

# NACS Newsletter

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## Manos Mavrikakis selected for the 2009 Paul H. Emmett Award in Fundamental Catalysis



Denmark. The primary research focus of Manos' group is the fundamental understanding of surface reactivity, using state-of-the-art first-principles methods, and extensively collaborating with experimental experts. Manos has coauthored more than 80 original publications. He is a member of the editorial board of *Surface Science* and of the *Annual Review of Chemical & Biomolecular Engineering*. Dr. Mavrikakis has pioneered the use of Density Functional Theory (DFT) methods in the screening of pure and alloy metal catalysts to discover which metals or alloys have potential to yield catalysts of improved activity and/or selectivity. Manos has been unique in having used theoretical methods to find new, interesting classes of systems and site-nanostructures. Key to his success here was the use of fundamental principles concerning the relationships between the energetics of certain key intermediates and the activation

I am pleased to announce that Professor Manos Mavrikakis has been selected for the 2009 Paul H. Emmett Award in Fundamental Catalysis. The award consists of a plaque and a prize. The purpose of the Award is to recognize and encourage individual contributions (under the age of 46) in the field of catalysis with emphasis on discovery and understanding of catalytic phenomena, proposal of catalytic reaction mechanisms and identification of and description of catalytic sites and species.

Since 1999 Manos has been with the Department of Chemical & Biological Engineering, University of Wisconsin - Madison. Manos is one of the world leaders in the area of computational chemistry in catalysis. He has also served as Visiting Professor, Department of Chemical Engineering, Technical University of Denmark, Lyngby,

barriers for the rate-controlling steps to make this screening procedure faster.

In particular, Manos demonstrated that possibility by identifying bimetallic alloys which bind atomic H as weakly as the noble metals (Cu, Au), but are able to break the H-H bond in H<sub>2</sub> more easily than noble metals. Such Near-Surface-Alloy (NSA) materials are ideal for low temperature, highly selective, H-transfer reactions (e.g., in pharmaceutical production), and energy related catalytic applications. Also, Manos's group systematically studied Oxygen Reduction Reaction (ORR) on a number of late transition metals, including bimetallic and ternary alloys of Pt. The result of that work was the construction of stable, ternary NSAs, which contain much less Pt, and  
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# Manos Mavrikakis selected for the 2009 Paul H. Emmett Award

(Continue from cover)

are up to a factor of four more active than pure Pt ORR electrocatalysts. Manos also has discovered many interesting aspects of catalytic reaction mechanisms that have inspired the field. In particular, very recently Manos' group has proposed a novel low-temperature reaction mechanism for the preferential oxidation of CO in the presence of H<sub>2</sub>, which explains the room-temperature reactivity of Ru-Pt core-shell nanoparticles. The specific nanoparticles were identified by Manos' group from first-principles as very active and selective PROX catalysts, and those predictions were confirmed upon synthesis and catalytic testing of the Ru-core Pt-shell nanoparticles. Manos also followed up his detailed gas-phase methanol decomposition DFT work with experiments and microkinetic modeling, to show that one can accurately predict experimental reaction rates directly from first principles. In the area of water gas shift catalysis, his efforts have led to a completely new water-gas shift reaction mechanism involving carboxyl species on Cu, Pt, and Au surfaces, which is quite general and may be applicable to other low temperature water-gas shift catalysts. Importantly, this mechanism is shown to be operational under realistic industrial water-gas shift

conditions.

Manos will give a plenary lecture and be recognized at the 2009 North American Catalysis Society meeting in San Francisco.

The Paul H. Emmett Award in Fundamental Catalysis is sponsored by the Davison Chemical Division of W.R. Grace and Company. It is administered by The North American Catalysis Society and is awarded biennially in odd numbered years. More information on this award, the awards process, and previous awardees can be found inside the Awards folder on the NACS home page: [www.nacatsoc.org](http://www.nacatsoc.org).

**John Armor,**

President of The North American Catalysis Society

## **Award Citation:**

*For his elucidation of the fundamental aspects of the surface chemistry for well-established catalytic processes, and his leadership in the use of Density functional Theory to set directions for future research in the search for new catalysts and new catalytic processes.*

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# Enrique Iglesia is the First Tanabe Prize Winner for Acid-Base Catalysis



**T**he international Acid Base Catalysis (ABC) group is proud to announce the awarding of the first Tanabe Prize for Acid-Base Catalysis to Professor Enrique Iglesia of the University of California at Berkeley.

