



Department of Chemistry Murray-Rust Research Group

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Semantic Physical Science

Workshop and Symposium on Semantic Physical Science, Unilever Centre for Molecular Science Informatics, Cambridge UK (2012-01-10/12)

Symposium presentations available online (2012-01-26)

The **symposium presentations** are now available on Vimeo (<http://vimeo.com/petemr/videos>) and via the UCS' Streaming Media Service (<http://www.sms.cam.ac.uk/collection/1208094>)

SYMPOSIUM PROGRAM (12 January 2012, 0930 - 1645)

0930 - 1000 - Coffee and Biscuits

1000 - 1010 - *Overview of the SPS symposium*

Peter Murray Rust, Department of Chemistry, University of Cambridge

Why we are supporting Semantic Science?

1010 - 1040

Bill Shelton - Pacific Northwest National Laboratory, Washington State, USA

1040 - 1110 - **Adventures in Semantic Materials Informatics**

Nico Adams, CSIRO, Melbourne, Australia

1110 - 1130 - Break

1130 - 1200 - **Semantic Crystallographic Publishing**

Brian McMahon - International Union of Crystallography (IUCr), Chester, UK

What are we doing in Semantic Science?

1200 - 1230 - **Service oriented science: Why good code matters for science and why a fundamental change in thinking is required**

Cameron Neylon - Science and Technology Facilities Council/Open Research Computation

1230 - 1300 - **On the use of CML in computational materials research**

Martin Dove - University of Cambridge/Queen Mary University London

Andrew Walker - University of Bristol

1300 - 1400 - Lunch

1400 - 1515 - *Working Group Reports*

1400 - 1430 - **The CML roadmap and further engagement with users, developers and publishers**

Marcus Hanwell - Kitware, USA

Group: Aileen Day, Clyde Davies, Martin Dove

1430 - 1445 - **Semantification of NWChem and AMBER codes**

Bert de Jong - PNNL

Group: Andrew Walker, Mark Williamson, Jon Tyzack

1445 - 1500 - **Semantifying NMR**

Nancy Washton - Pacific Northwest National Laboratory, Washington State, USA

Group: Cameron Neylon, Bill Shelton, Karl Mueller, Nico Adams

1500 - 1515 - **Semantic Repositories**

Jens Thomas

Group: Jorge Estrada, Erica Yang, Sam Adams

1515 - 1545 - Coffee Break

1545 - 1645 - *Next steps in the practice and publication of semantic science*

Publishers present: Nature, Royal Society of Chemistry (RSC), BioMedCentral, IUCr

1645 - Finish

Overview

We are running a hands-on workshop (January 10th/11th 2012) and symposium (January 12th 2012) on Semantic Physical Science, supported by EPSRC ("Pathways to Impact"). At these events, we will be investigating how semantic technologies (dictionaries, mark-up languages, ontologies, data-typing) can be applied to the capture, publication, preservation and re-use of data in the physical sciences (especially chemistry and materials science). We have invited 25 scientists (particularly from the fields of crystallography/solid state, analytical spectroscopy and computational chemistry; see list below) to a two-day workshop where we will review and create toolkits and protocols. We are delighted to see very great interest from national laboratories and national providers of services.

The results of the workshop and general talks on semantic principles will be presented at the full day symposium, which will be of particular interest to creators of chemical software, publishers, repository managers and funders who encourage data publication. The symposium is open to everyone without charge. The approximate program will be released shortly but some details will reflect the progress made in the preceding workshop. There will be significant time for discussion. If you wish to attend the symposium, please **email spsworkshop@gmail.com to register**; places are limited to 50 – first come, first served!

Please distribute this flyer to anyone who you feel may be interested in these events.

There may be one or two places still available in the workshop – please **email spsworkshop@gmail.com for information**.

Confirmed attendees:

Nico Adams (CSIRO), Simon Coles (University of Southampton), Clyde Davies (Microsoft), Bert de Jong (Pacific Northwest National Laboratory), Martin Dove (University of Cambridge/Queen Mary University of London), Jorge Estrada (Zaragoza Scientific Center for Advanced Modeling), Marcus Hanwell (Kitware), Marcus Kraft (University of Cambridge), Mahendra Mahey (JISC), Brian McMahon (IUCr), Karl Mueller (Pacific Northwest National Laboratory), Weerapong Phadungsukanan (University of Cambridge), Henry Rzepa (Imperial College), William Shelton (Pacific Northwest National Laboratory), Paul Sherwood (STFC Daresbury Laboratory), Michael Simmons (University of Cambridge), Christoph Steinbeck (EBI), Jens Thomas (STFC Daresbury Laboratory), Andrew Walker (University of Bristol), Alex Wade (Microsoft), Nancy Washton (Pacific Northwest National Laboratory), Mark Williamson (University of Cambridge), Erica Yang (Science and Technology Facilities Council)

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