Bio-ontologies SIG/ISMB'07

July 20, 2007

ART: An ontology based tool for the translation of papers into Semantic Web format

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2) Royal Society of Chemistry Publishing, UK;
3) University College London, UK .

Plan of the presentation

- Introduction to the ART;
- Related projects:
  - The Prospect project;
  - An ontology of experiments EXPO;
  - The ROAD project;
  - eBank.
- The ART project:
  - The ART system;
  - Examples.
- Discussion: An ontology of science.

The ART project (an ontology based ARticle preparation Tool)

- Translating scientific papers into a format with an explicit semantics.
- Explicit linking of repository papers to data and metadata.
- Creation of an example ‘intelligent’ digital repository.

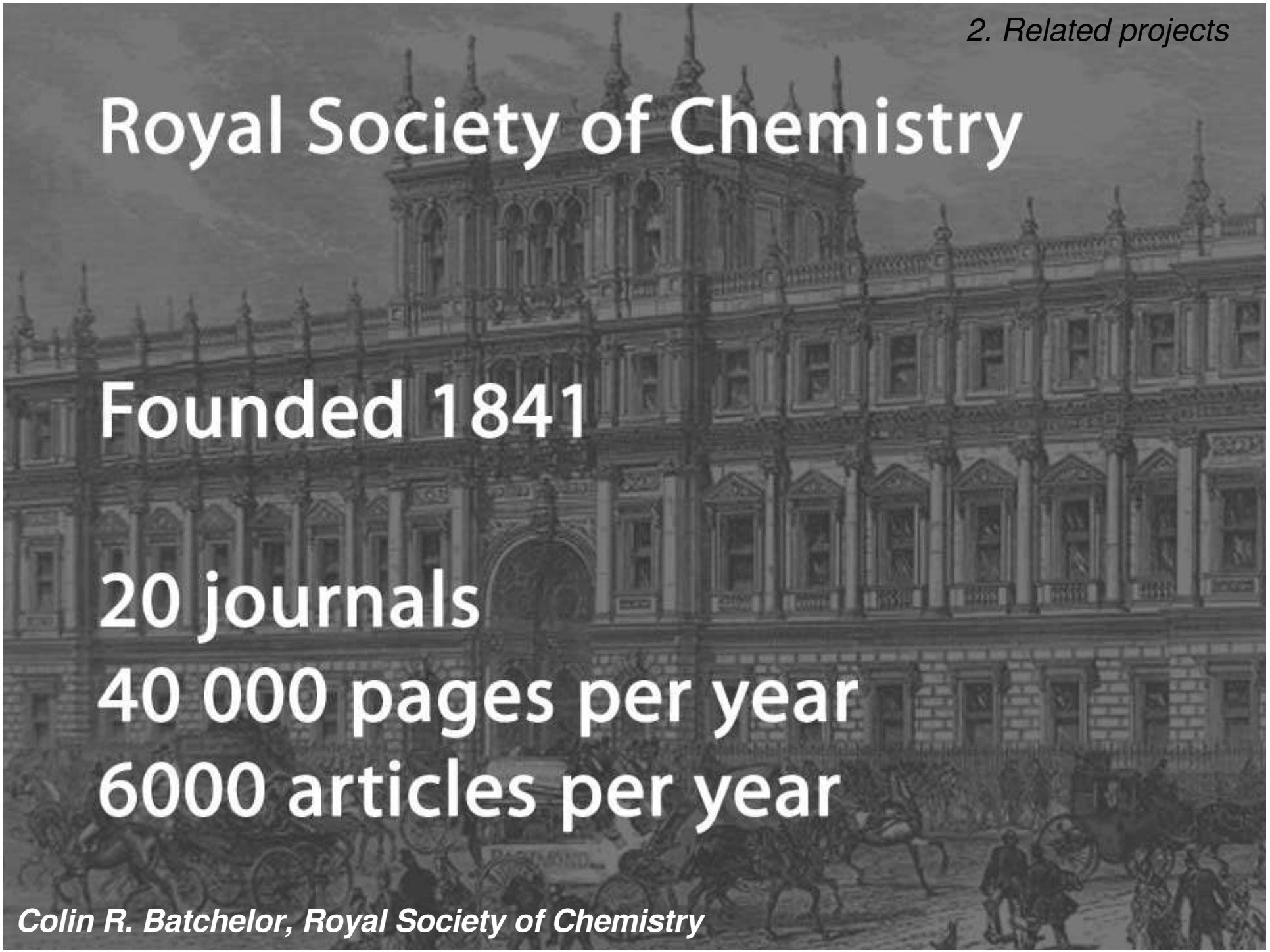
http://www.aber.ac.uk/compsci/Research/bio/art/

