

# COMBINATORIAL APPROACHES FOR NEW MATERIALS DISCOVERY

JANUARY 28-30, 2001 • WYNDHAM EMERALD PLAZA HOTEL • SAN DIEGO, CA, USA

**INFORMATICS AND  
SOFTWARE TOOLS**  
to Increase Efficiency  
of Throughput Optimization  
*Sunday, January 28, 2001*

• Data mining • Integration of databases with molecular modeling and statistics tools • Building the virtual libraries • Interoperability • Development of standards in hard- and software tools and their integration

**POST-WORKSHOP PANEL DISCUSSION**  
*Assessing the Importance of Information  
Technology and Modeling*

**SPECIAL  
PRE-CONFERENCE  
WORKSHOP**

The Knowledge Foundation's Combinatorial Materials Conference is regarded as one of the industry's leading events to further the development and implementation of advanced combinatorial methodologies and high throughput screening techniques for new materials discovery.

Combi 2001 features 37 internationally recognized academic, government and industry leaders who will share with you their latest working knowledge through key-note lectures, case studies, workshop and panel discussions on:

**Catalysts  
Polymers**

**Electronic & BioElectronic Materials  
Biomaterials  
Methodology & Instrumentation**

**Advances for new materials discovery and design strategies include:**

- New strategies for library synthesis and rapid catalyst characterization
- Efficient library production and handling
- Rapid analytical methods and properties evaluation
- Impact of HTS formulation and blending on performance and chemical space coverage
- Micro-reactor methods and their bottlenecks
- Effect of solid disk technology on synthesis
- Methodologies and instrumentation for HTS and parallel synthesis
- Advanced experiment design and automation
- Impact of modeling and simulation

*"The Combi 2001 conference will showcase the advances made by industry leaders in the application of combinatorial methodologies and high throughput screening techniques to new materials discovery and development."*

**Dr. Joseph C. Hogan, Jr.**  
Alveus Systems Inc.

**POST-CONFERENCE PANEL DISCUSSION:**

**Impact of Combinatorial Approaches on Material Science and High-Tech Industries**

- Scale-up and validation — small scale to industrial practice
- Impact on staff needs
- Minimum critical mass to practice — can small organizations compete effectively?
- Legal issues — is "combinatorial" intellectual property protectable?

Join your peers — ensure your presence at this annual event to gain the latest working insight into this ever-changing area of materials research and discovery.

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## AGENDA-AT-A-GLANCE

8:00	9:00	10:00	11:00	12:00	1:00	2:00	3:00	4:00	5:00	6:00	
<b>DAY 1 — Sunday, January 28, 2001</b>											
					<i>Workshop Registration</i>	<i>Pre-Conference Workshop: <b>INFORMATICS AND SOFTWARE TOOLS</b> To Increase Efficiency of Throughput Optimization</i>				<i>Cocktail Reception</i>	
<b>DAY 2 — Monday, January 29, 2001</b>											
<i>Conference Registration</i>	<b>MAIN CONFERENCE (all delegates participate)</b>										
<b>Catalysts I</b>				<b>Luncheon</b>	<b>Electronic &amp; Bioelectronic Materials</b>			<b>Method and Instru. for HTS</b>			
<b>DAY 3 — Tuesday, January 30, 2001</b>											
<b>MAIN CONFERENCE (all delegates participate)</b>											
<b>Polymers</b>				<b>Lunch</b>	<b>Biomaterials</b>			<b>Catalysts II</b>			
<b>NOTE: EXHIBITOR &amp; POSTER VIEWING AREAS OPEN THROUGHOUT CONFERENCE HOURS</b>											

### CALL FOR POSTERS

Industry and academic scientists are encouraged to submit poster titles for this event. One-page abstracts (8 1/2" x 11" with 1-inch margins) must be submitted no later than **December 20, 2000** for inclusion in conference documentation. Additional poster submissions will be accepted until **January 15, 2001** but may not be included in conference documentation. Note: If you are submitting a poster, you **MUST** be registered and paid in advance to ensure that a posterboard is reserved for you.

### EXHIBITS & SPONSORSHIPS

There is no better way to provide exposure for your organization as leaders in the industry than through conference sponsorships. Among other benefits, most sponsorship packages also entitle you to receive prominent exposure on premarketing materials - exposing your company to 10's of thousands of prospects prior to the program - in addition to the highly targeted audience we deliver at the event itself.

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may not have interest in the specific conference — but may well want information on your company.