The Tanabe Prize for Acid Base Catalysis is administered by the International Acid-Base Catalysis (ABC) Group and sponsored this year by the ExxonMobil Research and Engineering Co. It is named to honor the legacy and accomplishments of Professor Kozo Tanabe, who pioneered many of the modern concepts in acid-base chemistry. The prize will be presented at the ABC-6 Conference in Genova in May 2009 (6th world congress on Catalysis by Acids and Bases, Genova, Italy, 10-14 May 2009; <http://www.catalisidichep.unige.it/ABC-6.htm>). The award consists of a plaque, an honorarium, and travel expenses to attend the meeting and present a plenary lecture. The Tanabe prize recognizes substantial contributions to the field of acid and/or base catalysis. It may be presented to either a young person who has demonstrated unusual promise early in his/her career or to an individual of less than 56 years of age at the time of the ABC conference at any career stage, who has made significant contributions to the area within the six years preceding the award.

Enrique is being recognized for his pioneering contributions to the design and understanding of acid sites within specific structures and for his discovery of a new acid catalysis route with important industrial relevance, in particular for two of his more recent studies, the first on shape selective carbonylation and the second on heteropoly compounds.

His recent seminal discovery of shape selective carbonylation within microporous zeolites, in which unprecedented specificity for carbonylation reactions (very high rates of carbonylation along with selectivities to methyl acetate greater than 99% achieved for DME (dimethyl-ether) carbonylation). This significant increase in catalytic performance was shown to be the result of the unique structural and electronic topographies of 8-member ring channels. These highly active and selective zeolites are ideal replacements to the costly, highly toxic and corrosive iodide-promoted organometallic catalysts that are currently used in industry.

Also within the last five years Enrique has made a significant contribution to the area of heteropoly compounds as solid acids. Following the original contributions of Professor Misono, Enrique formulated exact composition-function relations with predictive value by addressing the reactivity of POM materials with varying composition and hence, acid strength, and measuring the corresponding kinetic and thermodynamic constants for elementary steps for alkanol dehydration reactions. In this work, the ubiquitous aggregation and incomplete environment dependent accessibility of POM clusters was minimized by dispersing the POM clusters on supports and probing accessibility before and during catalytic reactions using organic bases of varying polarity and size. His results, in collaboration with Professor M. Neurock's for calculations using DFT, have led to a quantitative assessment of structural and compositional effects on the intrinsic reactivity of Brønsted acid sites on Keggin-type POM materials. He showed that the effects of acid strength on the stability of cationic intermediates and transition states are partially compensated by the stabilization of the ion-pair at the transition state as acids become weaker and the anionic conjugate base acquires a higher charge density.



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# President's Letter

Let me summarize some of the key subjects discussed at our recent Board of Director's meeting held in Philadelphia during the August ACS meeting. The Board is made up of an elected representative from each of the 14 catalysis clubs/societies within the NACS. Four Directors-at-Large and the six elected NACS officers comprise the balance of the Board bringing the total attendance to 24 members. At this yearly Board meeting, we met for several hours to discuss many different subjects.

I brought up the topic of the upcoming Board elections (June 2009 in San Francisco) in order to stimulate thoughts about selecting future officers for the NACS. I announced that after almost 8 years (2 terms) as your President and a previous 7 years as the Treasurer, I would not be running for any elected office in 2009. In my retired mode and in my mid-sixties, I also believe it is important to bring in new leadership into the Society. If any member would like to become more involved in the national society's activities/operations, please feel free to contact me directly (nacatsoc@verizon.net).

Local clubs are reminded that they should apply for the NACS Local Club student travel awards which provide \$1,000. each year to any local clubs seeking to supplement travel for students to Spring local club meetings. Not many clubs are taking advantage of this opportunity. In 2007 the Chicago and Pacific clubs received awards; in 2008: Pittsburgh-Cleveland; Chicago; ORCS; Western States; and New York received awards. Information can be found in the last Newsletter and on the NACS web site [www.nacatsoc.org](http://www.nacatsoc.org).

The NACS has a large fund which supports the Keith Hall Educational Fund and it is administered by 4 "trustees". The Lead Trustee is, John Byrne; others on the Committee include, Chris Jones, Stu Soled, and Dick Gonzalez-Tom Degnan of ExxonMobil will now be filling in the balance of Gonzalez's 6 year term. John Byrne has been appointed to a second 6 year term as the lead trustee.

The Board discussed and unanimously approved the creation of a new NACS Award. The first Award will be announced in 2009.

NACS Award for Distinguished Service in the Advancement of Catalysis

Purpose: To recognize an individual (every two years with a \$5,000 prize) who advanced catalytic chemistry or engineering by significant service to the catalysis community in addition to the performance of outstanding technical accomplishments. Travel costs are provided to the meeting where the award is presented.

Rules of Eligibility: A nominee must have demonstrated extensive contributions to the advancement of catalysis during their career. Service activities recognized by the award may include roles such as teaching, mentoring, writing, editing, and leadership of meetings or organizations. An awardee must have made these contributions to the benefit of the North American catalysis community.

