

Year Three Report - Institute for Combinatorial Discovery (ICD)

Breakthroughs at the Interface of Chemistry, Biology, Materials Science, & Engineering

Overview: By developing approaches to construct and characterize massive numbers of materials concurrently, combinatorial science (*CombiSci*) is invaluable in solving complex problems with a vast search space. ISU's *ICD* aggressively applies these concepts to catalysts, biosystems, and other advanced materials. This report summarizes the *ICD*'s vision and Year Three accomplishments.

Vision: Aggressively advance ISU to a dominant global position in *CombiSci* by forming cross-disciplinary research teams from top ISU departments and by establishing strategic partnerships with national laboratories and industry. Core research areas include: catalysts, biomaterials, and nanomaterials, and the recent addition of informatics/statistics (Table 1).

Table 1. *CombiSci* methodology: focus areas and associated personnel (*ICD*-directed hires boldfaced).

METHODOLOGY	Research Foci		
	CATALYSTS	BIOMATERIALS	NANOMATERIALS
Library design	Nilsen-Hamilton, Hillier ^a , Larock, Kraus, Woo	Mallapragada, Narasimhan, Nilsen-Hamilton, Lin	Narasimhan, NEW2 , Hillier ^a , Jeffries-El , Shinar, Rajan
Library characterization	Schrader, Shanks	Sakaguchi, Porter, Pohl, Cornick, Woo, Lin, NEW1	Narasimhan, Porter, Shanks
High throughput screening	Yeung, Porter, Hillier ^a	Rajan , Olsen, Lin, Yeung, Porter, Zou ^b	Porter, Sundararajan, Zou ^b , NEW2

^aHillier (Assoc Prof; Chem/Bio Eng (2003)) - electrocatalysts; ^bQ. Zou (Assist Prof; Mech Eng (2004)) - nanopositioning/robotics

Year Three Accomplishments:

1. Faculty Searches

- Chemistry: A. Wheeler. Declined re stronger position and superior core research facilities at U Toronto
- Chemistry: M. Jeffries-El (Assist. Prof. Fall, 2005) - combinatorial synthesis of electronic plastics (organic light emitting diodes)
- Materials Science and Engineering: K. Rajan (Prof., Fall 2005) - informatics and high speed screening tools

2. NSF-IMI

As of July 1, 2005, ISU is now the home of NSF's Combinatorial Science and Materials Informatics Collaboratory (COSMIC). COSMIC, Director K. Rajan, is an informatics/data science infrastructure for integration with combinatorial experimentation and will be an integral component of the *ICD*. It supports international activities, for example, through: 1) informatics / high speed screening tools for assessing catalyst performance and chemistry from large scale combinatorial experiments and has a partnership with U of Saarlandes (Germany); and 2) databases and informatics techniques for aiding in the molecular design of nanomaterials. It also brings several new members to the *Industrial Partners Program* and to our external advisory team, including Boeing, Honeywell, and IBM. Other features: annual meeting (fall 2005), NSF site visit (2006), and merger of COSMIC and *ICD* seminar series.

3. Strategies to garner "Institute" level external research support, enhance visibility, and diversity partnerships

a) *NSF-IGERT*: Combinatorial Science at the Interface of Chemistry, Biology, and Engineering, declined, resubmission planned. b) *NSF-CRC*: New Platforms for Photoluminescence-Based Chemical & Biological Sensors, (pre- and full proposals; declined). c) *NSF-CBC*: Chemical Bonding Center for Single Molecule Science (pre- and full proposals; full proposal declined). d) *NSF-CRIF*: Integrated Instrumentation and Cyber Gateway for Nanomaterials Chemistry (\$6M/72 mo; pending). e) *NIH-CCNE*: Great Plains Center for Cancer Nanotechnology, (\$25M (\$5M/60 mo to ISU); pending). f) *W. M. Keck Foundation*: "W. M. Keck Laboratory for Combinatorial Science" (\$1.9M, preproposal pending). g) *NSF- Materials Digital Library Pathway*: Hub for Materials Education and Research (~\$3M-four year program led by Kent State U, and includes MIT, Michigan, and Purdue, pending). h) *Visibility*: Presentations at GRC, MRS, and ACS conferences, and textbook on Combinatorial Materials Science (Wiley). i) *Diversity Partnerships*: Kennedy-King College (Chicago), Southern U, Howard U and Jackson State U; Pioneer/Dupont as industrial partner.

4. Research Highlights

- Combinatorial design of biomaterials for stable, single-dose delivery of toxic vaccines: Materials effective in stabilizing encapsulated antigens for extended periods of time and capable of modulating the immune response have been discovered. Efforts include creation of libraries of novel biodegradable polymer adjuvants and tests of their conference of protective immunity.
- In vitro evolution of catalysts for green manufacturing of fine chemicals: Through a combination of molecular biology and inorganic chemistry, an innovative approach that produces catalytic activity as the dominant trait has been developed. This strategy has yielded ~500,000-fold enhancements in a range of organic coupling reactions.
- Preliminary tests in applying the inversion-based iterative-control technique have shown a 30-fold increase in lateral imaging speeds of scanning probe microscopes (SPM). These results directly translate to a 30-fold increase in throughput in efforts to apply SPM as a screening tool for nanometric material properties.

Plans for Year Four: 1) integration of *ICD* and COSMIC activities; 2) pursuit of faculty hires in analytical chemistry, nanomaterials, and/or biomaterials; 3) creation of a professorship in *CombiSci*; 4) develop basis for ERC proposal; and 5) develop MURI white papers (due August, 2005).