

# Short Introduction to a very certain point of View on the domain of Chemistry, a special focus on eLearning and on the development of a dynamic trajectories generator

An attempt for a partly scientific evening lesson, an  
insight into a great cooperation and a prospect on  
further developments in the field of eLearning  
mixed with components of edutainment

Richard Huber, FIZ CHEMIE

# Facts and Figures on FIZ CHEMIE



Scientific Research and Service Center

Founded in 11110111101

Our roots go back to 11100100110 with the establishment of the Chemischen Zentralblatt

1000110 ROI (GmbH)

1001000 employes, 111100% Scientists

Chemistry, Management of Knowledge and Information, Higher Education



Owners are:



# Short introduction to our special scientific domain: CHEMISTRY



How does a Chemist think?

# Short introduction to our special scientific domain: CHEMISTRY



How does a Chemist think?

Alcohol?

Some may at least know a correct chemical term



How does a Chemist think?

Alcohol?

**Ethanol**

## Live Demonstration



How does a Chemist think?

Alcohol?

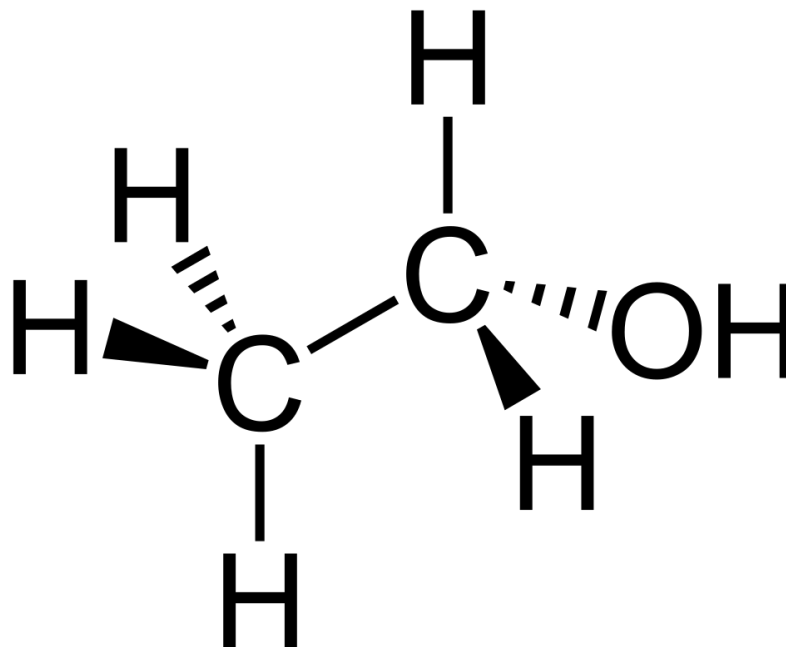
# Ethanol

# A short introduction to our special scientific domain: CHEMISTRY



How does a Chemist think?

Alcohol?

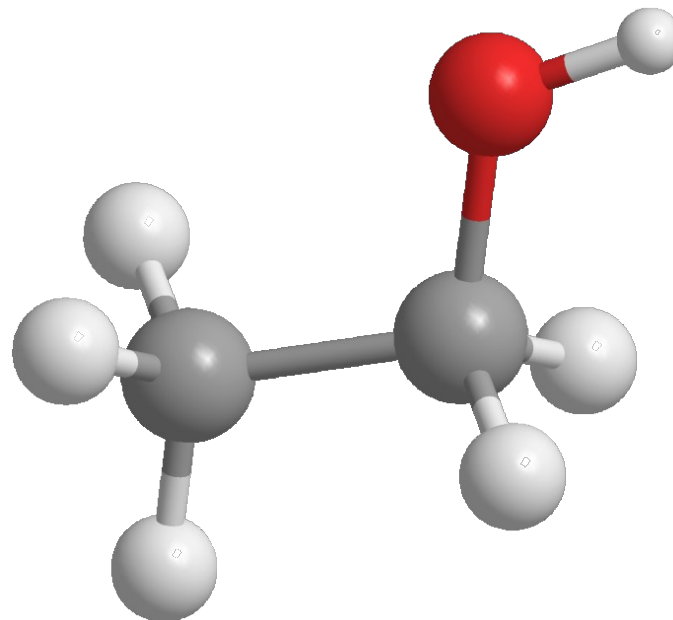
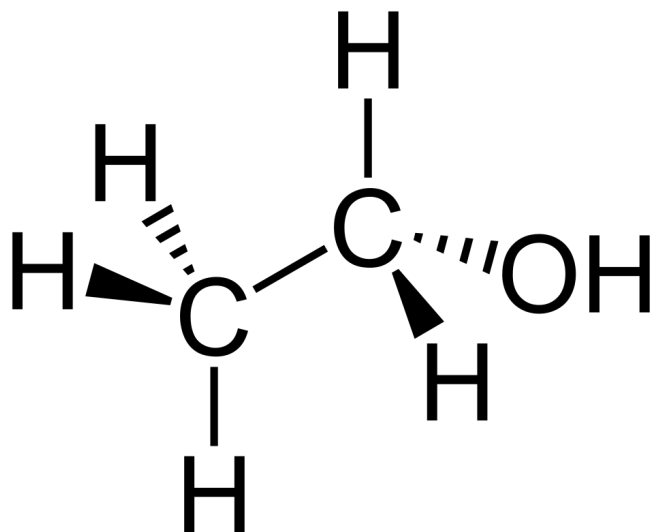


# Structures



**FIZ CHEMIE BERLIN**  
Fachinformationszentrum Chemie GmbH

Simply this way?



