Green Chemistry Education Webinar Series

Green Chemistry – Benign By Design

July 21, 2015

GC3 GREEN CHEMISTRY & COMMERCE COUNCIL
Business Mainstreaming Green Chemistry

What is the GC3?

- Cross-sectoral, B2B network of over 70 companies and other organizations
- Formed in 2005
- Collaboratively advances green chemistry across sectors and supply chains

Today's Speakers

JOHN WARNER

President & CTO,
Warner Babcock Institute for Green Chemistry

Green Chemistry: Benign by Design

John C. Warner
President and Chief Technology Officer
Warner Babcock Institute for Green Chemistry, LLC

warnerbabcock
institute for green chemistry

beyondbenign

Today' s Talk:

- Green Chemistry
- Product Design
- Zero and Big Numbers
- How it fits together
- Examples from WBI

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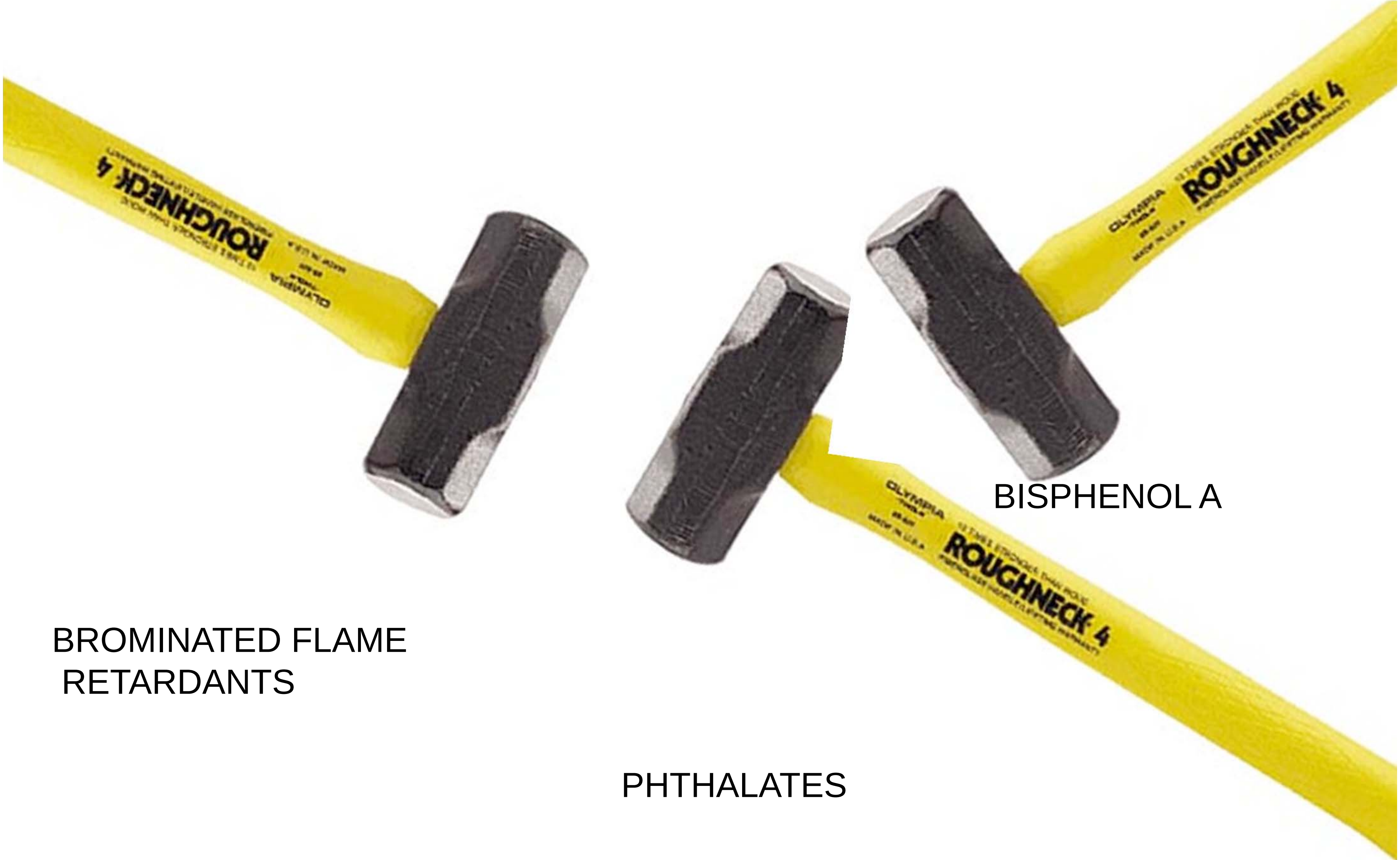
- Examples from WBI

BBC NEWS
The Washington Post
EPA Is Reconsidering
The New York Times
Child obesity is lin
to chemicals in plasti
TIME
The Poisoning of America
The Japan Times
Oceans awash in toxic seas of plastic
CNN.com
THE WALL STREET JOURNAL.
Yes, Bisphenol-A Does Enter the Body from Plastic Bottles
USA TODAY
5,000 evacuated after
hazardous Pa. acid spill
Chicago Tribune
Chicago's Toxic Air
THE SUNDAY TIMES
Household Dust Contains Highly Toxic Chemicals


WHACK A MOLE!


BISPHENOL A
BROMINATED FLAME
RETARDANTS
PHTHALATES

Asking the Right Questions

Why would a chemist
make a hazardous material?

How do we train chemists?

Every Year: (United States)

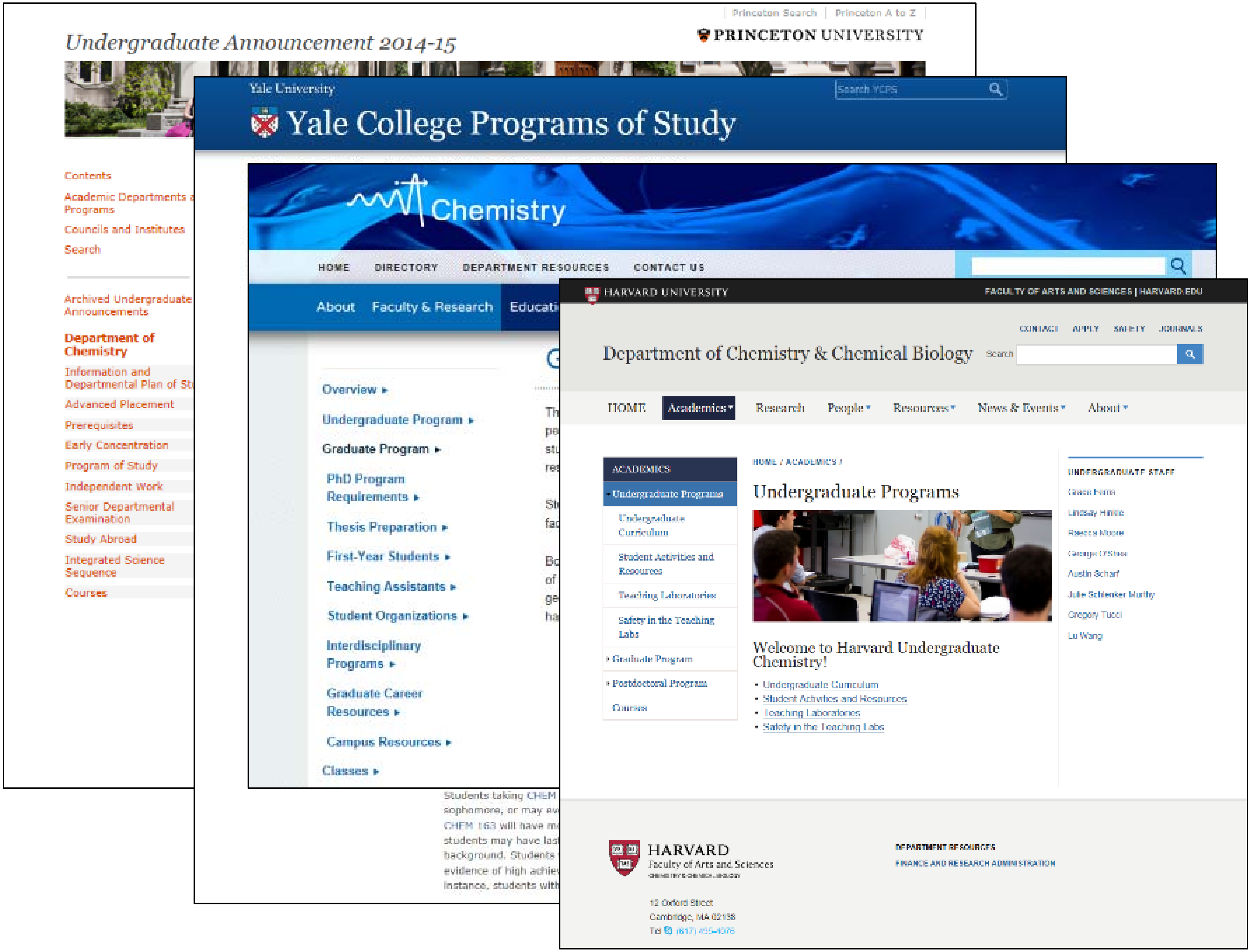
Chemistry and Chemical Engineering Graduates