Also with regard to all the NACS Awards, the following motion was approved unanimously and will take effect immediately for new awards:

Recipients of NACS Awards shall not have received a recent NACS Award or NACS Lectureship within the last 5 years

Edrick Morales (Commu-

nications Director) discussed the preparations underway for holding the Director-at-Large elections electronically via the WWW. He shared a proposal by the Creative Scanning Solutions, Inc. (CSS), which is a software consulting and data processing company located in Rochester, New York. CSS has provided a similar service to AIChE and ACS in the past. For electronic balloting to work for all the membership, we need reliable and current e-mail addresses for each member before mid-December. Local Club officers are responsible for getting current address information for their members to Edrick. More details on the election process will follow.

There was extensive discussion about how the NACS should deal with excess proceeds from a previous NAM meeting. Any excess proceeds will be shared with the local club operating the meeting and if proceeds are unexpectedly high, some of that excess shall be passed along to the organizers of the next NAM meeting in order to reduce future registration fees.

NAM Meetings: A summary report of the Houston 2007 NAM meeting was received. Bruce Gates reviewed progress on operations for the 2009 NAM meeting in San Francisco [[www.21nam.org](http://www.21nam.org)]. Galen Fischer summarized progress on the organization of the 22nd NAM meeting to be held in Detroit, MI in 2011. Preparations are beginning for the 23rd NAM meeting to be operated by the Tri-State Catalysis Club in 2013.

Your local club representative (to the NACS) has a draft of the full minutes of the Board meeting.

*John Armor, President*

# North American Meeting San Francisco, June 7-12, 2009

The 2009 NAM will take place at the Hyatt Regency Hotel, located directly on the Embarcadero waterfront in San Francisco. The meeting co-chairs are Enrique Iglesia, Charles Wilson, and Bruce Gates. Further information is available on the meeting website ([www.21nam.org](http://www.21nam.org)); the website is now open for registration. **April 1, 2009, is the deadline for early registration.**

The following industrial sponsors have already provided support for the meeting: Air Products, Avantium, BASF, BP, Chevron, ConocoPhillips, Eastman, Exxon-Mobil, Haldor Topsøe, Johnson Matthey, Lummus, Parr, Süd-Chemie and UOP.

Those wishing to become sponsors should be in contact with the Fund Raising Chair, Jon McCarty, whose email address is [JonGMcCarty@Eaton.com](mailto:JonGMcCarty@Eaton.com). Those interested in exhibits at the meeting should consult the web site.

The preliminary list of plenary and keynote speakers is as follows:

## Plenary Speakers

- Jeff Beck (ExxonMobil) – Houdry Award Winner
- Avelino Corma (University of Valencia) – Boudart Award Winner
- Manos Mavrikakis (University of Wisconsin) – Emmett Award Winner

## Confirmed Keynote Speakers (titles are tentative)

- Xinhe Bao (Dalian Institute of Chemical Physics) – *Catalysis of nano particles confined inside the channels of CNTs*
- Simon Bare (UOP) – *Unraveling the complexity of industrial catalysts using in-situ x-ray absorption spectroscopy*
- Charles Campbell (University of Washington) – *Which transition states and intermediates control catalyst activity, and how well do we know their energies?*

- Kazunari Domen (University of Tokyo, Japan) – *Efficient hydrogen evolution sites of photocatalysts for water splitting*
- Sonja Eisbouts (Albemarle Catalysts) – *FCC pretreatment (hydrotreating) catalysts*
- Wolfgang Hölderich (RWTH Aachen University) – *Chemicals production from renewable feedstocks*
- Yasuhiro Iwasawa (University of Tokyo) – *Active species and dynamic structures for selective catalysis on designed surfaces and nanoparticles*
- Michael Klein (Rutgers University) – *Modeling and control of complex reactions*
- John Lee (Dow, Retired) – *Research and development with modified mordenite zeolites*
- Johannes Lercher (Technical University Munich, Germany) – *Bifunctional catalysis on solid acids*
- Can Li (Dalian Institute of Chemical Physics) – *Characterization and reactivity of titania-based photocatalysts for environmental applications*
- Raul Lobo (University of Delaware) – *New mechanistic insights into the formation of zeolite catalysts*
- Tobin Marks (Northwestern University) – *Title to be announced*
- Richard Masel (University of Illinois) – *Formic acid fuel cells*
- Isabella Nova (Politecnico di Milano, Italy) – *Diesel NOx aftertreatment catalytic technologies: towards a convergence of the catalytic chemistry?*
- Ryong Ryoo (KAIST, Korea) – *Catalyst synthesis*
- Miguel Salmeron (Lawrence Berkeley National Laboratory) – *Structure and spectroscopy under ambient conditions of pressure and temperature: Novel techniques for fundamental studies in catalysis*
- Stuart Soled (ExxonMobil) – *Reversible and irreversible changes in Co Fischer-Tropsch catalysts during synthesis*
- Bert Weckhuysen (Utrecht University) – *Catalyst imaging by STXM and optical micro-spectroscopy*

