# Knowledge commons for green chemistry

## Collective solutions to information challenges in the substitution of hazardous chemicals

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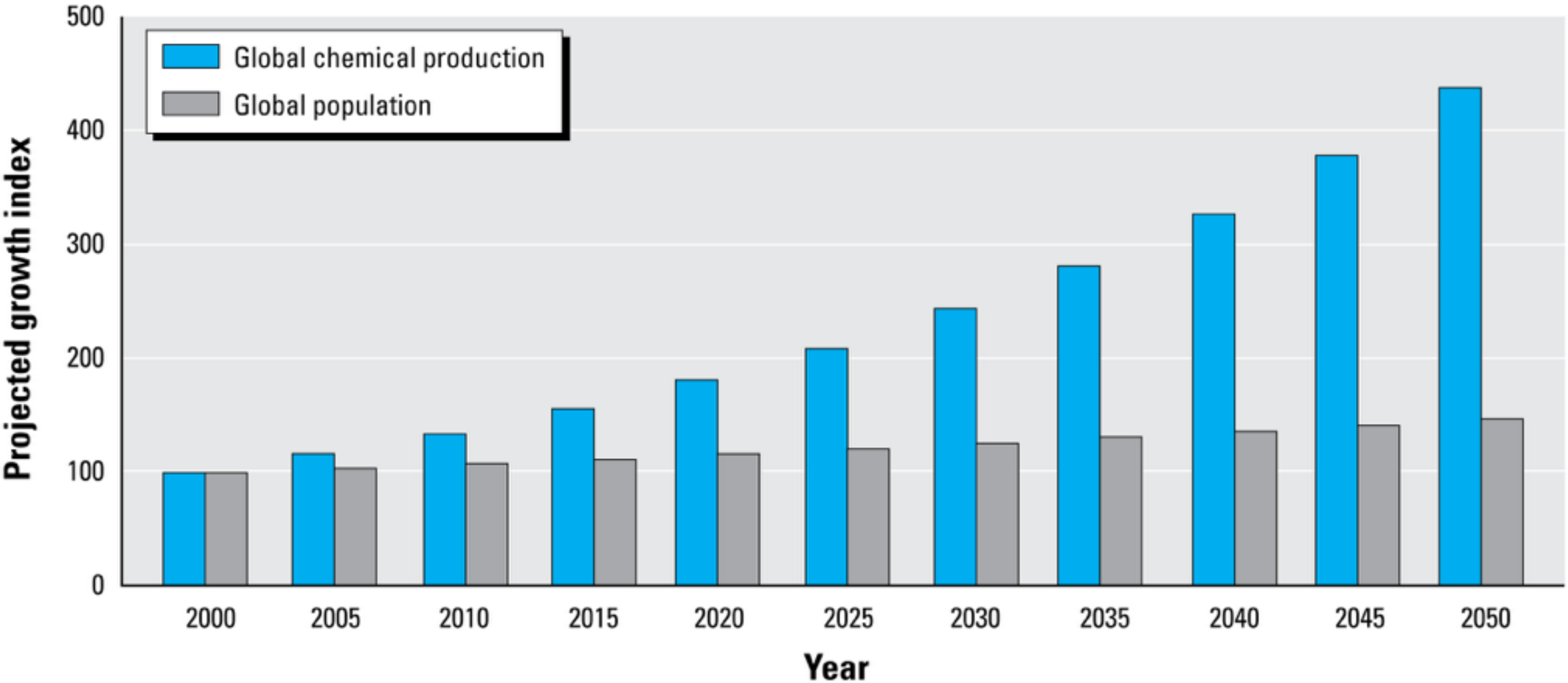


Wilson, M. P., & Schwarzman, M. R. (2009). Toward a New U.S. Chemicals Policy: Rebuilding the Foundation to Advance New Science, Green Chemistry and Environmental Health. *Environmental Health Perspectives, 117*(8), 1202–1209. http://doi.org/10.1289/ehp.0800404

Image: CDC

The 12 Principles of

# GREEN CHEMISTRY

Green chemistry is an approach to chemistry that aims to maximize efficiency and minimize hazardous effects on human health and the environment. While no reaction can be perfectly 'green', the overall negative impact of chemistry research and the chemical industry can be reduced by implementing the 12 Principles of Green Chemistry wherever possible.

## 1. WASTE PREVENTION

Prioritize the prevention of waste, rather than cleaning up and treating waste after it has been created. Plan ahead to minimize waste at every step.

## 2. ATOM ECONOMY

Reduce waste at the molecular level by maximizing the number of atoms from all reagents that are incorporated into the final product. Use atom economy to evaluate reaction efficiency.

## 3. LESS HAZARDOUS CHEMICAL SYNTHESIS

Design chemical reactions and synthetic routes to be as safe as possible. Consider the hazards of all substances handled during the reaction, including waste.

## 4. DESIGNING SAFER CHEMICALS

Minimize toxicity directly by molecular design. Predict and evaluate aspects such as physical properties, toxicity, and environmental fate throughout the design process.

## 5. SAFER SOLVENTS & AUXILIARIES

Choose the safest solvent available for any given step. Minimize the total amount of solvents and auxiliary substances used, as these make up a large percentage of the total waste created.

## 6. DESIGN FOR ENERGY EFFICIENCY

Choose the least energy-intensive chemical route. Avoid heating and cooling, as well as pressurized and vacuum conditions (i.e. ambient temperature & pressure are optimal).

## 7. USE OF RENEWABLE FEEDSTOCKS

Use chemicals which are made from renewable (i.e. plant-based) sources, rather than other, equivalent chemicals originating from petrochemical sources.