15,000 Undergraduate Degrees

3,000 Masters Degrees

3,000 Doctoral Degrees

50.9 % Women Undergraduate Degrees (2004)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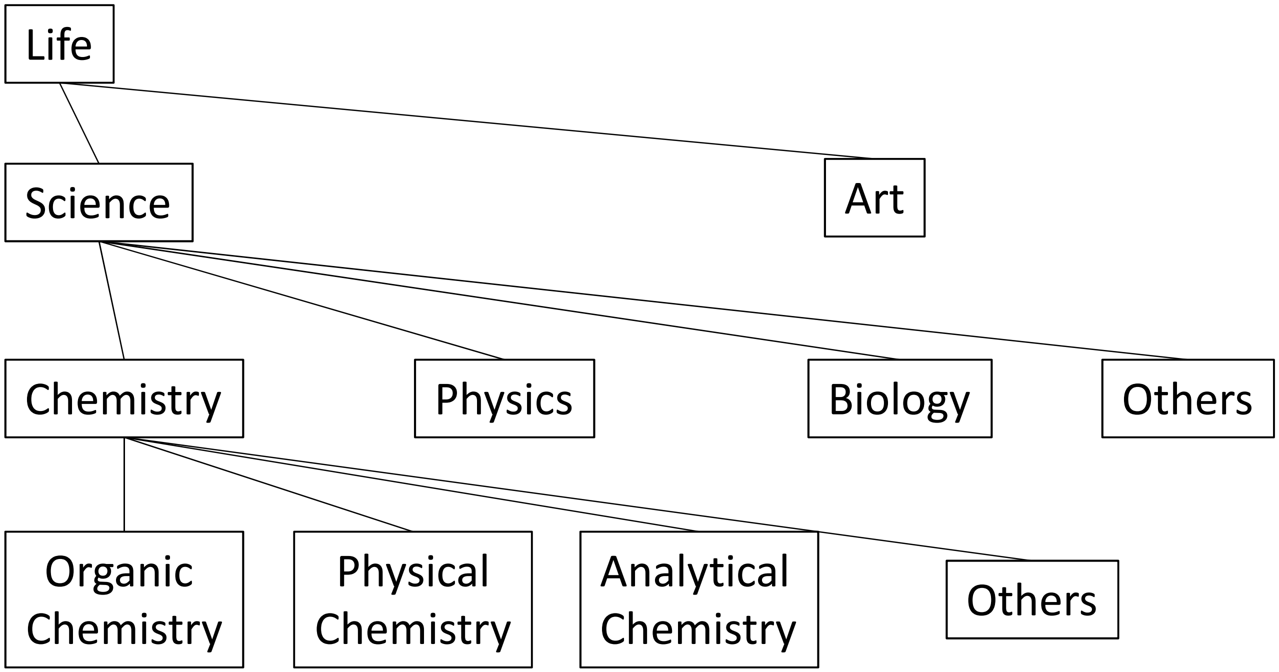
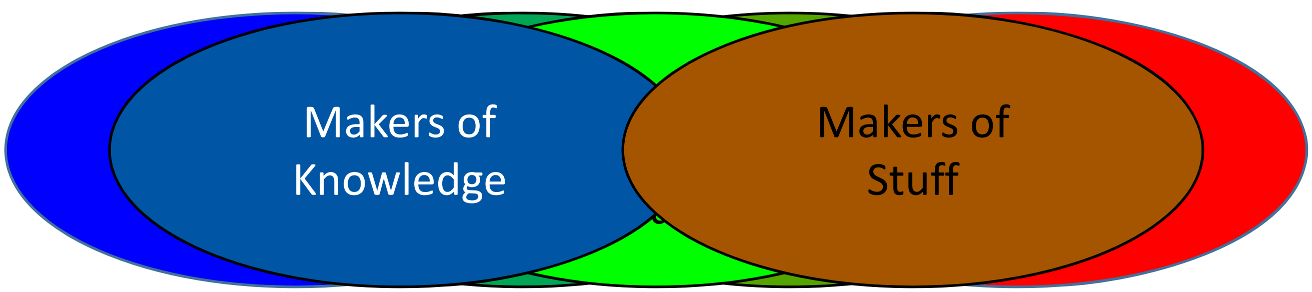
HARVARD
Faculty of Arts and Sciences
DEPARTMENT RESOURCES
FINANCE AND RESEARCH ADMINISTRATION
12 Oxford Street
Cambridge, MA 02138

To get a degree in Chemistry…

No universities require any demonstration of knowledge regarding toxicity or environmental impact!

This is not part of an
"epic battle of good and evil"


Life
Science
Art
Chemistry
Physics
Biology
Others
Organic Chemistry
Physical Chemistry
Analytical Chemistry
Others


Makers of Knowledge
Makers of Stuff

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 .

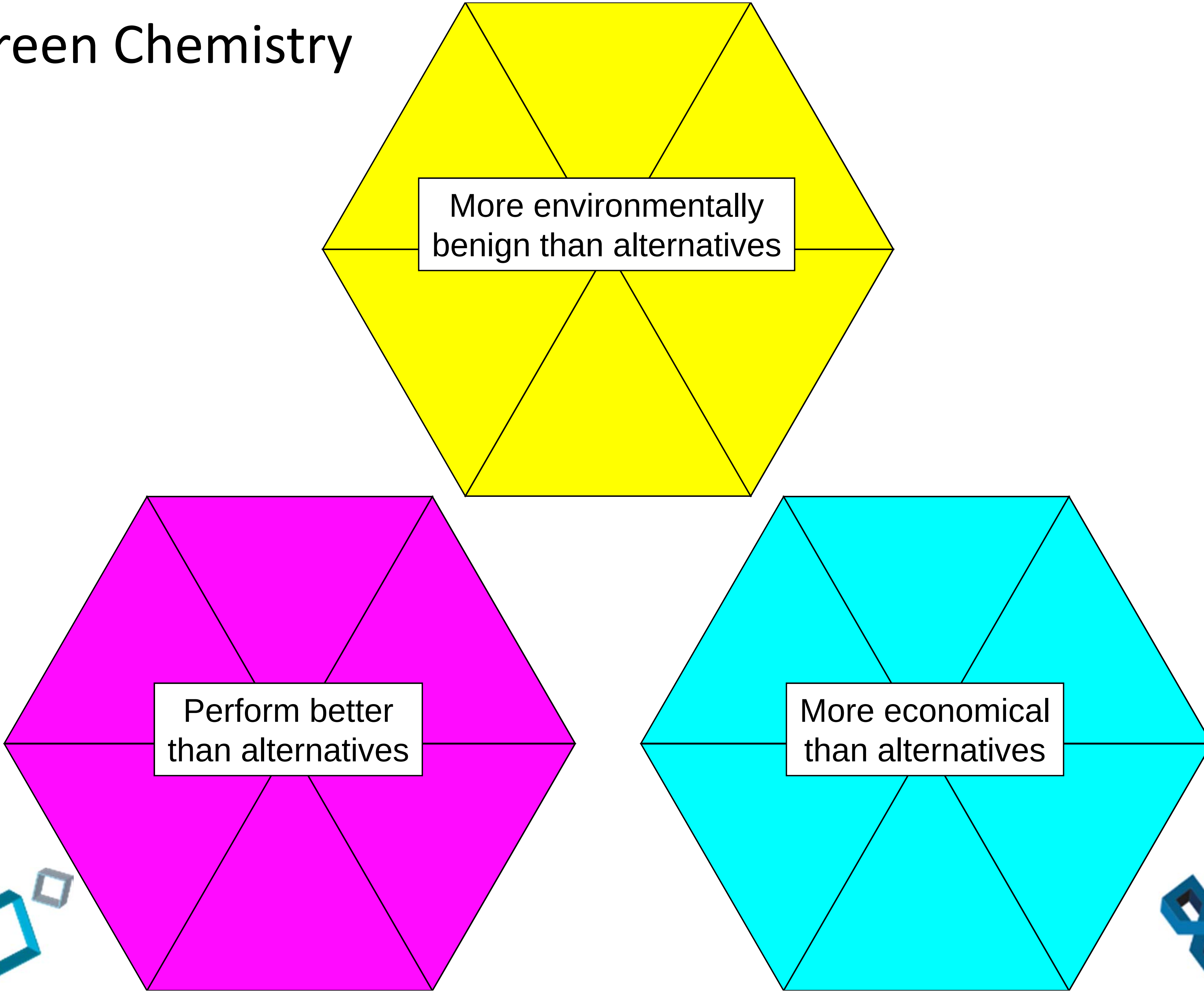
9. Catalysis. Catalytic reagents (as selective as possible) are superior to stoichiometric reagents.

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.