Nature Precedings : doi:10.1038/npre.2010.5407.1 : Posted 17 Dec 2010



## Our current products



CHEMISCHES  
ZENTRALBLATT  
SINCE 1830

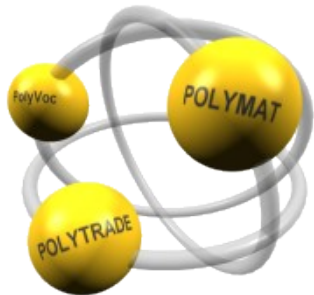


**CHEMGAROO**<sup>®</sup>  
EDUCATIONAL SYSTEMS



**FIZ CHEMIE BERLIN**

Fachinformationszentrum Chemie GmbH



**ChemInform**<sup>®</sup>

**INFOTHERM**<sup>®</sup>  
everyday science

# We're drowning in data, says pharma giant Roche

- **Drug maker says data volume is doubling every 15 months and “we don't know how to filter it”**

Press report from December 02  
2010

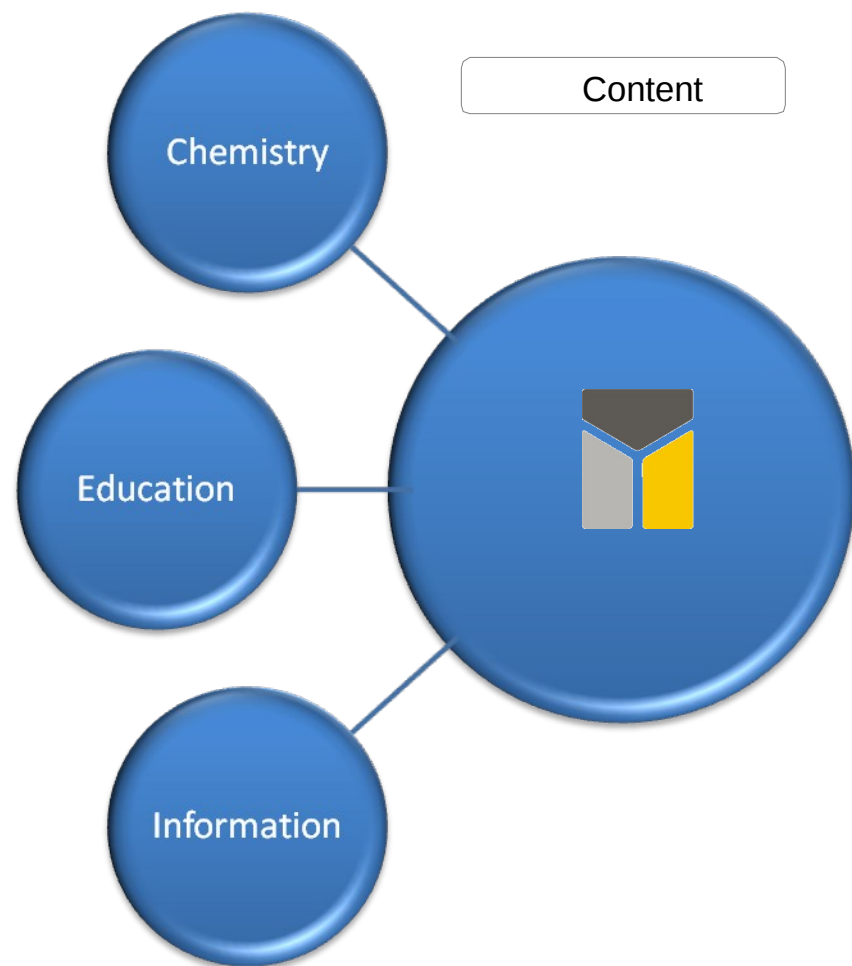
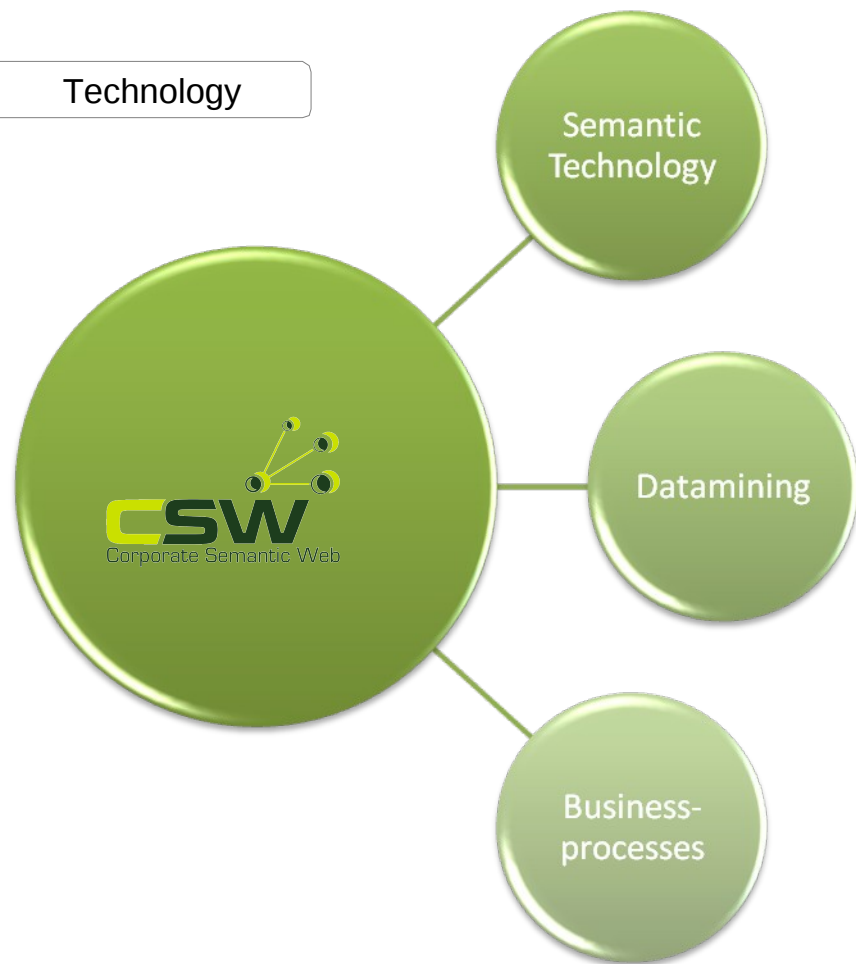
## How we (plan to) react