## 8. REDUCE DERIVATIVES

Minimize the use of temporary derivatives such as protecting groups. Avoid derivatives to reduce reaction steps, resources required, and waste created.

## 9. CATALYSIS

Use catalytic instead of stoichiometric reagents in reactions. Choose catalysts to help increase selectivity, minimize waste, and reduce reaction times and energy demands.

## 10. DESIGN FOR DEGRADATION

Design chemicals that degrade and can be discarded easily. Ensure that both chemicals and their degradation products are not toxic, bioaccumulative, or environmentally persistent.

## 11. REAL-TIME POLLUTION PREVENTION

Monitor chemical reactions in real-time as they occur to prevent the formation and release of any potentially hazardous and polluting substances.

## 12. SAFER CHEMISTRY FOR ACCIDENT PREVENTION

Choose and develop chemical procedures that are safer and inherently minimize the risk of accidents. Know the possible risks and assess them beforehand.

Green technological design should be informed by scientific knowledge of the environmental heath effects of chemicals and materials.

## Knowledge as a resource for decision-making

- **Understanding and assessing** the hazards of existing *and* "safer" technologies.
- **Guiding innovation and new solutions** in technology and design.
- **Informing and legitimizing action,** including regulation, business strategy, activism, and individual choices.

# Collective action for sustainability

- Scientific research
- Industry innovation
- Public policy
- Civil society

## How can we better mobilize scientific knowledge to advance green chemistry?

Knowledge commons definition and examples

Challenges in mobilizing knowledge

Framework for analyzing knowledge commons in green chemistry

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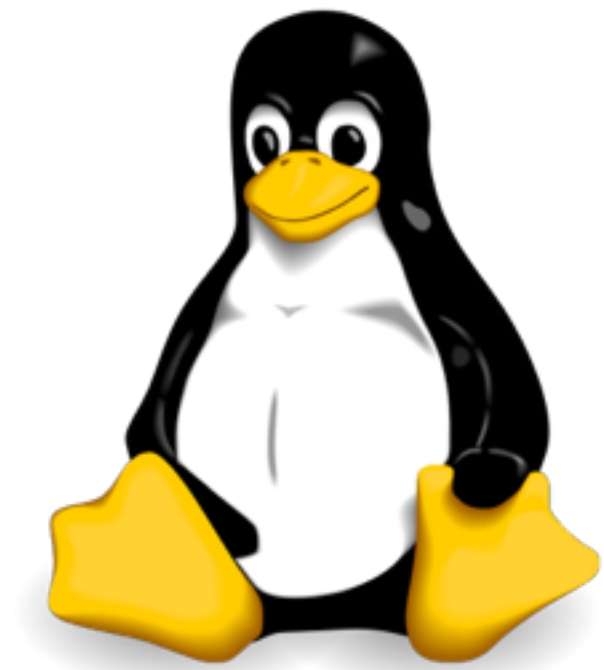
# What is a commons?

- **A pattern of institutional arrangements for sharing and co-producing resources among a community.**
- Not just resources: rules, infrastructures, social and technical systems.
- Not synonymous with “open access”, “free”, etc.
- **Governance** manages social dilemmas and reduces obstacles to sharing.

Hess, C., & Ostrom, E. (2007). *Understanding knowledge as a commons: from theory to practice.* Cambridge, Mass.: MIT Press.
Frischmann, B. M., Madison, M. J., & Strandburg, K. J. (Eds.). (2014). *Governing knowledge commons.* Oxford University Press.