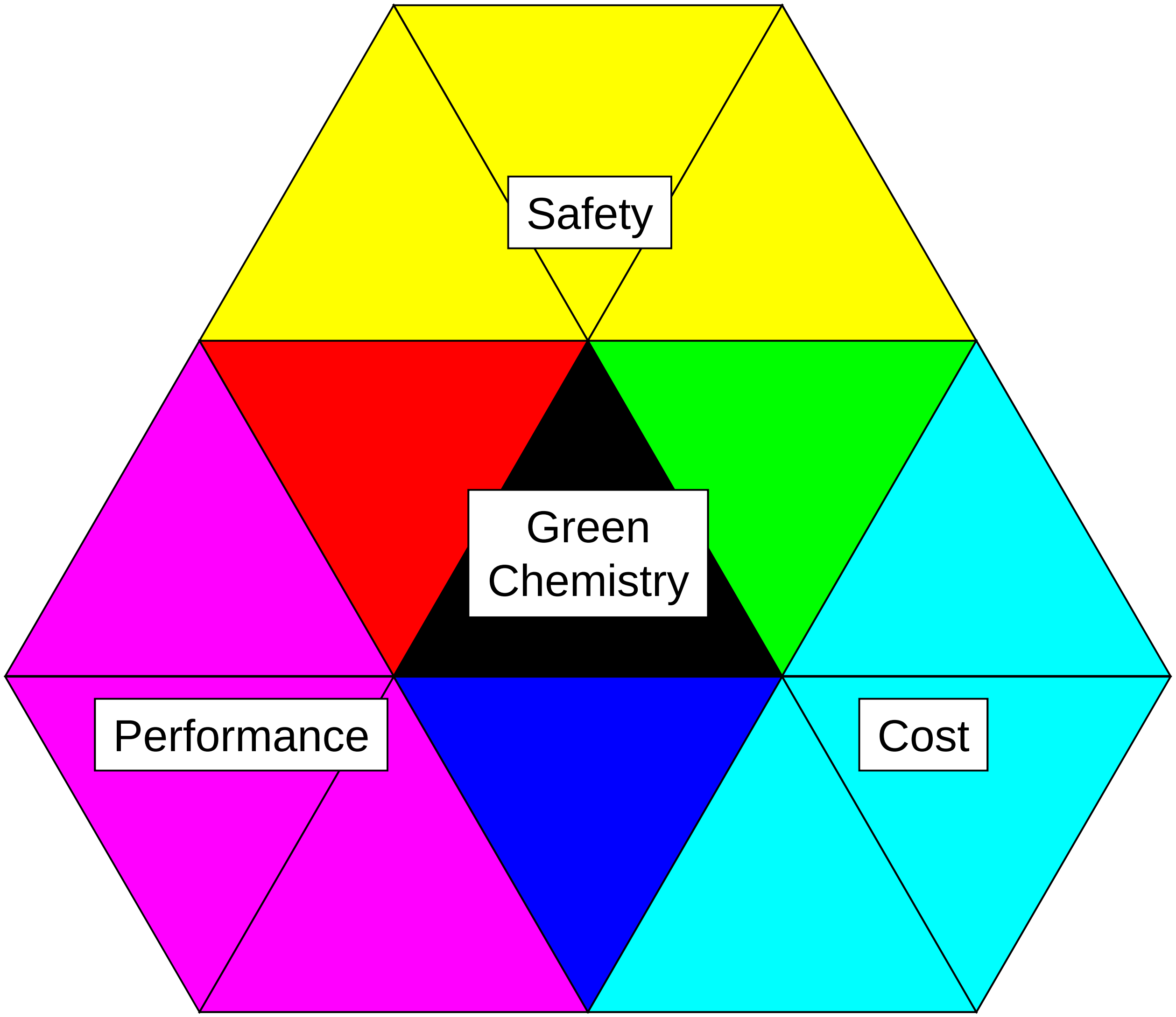
11. Real-time Analysis for Pollution Prevention. Analytical methodologies need to be further developed to allow for real-time in-process monitoring and control prior to the formation of hazardous substances.

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



Green Chemistry

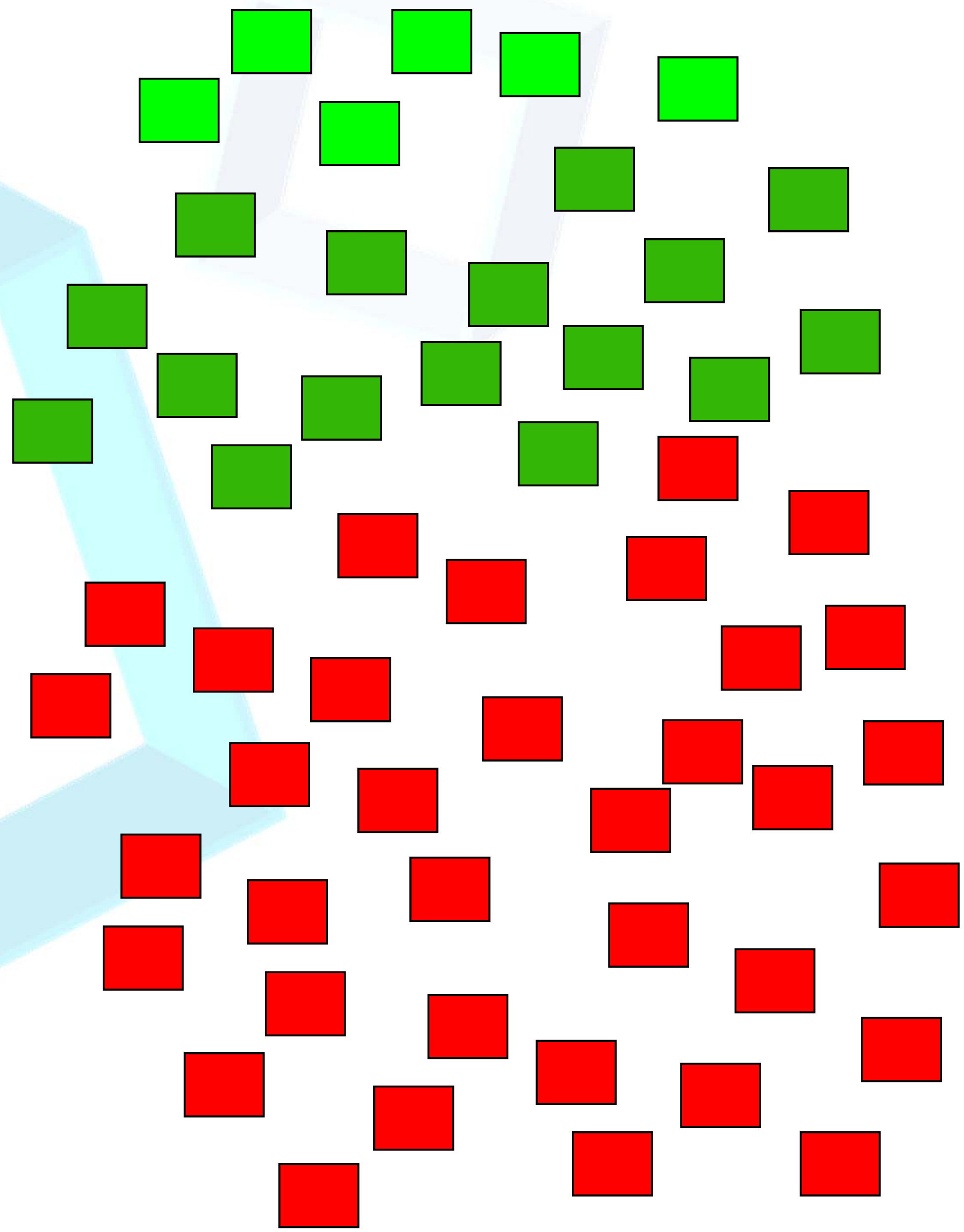


Of all the products and processes…

Maybe 10% are benign…

Maybe 25% have alternatives available…

65% Still have to be invented!



How does Green Chemistry fit into the big picture of Sustainability.

United States
Environmental Protection Agency

Learn the Issues | Science & Technology | Laws & Regulations | About EPA

Green Chemistry

Basics of Green Chemistry

On this page:

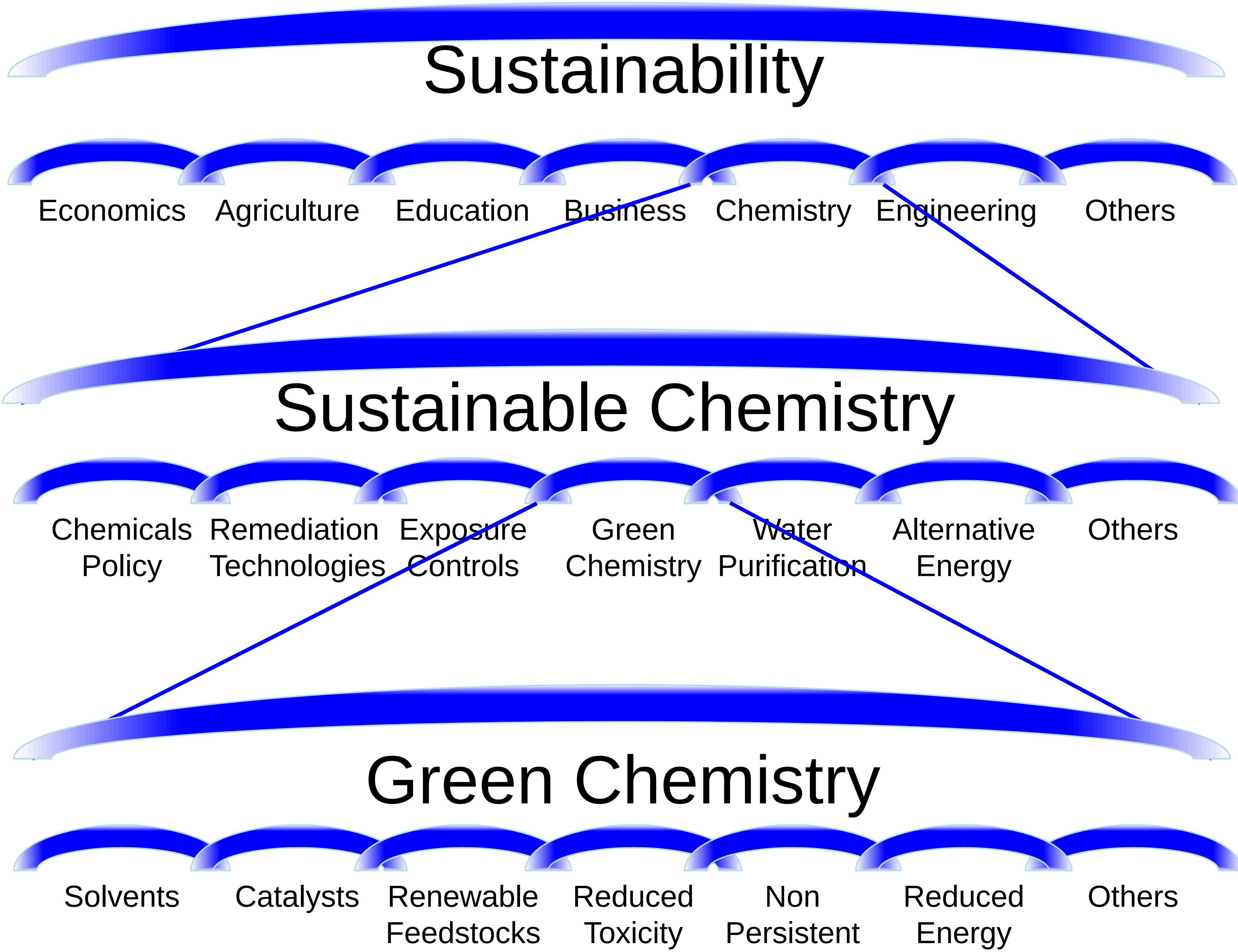
- Definition of green chemistry
- How green ch
- Green chemis
- Twelve princip
- Green chemis