Motivation:

- to improve information access;
- to provide semantic clarity and explicitness of represented information and knowledge;
- to promote the sharing of research results;
- to facilitate text mining and knowledge discovery applications.

www.ProjectProspect.org

Colin R. Batchelor, Royal Society of Chemistry



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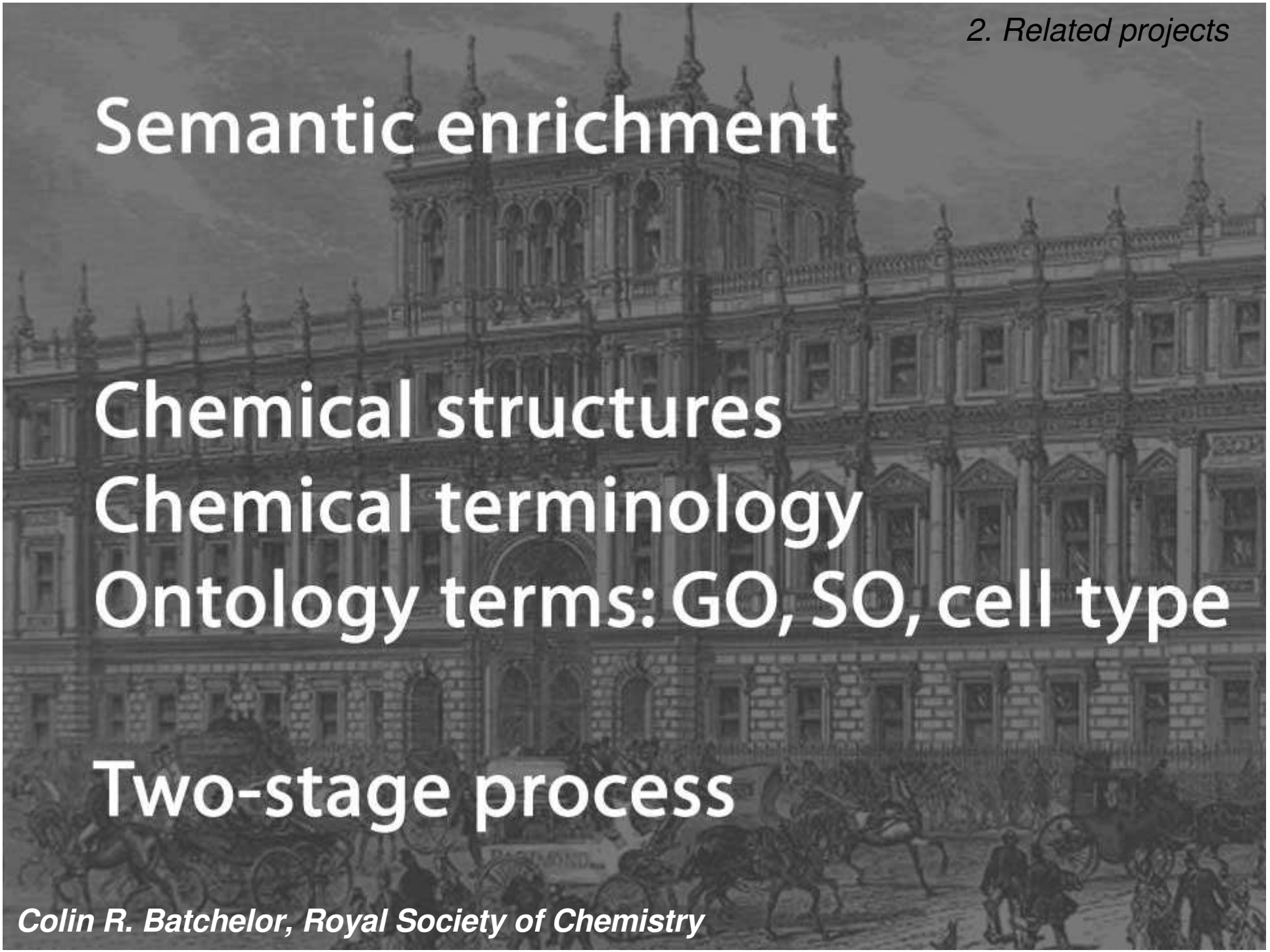