# Knowledge commons

- Free & open-source software
- Open science
- Open data, open knowledge, …

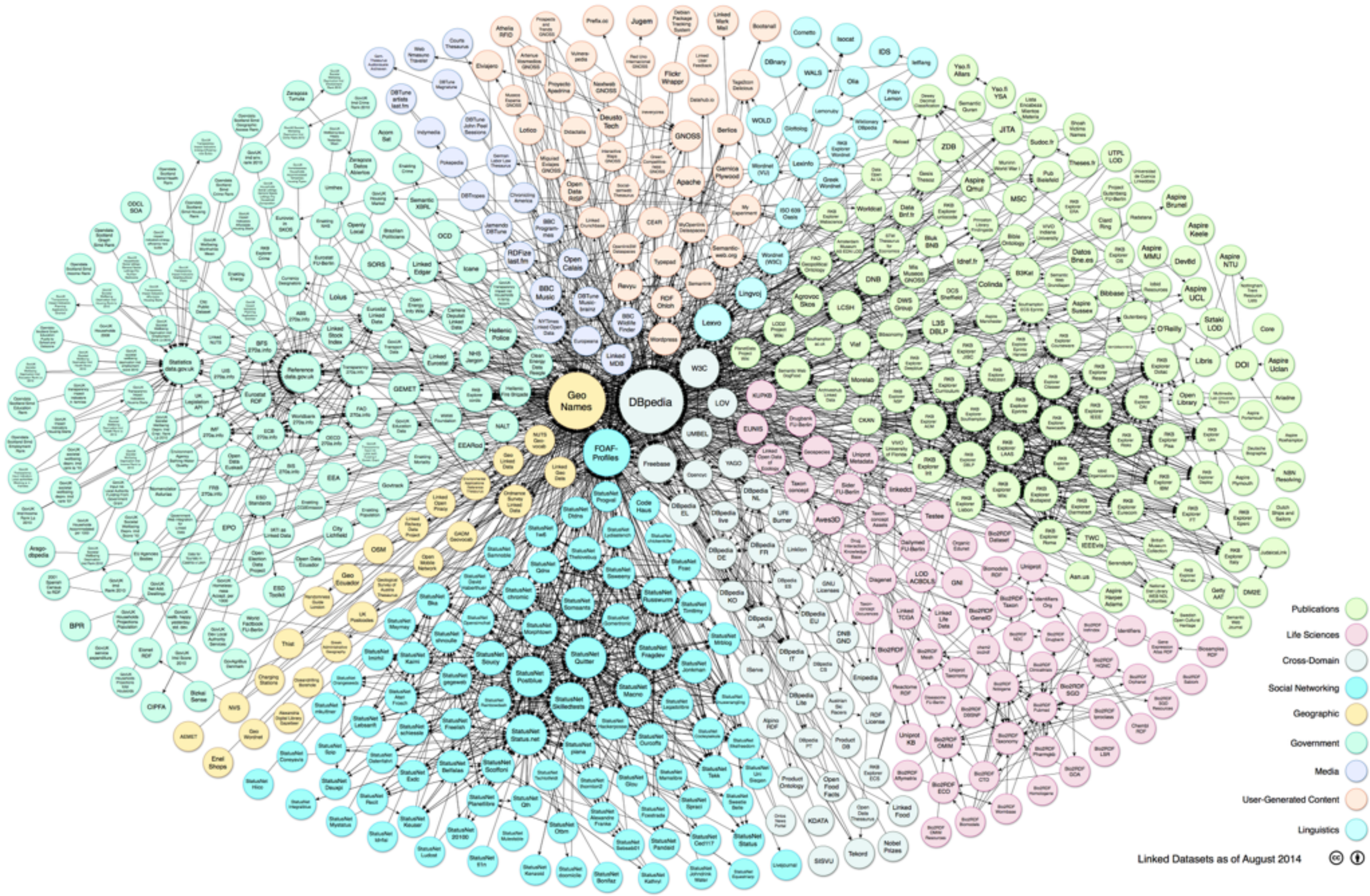


“Tux” by Larry Ewing, Simon Budig, & Anja Gerwinski

WIKIPEDIA
The Free Encyclopedia

The Wikimedia Foundation [CC BY-SA]

Schweik, C. M., & English, R. C. (2012). *Internet success: a study of open-source software commons.* Cambridge, Mass: MIT Press.
Nielsen, M. A. (2012). *Reinventing discovery: the new era of networked science.* Princeton, N.J.: Princeton University Press.
Open Knowledge. (2015). Open Definition 2.1. http://opendefinition.org/od/2.1/en/




Schmachtenberg, M., Bizer, C., Jentzsch, A., and Cyganiak, R. (2014). *Linking Open Data cloud diagram.* http://lod-cloud.net

Knowledge commons definition and examples

**Challenges in mobilizing knowledge**

Framework for analyzing knowledge commons in green chemistry

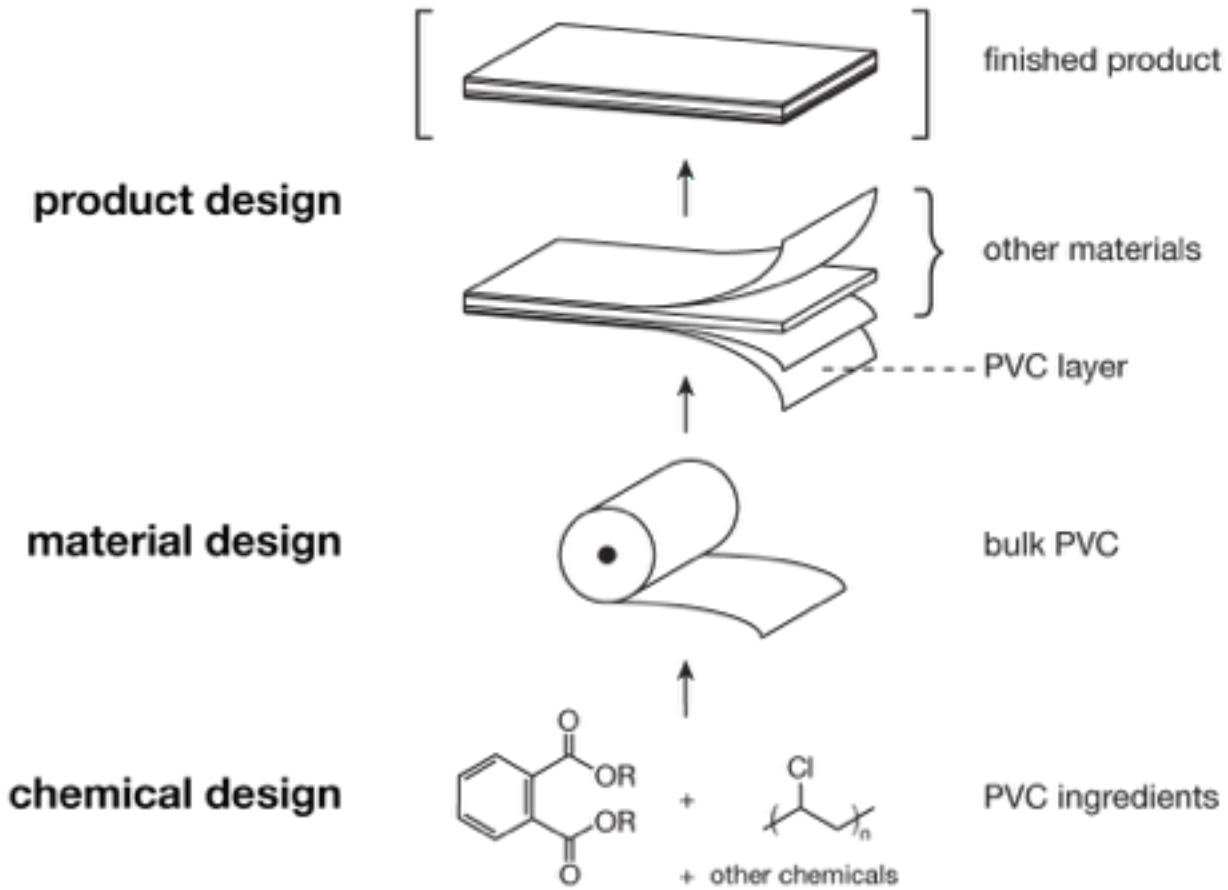
Technical, social, and political challenges in the mobilization of scientific knowledge are obstacles to advancing green chemistry.