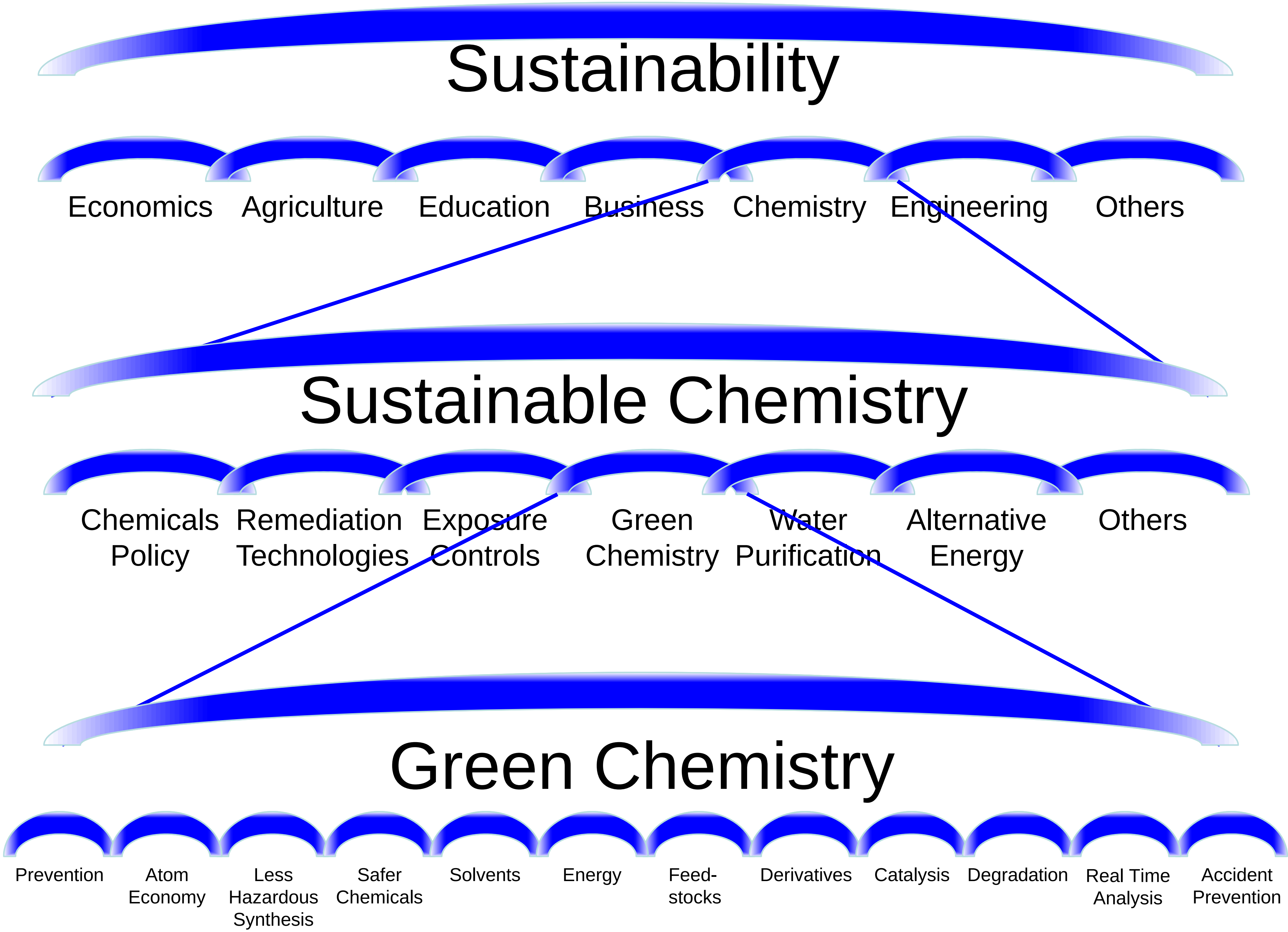
Green Chemistry is also known as sustainable chemistry.

Definition of green chemistry

Green chemistry is the design of chemical products and processes that reduce or eliminate the use or generation of hazardous substances. Green chemistry applies across the life cycle of a chemical product, including its design, manufacture, use, and ultimate disposal. Green chemistry is also known as sustainable chemistry.

Green chemistry:


Sustainability
Economics
Agriculture
Education
Business
Chemistry
Engineering
Others
Sustainable Chemistry
Chemicals Policy
Remediation Technologies
Exposure Controls
Green Chemistry
Water Purification
Alternative Energy
Others
Green Chemistry
Solvents
Catalysts
Renewable Feedstocks
Reduced Toxicity
Non Persistent
Reduced Energy
Others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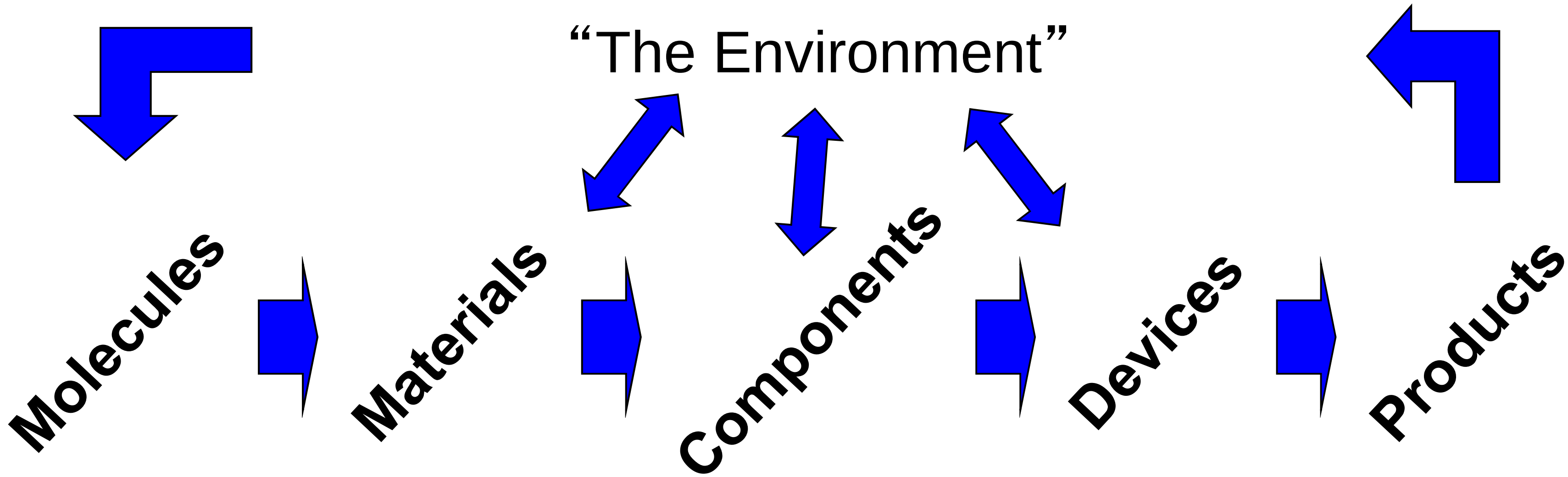
Exposure Controls
Green Chemistry
Water Purification
Alternative Energy
Others
Green Chemistry
Prevention
Atom Economy
Less Hazardous Synthesis
Safer Chemicals
Solvents
Energy
Feed-stocks
Derivatives
Catalysis
Degradation
Real Time Analysis
Accident Prevention

Where do products come from?