Colin R. Batchelor, Royal Society of Chemistry

Industry Track: 04
Project Prospect: Life Science Informatics at Royal Society of Chemistry Publishing

Sunday, July 22
4:50p.m. - 5:15 p.m.
Room: Hall M

Presented by: Colin R. Batchelor, Royal Society of Chemistry

HTML

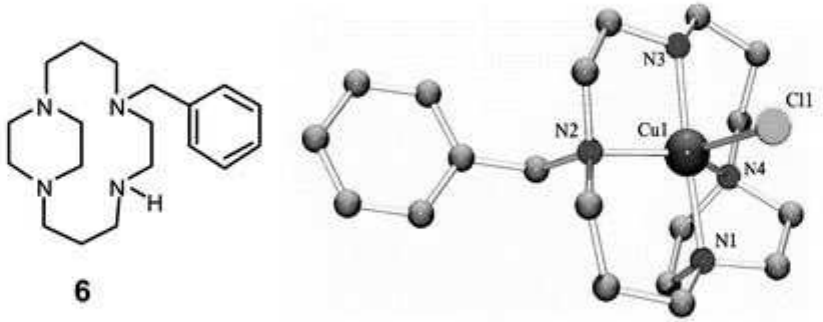

Fig. 1 Ball and stick representation of the X-ray crystal structure of the copper(II) complex formed with the benzyl derivative of the piperazine tetra-aza macrocycle. H-atoms and the $[CuCl_2]^-$ counter anion have been omitted for clarity.

Paramagnetic metal ions affect the fluorescence properties of their ligands[23] and fluorescence quenching has been used to [illegible] magnitude of the effect is expected to be reduced by an increased distance between the fluorophore and the chelated metal i[illegible]he fluorescence (approx. 75%) was observed on formation of $Cu\mathbf{5}Cl_2$; however, the fluorescence emission was still sufficient to [illegible]ogical systems.† Complex stability is also important. The copper(II) complex of a related piperazino cyclam macrocycle has been s[illegible]vorkers and shown to have a demetallation half life of >20 days in 1 M $HClO_4$.[25]

Cellular binding assays were carried out to determine whether the mono-macrocyclic fluorescent compounds interact wit[illegible]eptor. A T-lymphocyte cell line (Jurkat) that expresses high levels of the CXCR4 receptor was used. Compounds **5** and $Cu\mathbf{5}Cl_2$ were analysed for binding to the Jurkat cells by flow cytometry in competition with specific anti-CXCR4 monoclonal antibodies.

Two CXCR4-specific, monoclonal antibodies were used (mAbs 44716.111 and 44717.111), both of which bind to similar regions of the extracellular loop.[18] The binding assay was carried out by saturation of the receptors with a high concentration of compound (*ca.* 25 μM) followed by washing and introduction of the specific antibodies. The amount of antibody present on the cell surface was then quantified by addition of a secondary anti-mouse IgG fluoresceinated reagent by flow cytometry. The free macrocycle conjugate showed no shift from the positive control, suggesting that either no binding occurs or **5** is completely displaced by the antibodies [Fig. 2(A)]. The metal complex $Cu\mathbf{5}Cl_2$ binds and competes successfully with both antibodies showing a significant shift from the positive control [Fig. 2(B)].

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Ontology of scientific experiments EXPO

EXPO* v.1

http://sourceforge.net/projects/expo

2006 nomination for World Technology Award (software).