# Data gaps

- **Availability:** Large proportion of chemicals have not been tested for safety.
    - There are many health effects that require different tests.
- **Accessibility:** Restrictions and data 'silos'.
    - IP inhibits access to scientific data, even 'published'.
    - Limitations of public domain data infrastructures.

Judson, R., et al. (2009). The Toxicity Data Landscape for Environmental Chemicals. *Environmental Health Perspectives, 117*(5), 685–695. http://doi.org/10.1289/ehp.0800168
Wilson, M. P., & Schwarzman, M. R. (2009). Toward a New U.S. Chemicals Policy: Rebuilding the Foundation to Advance New Science, Green Chemistry and Environmental Health. *EHP, 117*(8), 1202–1209. http://doi.org/10.1289/ehp.0800404

# Communication of hazard information




Multiple levels of design and decision-making

Complex, global supply systems

**Inadequate flow of information**

**Information asymmetries**

Massey, R. (2008). *Sharing knowledge about chemicals: policy options for facilitating information flow.* Lowell Center for Sustainable Production. http://www.chemicalspolicy.org/downloads/OptionsforStateChemicalsPolicyReform.pdf
Scruggs, C. E., & Ortolano, L. (2011). Creating safer consumer products: the information challenges companies face. *Environmental Science & Policy, 14*(6), 605–614. http://doi.org/10.1016/j.envsci.2011.05.010
Scruggs, C. E., Ortolano, L., Schwarzman, M. R., & Wilson, M. P. (2014). The role of chemical policy in improving supply chain knowledge and product safety. *JESS, 4*(2), 132–141. http://doi.org/10.1007/s13412-013-0158-4

# Uncertainty and contestation

- **Interpretation of scientific evidence:** e.g., low-dose effects of endocrine disruptors.
- **Conventions:** Standards of safety, risk, etc.
- **Paradigms:** Definition of green chemistry, “sustainability”, …

Jasanoff, S. (1990). *The fifth branch: science advisers as policymakers.* Cambridge, Mass.: Harvard University Press.
Sarewitz, D. (2004). How science makes environmental controversies worse. *Environmental Science & Policy, 7*(5), 385–403. http://doi.org/10.1016/j.envsci.2004.06.001
Matus, K. J. M., Clark, W. C., Anastas, P. T., & Zimmerman, J. B. (2012). Barriers to the Implementation of Green Chemistry in the United States. *Environmental Science & Technology, 46*(20), 10892–10899. http://doi.org/10.1021/es3021777

Knowledge commons definition and examples

Challenges in mobilizing knowledge

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# Knowledge systems perspective

**The set of actors involved in knowledge activities**
that contribute to the governance of chemicals,
**and the flows of information among them.**

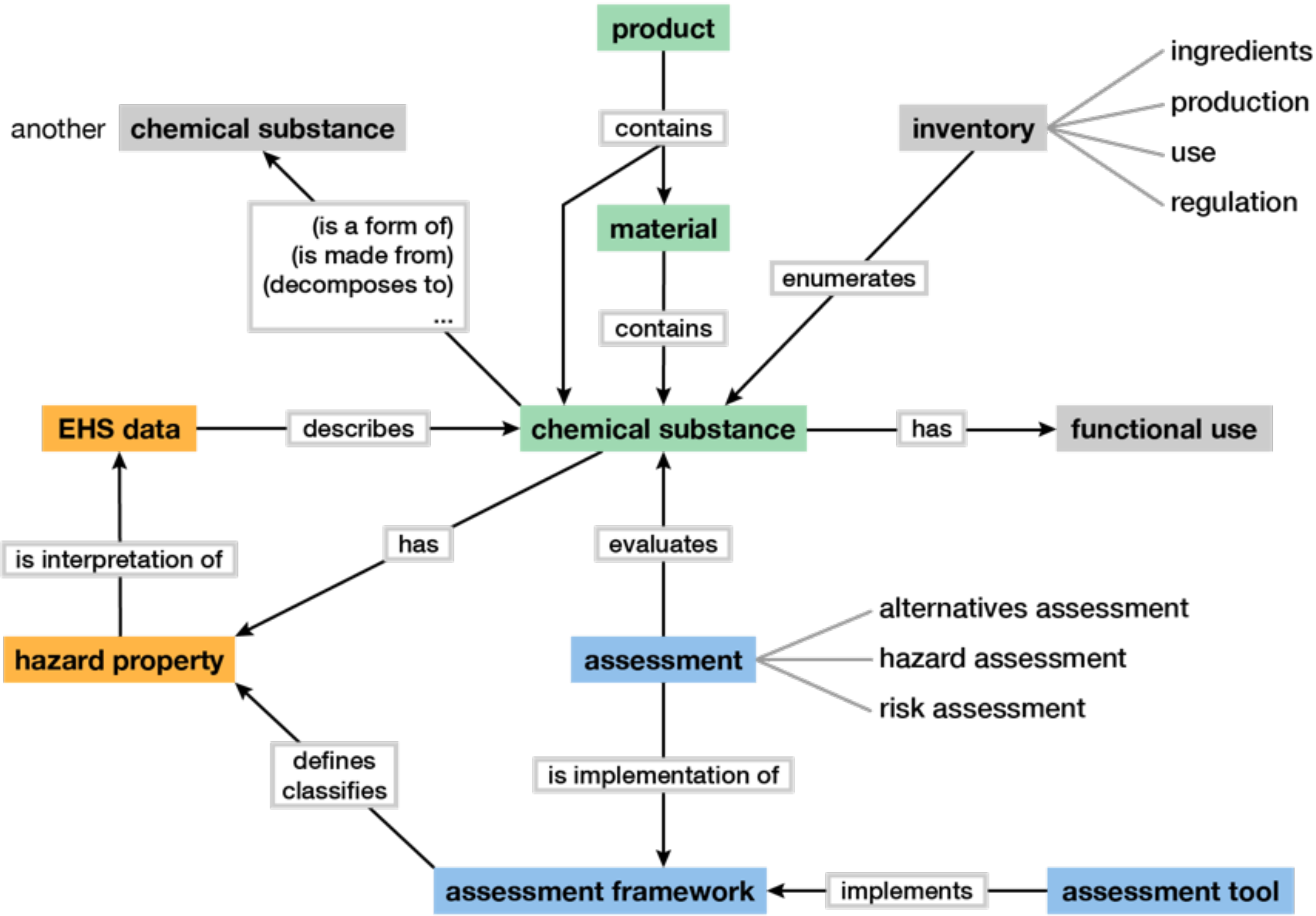
Cash, D. W., et al. (2003). Knowledge systems for sustainable development. *PNAS, 100*(14), 8086–8091. http://doi.org/10.1073/pnas.1231332100
McCullough, E. B., & Matson, P. A. (2011). Evolution of the knowledge system for agricultural development in the Yaqui Valley, Sonora, Mexico. *PNAS*. http://doi.org/10.1073/pnas.1011602108