Basic Research

Applied Research

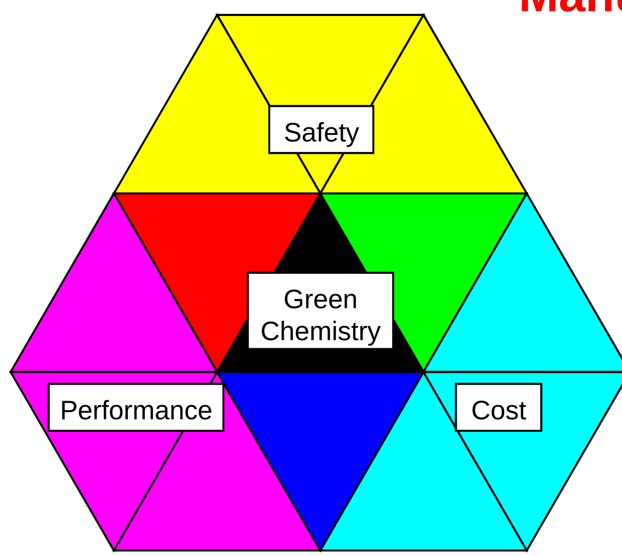
Development

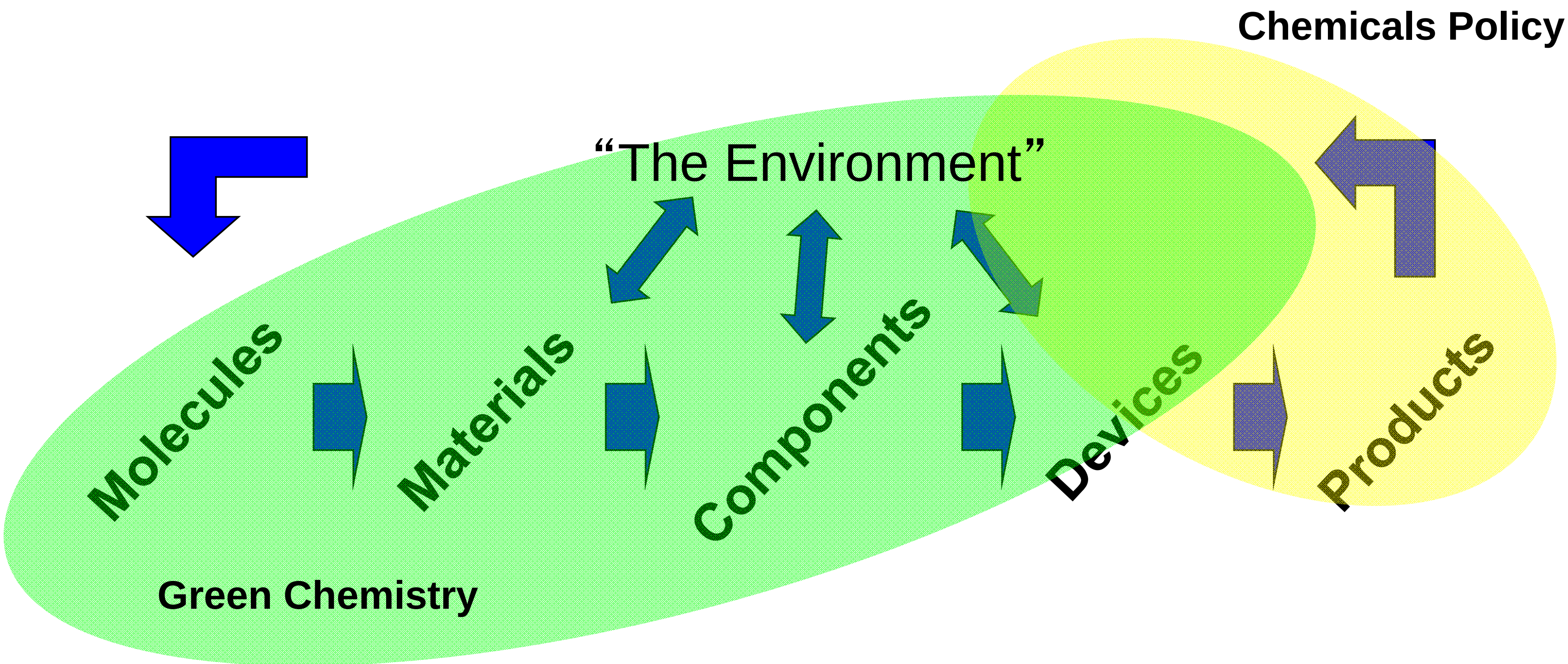
Manufacturing

Performance

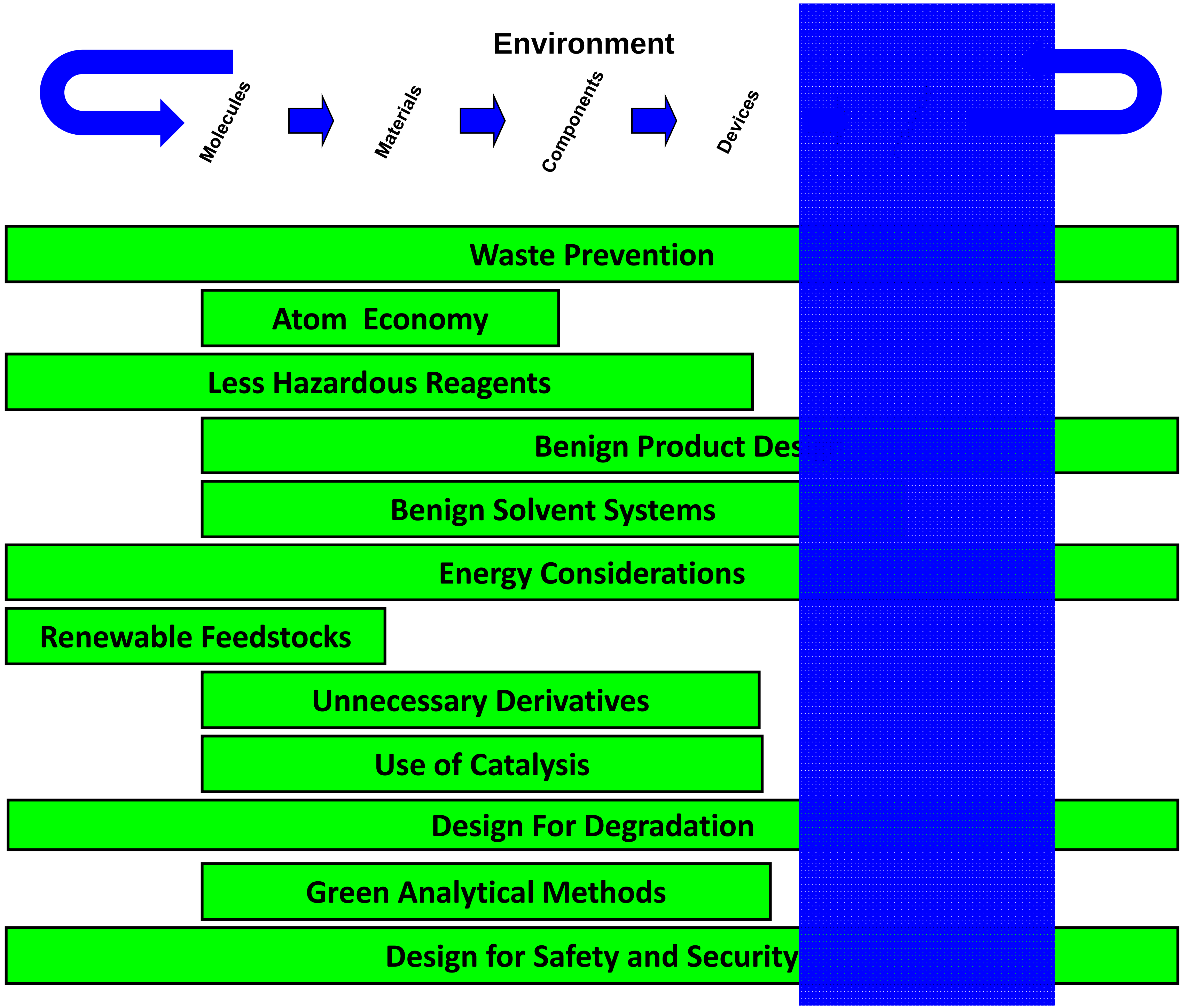
Economics

Social Implications

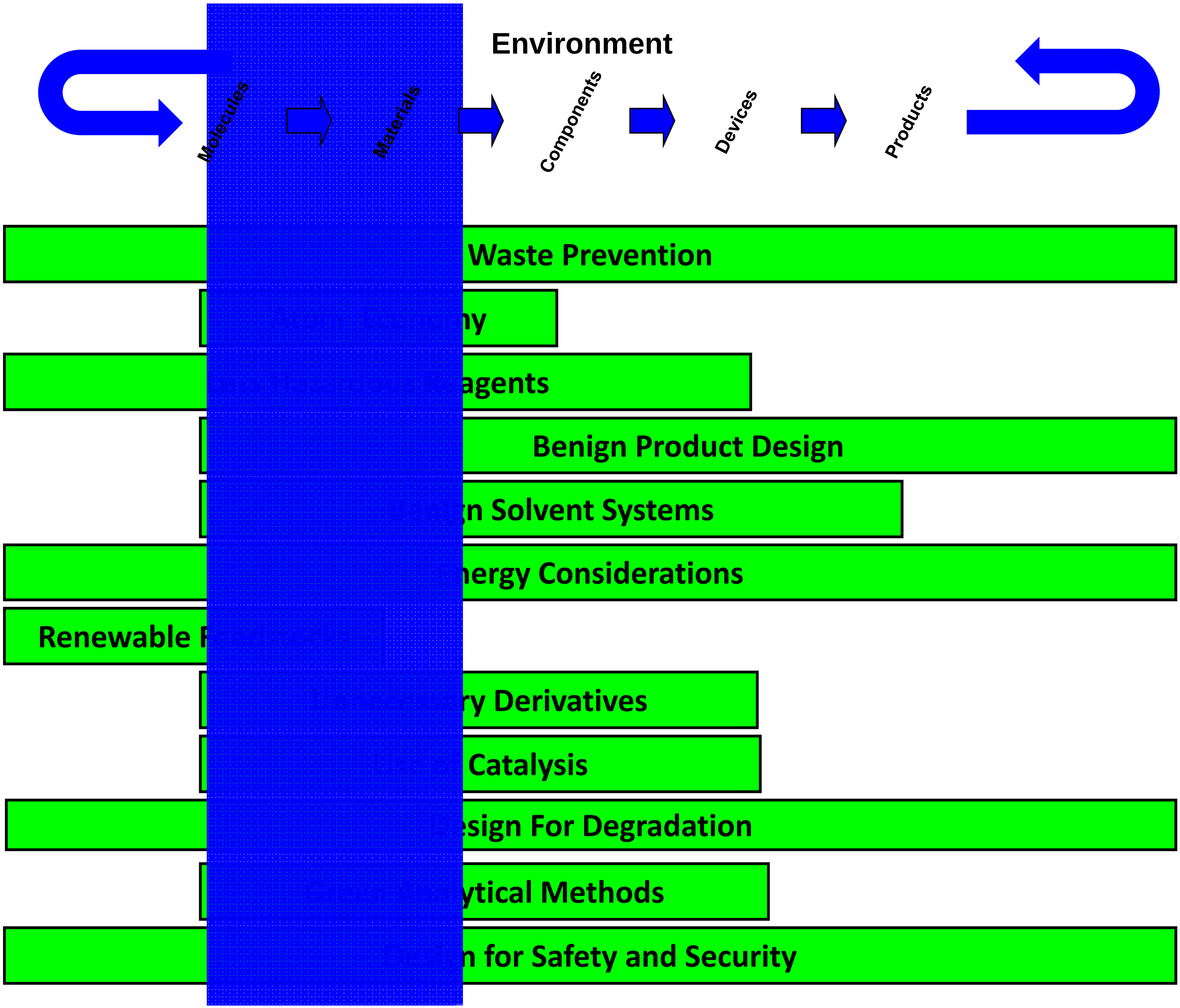



Chemicals Policy
“The Environment”
Molecules
Materials
Components
Devices
Products
Green Chemistry

How does Green Chemistry relate to Life Cycle Analyses?



Environment
Molecules
Materials
Components
Devices
Waste Prevention
Atom Economy
Less Hazardous Reagents
Benign Product Des
Benign Solvent Systems
Energy Considerations
Renewable Feedstocks
Unnecessary Derivatives
Use of Catalysis
Design For Degradation
Green Analytical Methods
Design for Safety and Security


Environment
Molecules
Materials
Components
Devices
Products
Waste Prevention
Benign Product Design
Solvent Systems
Considerations
Renewable
Derivatives
Catalysis
For Degradation
Methods