#### NETWORKING EVENT SPONSORSHIPS

These "mini" sponsorships offer representatives of your organization a dedicated opportunity to network with conference delegates - with your organization clearly recognized as the host of the event.

- Cocktail Receptions
- Luncheons
- Dinner Banquets
- Hospitality Suites

#### WORKSHOP SPONSORSHIPS

Your company may sponsor an instructional workshop (subject to approval) for delegates in conjunction with the conference. Highlight your organization's expertise! Delegate feedback indicates that these scientific/technical vehicles enhance retention of your organization's presence in their minds — increasing the potential for drawing customers long after the conference is over. See the Call for Papers for some proposed topic areas.

Call Craig Wohlers at (617) 232-7400 ext. 205 or email [cwohlers@knowledgefoundation.com](mailto:cwohlers@knowledgefoundation.com) today to for pricing information and customization options.

### HERE ARE JUST A FEW OF THE ORGANIZATIONS THAT HAVE BEEN REPRESENTED AT PAST COMBI MEETINGS:

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INFORMATICS AND SOFTWARE TOOLS  
to Increase Efficiency of Throughput Optimization

Sunday, January 28, 2001

1:00 Registration, Poster/Exhibit Set-Up &amp; Refreshments

2:00 Workshop Opening and Chairperson's Remarks

**Joseph C. Hogan, Jr., Ph.D., President and CEO,  
Alveus Systems Inc.**

2:15 Matinformatics — Better Decisions in Chemicals R&amp;D

**Michael J. Doyle, Ph.D., Director, Formulations  
Consortium, Materials Science QSAR and Informatics,  
Molecular Simulations, Inc.**

What properties are customers looking for in our products? Can we deliver them at lower cost, or with increased quality? What alternative processes can we use? Might other materials deliver the properties we need? How can we most efficiently test alternatives? What has been tried before and what did we learn? Typically, informatics tools must be tailored to the needs of the discipline being supported in particular to the peculiarities of the associated data. Thus many software vendors now offer specialist bioinformatics and cheminformatics tools that assist biotechnologists and drug discovery teams incorporating statistical tools that analyze and use that data enabling design of combinatorial libraries. In chemicals R&D, systematic storage and exploitation of data is much rarer. The informatics challenge in this area is significant because of the variety of relevant data and the range of materials, processes, and properties that must be modeled. However, a number of key trends are changing this situation. The result is the emergence of a discipline which, by analogy with those more established areas, we may term matinformatics.

2:50 Materials Informatics: Knowledge Acquisition for Materials Design

**John R. Rodgers, Ph.D., President, Toth Information  
Systems, Inc., Canada**

Combinatorial materials science is producing enormous amounts of experimental data which requires storage and analysis. Given the vast, available and existing resources of structure and property data it is possible to extract rules and regularities on the structure of materials and their properties. Using the results of such analysis it is possible to guide combinatorial experiments by first pointing the experimentalist to those areas of chemical space where there is a high probability of finding the material of interest. This informatics approaches coupled with *ab initio* quantum mechanical software will provide many of the necessary tools needed to guide combinatorial materials science experiments. The emergence of computational combinatorial materials science will provide new and faster ways for selecting candidate materials with specific properties for synthesis purposes.

3:25 Data Drowning — Knowledge Starvation

**Brian K. Southern, Ph.D., President, GSE Systems,  
VirtualPlant Inc.**

Combinatorial chemistry is creating reams of data and information enabling chemist and scientist to explore more and more of the available parameter space and expand the available information for existing and new science areas. This increase in available data has created a whole new dilemma on how to convert the data into information and ultimately into

knowledge. Not only is more information being made available due to high throughput screening techniques, but the areas and application of science have grown exponentially to create what is commonly referred to Data Drowning or Data Flooding. This is further complicated by the data being made available through varying sources of information and through different data structures. Turning this data into knowledge is what will be explored and the role of informatics for process chemistry (or proinformatics), data mining, modeling, simulation, and lab automation integrated with high speed experimentation and the various robotics, analytics, and chemical synthesis that can be achieved with this rapidly emerging technology segment. VirtualLab<sup>™</sup> from GSE Systems in partnership with Avantium Technologies will be used to demonstrate some of these advances and what the future can be for High Speed Experimentation and Simulation<sup>™</sup>.