# Types of knowledge resources

- **EHS information:** properties of chemicals
- **Inventories:** lists of chemicals
- **Standards:** including assessment frameworks
- **Tools:** to simplify knowledge tasks
- **Assessments:** knowledge for making decisions

For more on this, see http://kaios.net/research/organizing/

# Partial ontology of chemical hazard information

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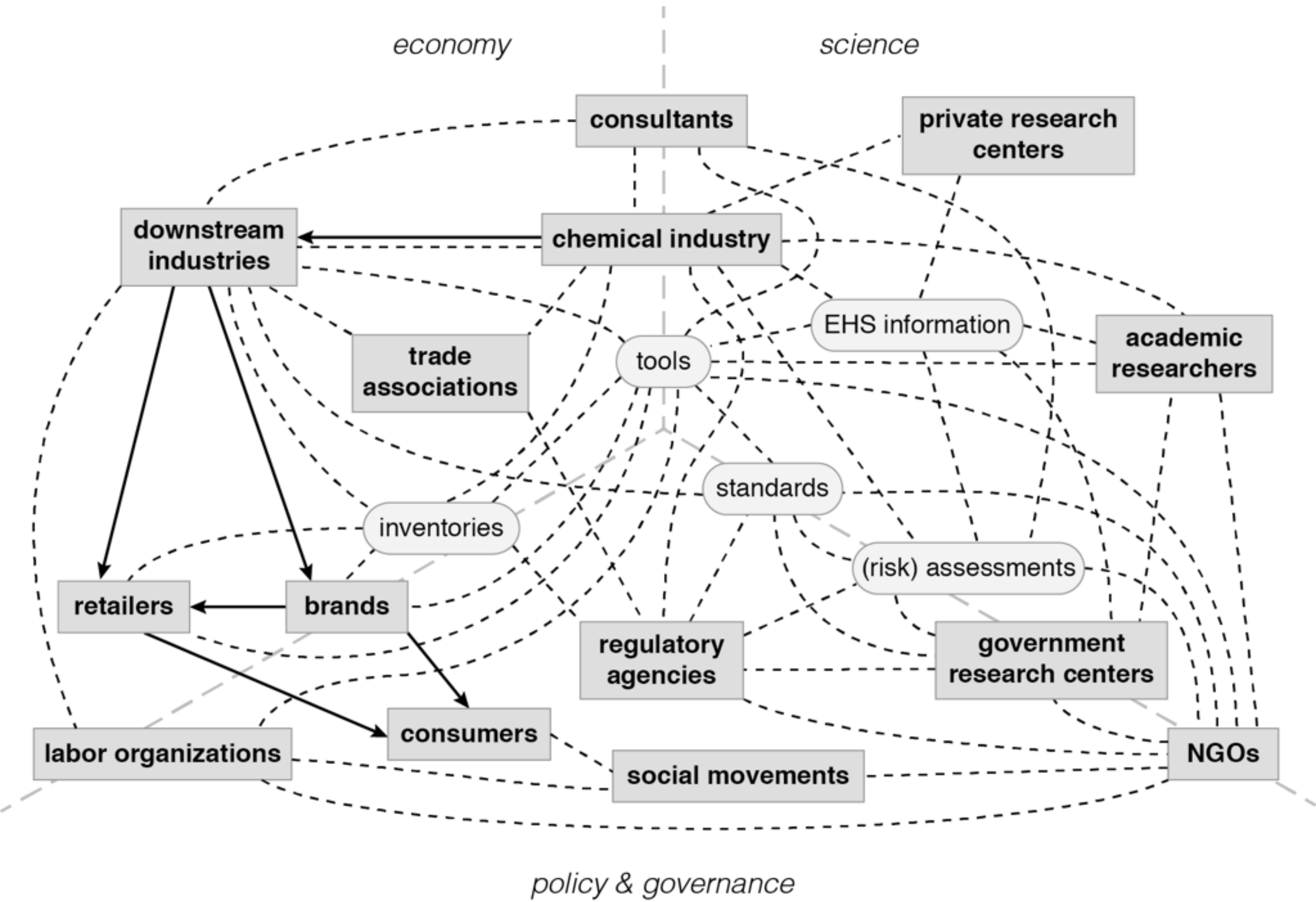



