Green Chemistry:
The Missing Element in Chemistry Education

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Disclaimer

Do Chemistry
1988-1997 Worked in Industry (Polaroid) for 10 years.

Teach Chemistry
1996-2007 Worked in Academia (UMASS) for 11 years.

Invent Chemistry
Over 250 Patents and Publications.

Invest in Chemistry
2007- Cofounded an Entrepreneurial For-Profit Company (WBI)

Manage Chemistry
1990 - Active in Green Chemistry (US EPA, CA DTSC, MA TURA)
Today’s Talk:

- Doing Chemistry
- Teaching Chemistry
- Inventing Chemistry
- Investing in Chemistry
- Managing Chemistry
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For over 180 years of “Modern Chemistry”...

But Nature...

Heat things under high temperature

Runs reactions at “room” temperature

Apply high pressures

Runs reactions at ambient pressure

Use organic solvents

Uses water as a solvent
A thermometer is a molecular speedometer...
Molecular reactivity is based on specific geometries.

Most molecular collisions do not result in a chemical reaction.

By heating up a reaction, or putting it under pressure, we increase the velocity of the molecules, and thus the frequency of the collisions.

This increases both the non-productive and reaction producing collisions.

There is NEVER a REACTIVE COLLISION in Nature!

In nature, molecules for the most part first from some form of complex or assembly, that orients the reactive orbitals.

I called this Non-Covalent Derivatization.
Green Chemistry is the **design** of chemical products and processes that reduce or eliminate the **use** and/or **generation** of hazardous substances.
The Twelve Principles of Green Chemistry

1. **Prevention.** It is better to prevent waste than to treat or clean up waste after it is formed.

2. **Atom Economy.** Synthetic methods should be designed to maximize the incorporation of all materials used in the process into the final product.

3. **Less Hazardous Chemical Synthesis.** Whenever practicable, synthetic methodologies should be designed to use and generate substances that possess little or no toxicity to human health and the environment.

4. **Designing Safer Chemicals.** Chemical products should be designed to preserve efficacy of the function while reducing toxicity.

5. **Safer Solvents and Auxiliaries.** The use of auxiliary substances (solvents, separation agents, etc.) should be made unnecessary whenever possible and, when used, innocuous.

6. **Design for Energy Efficiency.** 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. **Use of Renewable Feedstocks.** A raw material or feedstock should be renewable rather than depleting whenever technically and economically practical.

8. **Reduce Derivatives.** Unnecessary derivatization (blocking group, protection/deprotection, temporary modification of physical/chemical processes) should be avoided whenever possible.

9. **Catalysis.** Catalytic reagents (as selective as possible) are superior to stoichiometric reagents.

10. **Design for Degradation.** Chemical products should be designed so that at the end of their function they do not persist in the environment and instead break down into innocuous degradation products.

11. **Real-time Analysis for Pollution Prevention.** 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. **Inherently Safer Chemistry for Accident Prevention.** Substance and the form of a substance used in a chemical process should be chosen so as to minimize the potential for chemical accidents, including releases, explosions, and fires.
Green Chemistry

More environmentally benign than alternatives

Perform better than alternatives

More economical than alternatives
Green Chemistry

- Safety
- Green Chemistry
- Performance
- Cost
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Of all the products and processes...

Maybe 10% are benign...

Maybe 25% have alternatives available...

65% Still have to be invented!
Carbon-Carbon Bonds
Oxidations
Reductions
Hydroxylations
Polymer Syntheses

Traditional Processes

Green Alternatives
How does Green Chemistry fit into the big picture of Sustainability.
Green Chemistry is also known as sustainable chemistry.
Let's talk about nothing:

There are two issues with the use of “free” and “zero”:

(1) What does “chemical free” mean?
“BPA Free”:

(2) Can we ever have an “anything” free product?

BPA in cash register receipts....

No BPA added in the coating...

Unavoidable trace amounts of BPA in the paper!!!!

So what does “BPA-Free” mean?
Is it achievable?
"Nothing" and Big Numbers:

55 Gal Drum water
6.97 x 10^{27} Molecules of water

Teaspoon of sugar
7.93 x 10^{21} Molecules of sugar  1.14 ppm

Grain of sugar
5.22 x 10^{17} Molecules of sugar  50.6 ppt

Nanogram of sugar
1.76 x 10^{12} Molecules of sugar
176 Billion molecules of sugar

Amedeo Avogadro
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John Warner’s 5 Elements of Innovation

1. All innovation begins with science fiction

2. Innovation happens not within the field of focus but in the periphery.

3. Encyclopedic knowledge inhibits innovation in the absence of intuitive knowledge.

4. The ability to innovate is simultaneously proportional to wisdom and the tolerance of intellectual risk.

5. Innovation is orthogonal to complexity.
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Renovation
The 2011 World Science Fiction Convention
August 17-21, 2011, Reno, Nevada
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It’s a Fan!