4:00 Refreshment Break, Exhibit and Poster Viewing

4:30 Vestigial LIMS

**David B. Nicolaidis, Ph.D., FAST Product Manager,  
Molecular Simulations Ltd., United Kingdom**

The power of laboratory information management systems (LIMS) to capture and manage information defining experimental tests and test conditions, as well as the raw data coming from the Instruments themselves, is certain to become an important part of any integrated informatics solution for combinatorial chemistry. However, on closer examination it is how these capabilities integrate with other crucial parts of the Solution which will determine its success in practice. In this talk we will focus on how a generic LIM system will interoperate with existing statistical analysis, design of experiment, and formulations data mining tools, in the context of FAST, the Formulation Assisting Software Toolkit of MSI. Additional examples will be based on ongoing development of a prototype for a combinatorial catalysis informatics system.

5:05 Frequency Pattern Mining: An Informatics Tool for Materials Science

**Krishna Rajan, Sc.D., Professor, Dept. of Materials  
Science and Engineering/ Faculty of Information  
Technology, Rensselaer Polytechnic Institute\***

The basic premise of our materials informatics efforts is that there is a wide class of data mining methods, where the prime goal is to find the frequent substructures in a collection of larger structures. Examples of such structures include frequent sets, sequences, trees and graphs. Even though the structures become more complex, and may need special techniques for non-duplicate structure enumeration or for computing frequency, they are amenable to a common mining paradigm. In this presentation, we provide examples of using Frequent Pattern Mining as a tool for searching for structure-property relationships in materials. \* *In collaboration with M. Zaki, Rensselaer Polytechnic Institute*

5:40 Post-Workshop Panel Discussion

**Assessing the Importance of Information Technology  
and Modeling**

6:15

Opening Night Networking  
Reception in Exhibit Area  
(all conference participants are invited)

\*cash bar

*"I have attended each of The Knowledge Foundation's Combi meetings and I have noticed that they bring together a diverse audience of speakers and presenters illustrating major breakthroughs in such rapidly expanding field as combinatorial materials science and stimulating a lot of useful discussions."*

Prof. Joachim Kohn, Rutgers University

Monday, January 29, 2001

10:30 New Developments in Combinatorial Catalysis

8:00 Registration, Poster/Exhibit Set-Up, Coffee and Danish

8:45 Chairperson's Opening Remarks

*Joachim Kohn, Ph.D., Professor, Wright Labs/Dept. of Chemistry, Board of Governors, Rutgers University***9:00 KEYNOTE ADDRESS — Results and Commercialization - Progress in the Practice of Combinatorial Materials Science***Peter E. Cohan, Ph.D., Vice President, Discovery Tools, Symyx Technologies, Inc.*

Application of high throughput design, parallel synthesis, high throughput screening and data analysis is now being practiced across a range of materials science applications, including catalysts, polymers, and electronic materials. A number of organizations have invested in developing programs in specific fields and some programs have yielded results that are moving towards commercialization. What are the success factors necessary to achieve sustainable high throughput workflows that deliver the desired results? We will discuss the key factors learned in the implementation of successful high throughput programs at Symyx and other firms. These success factors span the technical, including overall workflow, design, synthesis, sample preparation, properties screening, instrument and software integration, databasing, data management, and data mining functions, as well as economic and cultural components.

*Selim Senkan, Ph.D., Professor and Chairman, Dept. of Chemical Engineering, University of California, Los Angeles*

Combinatorial catalysis is a methodology and sets of tools where large diversities of solid state catalytic materials are prepared, processed and tested in a highly parallel fashion. Combinatorial catalysis also embodies microfabrication, robotics, automation, computational chemistry, and large scale information management (informatics), and as such represents a new paradigm in catalytic reaction engineering. The integration of all the components of combinatorial catalysis is the ultimate goal of this field, enabling the intelligent planning and execution of highly parallel catalyst discovery and optimization experiments. Initial integration of library synthesis and high throughput screening is realized as evidenced by a number of publications in these fields. Significant progress is also being made on the development of software to organize and analyze the resulting data that would then provide an automatic feedback to the design of new generations of libraries of catalytic materials. Summary of recent research in all of these areas will be provided with examples in VOC and NO<sub>x</sub> control catalysis.

11:00 Refreshment Break, Exhibit and Poster Viewing

**11:30 Combinatorial Chemistry in Catalysis and Materials Research — An Academic Experience** Case Study*Wilhelm F. Maier, Ph.D., Professor, Head of Research Group, Max-Planck-Institut für Kohlenforschung, Germany*

Combinatorial research in an academic environment is not only exciting and rewarding but significant problems and limitations have to be faced. Our research group has developed a variety of methods and tools to perform combinatorial catalyst research (library synthesis, library characterization and performance testing), such as emissivity corrected IR-thermography, spatially resolved MS, spatially resolved hydrothermal as well as sol-gel library synthesis and characterization methods. These methods will be briefly reported and their advantages and known challenges will be discussed. The strength and shortcomings of the academic approach for combinatorial materials science and its potential for industrial and small business applications will be addressed.