Inspired by: McCullough, E. B., & Matson, P. A. (2011). Evolution of the knowledge system for agricultural development in the Yaqui Valley, Sonora, Mexico. *PNAS*. http://doi.org/10.1073/pnas.1011602108

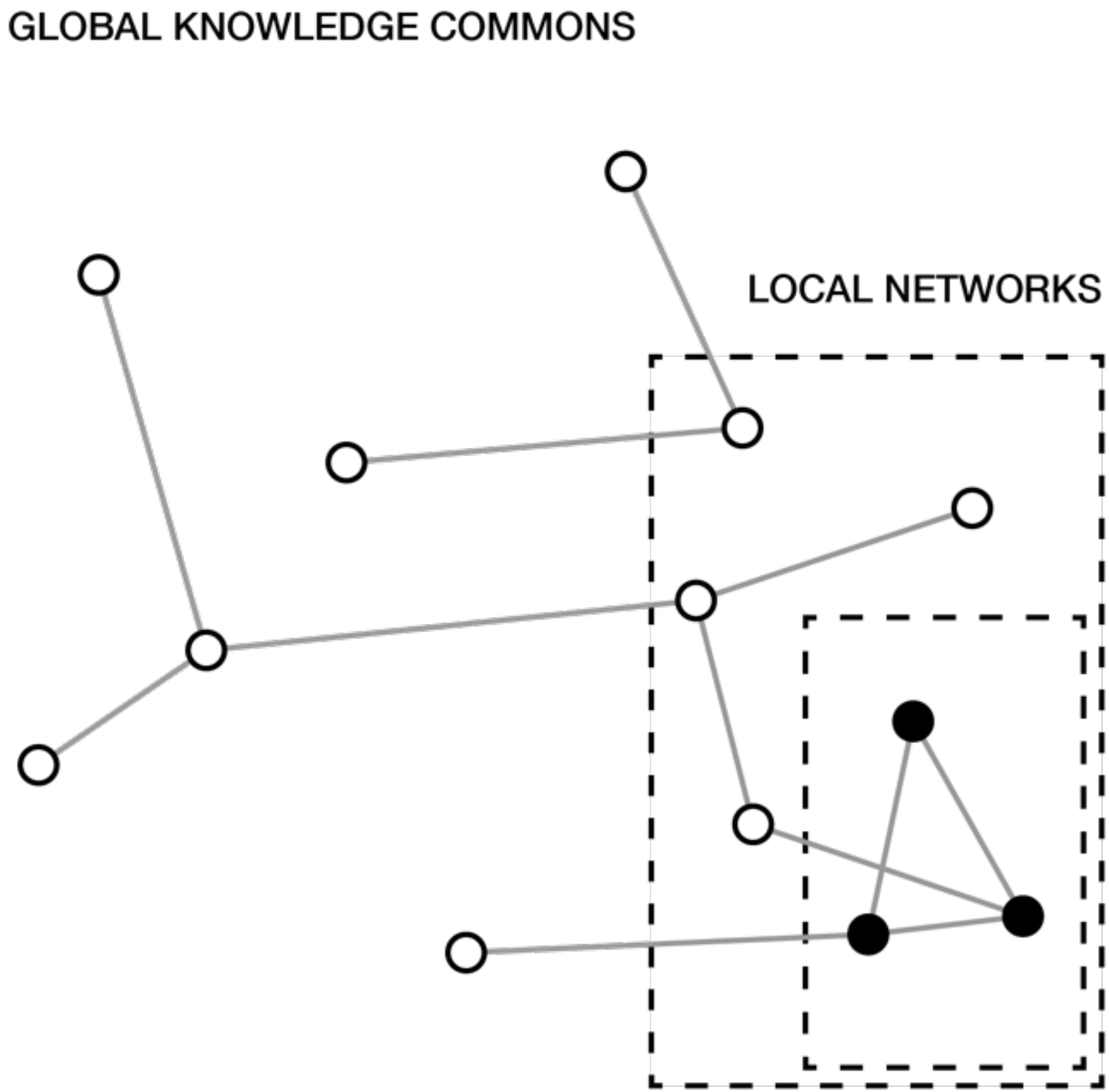
# New features of knowledge production?

- **Participatory** modes of production and validation, involving **multiple communities & stakeholder groups.**
- **Multi-directional flows** of information.
- **Diversified expert groups:** “extended peer review.”
- **Transparency** of knowledge resources.

Nowotny, H., Scott, P., & Gibbons, M. (2001). *Re-thinking science: knowledge and the public in an age of uncertainty.* Cambridge, UK: Polity.
Iles, A. (2011). Greening chemistry: Emerging epistemic political tensions in California and the United States. *Public Understanding of Science, 22*(4), 460–478. http://doi.org/10.1177/0963662511404306