for Safety and Security

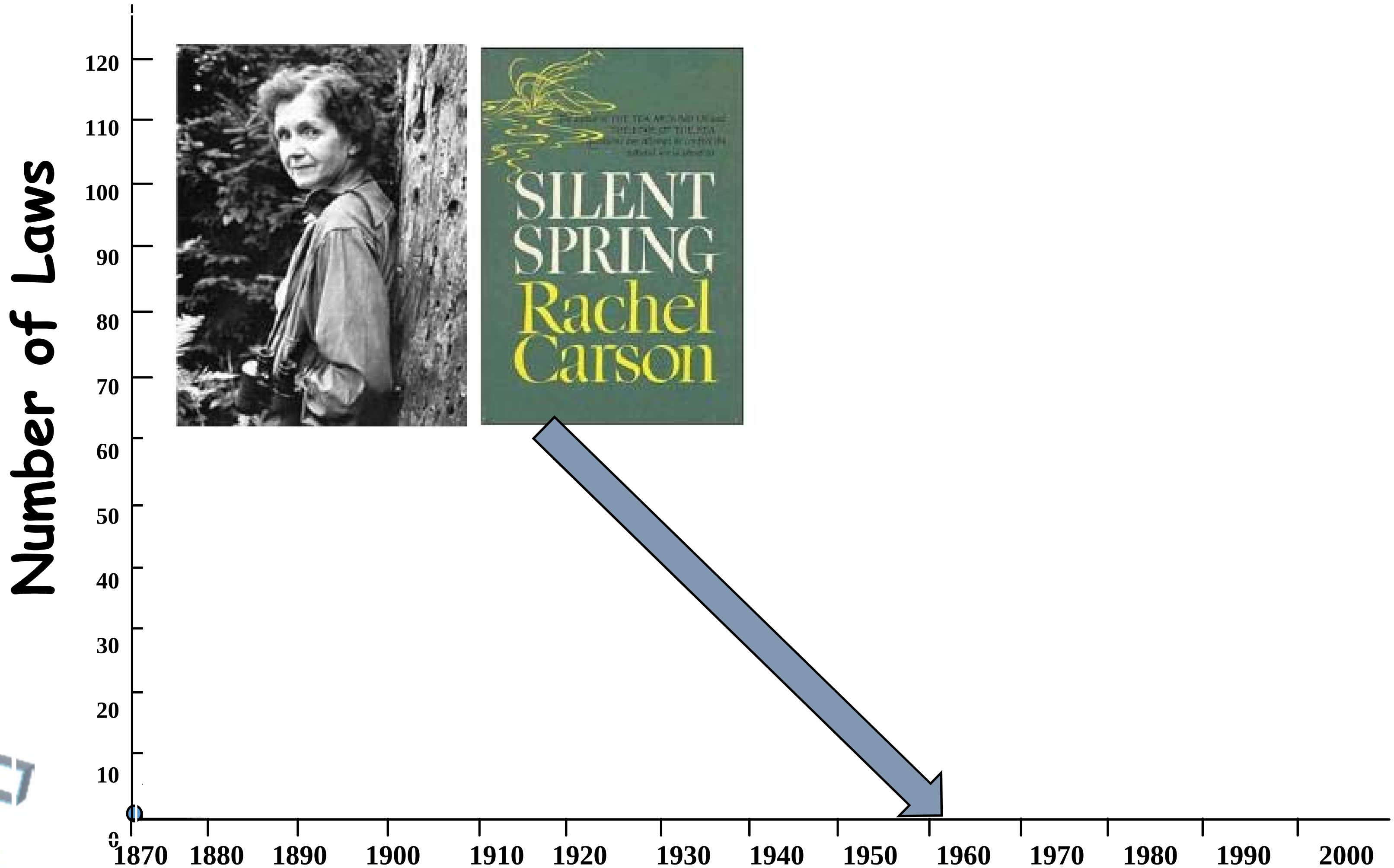
Chemists have ALWAYS cared about Human Health and the Environment.

Risk = Exposure x Hazard

The cost of using hazardous materials:

Storage
Transportation
Treatment
Disposal
Regulatory Costs
Liability
Worker Health and Safety
Corporate Reputation
Community Relations
New Employee Recruitment

Environmental Regulations



Traditional Processes

Green Alternatives

Today's Talk:

- Green Chemistry
- Product Design
- Zero and Big Numbers
- How it fits together
- Examples from WBI

Product Design

Identify and prioritize key attributes

Design/plan metrics and tools to evaluate

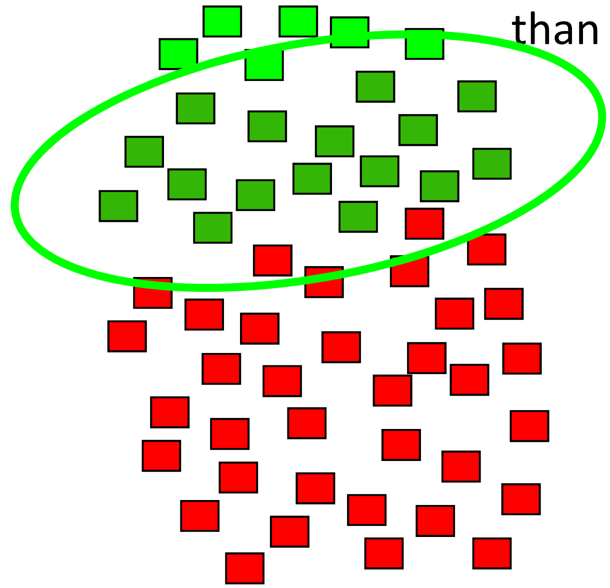
Identify possible existing materials

Measure/Quantify performance of materials

If acceptable materials are found –> Make Product

If acceptable materials are not found -> Invent new technology

This will happen less than 25% of the time.