**12:00 Catalytic Reaction Engineering Approaches to High Throughput Methodologies***Jan J. Lerou, Ph.D., Vice President and Chief Technology Officer, Catalytica NovoTec, Inc.*

High throughput approaches to finding new or improved catalysts have been accepted by the industry and are believed to be not only viable but also essential. Next, the attention has to be focussed on the exploitation of the leads of these high throughput catalyst synthesis and testing cycles to realize the full potential of this methodology. This presentation will give an outline of how catalytic reaction engineering approaches could support this effort.

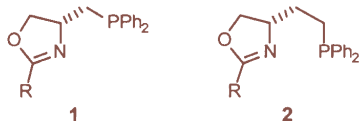
**12:30 Discovery of Polymer-Supported Catalysts Using a New Colorimetric Assay***James Morken, Ph.D., Professor and Shelley C. Danek, Research Associate, Venable and Kenan Laboratories, University of North Carolina at Chapel Hill*

A new assay to screen for novel catalysts for phosphate ester cleavage, based upon deposition of color on a solid support bearing an active catalyst has recently been tested. A series of a polymer-bound ligand were synthesized, complexed to gadolinium, and screened for activity. Using our assay, a number of potential catalysts were isolated, characterized and studied. These results and their interpretations will be presented.

1:00 Luncheon hosted by The Knowledge Foundation

**ELECTRONIC AND BIOELECTRONIC MATERIALS****1:55 Chairperson's Remarks***Krishna Rajan, Sc.D.***CATALYSTS I****9:30 High Throughput Screening of Catalyst Libraries***Kevin Burgess, Ph.D., Professor, Dept. of Chemistry, Texas A & M University*

Ligand availability is the rate-limiting step in formation and testing of catalyst libraries for optimizing asymmetric transformations. Our first approach to this problem is divergent syntheses of ligand libraries via conventional solution phase methods. In work that is now published, a set of ligands 1 were prepared in this way, and tested in allylation reactions. The results were very encouraging (up to 93 % ee) but did not match the performance of the best results in the literature. Ligand design 2 was formulated as an improvement on the basis of various considerations and experimental observations. A small ligand set 2 has now been prepared and tested in some asymmetric reactions. This talk will describe several preparations of those ligands, and some of their applications.

**10:00 High-Speed Experimentation & Simulation: A Paradigm Shift in Catalysis and Process R & D***Ian E. Maxwell, Ph.D., Managing Director, Avantium Technologies BV, The Netherlands*

Integrated High-Speed Experimentation & Simulation (HSE & S) technology can be described as a combination of enabling technologies that are deployed to screen for new catalysts and optimal process conditions at high throughput rates by integrating the use of robotic synthesis, reactor miniaturization, parallelism, high-speed functionality techniques and informatics/simulation. Clearly, this approach has the potential for enormous time savings in research and development, thus enabling industry to bring new catalysts, processes and products to the market at lower cost and, more importantly, dramatically shorten the development time. It also increases the chances of technical success and innovation through greater parameter diversity in the catalyst/process screening phase.

## 2:00 Active Microelectronic Arrays for Combinatorial Library Screening and Other Applications

**Michael J. Heller, Ph.D., Chief Technical Officer, Nanogen\***

Nanogen has developed a microelectronic chip based system (Molecular Biology Workstation and NanoChip™) for single nucleotide polymorphism (SNP) analysis, pharmacogenomic research, DNA diagnostics and more recently for drug discovery applications. A variety of active microelectronic chips including 25, 100, 400, and 10,000 test sites have been fabricated. In collaboration with Aventis, Nanogen is now utilizing its 10,000 test site active array device to investigate a novel process for screening very large combinatorial peptide libraries. The peptides in these libraries are linked to a unique nucleic acid like pairing molecule called pRNA, which allows supramolecular structures and complexes to form. These combinatorial libraries and sub-libraries are composed of 10,000 different hexamer peptides, which have the potential to produce a trillion ( $10^{12}$ ) different supramolecular binding structures. These peptide libraries are now being screened on the 10,000 site active CMOS array for unique three-dimensional ligand-binding complexes and for ultimate development of the array as a molecular descriptor device for drug discovery applications. \*In collaboration with R. Anderson, R. Gelbart, S. Miick, B. McGowan, and M. Fiechtner, Nanogen