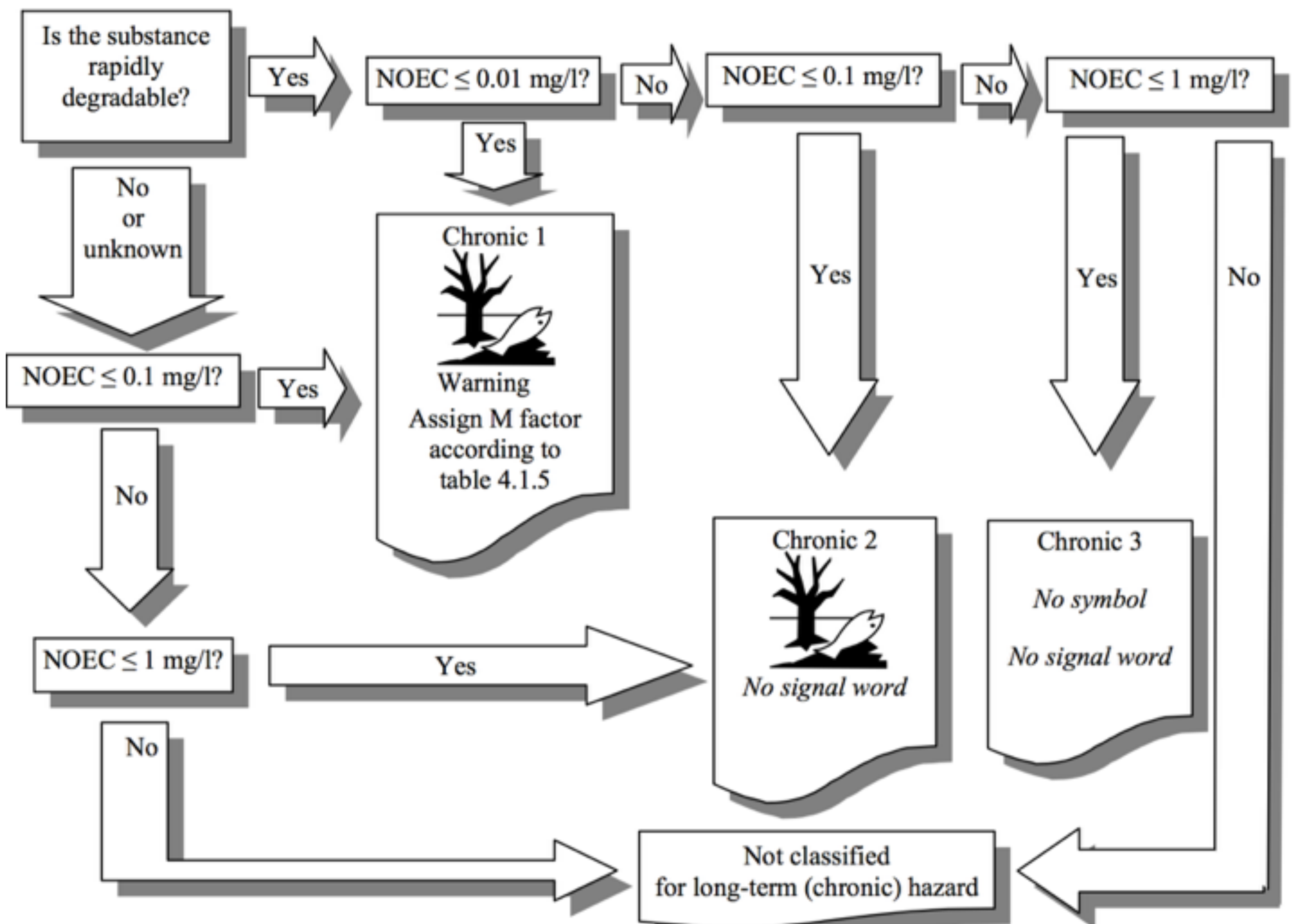
How do knowledge commons shape the production and validation of knowledge about chemicals and environmental health?

We can identify cases of knowledge commons among green chemistry efforts.


GLOBAL KNOWLEDGE COMMONS
LOCAL NETWORKS

# Case: Alternatives assessment

4.1.5.2.2 *Decision logic 4.1.3 (b) for substances (when adequate chronic toxicity data are available for all three trophic levels)*[5]




UNECE. (2015). *Globally harmonized system of classification and labelling of chemicals (GHS) (6th Revised Edition).* http://www.unece.org/trans/danger/publi/ghs/ghs_rev06/06files_e.html

# Case: Alternatives assessment

**Acute Aquatic Toxicity (AA)**

| Information Type | Measurement | | Very High (vH) | High (H) | Moderate (M) | Low (L) | |
|---|---|---|---|---|---|---|---|
| Data | GHS Criteria & Guidance | | GHS Category 1 | GHS Category 2 | GHS Category 3 | Sufficient data available and not classified | |
| Guidance Values (see GHS for further information) | $LC_{50}$ or $EC_{50}$ (mg/L) | | ≤1 | >1 to 10 | > 10 to 100 | >100 | |
| A Lists | DSL | Screening | *iT non-human* *Note: Could be based on acute or chronic aquatic toxicity. Only assess here if the classification is based on acute aquatic toxicity.* | | | | |
| | EU H-statements | Authoritative | H400 | | | | |
| | EU R-phrases | Authoritative | R50 | R51/53 | R52/53 | | |
| | GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan) | Screening | Category 1 | Category 2 | Category 3 | "Not Classified" | |
| B Lists | EU R-phrases | Authoritative | | R51 or R52 | | | |

**Chronic Aquatic Toxicity (CA)**

| Information Type | Measurement | | Very High (vH) | High (H) | Moderate (M) | Low (L) | |
|---|---|---|---|---|---|---|---|
| Data | GHS Criteria & Guidance | | | | GHS Category 4 | | |
| | Guidance Value (mg/L) | | ≤0.1 | >0.1 to 1.0 | > 1.0 to 10 | >10 | |
| A Lists | DSL | Screening | *iT non-human* *Note: Could be based on acute or chronic aquatic toxicity. Only assess here if the classification is based on chronic aquatic toxicity.* | | | | |
| | EU H-statements | Authoritative | | | H413 | | |
| | EU R-phrases | Authoritative | | | R53 | | |
| | GHS-[COUNTRY]* Lists (*Korea, Japan, Indonesia, Australia, Europe, New Zealand, and Taiwan) | Screening | | | Category 4 | | |
| B Lists | DSL | Screening | iT non-human *Note: Could be based on acute or chronic aquatic toxicity. Only assess here if the classification is based on chronic aquatic toxicity.* | | | | |