- Providing high quality data (Relevance of Quality)
- Personalized user access to data by providing individual sets of tool
- Personalized data sets
- HCI that learns to know its users and the related preferences

## How we (plan to) react

- Providing high quality data (Relevance of Quality)
  - Personalized user access to data by providing individual sets of tool
  - Personalized data sets
  - HCI that learns to know its users and the related preferences

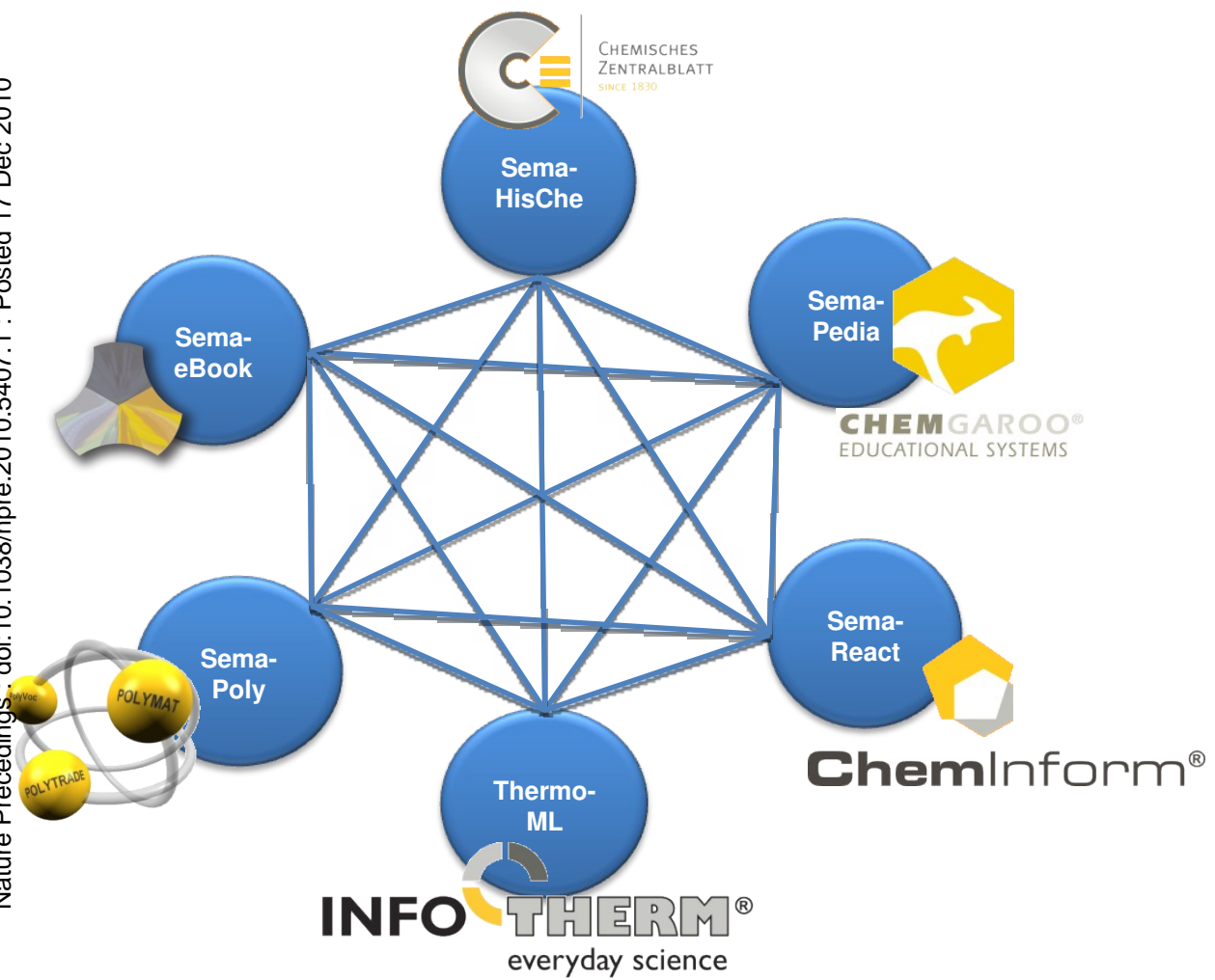