## 2:30 Exploring Complex Material Systems by High Throughput Screening of Combinatorial Materials Chips

**Xiao-Dong Xiang, Ph.D., Staff Scientist, Lawrence Berkeley National Laboratory**

Conventional approaches to mapping phase diagrams or exploring new materials is to make and characterize samples of discrete composition one at a time. Since 1994, in an effort to speed up this process, we have fabricated "combinatorial materials chips" (CMCs) in a format of "discrete material chip" and "continuous phase diagrams" (CPDs) using thin film deposition of elemental precursors through "combinatorial masks" or linear shutters. Followed by proper annealing processes, thousands of distinct compounds or an entire continuous ternary phase-diagram can be formed, in either polycrystalline or more often epitaxial thin film format, on a small (e.g. inch<sup>2</sup>) substrate. Various physical properties, including electrical impedance, optical, magnetic and structural properties, of these compounds are then mapped using various imaging instruments. We are routinely applying this approach to explore and optimize existing function materials and to study materials phase diagrams. Application areas include exploring ferroelectrics/dielectrics, electro-optical, luminescent, piezoelectric, magnetic materials and highly-correlated condensed matter systems. I will discuss some of recent studies on phase diagram mapping on oxides and metal alloys.

## 3:00 Combinatorial and Spread Techniques in the Fabrication of Organic Light-Emitting Devices

**Ghassan E. Jabbour, Ph.D., Professor, Optical Sciences Center & Dept. of Materials Science and Engineering, University of Arizona**

We will present the use of combinatorial and spread techniques in the fabrication and optimization of organic light-emitting devices. In particular, the use of these techniques in studying the effects of inorganic buffer layers on device performance using aluminum cathodes. We will discuss also the usefulness of combinatorial techniques in the optimization of the active layers in these devices. Using spread techniques, we can also study the effects of the metal cathode thickness on device performance. In this regard, we will highlight the electroluminescent characteristics of organic light-emitting devices having cathodes with various thickness.

## 3:30 Combinatorial Approaches to Thin Film Device

**Qi Wang, Ph.D., Senior Engineer, National Renewable Energy Laboratory**

Combinatorial approaches have been used to speed up the process of research and optimization of thin film devices, such as  $\alpha$ -Si:H n-i-p thin film solar cells. The combination of different n-type layers, intrinsic-layers, and p-type layers are deposited on a single substrate so that the effect of multi-variables, such as layer thickness, dopant level, and substrate temperature, on the device performance can be studied quickly. In the current

system, one hundred different devices can be made in a single day compared to a couple of devices using the conventional approach.

## 4:00 Microdispensing for Combinatorial Synthesis

**David B. Wallace, Ph.D., Vice President, Technology Development, MicroFab Technologies, Inc.**

Ink-jet printing technology allows for the creation of individual fluid volumes in the 1 pL-1 nL range at rates up to 10,000 per second. These droplets can be dispensed under digital control onto features in the 25  $\mu$ m to 1 mm range. Multiple fluids dispensing onto multiple sites can be used in combinatorial synthesis applications to rapidly create a large range of combinations in a small area using a limited amount of material. Application to DNA, peptide, aroma, and flavor synthesis will be discussed.

## 4:30 Refreshment Break, Exhibit and Poster Viewing

### METHODOLOGY AND INSTRUMENTATION FOR HTS

## 4:55 Chairperson's Remarks

**Ian E. Maxwell, Ph.D.**

## 5:00 EPR as a Tool for High Throughput Structural Screening of Crystal Chemistry

**Krishna Rajan, Sc.D.\***

One of the major challenges in combinatorial materials science is the ability to conduct structural characterization at a variety of length scales. One of the primary reasons for this problem is the ability to gather crystal structure as well as coordination chemistry and site occupancy. Techniques such as electron diffraction do not easily lend themselves as a primary screening technique while conventional X-ray diffraction does not provide details on local atomic environments and coordination chemistry. In this presentation we describe the use of Electron Paramagnetic Resonance as a tool that is well suited for high throughput screening for structural information ranging from sub-atomic structural information such as electronic exchange interactions, valence state, coordination chemistry to microporosity. Some examples are given from combinatorial type studies. \*In collaboration with C. Suh, R. K. MacCrone Rensselaer Polytechnic Institute

