


**WILLIAM H. NICHOLS MEDAL — DISTINGUISHED  
SYMPOSIUM AND AWARD BANQUET**

**Symposium: Mass Spectrometry: New Ways to Probe Molecular Structure and Reactivity**

*Award Recipient:* **PROFESSOR ALAN G. MARSHALL**  
 Ion Cyclotron Resonance Program  
 National High Magnetic Field Laboratory  
 Florida State University, Tallahassee, FL

**PROGRAM**

- 1:30 PM **Welcome** Professor JaimeLee Iolani Rizzo  
 2012 Chair, ACS, New York Section  
 Pace University, NYC
- 1:35 PM **Opening of the Distinguished Symposium** Professor Philip H. Mark  
 2012 Chair-elect, ACS, New York Section  
 Nassau Community College - SUNY
- 1:45 PM **Accelerated Chemical Reactivity Implemented Using Mass Spectrometry** Professor R. Graham Cooks  
 Purdue University

This presentation deals with studies of chemical reactions in solution and at surfaces that are facilitated by the new ambient ionization methods of mass spectrometry. These analytical methods like desorption electrospray ionization (DESI) and paper spray ionization (PS-MS) have facilitated experiments based on reactions occurring outside the mass spectrometer at atmospheric pressure. This talk covers reactions occurring (i) in charged microdroplets generated by spray ionization, (ii) between dry organic ions and reagents on surfaces and (iii) between compounds on paper and surrounding gaseous ions. These unusual media are shown to be effective in driving and accelerating organic reactions. Bimolecular solution phase and heterogeneous reactions are a recent component of the subject, and the possibility of scaling up reactions under these conditions is noteworthy.

- 2:30 PM **Searching for Short-Lived Intermediates in Liquid Chemical Reactions** Professor Richard N. Zare  
 Stanford University

Without measurement we cannot have science, and nothing so much stimulates new measurements as inventing and perfecting new measurement devices. In this presentation I wish to describe some new directions being developed in my laboratory for the use of desorption electrospray ionization (DESI), an ambient ionization technique for mass spectrometry, which was first introduced by Prof. R. Graham Cooks and co-workers, Department of Chemistry, Purdue University. I will stress the use of DESI to record transient intermediates of solution-phase chemical reactions on the millisecond time scale. I will also describe some uses of DESI imaging to examine healthy and diseased tissue. This work has been primarily carried out by Dr. Richard H. Perry and Dr. Ali Ismail under the support of the Air Force Office of Scientific Research.

- 3:15 PM **Coffee Break**

- 3:45 PM **Mass Spectrometry Enables Chemical Footprinting and New Understanding about Proteins** Professor Michael L. Gross  
 Washington University

Our goal is a rapid, sensitive, and specific means of determining protein interactions, folding, and unfolding by using chemical footprinting coupled with MS. Driving this approach is the wide availability of mass spectrometers for analytical proteomics; these should also be applicable to protein footprinting. To this end, we are developing fast photochemical oxidation of proteins (FPOP) and hydrogen/deuterium exchange to interrogate protein interactions, interfaces, and dynamics of folding/unfolding. We will illustrate the potential of H/DX and FPOP with applications to the ApoE family of proteins, a family with important implications in Alzheimers and other diseases.

4:30 PM **Mass: The Universal Chemical Currency** **Professor Alan G. Marshall**  
**NICHOLS MEDALIST**

It is now possible to produce, intact, a gas-phase ion, often under ambient conditions, from almost any molecule, including many not isolable or stable in solution. Ultrahigh resolution and mass accuracy enable determination of elemental composition (C<sub>x</sub>H<sub>y</sub>N<sub>z</sub>O<sub>w</sub>S<sub>v</sub>...) for mixtures as complex as petroleum crude oil, peptide amino acid composition and sequence for protein identification, nature and site(s) of protein post-translational modification(s), and mapping of binding surfaces in bio-macromolecular complexes. Recent advances in high-end instrumentation will be described, and applied to problems ranging from the Deepwater Horizon oil spill to identification of drug targets in protein assemblies. Work supported by NSF NIH (R01 GM78359), NSF Division of Materials Research through DMR-06-54118, NSF CHE-10-49753, NSF CHE-1016942, and the State of Florida.

5:45 PM **Social Hour**

6:45 PM **William H. Nichols Medal Award Dinner**

**Date: Friday, March 16, 2012**

Times: Registration 1:00 PM

Symposium 1:30 PM – 5:30 PM

Reception 5:45 PM

Award Dinner 6:45 PM

Place: Crowne Plaza Hotel, White Plains, NY

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