# Introducing a strategic cooperation



Nature Precedings : doi:10.1038/npre.2010.5407.1 : Posted 17 Dec 2010

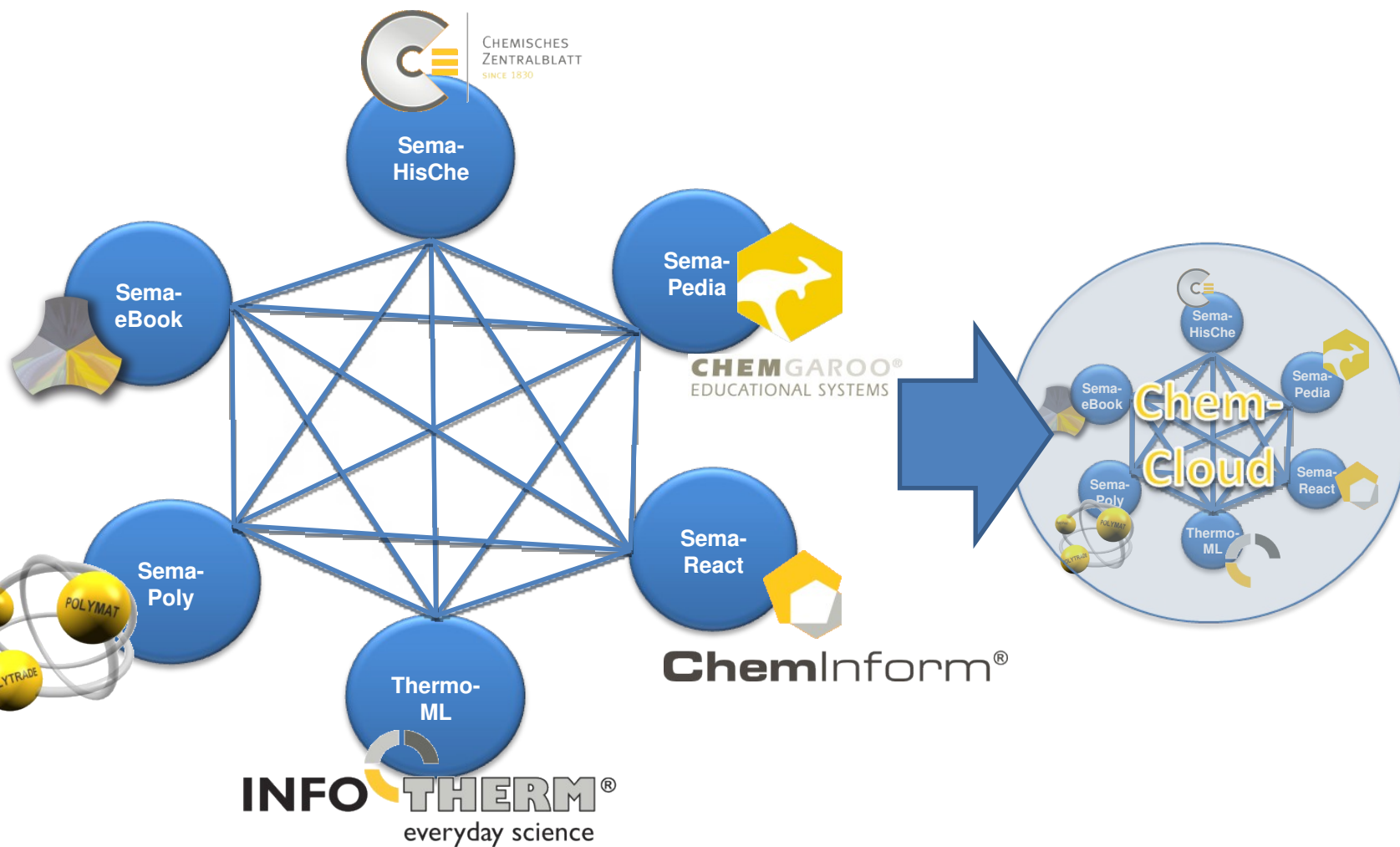
# Building specialized Ontologies

Nature Precedings : doi:10.1038/npre.2010.5407.1 : Posted 17 Dec 2010



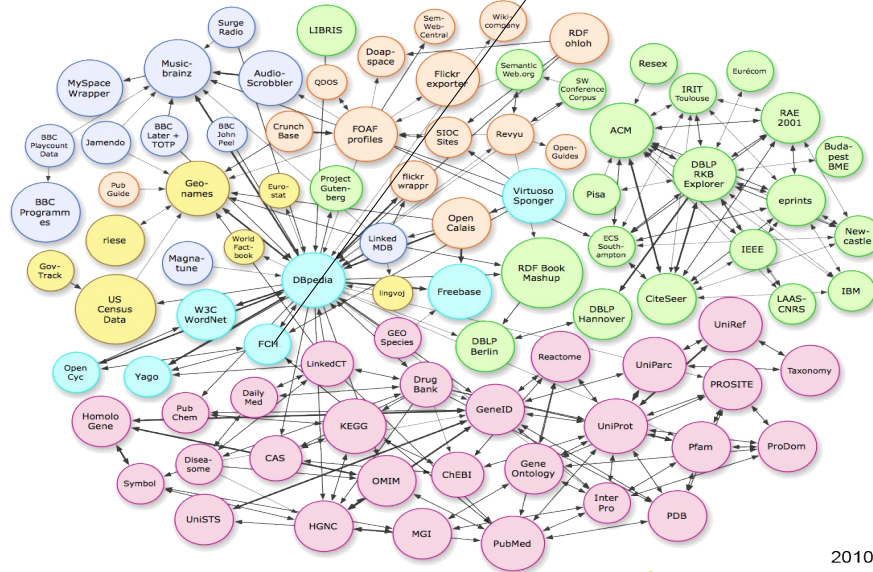
# Combine subject related Ontologies to one large Chemistry Ontology

Nature Precedings : doi:10.1038/npre.2010.5407.1 : Posted 17 Dec 2010



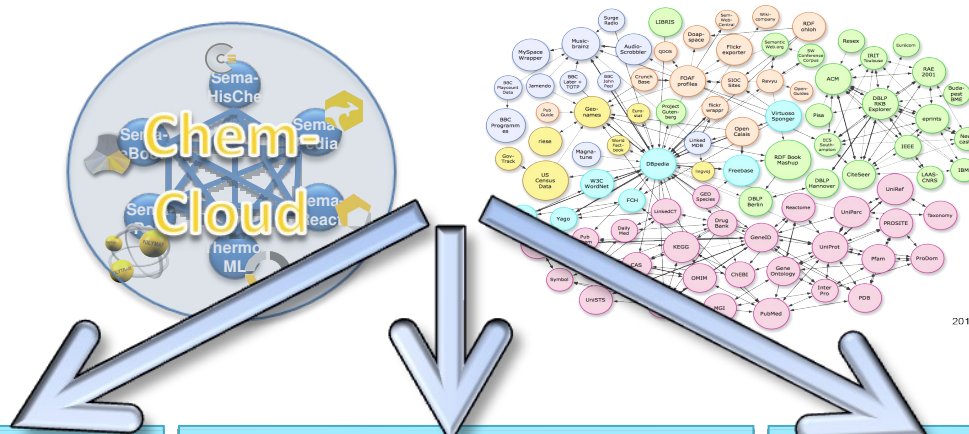
# Transferring that Chemistry Ontology into the Linked Data Cloud