## 5:30 Combinatorial Approaches for New Material Discovery — Based On Multivariate Methods

**Torbjörn Lundstedt, Ph.D., Professor, Melacure Therapeutics AB, Sweden\***

We employ a strategy for constructing combinatorial libraries with optimal information while still taking experimental feasibility into account. The objective is to provide optimal chemical diversity with a moderate number of compounds, plus adequate depth and width of the response testing. The strategy is based on a multivariate characterisation of the synthesis starting materials (building blocks), Principal Component Analysis (PCA), multivariate design, and Multivariate Quantitative Structure-Property Relationships (M-QSPR). The strategy applies both to solid phase synthesis, libraries in solution, polymers, tablet formulation. Examples from combinatorial chemistry and combinatorial pharmacy will be presented. \*In collaboration with A. Skottner, C. Post and P. Andersson, Melacure Therapeutics AB

## 6:00 Sandia's $\mu$ ChemLab™ Program

**Al Sylwester, Ph.D., Manager, Catalysis and Chemical Technologies, Sandia National Laboratories\***

Sandia National Labs is developing a fully self-contained, hand-held,  $\mu$ ChemLab™. The  $\mu$ ChemLab™ combines microfabricated gas and liquid chromatographic multi-channel modules with "on-board" detection, data reduction, communications and a power source. Key features of  $\mu$ ChemLab™ have been chosen to be consistent with counter-terrorism/first responder applications - an area of interest to numerous federal agencies. An overview of the  $\mu$ ChemLab™ program - including potential applications in high throughput analysis will be provided. \*Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

## 6:30 High Throughput Synchrotron X-ray Micro-Characterization

**Eric D. Isaacs, Ph.D., Member Technical Staff, Bell Laboratories, Lucent Technologies**

Combinatorial synthesis has the potential for revolutionizing new materials discovery in a range of disciplines from biotechnology to materials science because of the efficient and systematic way in which it searches for new materials. Whether a combinatorial library of solid state films can yield useful electronic materials depends on the accurate and rapid characterization of up to thousands of ultra-low volume films. In particular, X-ray characterization is essential for identifying material phase and composition. Characterization of the ultra-low mass films that are the basic constituents of combinatorial libraries has required novel adaptations of X-ray microbeam techniques, such as mirrors to focus polychromatic X-ray beams to 0.5  $\mu\text{m}$ . In this talk we will describe several of these microbeam techniques and their applications to characterize combinatorial solid state systems including rare earth activated phosphors and high- $T_c$  superconductors. \*In collaboration with: G. Aepli, X.-D. Xiang, X.-D. Sun, P. Schultz, R. Haushalter, W. Yun, D. Manchini

7:00 End of Day One

## Tuesday, January 30, 2001

7:45 Coffee and Danish and Poster/Exhibit Viewing

### POLYMERS

#### 8:25 Chairperson's Remarks

**Eric G. Derouane, Ph.D., Professor, Director, Leverhulme Centre for Innovative Catalysis, The University of Liverpool, United Kingdom**

#### 8:30 Combinatorial Approaches for Polymer Design: An Overview and a Case Study Involving Polyarylates

**Joachim Kohn, Ph.D.**

#### Case Study

Pioneering research has already established the utility of combinatorial approaches in the design and synthesis of novel polymers. This area of research is now experiencing significant growth and over the last few years, key publications and patents have described the combinatorial design of both free radical and condensation type polymers. These recent developments will be reviewed and the differences between the various approaches will be highlighted. In the second part of the presentation, a case study will be presented using the library of polyarylates as an example. These polyarylates are degradable, non-toxic polymers whose structure and properties was optimized efficiently using a combinatorial design.

#### 9:00 Novel High Loaded Spacer Polymers in Combinatorial Synthesis

**Wolfgang E. Rapp, Ph.D., CEO, Rapp Polymere GmbH, Germany**

Solid phase reactions and polymer supported reactions are widely used in combinatorial chemistry. We have developed HypoGels as a novel high loaded spacer polymer for organic synthesis. Short oligoethyleneglycols are grafted into a polystyrene matrix to form a hydrophobic, high loaded spacer modified polymer support which combines the advantage of a sacermmodified resin with high capacity. TentaPore and ScavengePore are novel spacermodified macroporous resins which are used as scavenger resins and polymer supported reagents. The use of these resins in combinatorial organic chemistry as well as their novel properties will be discussed in detail.

#### 9:30 Auxiliaries for Solution-Phase Combinatorial Chemistry in a Novel Shape: Monolithic Discs with Functionalized Pores

**Frantisek Svec, Ph.D., Senior Researcher, Dept. of Chemistry, University of California at Berkeley**

Functionalized porous monoliths in the shape of macroscopic discs with reactive polymer chains grafted to the inner pore surfaces will be described. The flow-through application of these discs in "reactive

filtration", a simple process enabling removal of excess of reagent from solution, and as solid-phase acylating reagent will be demonstrated.