Soldatova, LN & King, RD (2006) An Ontology of Scientific Experiments. Journal of the Royal Society Interface **3/11: 795-803.*

eBank

Aims to provide a technological solution to the access and curation of digital resources:

http://www.ukoln.ac.uk/projects/ebank-uk/

The project is being led by UKOLN in partnership with the Intelligence, Agents & Multimedia Group, Department of Electronics & Computer Science, and the Department of Chemistry, University of Southampton and the Digital Curation Centre:

http://www.dcc.ac.uk/

ROAD (Robot-generated Open Access Data) project

http://www.jisc.ac.uk/whatwedo/programmes/programme_rep_pres/road.aspx

ART as an authoring tool

- ***Assist:*** help the user to identify the high level concepts about an investigation in the text. (i.e. hypothesis, object of investigation, conclusion) and domain ontology entities.
- ***Explain:*** provide examples and explanations if necessary.
- ***Represent:*** help the author to represent his/her research results directly in OWL format. The system will ask to input required metadata about the research.

Support for ontologies

- **OBI** (Ontology for Biomedical Investigations)
  i.e. <investigation>, <objective>, <conclusion>.
- **EXPO** (Ontology of scientific experiments)
  i.e. <hypothesis>, <method>, <result>.
- An **ART**-extension
  i.e. <analytical method>, <model>, <equation>.
- Domain ontologies
  - **ChEBI** (Chemical Entities of Biological Interest);
  - **REX** (ontology of physico-chemical methods and properties);
  - **FIX** (ontology of physico-chemical processes);
  - An **ART-d**omain extension.

an ontology for the ART system (a fragment):

- Investigation component
  - Hypothesis of investigation
  - Experiment
  - Goal of investigation
  - Object of investigation
  - Result of investigation
  - Model
  - Technology
  - Motivation
  - Experiment component
  - Problem analysis
  - Example
  - Method of investigation
    - Analytical method
    - Observational method
    - Experimental method
- Linguistic component
  - Paper section
    - Title
    - Abstract
    - Introduction
    - Experimental
    - Results and discussion
    - Conclusion
  - Paper
  - Representation

ART as a translator

- ***Annotate:*** ontology-based markup of the input text;
- ***Recognize:*** automatically find a concept/ synonym in the text;
- ***Get feedback:*** from a user;
- ***Link:*** concept/ synonym in the text to the external source;
- ***Generate***: summary; RSS feed.