Nature Precedings : doi:10.1038/npre.2010.5407.1 : Posted 17 Dec 2010





# Building new Business Processes



## Semantic Thermodynamics (SemaThermo):

- Semantic version of InfoTherm database
- Better Performance of integrated Thesaurus
- Increased amount of hits
- Relationship between trivialname and scientific vocabulary
- Relations to associated expressions

BP



## Semantic Chemistry Education (SemaPedia):

- Personalized learning environment
- Identification of chemical entities
- Parsing existing metadata
- Improved search functions
- Personalized didactics
- Dynamic assembly of pages and units
- Personalized teaching path
- Platform adjusting to individual skills

BP



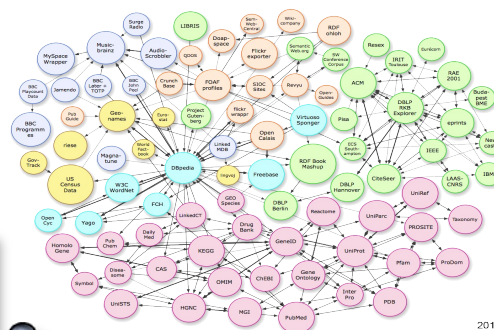
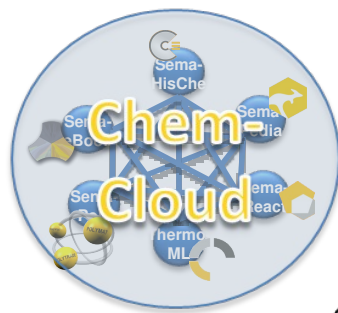
## Semantic Polymers (SemaPoly):

- Portal for chemists and engineers
- New version of FIZ CHEMIE Poly-Databases
- Relationship between trivialname and scientific vocabulary
- Different user levels
- Role- and personalisation methods
- 5.000 Suppliers, 19.000 commercial products, dictionary with 124.000 plastics, 20.000 trade products, 1.100 manufacturers

BP



# Building new Business Processes



2010

## Semantic Thermodynamics (SemaThermo):

- Semantic version of InfoTherm database
- Better Performance of integrated Thesaurus
- Increased amount of hits
- Relationship between trivilanname and scientific vocabulary
- Relations to associated expressions

BP



## Semantic Chemistry Education (SemaPedia):

- Personalized learning environment
- Identification of chemical entities
- Parsing existing metadata
- Improved search functions
- Personalized didactics
- Dynamic assembly of pages and units
- Personalized teaching path
- Platform adjusting to individual skills

BP



## Semantic Polymers (SemaPoly):

- Portal for chemists and engineers
- New version of FIZ CHEMIE Poly-Databases
- Relationship between trivilanname and scientific vocabulary
- Different user levels
- Role- and personalisation methods
- 5.000 Suppliers, 19.000 commercial products, dictionary with 124.000 plastics, 20.000 trade products, 1.100 manufacturers

BP



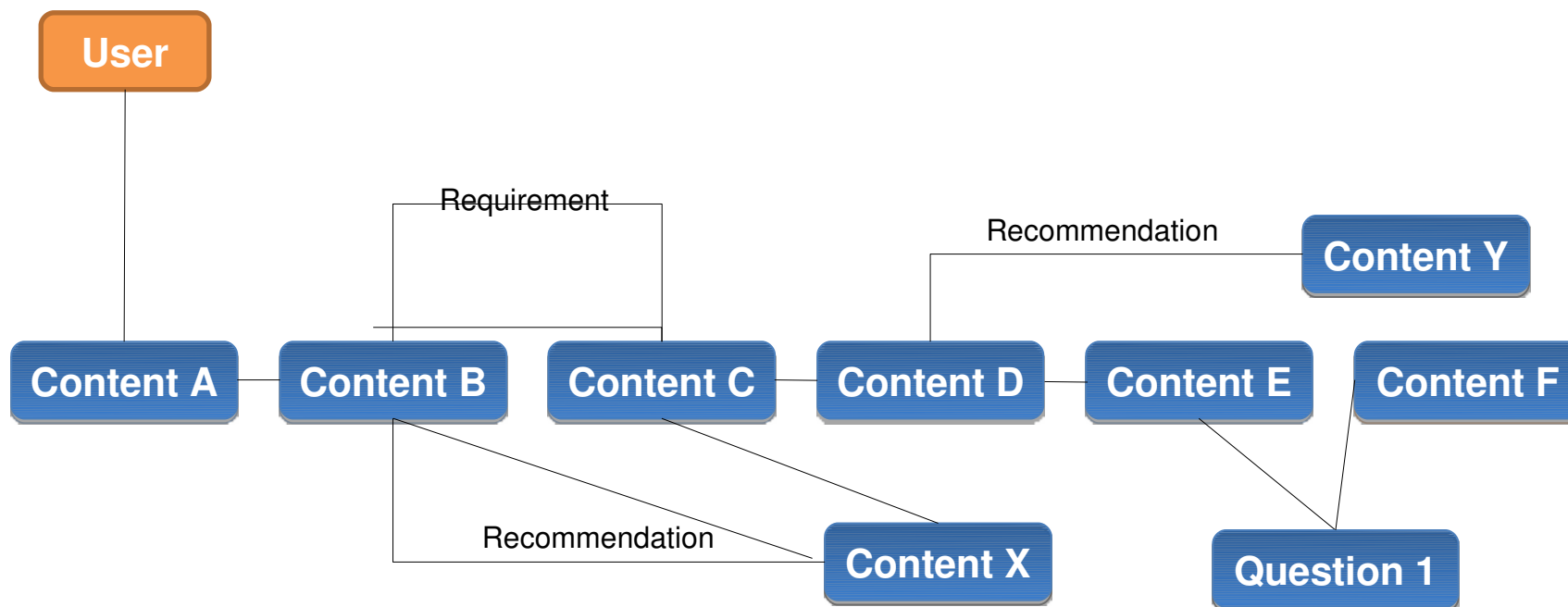
- Collection of 1.700 multimedia eLearning lessons in the subject of Chemistry and related sciences
- Some 18.000 interactive content pages with approx. 25.000 media elements
- 4 Million users during last 12 months,
- Homogenous target group - students, teachers (schools and universities), trainers
- Localization: Currently German spoken areas
- Open platform concept without registration
- Teaching paths are coded with the content by the initial authors
- XML-based
- Guided bulletin board