10:00 Refreshment Break, Exhibit and Poster Viewing

#### 10:30 Novel Polymers — A Systems Engineering Approach at the Molecular Level

**Joseph C. Hogan, Jr., Ph.D.**

A general approach to the design, development and production of novel polymers is outlined. This approach is based on the convergent and combinatorial processing of hierarchical sets of chemical components, reactions and processes to produce arrays of polymers having modulated properties. The lessons learned from high throughput pharmaceutical discovery are discussed, together with the implications for polymer applications and markets.

#### 11:00 Combinatorial and High Throughput Screening (HTS) for Polymer Coatings

**Alamgir Karim, Ph.D., Group Leader, Multivariant Measurement Methods Group, Polymers Division, National Institute of Standards and Technology\***

Recent success of combinatorial and high throughput methods in the pharmaceuticals research arena has spawned similar activity and excitement in the discovery and synthesis of new inorganic materials, catalysts, and organic polymers by combinatorial methods. Likewise, the combinatorial method can be adapted for rapid scanning of material properties for fundamental studies or industrial applications. It can also be used to validate physical models in a high throughput fashion. The material properties of polymeric coatings and the effects of processing variables such as composition, temperature, and thickness are readily studied by combinatorial methods. Polymeric coatings play an important role in many industrial applications such as automotive, electrical, aerospace industries where their stability and integrity is of fundamental importance. \*In collaboration with E.J. Amis, NIST

#### 11:30 Development Of New Resins for Combinatorial Synthesis

**Kim D. Janda, Ph.D., Ely R. Callaway Professor of Chemistry, Departments of Chemistry and Molecular Biology, The Scripps Research Institute**

Abstract not available at time of print.

#### 12:00 KEYNOTE ADDRESS

#### Economic Impact of Combinatorial Chemistry on Industry and Society

**John D. Hewes, Ph.D., Program Manager, Advanced Technology Program, National Institute of Standards and Technology**

U.S. industry has indicated that the National Institute of Standards and Technology (NIST) Advanced Technology Program (ATP) has a significant role to play in the area of high throughput R&D or combinatorial methods. ATP can catalyze the development of lower-cost hardware and software tools to bring leading-edge, generic technologies to more industries, and can facilitate the integration of hardware and software systems. The ATP is currently funding extra mural research projects in high throughput discovery of catalysts and polymer coatings, with project budgets of \$40M through 2004. The ATP is also funding intramural research at the NIST Measurement and Standards Labs in six areas-scanning microwave microscopy of BST thin layer dielectrics; scanning X-Ray (NEXAFS) studies of supported catalysts; micro-reactors and micro-sensors; genetic programming for data mining and visualization; and two-dimensional mid- and far-FTIR Imaging. This presentation will highlight results from the intra- and extramural ATP research projects, as well as detail economics studies that are ongoing at the ATP.

12:30 Lunch on your own

#### 1:30 Chairperson's Opening Remarks

**Richard C. Willson, Ph.D., Associate Professor of Chemical Engineering, Biochemical & Biophysical Sciences, Dept of Chemical Engineering, University of Houston**

## BIOMATERIALS

### 1:35 Combinatorial Materials Science for Bio-Materials Science

**Eric J. Amis, Ph.D., Chief, Polymers Division, National Institute of Standards and Technology**

The range of variables in materials science is clearly broad enough to inspire combinatorial approaches for characterization and optimization of materials and processes. For materials designed to function in a biological system the scope of the issues is staggering. Our work has focused on two aspects of this problem. We are developing combinatorial approaches to characterize both the materials properties and the biological response of biomaterials. Our libraries are designed to explore processing parameters as well as traditional composition space, and to use assay methods inspired by the intended applications for the materials.

### 2:05 Combinatorial Shortcuts to Understanding Gene Function

**Joel S. Bader, Ph.D., Director of Bioinformatics, CuraGen Corporation**

The relationship between one's susceptibility to complex diseases, including cancer, heart disease, and diabetes, and the underlying 100,000 genes one has inherited, each with several common variants, is a problem of enormous combinatorial complexity. We describe new approaches that we have implemented to scan for associations between genetic variants and these medically relevant characteristics.