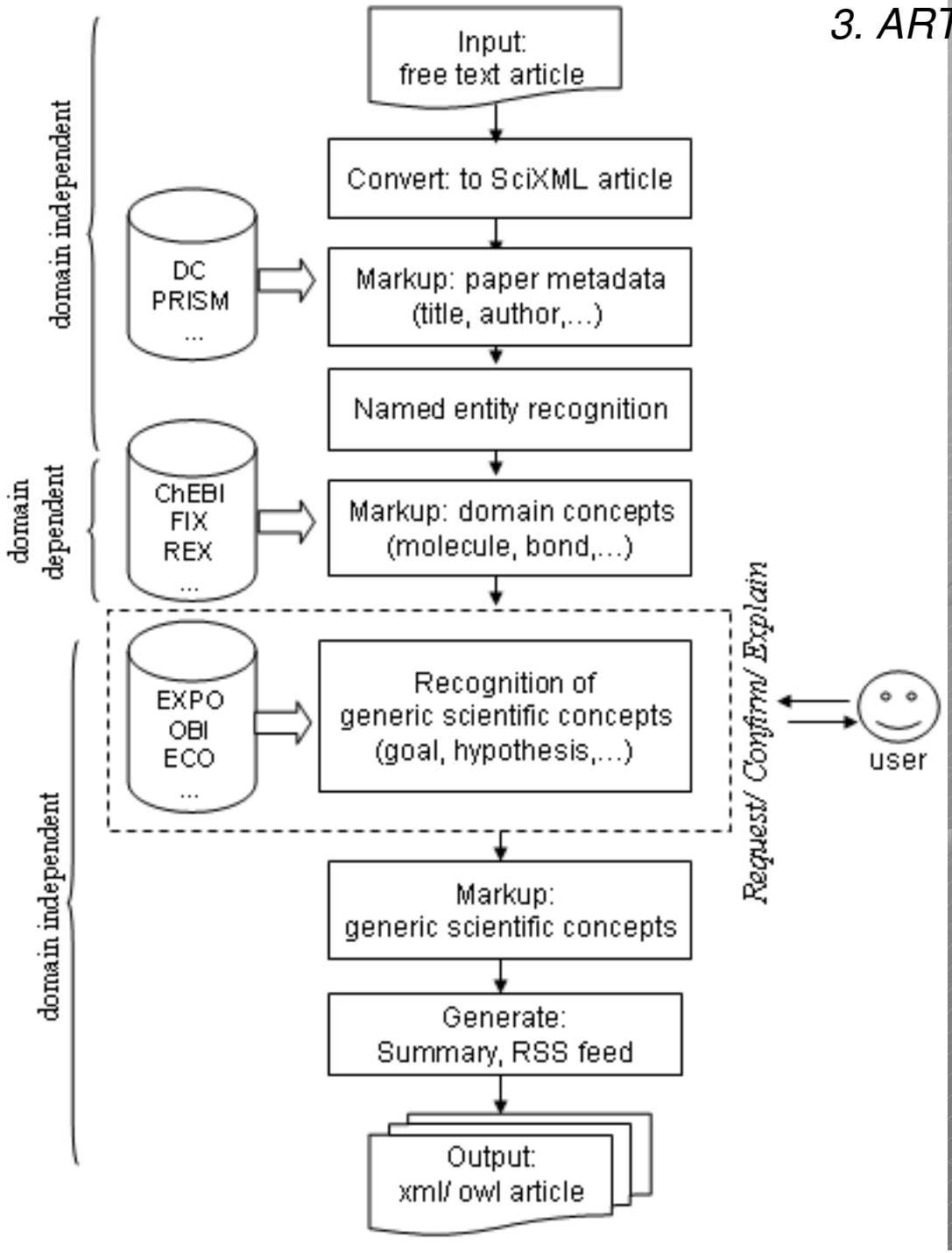
Methodology

- ‘supervised search’;
- machine learning:
  - concepts recognition;
  - features: ‘zoning’ (i.e. “aim”, “own”); meta-discourse markers (i.e. “this paper is aimed at…”);
- interactive learning;
- evaluation of the system: survey of generated summaries; text mining application.

Concepts for automatic recognition:

<motivation for investigation>
<goal of investigation>
<object of investigation>
<hypothesis>
<method>
<model>
<experiment>
<observation>
<result>
<conclusion>

A flow diagram for the ART system



A fragment of an annotated article

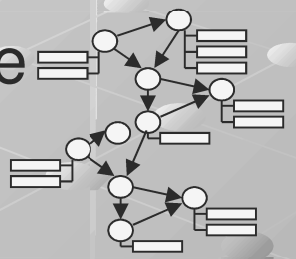
<EXPO: investigation> *map to*
<DC: title> *map to*
<OBI: investigation>
The physical origin of large covalent-ionic resonance energies in some two-electron bonds.
<EXPO: goal>
"studying in detail all the aspects of bond formation in a series of molecules that each display a range of bonding features: H2 and C2H6 as members of the classical family of covalent bonds, Cl2 as a bond exhibiting significant CS character, and the series N2H4, H2O2, and F2 as molecules exhibiting increasing CS character from left to right of the periodic table."
<EXPO: object of investigation> *map to*
<OBI: investigation object role>
characteristics of CS bond in H2, C2H6, Cl2, N2H4, H2O2, F2 molecules
<EXPO: method>
valence bond calculation on two levels:
valence-bond-self consistent field (VBSCF)
breathing-orbital valence bond (BOVB)

Ontology of science

e-Science

Ontology of science

(formalization of scientific methods, technologies, infrastructure of science)



- Controlled vocabulary for science;
- Formalized computational representation of scientific investigations;
- Unified standard for representation, annotation, storage, and access to experimental results;
- Automated reasoning over experimental data and conclusions.

Summary

- The ART tool;
- An ontology support;
- An example repository of papers in OWL.

Acknowledgements

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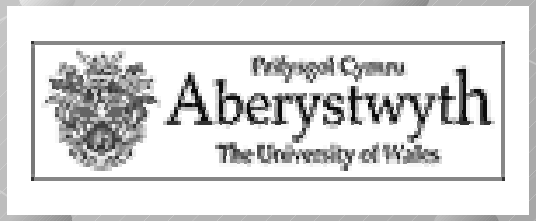

Osaka University, Japan

Thank you