[www.chemgapedia.de](http://www.chemgapedia.de)

# Teaching-Paths (trajectories) in ChemgaPedia (today)

## Hardcoded paths (static, generic)



# Current representation inside Chemngapedia

Nature Precedings : doi:10.1038/npre.2010.5407.1 : Posted 17 Dec 2010

Mindmap - Chemngapedia - Mozilla Firefox  
 http://www.chemngapedia.de/vsengine/mindmap/de/topics.mm.html

Navigation: Mindmap, Html Seite  
 Volke: Lerneinheit, Seite, Glossar, Biographie  
 Fachgebiet: Chemie, Biochemie, Pharmazie, Mathematik, Physik

Legende ausblenden

Chemngapedia

- Chemie
  - Allgemeine Chemie
  - Anorganische Chemie
  - Organische Chemie
  - Physikalische Chemie
  - Analytische Chemie
  - Technische Chemie
  - Makromolekulare Chemie
    - Einführung
    - Polymere
    - Reaktionsmechanismen
    - Copolymerisation
    - Polymerisationsverfahren
    - Reaktionstechnik
    - Polymeranalytik
    - Polymereigenschaften
    - Polymerverarbeitung
    - Anwendungen
    - Funktionspolymere
    - Polymere Netzwerke
    - Spezielle Architekturen
  - Theoretische Chemie
  - Chemieinformation
  - Chemoinformatik
  - Umweltchemie
  - Toxikologie
- Pharmazie
- Physik
- Mathematik
  - Zahlen
  - Vektoren
  - Zahlenfolgen und Reihen
  - Funktionen
  - Differenzialrechnung von Funktionen einer Variablen
  - Differenzialrechnung von Funktionen mehrerer Variablen
  - Integration von Funktionen einer Variablen
  - Integration von Funktionen mehrerer Variablen
  - Kombinatorik
  - Verteilungen und Wahrscheinlichkeiten
  - Optimierung
  - Lineare Algebra
  - Funktionsdarstellung durch Reihen und Integrale
  - Gewöhnliche Differenzialgleichungen
  - Partielle Differenzialgleichungen
  - Elementare Operatoralgebra
  - Spezielle Module
- Biochemie
  - Chemische Grundlagen
  - Biologische Grundlagen
  - Stoffwechsel
  - Signal- und Stofftransport
    - Botenstoffe
    - Neurotransmission
    - Hormone
    - Rezeptoren
    - Transportprozesse
  - Proteinbiosynthese
  - Arbeitsmethoden
  - Medizinische Chemie und Biochemie

Übertragen der Daten von www.chemngapedia.de...

## Advantages and Disadvantages of anonymous educational platforms

User



- ❖ Anonymous,
- ❖ Self conducted learning



- ❖ only static paths
- ❖ no personal environment
- ❖ no save mechanism for path and advantage

Hoster
















- ❖ minimized administration needs
- ❖ high numbers of users



- ❖ limited feedback
- ❖ only anonymous data
- ❖ Methods of EDM rarely useful

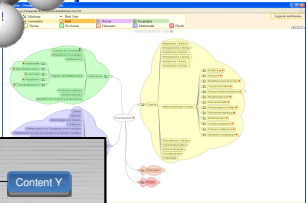
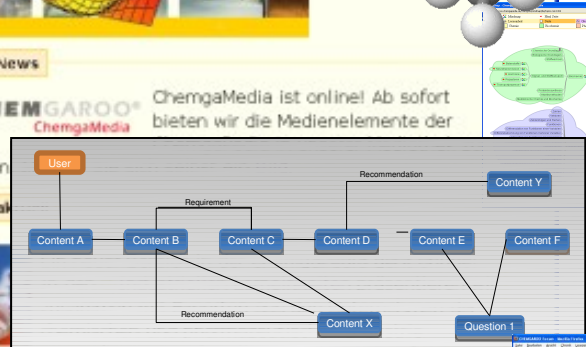
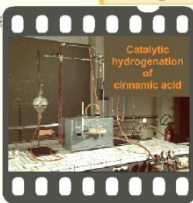
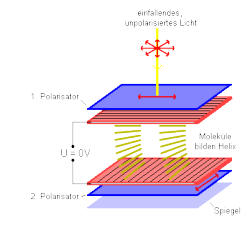
## Our wishlist for an eLearning future<sup>®(\*1)</sup>

-  Dynamic role module
-  Advanced communication tools
-  Tools for collaborative learning
-  Individual dynamic page creation and path recommendations
-  Personalized Working environment with individually selectable set of tools
-  Dynamic selection of scientific precision by the user
-  Personal workspace to save paths, learning advantages and preferences
-  Tools to analyse/compare current userbehavior and userdata with background eLearning ontologies
-  Non-invasive integration of applications which require registration to gain user data
-  Platform that allows different didactic models like explorative access to teaching information or classic
-  „booklike“ learning
-  Dynamic tools and environment for authors
- 

(\*1) Registered trademark by Santa Clause

# Screenshot of current platform

Nature Precedings : doi:10.1038/npre.2010.5407.1 : Posted 17 Dec 2010





# Screenshot of first pre-alpha Version of prototype of a semantic based ChemgaPedia

Nature Precedings : doi:10.1038/npre.2010.5407.1 : Posted 17 Dec 2010

The screenshot shows a Mozilla Firefox browser window with the address bar displaying `http://paschke-101.fiz-chemie.de/chem/index.html`. The main content area features a semantic network diagram centered on a node labeled "organische C". This central node is connected to four other nodes: "Thiolalkohol" (top), "Thiol" (bottom), "Kohlenwasser" (left), and "Term" (right). The "Term" node is further connected to a cluster of related terms: "chemische S", "anorganische", "chemisches", "Element", and "Organometal".