Performance and Cost

Step	Sources	Output
Identify and prioritize key attributes	Industry Standards Voice of Customer Business Economics	Color stability in light Stability to cold and heat Cost
Design/plan metrics and tools to evaluate	ASTM Tests In-house historical Customer Supplied	Z% fading in Y amount of time under X amount of intensity < W number of cracks > V mm in length after U hours at T ^{o}C Less that S$/gallon
Identify possible existing materials	Pre-existing supplier relationships Product development intelligence Supply chain sales and marketing	Material A Material B Material C
Measure/Quantify performance of materials	In house testing Supplier testing 3rd Party testing	Material A: S, T, U, V, W, X, Y, Z Material B: S’, T’, U’, V’, W’, X’, Y’, Z’ Material C: S”, T”, U”, V”, W”, X”, Y”, Z”
If acceptable materials are not found -> Invent new technology	In house R&D Supplier R&D University/Government 3rd Party R&D	

Performance, Cost, Safety and Sustainability

Identify and prioritize key attributes

- Industry Standards
- Voice of Customer
- Business Economics
- Regulatory Agencies
- NGOs

→

- Color stability in light
- Stability to cold and heat
- Cost
- Safety (Mutagenicity, Endocrine Activity, Hepatotoxicity…)
- Sustainability (Energy Usage, Renewables Usage…)

Design/plan metrics and tools to evaluate

- ASTM Tests
- In-house historical
- Customer Supplied
- Government Agencies
- 3rd Party Organizations

→

- Z% fading in Y amount of time under X amount of intensity
- < W number of cracks > V mm in length after U hours at T ^{o}C
- Less that S$/gallon
- > R mg/kg on Ames Test
- > Q mg/kg on Tier three TiPED assay
- < P% mitochondrial damage with CM-H2DCFDA probe
- < N BTU per manufactured unit
- > M % Biobased Carbon (ASTM D6866)

Identify possible existing materials

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

→

- Material A
- Material B
- Material C

Measure/Quantify performance of materials

- In house testing
- Supplier testing
- 3rd Party testing
- Government Labs

→

- Material A: S, T, U, V, W, X, Y, Z, M, N, P, Q, R
- Material B: S’, T’, U’, V’, W’, X’, Y’, Z’, M’, N’, P’, Q’, R’
- Material C: S”, T”, U”, V”, W”, X”, Y”, Z”, M”, N”, P”, Q”, R”

If acceptable materials are not found -> Invent new technology

- In house R&D
- Supplier R&D
- University/Government
- 3rd Party R&D

A deliverable attribute must be:

Quantifiable

Color doesn’t fade.

Achievable

Color NEVER fades (IS NOT achievable)
Color only fades a little over a certain period of time (IS achievable)

Measurable

Optical density decreases by less than 10% after
48 hours with 20000 lumens solar simulator.

Today's Talk:

- Green Chemistry
- Product Design
- Zero and Big Numbers
- How it fits together
- Examples from WBI

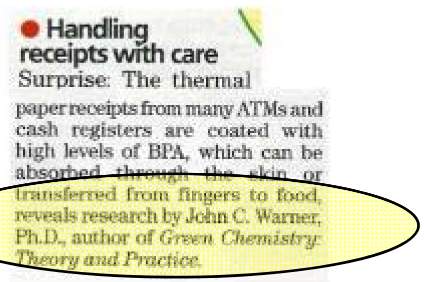
Lets talk about nothing:

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?



● Handling receipts with care
Surprise: The thermal paper receipts from many ATMs and cash registers are coated with high levels of BPA, which can be absorbed through the skin or transferred from fingers to food, reveals research by John C. Warner, Ph.D., author of *Green Chemistry: Theory and Practice.*

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 9 7 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

6.97×10^{27} Molecules of water

7 9 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Teaspoon of sugar

7.93×10^{21} Molecules of sugar 1.14 ppm

Grain of sugar

3 5 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

5.22×10^{17} Molecules of sugar 50.6 ppt

Nanogram of sugar

1.76×10^{12} Molecules of sugar

1 7 6 0 0 0 0 0 0 0 0 0 0

176 Billion molecules of sugar

Amedeo Avogadro

Today's Talk:

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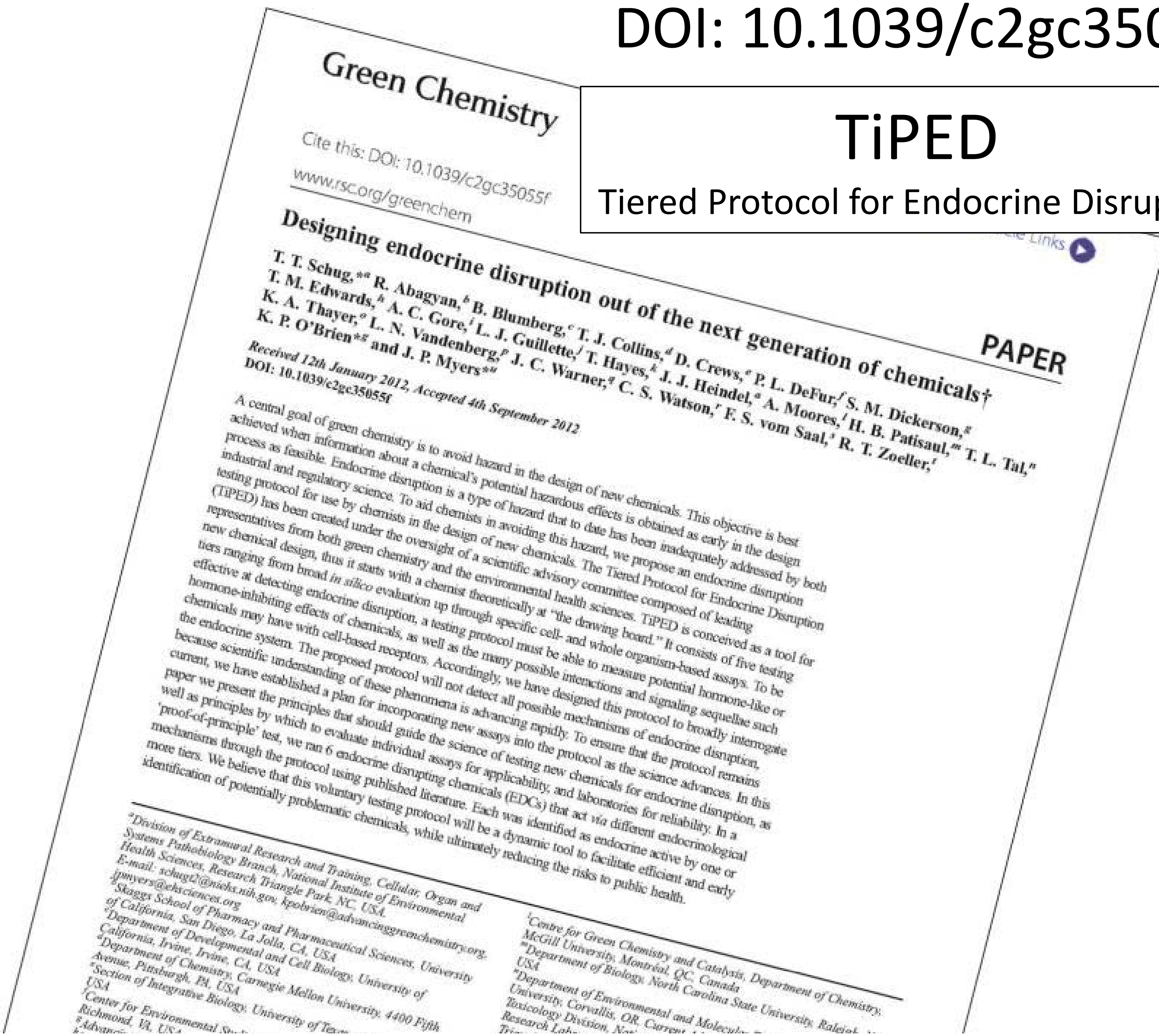
The ability to invent & design solutions to a problem is directly proportional to the quality of the description of success.

Quantifiable
Achievable
Measurable

DOI: 10.1039/c2gc35055f

TiPED

Tiered Protocol for Endocrine Disruption


Green Chemistry

Cite this: DOI: 10.1039/c2gc35055f

www.rsc.org/greenchem

PAPER

Designing endocrine disruption out of the next generation of chemicals†

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DOI: 10.1039/c2gc35055f

A central goal of green chemistry is to avoid hazard in the design of new chemicals. This objective is best achieved when information about a chemical's potential hazardous effects is obtained as early in the design process as feasible. Endocrine disruption is a type of hazard that to date has been inadequately addressed by both industrial and regulatory science. To aid chemists in avoiding this hazard, we propose an endocrine disruption testing protocol for use by chemists in the design of new chemicals. The Tiered Protocol for Endocrine Disruption (TiPED) has been created under the oversight of a scientific advisory committee composed of leading representatives from both green chemistry and the environmental health sciences. TiPED is conceived as a tool for new chemical design, thus it starts with a chemist theoretically at "the drawing board." It consists of five testing tiers ranging from broad *in silico* evaluation up through specific cell- and whole organism-based assays. To be effective at detecting endocrine disruption, a testing protocol must be able to measure potential hormone-like or hormone-inhibiting effects of chemicals, as well as the many possible interactions and signaling sequellae such chemicals may have with cell-based receptors. Accordingly, we have designed this protocol to broadly interrogate the endocrine system. The proposed protocol will not detect all possible mechanisms of endocrine disruption, because scientific understanding of these phenomena is advancing rapidly. To ensure that the protocol remains current, we have established a plan for incorporating new assays into the protocol as the science advances. In this paper we present the principles that should guide the science of testing new chemicals for endocrine disruption, as well as principles by which to evaluate individual assays for applicability, and laboratories for reliability. In a 'proof-of-principle' test, we ran 6 endocrine disrupting chemicals (EDCs) that act *via* different endocrinological mechanisms through the protocol using published literature. Each was identified as endocrine active by one or more tiers. We believe that this voluntary testing protocol will be a dynamic tool to facilitate efficient and early identification of potentially problematic chemicals, while ultimately reducing the risks to public health.

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[m]Department of Biology, North Carolina State University, Raleigh,
USA
[n]Department of Environmental and Molecular
University, Corvallis, OR. Current
Toxicology Division,
Research

Safety and Sustainability

Identify and prioritize key attributes

- Industry Standards
- Voice of Customer
- Business Economics
- Regulatory Agencies
- NGOs

Chemicals Policy

Design/plan metrics and tools to evaluate

- ASTM Tests
- In-house historical
- Customer Supplied
- Government Agencies
- 3rd Party Organizations

Toxicology and Environmental Health Sciences

Identify possible existing materials

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

Alternatives Assessment

Measure/Quantify performance of materials

- In house testing
- Supplier testing
- 3rd Party testing
- ment Labs

Green Chemistry

If acceptable materials are not found -> Invent new technology

- In house R&D
- Supplier R&D
- University/Government
- 3rd Party R&D

We can’t sit on our hands waiting for all the criteria to be sorted out.

