

Interfacial and Processing Sciences  
**News Notes**

August 1999, Issue 1

**Environmental and Molecular Sciences Laboratory  
Pacific Northwest National Laboratory**

*News Notes, established to help keep our Users and others who have had a connection with us up-to-date on activities, events, capabilities, and interesting results, including short summaries of the work of users.*

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This issue includes:

- **New Associate Director for I&PS**
- **Users Meeting a Success**
- **New Program Funding to Link Undergraduates to DOE Labs**
- **AVS and QSA-8 Conferences Coming Up in October 1999**
- **Research Highlights**
- **I&PS Scientist Promoted to Level V**

**Bill Rogers to be I&PS Associate Director**

As of September 1, 1999, Dr. J. W. (Bill) Rogers, Jr. will be joining PNNL as the Associate Director for Interfacial and Processing Sciences. Bill has been Chairman and Professor of Chemical Engineering at the University of Washington. His recent research interests have included fundamental studies involving chemical vapor deposition of electronic materials. In the words of EMSL Director Jean Futrell, "In his new role, Bill will provide scientific leadership and administration for an organization focused on surface science, materials, sensors, and waste processing research, utilizing a large complement of advanced scientific instrumentation useful for collaborative research."

Acting Associate Directors of I&PS Chuck Peden and Don Baer are delighted to have Bill take over the management of a productive and often groundbreaking organization.

**Successful EMSL Users Meeting**

The first EMSL Users Meeting was very successful with over 250 researchers attending. Of particular importance to I&PS was the oxide symposium and the Surface Analysis tutorial. Both attracted large audiences and were very well received. Several researchers became EMSL users as a result of the tutorial. We were delighted both by the number of people participating and the quality of the interactions.

**New DOE Program (FaST) to Link DOE Labs and Small Colleges**

The U.S. Department of Energy, through its Office of Science, will be launching (in Fiscal Year 2000) a multi-phase, multi-faceted pilot program, the Faculty and Student Teams ("FaST")

initiative. This new program will improve undergraduate education through research while transforming and enhancing the relationships of select colleges and universities with DOE's science laboratories, including PNNL. Of particular interest in this initiative will be establishing or expanding interactions with smaller academic institutions having limited prior research activity (that is, those receiving less than \$1 million in annual Federal R&D funding) or those serving populations underrepresented in the fields of science and technology.

Through a competitive process, faculty and student teams will be selected for laboratory research appointments during the summer of 2000. Concurrent professional-development workshops on proposal writing, communication, and other topics will be offered. At the conclusion of the on-site appointments, participants will be afforded opportunities to continue (in FY2001) their research relationships through sustained collaborations (including those mediated by Internet-based technologies) among the respective laboratories and campuses. For more detailed information see [http://www.ORAU.gov/DOE\\_FaST](http://www.ORAU.gov/DOE_FaST).

### **Upcoming AVS meeting and Quantitative Surface Analysis topical conference**

Users of surface science methods who are not normally part of the surface and interface community may want to take advantage of the American Vacuum Society meeting that is scheduled for October 25-29, 1999 in Seattle, Washington. Highlights will include:

- Many technical talks on surface science and applied surface science
- Short courses on surface analysis methods and vacuum technology

In addition, the Quantitative Surface Analysis topical conference (QSA-8) will be held at the Best Western Park Plaza, Puyallup, WA on Friday and Saturday, October 22-23, 1999, just prior to the International Symposium of the American Vacuum Society in Seattle (October 25-29). This topical conference will provide a forum for discussion on the quantitative aspects of surface analysis and on assessments of uncertainty.

Topics of interest include reference data, reference materials, instrument calibration and performance, software, databases, reference procedures, and applications of quantitative surface analysis. The focus will be on techniques in common use (AES, XPS, SIMS, and sputter-depth profiling) and on improved or emerging techniques. Six invited papers will each be followed by an extended discussion period.

Information on both conferences is available at [www.vacuum.org](http://www.vacuum.org) and [www.vacuum.org/topicalconf.html](http://www.vacuum.org/topicalconf.html).