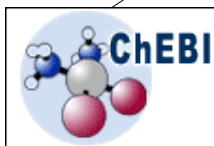
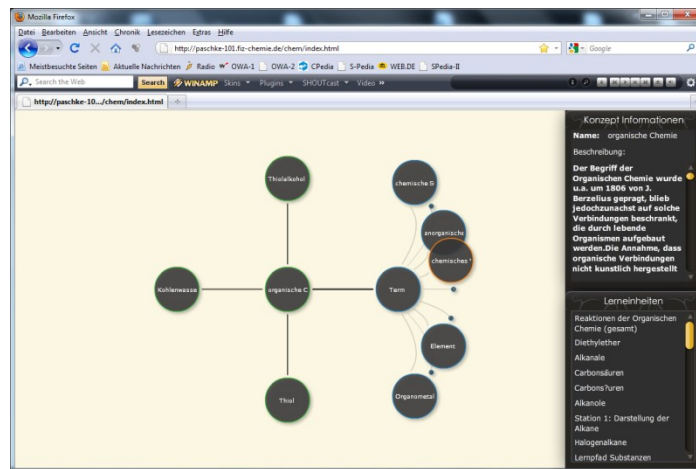
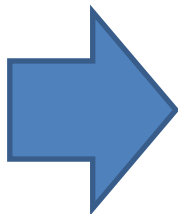
On the right side of the browser, there is a sidebar with two sections:

- Konzept Informationen**
  - Name: organische Chemie
  - Beschreibung:
  - Der Begriff der Organischen Chemie wurde u.a. um 1806 von J. Berzelius geprägt, blieb jedoch zunächst auf solche Verbindungen beschränkt, die durch lebende Organismen aufgebaut werden. Die Annahme, dass organische Verbindungen nicht künstlich hergestellt
- Lerneinheiten**
  - Reaktionen der Organischen Chemie (gesamt)
  - Diethylether
  - Alkanale
  - Carbonsäuren
  - Carbons?uren
  - Alkanole
  - Station 1: Darstellung der Alkane
  - Halogenalkane
  - Lernpfad Substanzen

# A first Version of a prototype

## XML -> RDF

## Chemical entity Identification



## Internals

- Align our ontology with ChEBI and PubChem schemata from Biio2RDF
- Enrich ChemgaPedia content with chemical identifiers and classifications
- Improved search functionality (new and more precise data)
- Enhance ChemgaPedia content with related content from DBPedia (Germany)
- Based on the Open Semantic Framework
- Core part is StructWSF (web service framework with access to triple store)
- The GUI is implemented with DRUPAL (Open Source CMS) and the con Struct component
- Faceted Search functionality

## Two steps

### PROTOTYPE/ DEMONSTRATOR

#### Prototype Functionality:

- Chemistry Ontology
- Based on expertise of authors
- eLearning orientated selection and modelling
  
- eLearning Ontology
- Based on existing metadata
- Content related concepts/relationships

#### Prototype Features:

- Ontology based copy of ChemgaPedia
- XML -> RDF converters
- Identification of chemical entities
- Parsing existing metadata
- Improved search functions

### DYNAMIC E-LEARNING TRAJECTORIES (DELTS)

#### DeLTs idea:

Collecting user information by offering value added services and transferring concepts and recommendations from certain user groups to all users of ChemgaPedia

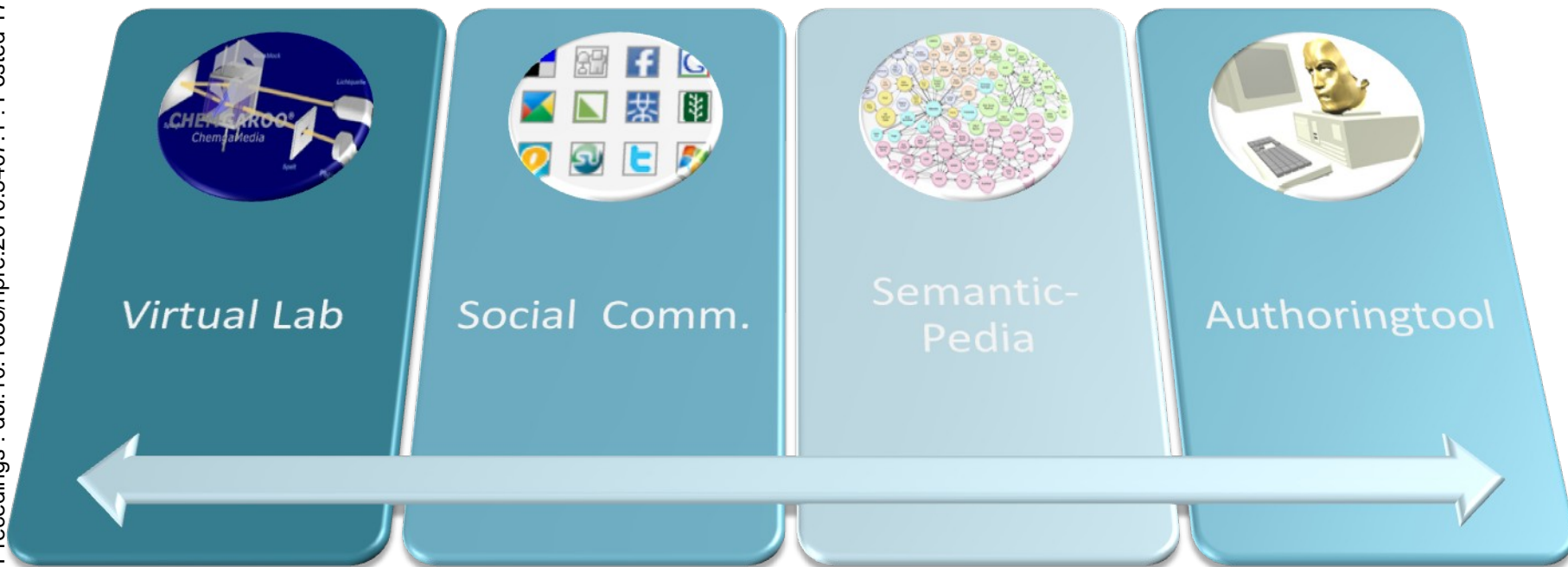
#### DeLTs aims:

- Personalized didactics
- Dynamic assembly of pages and units
- Personalized teaching path
- Platform adjusting to individual skills

#### DeLTs requirements:

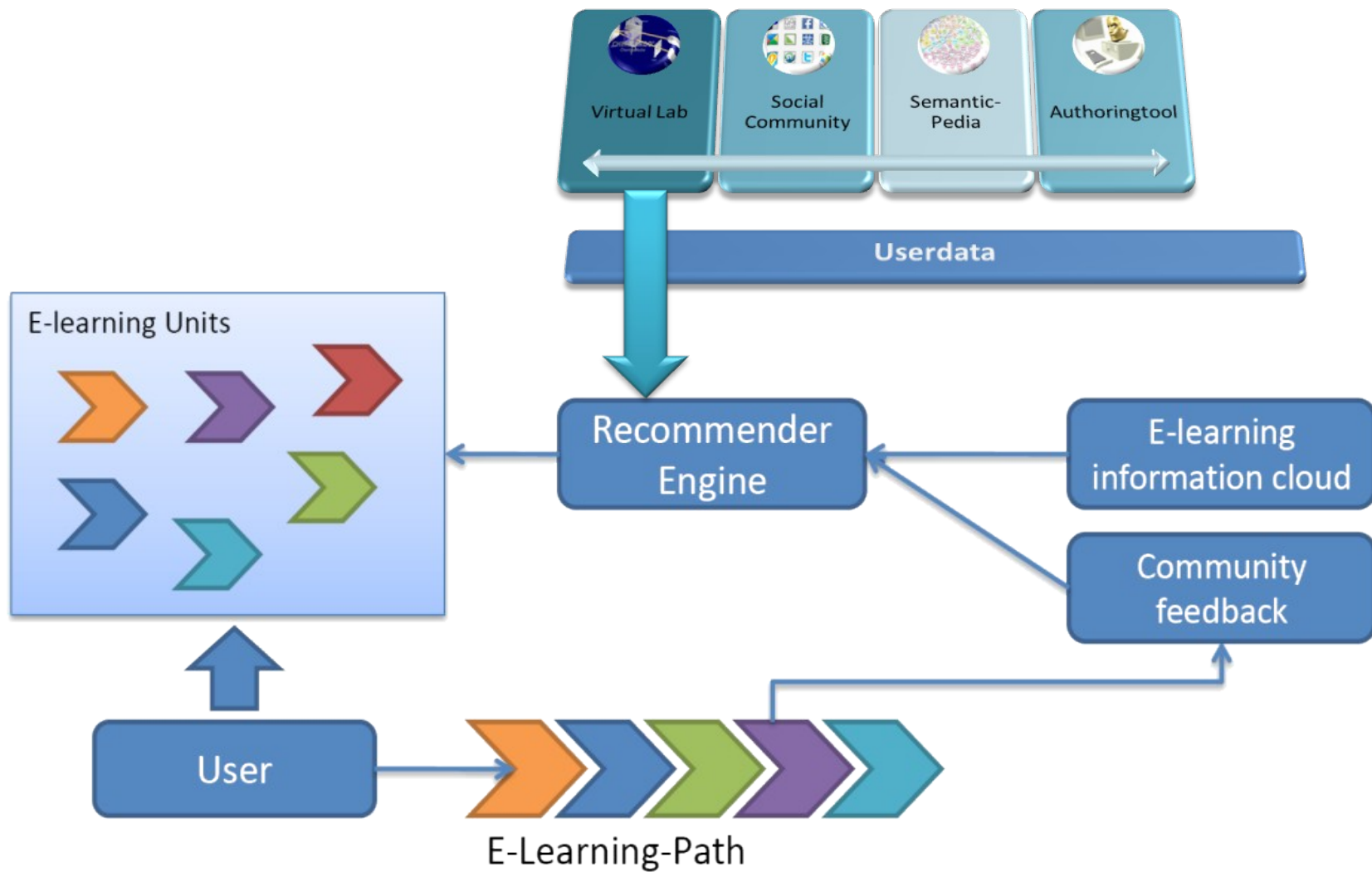
- Registration process
- Knowledge level
- Level of experience
- Personal background
- Performance
- Preferred didactics
- Personal skills
- Age, gender, origin, ...

## Value added Services to generate user data



Nature Precedings : doi:10.1038/npre.2010.5407.1 : Posted 17 Dec 2010

# From Value added Services to Dynamic eLearning Trajectories (DeLTs)



Nature Precedings : doi:10.1038/npre.2010.5407.1 : Posted 17 Dec 2010

## Credits

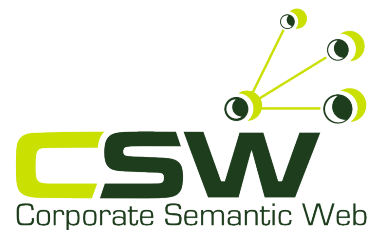
Richard Huber, Kirsten Hantelmann

**FIZ CHEMIE**



Alexandru Todor, Sebastian Krebs, Ralf Heese, Adrian Paschke

**Freie Universität Berlin**



# Thank You for your interest

## Don't miss to see our poster presentation

