

*You are
Cordially invited
to attend*

The 43rd Annual

Harry G. Fair Memorial Lecture in Chemical Engineering 2017

**Thursday, March 23, 2017
Seminar – 1:45 P.M.
Room M-204
Sarkeys Energy Center
100 East Boyd
University of Oklahoma
Norman, Oklahoma**

Coffee and refreshments
will be served.

Accommodations on the basis of disabilities are
available by calling (405) 325-5811.


The University of Oklahoma is an equal
opportunity institution. 1/17

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Harry G. Fair Memorial Lecturers

2017	Philippe Sautet, University of California, Los Angeles
2016	Nicholas L. Abbott, University of Wisconsin-Madison
2015	Antonios G. Mikos, Rice University
2014	Mark E. Davis, California Institute of Technology
2013	Alexis T. Bell, University of California, Berkeley
2012	Charles Zukoski, University of Illinois
2011	Peter C. Stair, Northwestern University
2010	Juan J. de Pablo, University of Wisconsin-Madison
2008	Donald R. Paul, University of Texas at Austin
2007	David Mooney, Harvard University
2007	John Prausnitz, University of California, Berkeley
2006	George Georgiou, University of Texas at Austin
2005	James A. Dumesic, University of Wisconsin
2004	Robert C. Armstrong, Massachusetts Institute of Technology
2003	Nicholas Peppas, University of Texas at Austin
2002	Richard C. Alkire, University of Illinois
2001	Ralph T. Yang, University of Michigan
2000	Enrique Iglesia, University of California, Berkeley
1999	George Stephanopoulos, Massachusetts Institute of Technology
1998	Stuart L. Cooper, University of Delaware
1997	Keith E. Gubbins, Cornell University
1996	H. Scott Fogler, University of Michigan
1995	Gary L. Haller, Yale University
1994	Christopher W. Macosko, University of Minnesota
1993	Larry V. McIntire, Rice University
1992	Dan Luss, University of Houston
1991	E. N. Lightfoot, University of Wisconsin
1990	George A. Samara, Sandia National Labs
1989	James Wei, Massachusetts Institute of Technology
1988	C. Judson King, University of California, Berkeley
1987	Eli Ruckenstein, SUNY Buffalo
1986	Stuart W. Churchill, University of Pennsylvania
1985	John M. Campbell, John M. Campbell & Co.
1984	Richard G. Askew, Phillips Chemical Co.
1983	B. H. Sellers, Sellers Chemical Co.
1982	Lynn T. Reed, Warren Petroleum Co.
1981	Robert S. Purgason, Perry Gas Processors
1980	A. B. Slaybaugh, Conoco Inc.
1979	Charles R. Perry, Perry Gas Cos.
1978	Raymond W. Lowe, E. I. DuPont de Nemours
1977	Laurance S. Reid, Ball-Reid Engineers Inc.
1976	Harry L. Blomquist Jr., Coastal States Gas Co.
1975	Stanley Learned, Phillips Petroleum Co.

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 **The UNIVERSITY of OKLAHOMA**
Gallogly College of Engineering
School of Chemical, Biological and Materials Engineering

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Harry G. Fair Memorial Lecture in Chemical Engineering 2017



Philippe Sautet

Chemical and Biomolecular Engineering
And California NanoSystems Institute
University of California, Los Angeles
Los Angeles, California, USA

Structure-Activity Relations In Heterogeneous Catalysis -- A View from Computational Chemistry



Harry G. Fair

Each year, a special lecture is given in memory of Harry G. Fair, an outstanding OU alumnus. Fair was born in Okmulgee, Oklahoma, on June 3, 1916, and earned his bachelor of science degree in chemical engineering in 1939. He joined Phillips Petroleum Company in 1939 and worked his way up to vice president for supply and transportation, with responsibility for worldwide exchange of crude oil and all transportation facilities. In 1966, Fair joined M. W. Kellogg Company as executive vice president in charge of all engineering activities. He was named executive vice president of Coastal States Gas Corporation in 1971, a post he held until his death on July 27, 1974. A member of a number of professional societies and a licensed professional engineer, Fair was active in service to society and his alma mater.

This lecture is made possible by the Harry G. Fair Memorial Fund established by his widow, Jane Swift Fair. Arrangements for the lecture are made by the School of Chemical, Biological and Materials Engineering in OU's College of Engineering.

Structure-Activity Relations In Heterogeneous Catalysis -- A View from Computational Chemistry

Philippe Sautet

Chemical and Biomolecular Engineering
University of California, Los Angeles
Los Angeles, California, USA

The understanding of the catalytic properties of nanoparticle catalysts and the design of optimal composition and structures demands fast methods for the calculation of adsorption energies. By exploring the adsorption of O and OR ($R=OH$, OOH , OCH_3) adsorbates on a large range of surface sites with 9 transition metals, we propose new structure sensitive scaling relations between the adsorption energy of two adsorbates that are valid for all metals and for all surface sites. This opens the way for a new class of activity volcano plots where the descriptor is not an energy but a structure-related descriptor. In addition, to better grasp finite size effects in the nanoparticles, a generalized coordination number is proposed as a leading descriptor for the adsorption strength.

Simple descriptors as generalized coordination show a strong predictive potential exemplified in the design of optimal oxygen reduction reaction catalysts, with strong impact on efficient storage of energy.

In a second part, smaller clusters (Pt_{13}) will be considered, supported on a γ -alumina surface. We will show how the structure of the cluster is modified upon interaction with the support. The system will then be submitted to a pressure of H_2 . The cluster is covered by a high coverage of H atoms (up to 3H per surface Pt) and its structure is modified, with strong implications on its reactivity.

Finally I will show how the ordering of the surface of an alloy between Ag and Pd is modified between vacuum and a gas phase of acetylene. The molecule hence create the active site on the alloy surface for its own reactivity.

Philippe Sautet Biography

Philippe Sautet has studied at "Ecole Polytechnique" in Paris and defended his doctorate in Theoretical Chemistry at Orsay University (Paris XI) in 1989. He then entered CNRS – Centre National de la Recherche Scientifique at the Institute of Research on Catalysis in Lyon, where he developed and lead a group devoted to the applications of theoretical chemistry to heterogeneous catalysis. He spent a sabbatical at University of California, Berkeley. After being the director of the laboratory of Chemistry at the ENS of Lyon for 8 years, he was director of the "Institut de Chimie de Lyon", a cluster of chemistry laboratories in Lyon, from 2007 to 2015. Philippe Sautet is now Professor at the Chemical and Biomolecular Engineering department of UCLA.

His research interests are in the theory of the electronic structure at the interface between a solid surface and molecules and the modeling of elementary steps of heterogeneous catalysis. His work on the simulation of the atomic scale image of surfaces obtained with the scanning tunneling microscope brought him to international attention. He is worldwide recognized for his theoretical study at the molecular scale of catalysts and catalyzed reactions.

He has published over 300 scientific papers. The impact of his research is illustrated by more than 100 invited lectures at conferences and by a H factor of 58. He received several awards including the silver medal of CNRS in 2007, the Paul Pascal Prize of the French Academy of Science in 2008 and the Pierre Süe Grand Prize of the French Chemical Society in 2012. He was elected at the French Academy of Science in 2010. In addition, France distinguished him as "Chevalier de l'Ordre National du Mérite" for his action in research and research organization and as "Chevalier de l'ordre des palmes académiques" for his teaching and action towards students. He is nominated in several councils or committees and is associate editor of ACS Catalysis, an international journal published by the American Chemical Society.