It’s a Wall!

It’s a Spear!

It’s a Snake!

It’s a Rope!

It’s a Tree!
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Encyclopedic Knowledge

Dilbert

Wow! You have three Masters degrees and a PhD!

Yes, it's all very impressive, but interestingly, I have no common sense whatsoever.

That's not the sort of thing you should say during a job interview.

I don't see why not.
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Daniel Shechtman, who has won the chemistry Nobel for discovering quasicrystals, was initially lambasted for 'bringing disgrace' on his research group.

"His discovery was extremely controversial. In the course of defending his findings, he was asked to leave his research group," the Nobel committee at the Royal Swedish Academy of Sciences said in a statement.

A remarkable mosaic of atoms

In quasicrystals, we find the fascinating mosaics of the Arabic word reproduced at the level of atoms: regular patterns that never repeat themselves. However, the configuration found in quasicrystals was considered impossible, and Dan Shechtman had to fight a fierce battle against established science. The Nobel Prize in Chemistry 2011 has fundamentally altered how chemists conceive of solid matter.

On the morning of 8 April 1982, an image counter to the laws of nature appeared in Dan Shechtman's electron microscope. In all solid matter, atoms are believed to be packed inside crystals in symmetrical patterns that can be repeated endlessly, over and over again. To scientists, this repetition was required in order to obtain a crystal.

Shechtman's image, however, showed that the atoms in his crystal were packed in a pattern that could not be repeated. Such a pattern was considered impossible as creating a solid using only pentagonal polygons, when a sphere nested with hexagonal polygons. His discovery was extremely controversial. In the course of defending his findings, he was asked to leave his research group. However, his battle eventually forced scientists to reconsider their conception of the very nature of matter.

Aperiodic mosaics, such as those found in the medieval Islamic mosaics of the Alhambra Palace in Spain and the Darb-i Imam Shrine in Iran, have helped scientists understand what quasicrystals look like at the atomic level. In those mosaics, as in quasicrystals, the patterns are regular - they follow mathematical rules - but they never repeat themselves.

When scientists describe Shechtman's quasicrystals, they use a concept that comes from mathematics and art: the golden ratio. This number had already caught the interest of mathematicians in Ancient Greece, as it often appeared in geometry. In quasicrystals, for instance, the ratio of various distances between atoms is related to the golden mean.
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**Science**

- **Explore**
  - Observe and define structure and dynamics.
- **Basic Research**
- **Understand**
  - Identify and characterize impact of changes of structure on dynamics and dynamics on structure.
- **Parameterize**
  - Design alterations in structure and/or dynamics to purposefully control response.
- **Create**
  - Create a potentially useful prototype.

**Business**

- **Explore**
  - Observe and define a product and market.
- **Market Analysis**
- **Understand**
  - Identify and characterize market history and likely future trends.
- **Parameterize**
  - Design potential products and assess potential markets and parameters for success.
- **Create**
  - Develop a potentially successful product.
- **Develop**
- **Commercialize**
  - Commercialize a successful product.
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Safety and Sustainability

Identify and prioritize key attributes
- Industry Standards
- Voice of Customer
- Business Economics
- Regulatory Agencies
- NGOs

Design/plan metrics and tools to evaluate
- ASTM Tests
- In-house historical
- Customer Supplied
- Government Agencies
- 3rd Party Organizations

Identify possible existing materials
- Pre-existing supplier relationships
- Product development intelligence
- Supply chain sales and marketing
- Alternatives Assessment

Measure/Quantify performance of materials
- In house testing
- Supplier testing
- 3rd Party testing
- Government Labs

If acceptable materials are not found -> Invent new technology
- In house R&D
- Supplier R&D
- University/Government
- 3rd Party R&D
Elements of Safer Chemicals Policy

Element 1. Move from a list based system to an assay based system.
   - Focusing on assays avoids unfortunate substitutions.
   - Identifying criteria of success allows companies to invest strategically.

Element 2. Move from a molecule based system to a product based system.
   - Some “ingredients” disappear and some molecules appear during manufacturing.
   - Avoids disclosing trade secrets.

Element 3. Identify and disclose results of assays.
   - Allows consumers quantitative assessments to base decisions.
   - Provides a framework for advocacy groups to communicate effectively.