### **Research Highlights**

- *I&PS Staff Contribute to Work Honored with a Presidential Green Chemistry Award*  
Biofine, a small Massachusetts company, has developed an economical process to turn paper mill waste into levulinic acid, an important, multipurpose chemical. Using a Pacific Northwest National Laboratory (PNNL) patented process, Biofine then will be able to process the levulinic acid to make an alternative fuel component which can be used with ethanol and natural gas liquids to create a cleaner burning fuel for cars and trucks. This combination of technologies has earned a Presidential Green Chemistry Challenge Award for Biofine, PNNL, and the other team members, The New York State Energy Research and Development Authority, Merichem and the National Renewable Energy Laboratory.

"This process is exciting because we have the ability to go from renewable, plant-based feed stocks to a high-value product on a commercial scale, and Biofine's cost projections suggest that

the whole process can be profitable, even when competing against historically low oil prices," says Doug Elliott, of Pacific Northwest's Chemical Process Development Group. Todd Hart and Yong Wang of the I&PS group along with other PNNL staff, John Frye, Gary Neuenschwander, and Alan Zacher, also participated in the project.

President Clinton established the Green Chemistry Challenge Awards in 1995 to recognize outstanding chemical technologies that incorporate green chemistry principles into chemical design, manufacture and use. This year, a panel selected by the American Chemical Society chose only four companies and one academic team from among 152 entries to receive the awards.

See <http://www.pnl.gov/news/1999/horizon.htm> for more information on this technology.

- *New Molecular Environmental Science Synchrotron Beamline Funded*

I&PS scientist, Scott Chambers, recently contributed to a proposal for a soft to medium-hard, x-ray beamline to do molecular environmental science at the Advanced Light Source at Lawrence Berkeley National Laboratory (LBNL). The proposal has been funded by Department of Energy, Office of Basic Energy Sciences, Divisions of Chemical Sciences and Materials Sciences to the tune of 6M\$ (9.2 M\$ was requested). The effort involved several people, but was spearheaded by David Shuh (LBNL) and I&PS collaborator, Gordon Brown (Stanford University). Scott and Greg Herman (EMSL/I&PS) attended a hardware planning meeting at Berkeley on August 4.

- *Hydrosilylation in Polymer Synthesis Featured in May 99 Issue of PolymerNews*

Jay Grate's work on hydrosilylation as a versatile reaction for polymer synthesis was the Feature Article in the May issue of Polymer News (Vol. 24, pg. 149), with highlights of the work also appearing on the cover of that issue. The hydrosilylation reaction involves the addition of a silicon hydride across a carbon-carbon double bond. With this approach, a variety of novel architectures and functionalized polymers can be prepared. A particular interest of Grate's work in this area has been for the synthesis of sorbent polymers with tunable chemical and physical properties that are then useful for chemical sensor applications.

- *EMSL Collaboration Yields Detailed Oxide Surface Structure Information*

Recent results from an EMSL collaboration between Juerg Osterwalder (University of Zurich) and Greg S. Herman (I&PS) have indicated that there is a small but significant dispersion in the gap-state emission due to bridging-oxygen vacancies on TiO<sub>2</sub>(110). Typical models suggest that these types of defect states are localized at the cation sites (Ti<sup>3+</sup>), and therefore should not have dispersion. Experimental results suggest that the extra electron at the vacancy site is in fact delocalized, and may influence the chemistry at the defective surface. Two-dimensional Fermi-surface mapping suggests that the largest contribution to this gap-state is due to emission from the Ti 3d<sub>z<sup>2</sup></sub> orbital. TiO<sub>2</sub> can be used as a photocatalyst for waste decomposition and the nature of surface defects will influence the relevant surface chemistry.

### **Jay Grate Promoted to Scientist and Engineer V**

I&PS scientist, Jay Grate, was recently appointed to one of the highest technical positions at Pacific Northwest National Laboratory, the Scientist and Engineer V rank. Grate's promotion is in recognition of his sustained outstanding contributions and international reputation in his primary research areas, chemical sensors and microanalytical chemistry. Promotion to this prestigious position at PNNL entails an extensive external peer review that assesses the impact of the individual's scientific accomplishments, their technical leadership and mentoring skills, as well as their impact on the business of the laboratory.

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