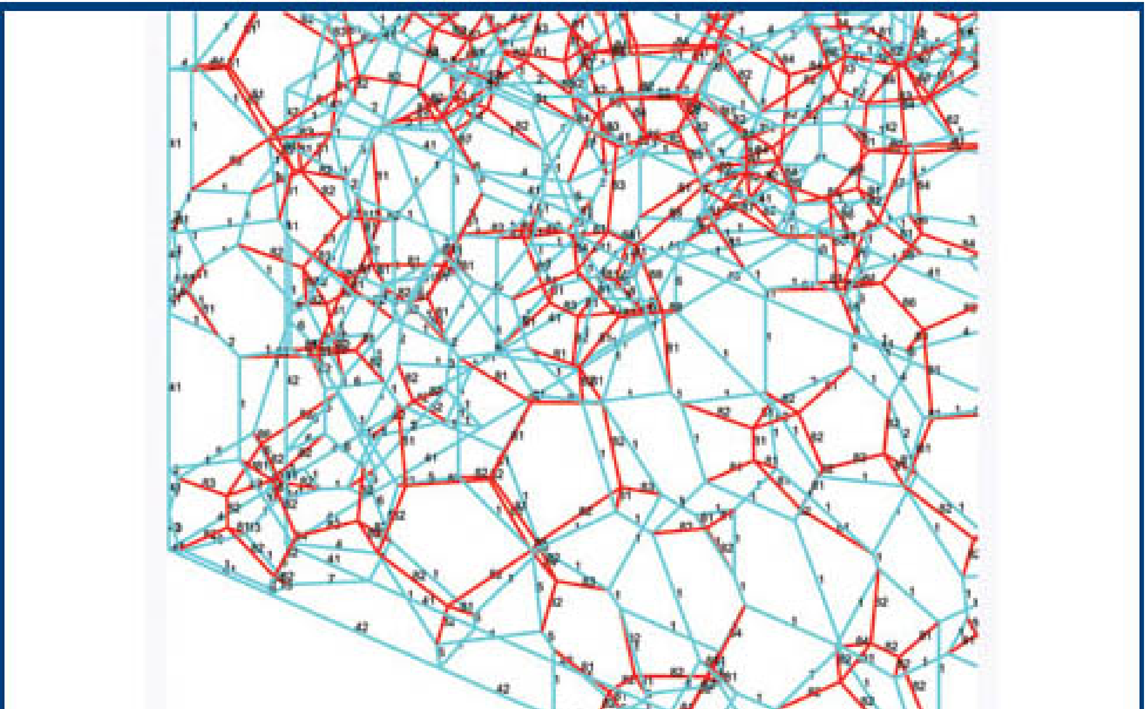
SEM micrographs of some other irregular cellular networks (all with high structural efficiencies):

(a) cork (b) balsa (c) sponge (d) cancellous bone (e) coral (f) cuttlefish (g) iris leaf (h) stalk of a plant

Ref. 14



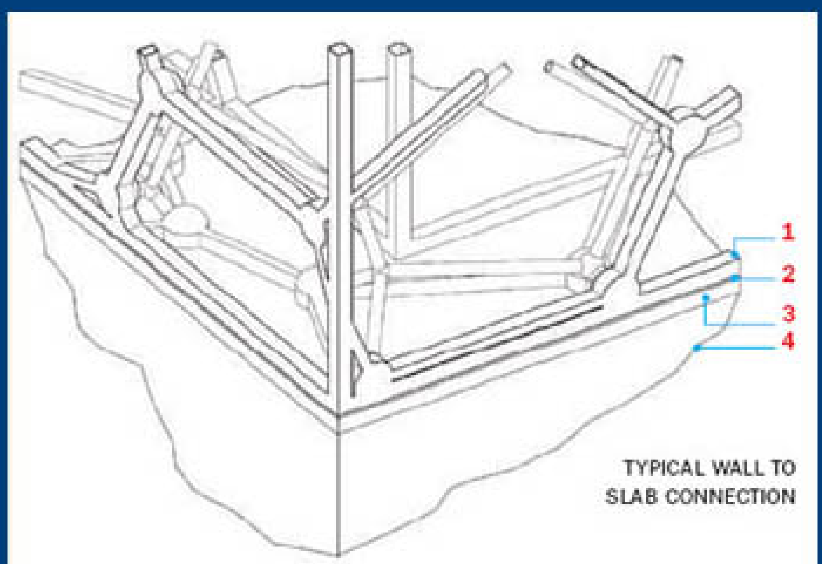

Water Cube
1: Freedom Case 1
Global XYZ [Cartesian]
10909[0] Nodes
22167[0] Beams
0[0] Plates
0[0] Bricks
0[0] Links
0[0] Vertices
0[0] Faces
m
kN
kg
Pa
K
J
(-58,0,-30)
Model
Z
Y
X



Software that Arup developed helped designers optimize and size these components (above) and generate a 3D model as well as traditional 2D construction documents (below).

