

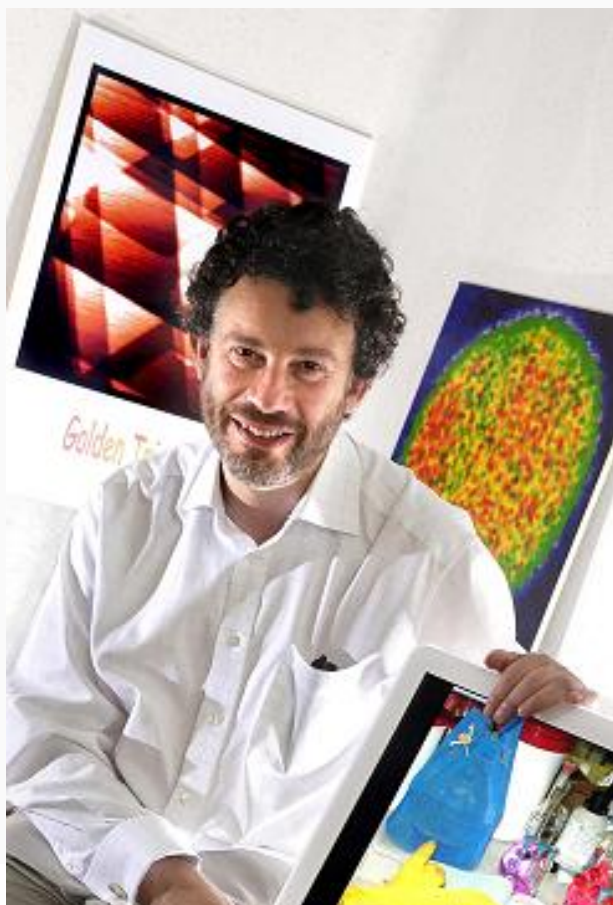
Jeremy Frey: The CombeChem project: From smart labs to smart papers

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Abstract

In this paper we will discuss the CombeChem Project's (www.comebchem.org) "end-to-end" management of laboratory chemical information from its creation in the laboratory, digital capture of information from equipment and people in a laboratory context, the analysis of the information and its dissemination. Throughout these processes we show how maintaining the links to the original data provides the necessary provenance and how this process is mediated by appropriate middleware. The examples will show how the project has made use of grid-enabled equipment, pub-sub systems for laboratory monitoring, and repositories to underpin both data management and dissemination. All the components are integrated together using semantic web technologies with the recent use of the Blog & Web 2.0 metaphors being particularly appealing to the student community.

About the speaker



Dr. Jeremy Frey is a Reader in the School of Chemistry at the University of Southampton, UK. He is committed to a collaborative and interdisciplinary approach to chemical research. The interactions with Physics, The Opto-Electronics Research Centre (ORC), Electronics and Computer Science Departments have been particularly fruitful.

His research is based on the use of laser spectroscopic techniques to probe molecular structure reactivity and dynamics and organization in a variety of environments from single molecules, molecular beam kinetics and photochemistry, to the study of interfaces and surfaces with interfacial non-linear spectroscopy.

As part of his current research he is involved with the UK e-Science programme as PI of the CombeChem project looking at the ways in which e-Science and Grid infrastructure can be developed to provide support for and carry out chemical research, for example in



Electronic Laboratory Notebooks (ELNs) with the Smart Tea Project, generating and applying a “Semantic Chemical Grid” and applying Web 2.0 & Social Network ideas with Chemical Blogs and related technologies.

Fundamental to the ideas of “Publication @ Source” for scientific data is his work on the interaction of e-print repositories with chemistry in the work on the e-Bank & e-Crystals projects.

His most recent laser research, involving higher order non-linear effects, is as the PI of a Basic Technology project to generate a nanoscale ultra short pulse of x-ray source using ultrashort-pulsed lasers and fibre technology aimed at probing the shape of single large molecules of biological significance, such as enzymes, using x-ray scattering and x-ray spectroscopy.

He is the chair of the UK e-Science User Group and in 2005/6 held a visiting Fellowship at the Centre for Mathematics and its Applications at ANU.

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