### 2:35 Human Receptor Sensors to Discover Target Based Chemical Space

**Tauseef R. Butt, Ph.D., Vice President of R&D, LifeSensors Inc.**

Chemical space is vast but the space in the context of a biological target is restricted. Ligand dependent human receptors that play important role in therapeutics and diagnostics are good model systems for uncovering a defined chemical target space. It is possible to screen chemical libraries using the receptor binding assays in high throughput fashion. However, this data is less valuable as we do not know the impact of this binding on receptor function. We have developed ligand dependent functions for many of the human nuclear receptor super family such as human estrogen, androgen, thyroid hormone, vitamin D, and some orphan receptors. Development of ultra-sensitive and high throughput simple cell-based sensors is ideal to discover and refine a targeted chemical space in the context of important human physiology. This talk will describe the use of several human receptor sensors to screen chemical libraries. Integration of biological sensors with combinatorial chemistry platforms and informatics will be discussed.

## CATALYSTS II

### 3:05 Chairperson's Remarks

**Peter E. Cohan, Ph.D.**

### 3:10 Combinatorial Approaches to Heterogeneous Catalysis: A Case Study within the European Consortium "COMBICAT"

**Claude Mirodatos, Ph.D., Research Director, Recherches sur la Catalyse - CNRS, France**

Case Study

This communication will present the running research developed in an academic laboratory within a consortium of 11 European partners from 7 countries settled to assess the potentiality of combinatorial chemistry applied to heterogeneous catalysis. On the basis of different probe reactions, the optimization loops including HTS equipment and data management via genetic algorithms will be presented as a case study.

### 3:40 Organometallic Combinatorial Chemistry

**Olivier Lavastre, Ph.D., UMR CNRS - Université De Rennes, France**

Combinatorial chemistry applied to catalysis and materials science is a very efficient tool to detect new catalysts and new generations of material precursors. Several examples of these different aspects will be presented: 1) Detection of the best catalyst from a specific ligand library : the aminophosphine-

phosphinite ligands were already described for the hydrosilylation of ketones. The synthesis, by the split and pool strategy, of a NP-OP ligand library allowed us to detect a new rhodium catalyst . 2) Fast discovery of new generations of catalysts : the parallel approach, which led to combining ligands and metals salts to generate 96 potential catalysts (8X12 well plate format) , associated to a colorimetric screening test was particularly efficient to find a completely new and unexpected iridium-based catalyst for the allylic alkylation. 3) A new approach for a fast synthesis and evaluation of fluorescent conjugated polymers.

### 4:10 Refreshment Break, Exhibit and Poster Viewing

### 4:40 Combinatorial Heterogeneous Catalysis

**Robert Schlögl, Prof. Dr., Director, Dept. of Chemistry, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany**

Selective oxidation of small organic molecules is a key technology in chemical industry. Many heterogeneous catalysts systems are based upon multi-element multi-phase oxide mixtures. The development of these catalysts is difficult and time-consuming and despite enormous efforts the results are still far from satisfactory. This presentation will look into latest achievements and trends of conventional vs. combinatorial approach of developing the heterogeneous catalysts. It will be shown that the most promising strategy would be a reasonable superposition combination of both methods. Illustrations of this statement will be provided using a molybdenum-vanadium-tungsten oxide system as development model for acrolein oxidation.

### 5:10 Automated Combinatorial Chemistry Equipment for Performing and Evaluating Catalytic Reactions

**James Harness, Ph.D., Chief Scientist, Mettler-Toledo Bohdan, Inc.**

The use of combinatorial chemistry techniques has proven to be an effective approach in speeding up the discovery and development of new chemical entities for the pharmaceutical industry. For several years now, these techniques have been finding applications outside of their original pharmaceutical uses and the material sciences area has rapidly been discovering how useful this way of thinking can be for their discovery purposes. As a result, the demand for combinatorial-related equipment has spawned the development of new chemistry equipment for developing and monitoring reactions, particularly in the catalysis area. The details of the reaction equipment and reaction monitoring processes, along with the support automation, will be described during this presentation.

### 5:40 Shifting Gears In Discovery Research — An Industrial Perspective

**Troy J. Campione, Ph.D., Vice President, Business Development - Commodity Applications, Symyx Technologies**

Skepticism over the applicability of combinatorial high throughput approaches to the area of heterogeneous catalysis persists. Much of the chemical industry has adopted a "wait and see" attitude and active players have been few. An industrial perspective on combinatorial materials science's emerging role in commodity chemicals R&D will be given.

### 6:10 PANEL DISCUSSION

#### Impact of Combinatorial Approach on Materials Science and High-Tech Industry

#### Discussion Panelists

**Eric G. Derouane, Ph.D., Joachim Kohn, Ph.D., and Richard C. Willson, Ph.D.**

### 6:45 Chairperson's Remarks and Close of Conference.

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