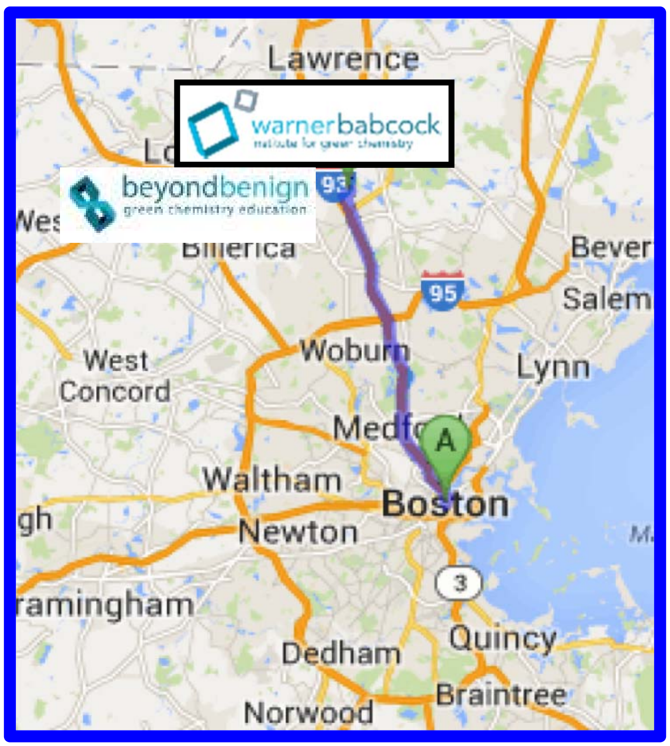
While zero may not be achievable from a regulatory perspective…

From an innovation and design perspective, it will always point us in the right direction.

Today's Talk:

- Green Chemistry
- Product Design
- Zero and Big Numbers
- How it fits together
- Examples from WBI

John Warner Amy Cannon Jim Babcock Joe Pont, CEO



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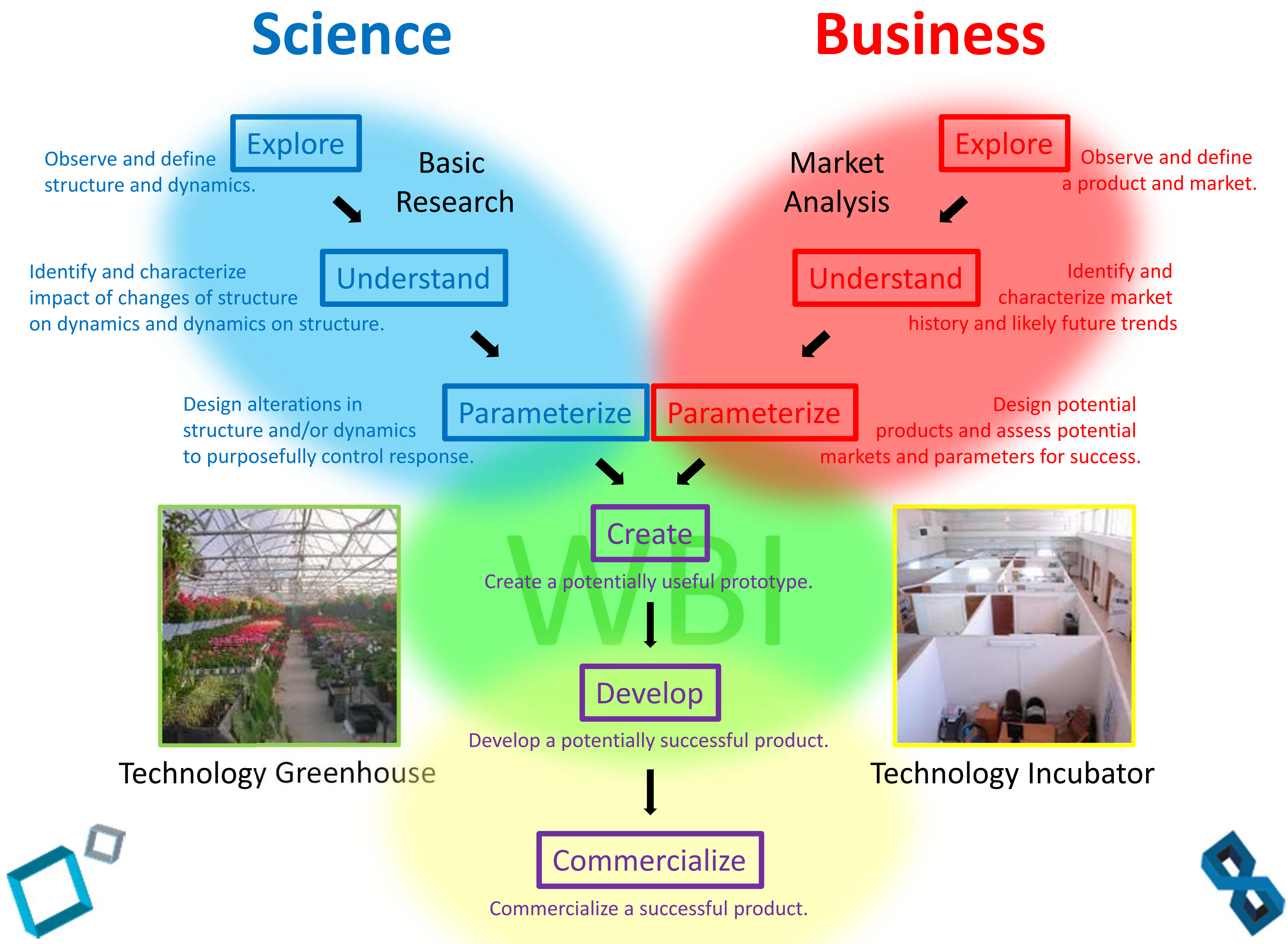

Science
Business
Explore
Observe and define structure and dynamics.
Basic Research
Understand
Identify and characterize impact of changes of structure on dynamics and dynamics on structure.
Parameterize
Design alterations in structure and/or dynamics to purposefully control response.
Market Analysis
Explore
Observe and define a product and market.
Understand
Identify and characterize market history and likely future trends
Parameterize
Design potential products and assess potential markets and parameters for success.
WBI
Create
Create a potentially useful prototype.
Develop
Develop a potentially successful product.
Commercialize
Commercialize a successful product.
Technology Greenhouse
Technology Incubator

Hairprint: Hair Color Restoration

Increased Recycled Asphalt
And Lower Temperature Process

COLLABORATIVE AGGREGATES LLC

Alberta Innovates Technology Futures

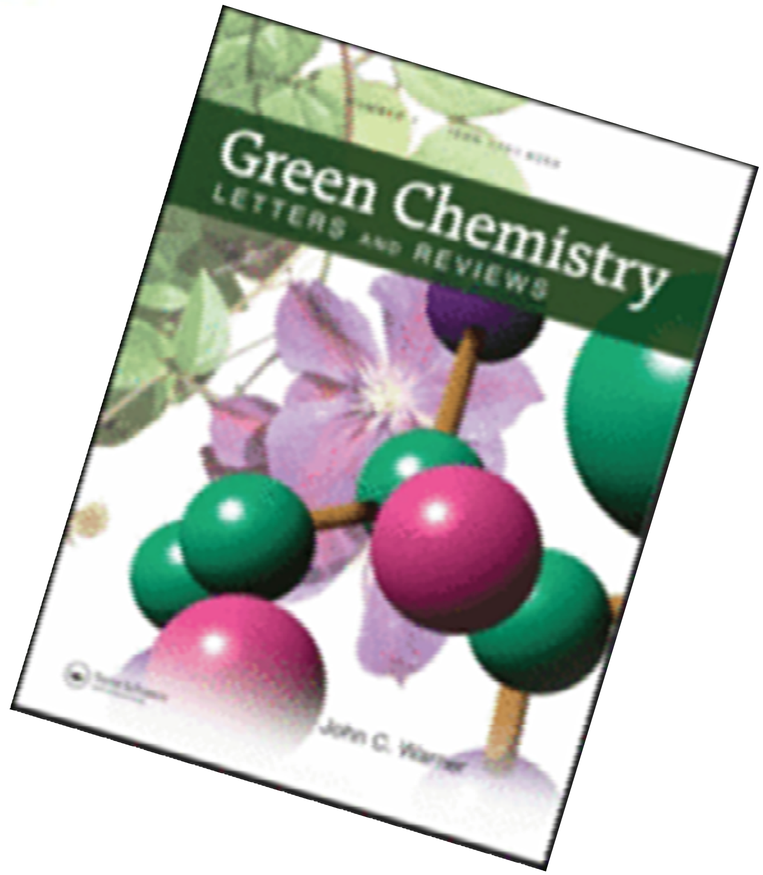
COLLABORATIVE AGGREGATES LLC

Formaldehyde Free
Wood Composite Adhesives

Reuse of Ocean Plastics

warner babcock
institute for green chemistry

beyond benign
a warner babcock foundation



john.warner@warnerbabcock.com

amy_cannon@beyondbenign.org

Thanks for joining us!

For more information about the GC3:

www.greenchemistryandcommerce.org

GC3 GREEN CHEMISTRY & COMMERCE COUNCIL

Business Mainstreaming Green Chemistry