**Persistence (P)**

| Information Type | Media & Measurement | List Type | Very High (vH) | High (H) | Moderate (M) | Low (L) | Very Low (vL) |
|---|---|---|---|---|---|---|---|
| Data | **Soil or Sediment** (1/2 life in days OR Result) | | >180 or recalcitrant | >60 to 180 | 16 to 60 | < 16 OR GHS "Rapid degradability" | Meets 10-day window in "Ready Biodegradation Test" |
| | **Water** *(1/2 life in days OR Result)* | | > 60 or recalcitrant | > 40 to 60 | 16 to 40 | < 16 OR GHS "Rapid degradability" | Meets 10-day window in "Ready Biodegradation Test" |
| | **Air** *(1/2 life in days OR Result)* | | > 5 or recalcitrant | >2 to 5 | | < 2 | |
| | **Long-Range Environmental Transport** | | | Evidence | Suggestive Evidence | | |
| B Lists | DSL | Screening | Persistent (P) | | | | |

**Bioaccumulation Potential (B)**

| Information Type | Measurement | | Very High (vH) | High (H) | Moderate (M) | Low (L) | Very Low (vL) |
|---|---|---|---|---|---|---|---|
| Data | **BAF** (Bioaccumulation Factor) | | > 5000 | > 1000 to 5000 | > 500 to 1000 | > 100 to 500 | ≤ 100 |
| | **BCF** (Bioconcentration Factor) | | > 5000 | > 1000 to 5000 | > 500 to 1000 | > 100 to 500 | ≤ 100 |
| | **Log Kow** *(Log octanol-water partition coefficient)* | | > 5.0 | > 4.5 to 5.0 | > 4.0 to 4.5 | | ≤ 4 |
| | **Monitoring Data** *(Presence in humans or wildlife)* | | | Evidence | Suggestive Evidence | | |
| A Lists | DSL | Screening | *Bioaccumulative (B)* | | | | |

Clean Production Action. (2014). *GreenScreen Method.* http://www.greenscreenchemicals.org/method/full-greenscreen-method

**GHS**

Hazard classification system

SAFER CHOICE
Meets U.S. EPA Safer Product Standards
epa.gov/saferchoice

Chemical & product safety standard

GREEN SCREEN FOR SAFER CHEMICALS

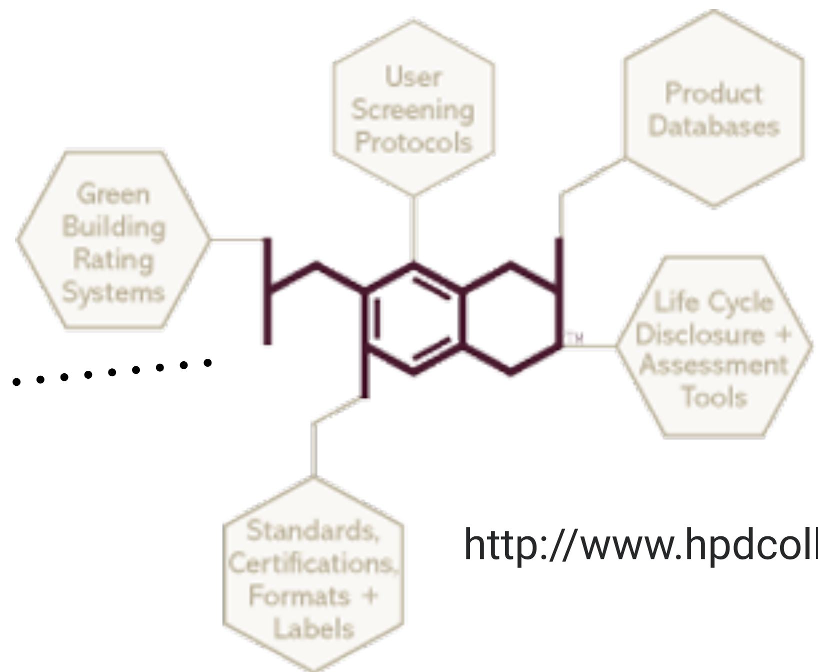
Comparative chemical hazard assessment framework

http://www.greenscreenchemicals.org/

Substitution knowledge base

SUBSPORT
Substitution Support Portal

http://www.subsport.eu/




Pharos

https://www.pharosproject.net/

Chemical hazard assessment database & Product selection tool

http://www.hpdcollaborative.org/

Product ingredient disclosure open standard

# Goals of knowledge commons in green chemistry

- Make the work **more effective, efficient.**
- **Build consensus and momentum** toward solutions.
- **Correct information asymmetries** in the chemicals market and downstream industry markets by **institutionalizing transparency.**
  - *While also protecting private knowledge.*

# Commons and the mobilization of knowledge

| Major knowledge challenges | Commons innovations |
| --- | --- |
| Knowledge gaps | Increase access |
| Inadequate information flows | Multi-directional flows |
| Uncertainty and contestation | Transparency and participation |

The commons presents opportunities for mutual benefit across society in overcoming barriers to sustainable transformation.

# Mahalo nui loa


- **National Science Foundation**
  - “Systems Approach to Green Energy” (SAGE) integrative graduate traineeship
- **Berkeley Center for Green Chemistry**
  - http://bcgc.berkeley.edu/
- **Department of Environmental Science, Policy, and Management (ESPM), UC Berkeley**




Slides available: http://kaios.net/talks