1. Base of space frame
2. Steel plate
3. Steel angle
4. Concrete slab

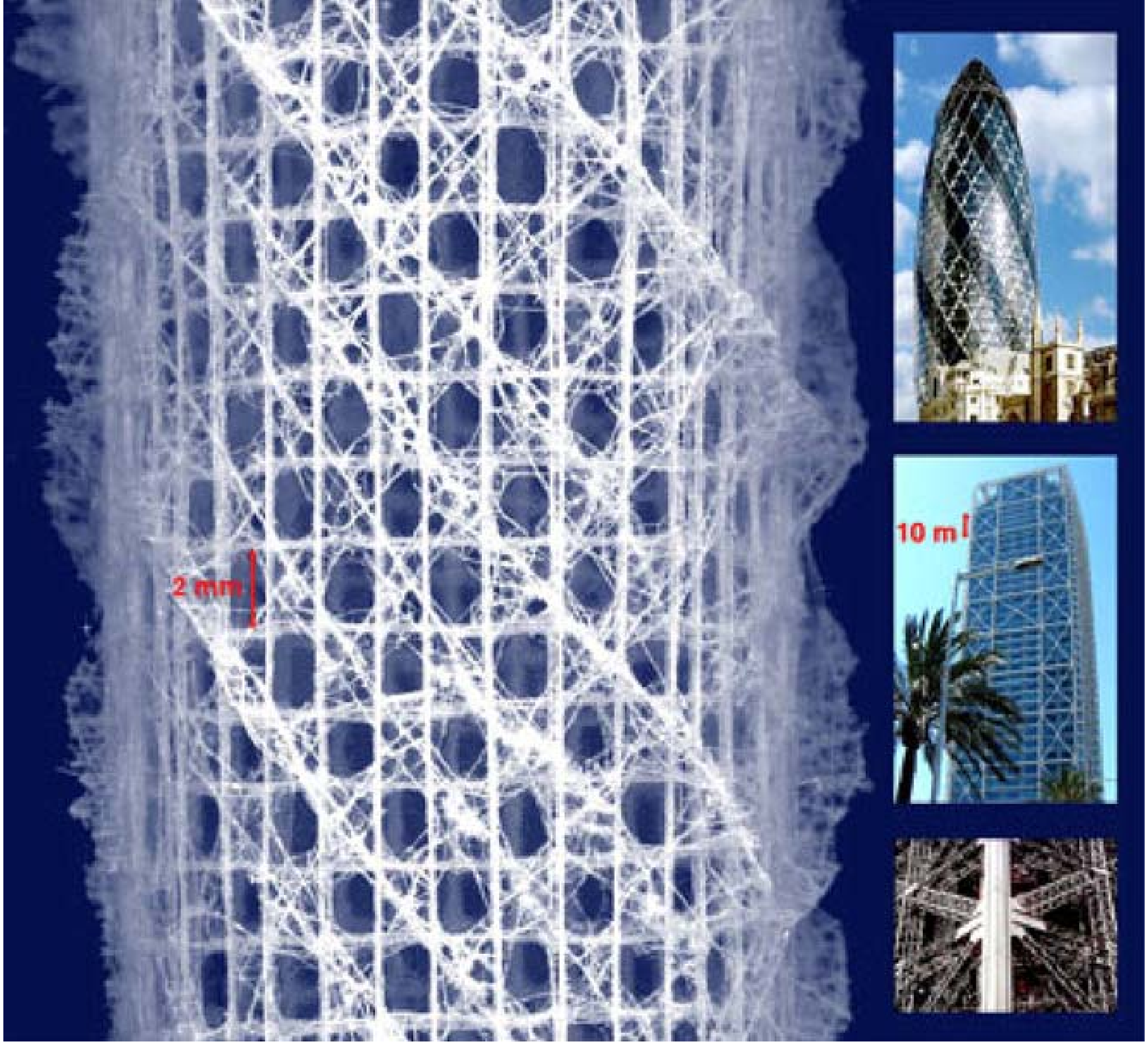
Drawings courtesy Arup



The rapid maturation of computational engineering software has made it possible to implement complex Biomimetic structural designs
such as those developed for the Water Cube.

The availability of BIM tools means that non-linear or irregular architectural forms no longer pose such a significant construction

challenge



Skeleton of the deep sea sponge *Euplectella* compared to various modern architectural forms

Ref. 18

So, how do ensure that we do the right things right from the start?

- Molecular perspective
- Environmental Health perspective
- Engineering perspective
- Construction perspective
- Architecture perspective
- Design perspective
- Operations and maintenance perspective
- Occupant perspective

EXPAND

- Design-Build concept to include chemists and material scientists
- Redefining “performance”
- Opportunities for adaptation, evolution, dynamic response within a “static” structure
- Integration of resiliency
- “Green Building” to address hazard reduction and sustainability at the molecular level

Final Thoughts

- The compass is more important than the speedometer.
- The accomplishments of Green Chemistry thus far are a fraction of what is possible in the future.
- A design framework that incorporates inherent sustainability can facilitate transformative innovation.
- Molecular Design-Build because we can.
- Molecular Design-Build because we must.

- End