21<sup>st</sup>  
NAM

San Francisco,  
California 2009

[www.21nam.org](http://www.21nam.org)

#### Web Links

- Chicago - [www.catalysisclubchicago.org](http://www.catalysisclubchicago.org)
- Mexican Academy of Catalysis - [www.acat.org.mx](http://www.acat.org.mx)
- NACS - [www.nacatsoc.org](http://www.nacatsoc.org)
- New York - [www.nycsweb.org](http://www.nycsweb.org)
- ORCS - [www.orcs.org](http://www.orcs.org)
- Philadelphia - [www.catalysisclubphilly.org](http://www.catalysisclubphilly.org)
- Pittsburgh-Cleveland - [www.pitt.edu/~gveser/PCCS](http://www.pitt.edu/~gveser/PCCS)

## Clubs & Societies News

### Catalysis Division, Chemical Institute of Canada

The 20th Canadian Symposium on Catalysis, a biannual meeting of the Catalysis Division of the Chemical Institute of Canada, was held on June 15-18, 2008 in Kingston Ontario, Canada. The theme of the symposium was Clean Air, Climate Change and Catalysis organized by Professor Brant Peppley of Queen's University, Ontario, Canada. The meeting was held at the Waterfront Holiday Inn which provided a view of the Kingston harbor and was in the heart of the historic district of the city. The meeting was very successful and there were 114 delegates from 9 countries. The highlight of the meeting included 5 plenary lectures: Professor Manfred Bochman from the University of East Anglia, UK lectured on "Catalysis by Organometallics", Professor Tom Ziegler from the University of Calgary lectured on "Computational Methods in Studies of Catalytic Processes", Dr. Robert Farrauto of BASF, 2008 Ciapetta Award lecturer, lectured on "Combining Industrial and Fundamental Research for Commercial Success", Dr. Fred Wagner of General Motors Corporations lectured on "Oxygen Reduction Catalysis for PEM Fuel Cells", Professor Flora Ng from the University of Waterloo, recipient of the 2008 Chemical Institute of Canada Catalysis Award, lectured on "Catalysis for Green Chemical Processes". We would like to thank our sponsors, Imperial Oil, DuPont of Canada,

Queen's University (Office of Research Services and the Department of Chemical Engineering). The Technical Exhibition was organized by Peter Byrne (Representative of Altamira and Autoclave Engineers) which included Altamira Instruments, Autoclave Engineers, Spectra Research Corporation and Varian Instruments. The Canadian Catalysis Foundation also sponsored travel awards for students and postdoctoral fellows to present papers/posters at the meeting.

During the symposium, new officers for the Catalysis Division for 2008-2010 were elected at the Annual Business Meeting of the Catalysis Division. The next Canadian Symposium on Catalysis will be held in Banff, Alberta, May 9-12, 2010. The theme for the meeting will be "Catalyzing a Sustainable Future". More details will be forthcoming.

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# Clubs & Societies News

## Catalysis Club of Chicago

### 2008 Herman Pines Award

**D**r. Aleksey Yezerets of the Catalyst Technology & Emissions Chemistry Department, Corporate R&D, Cummins Inc., is the recipient of the 2008 Herman Pines Award in Catalysis. The award, sponsored by UOP, the Northwestern University and the Catalysis Club of Chicago is presented annually at the Spring Symposium of the Catalysis Club of Chicago in recognition of outstanding contributions in the field of catalysis. Dr. Aleksey Yezerets received a plaque, a cash award and delivered the keynote address entitled "Catalysis for Clean Diesel Power".

### Herman Pines Award Nominations

Hello Catalysis Community!

The Catalysis Club of Chicago is soliciting nominations for the Herman Pines Award for outstanding research in the field of catalysis. The Award, co-sponsored by UOP and the Catalysis Club of Chicago, is given annually and is alternating between Academic/National Laboratory and Industrial researchers. The Award will be presented at the 2009 Catalysis Club of Chicago Spring Symposium and consists of a plaque, a cash award of \$1,000 and reimbursement for travel and lodging for the Spring Symposium where the recipient will deliver the plenary address.

The recipient will be chosen based on the following criteria:

- Importance of catalysis research completed in the past five years.
- Alternation of the award between industrial and academic/national laboratory researchers. For year 2009, nominations are sought for candidates from the ACADEMIA or NATIONAL LABORATORIES.
- Recipient must be a resident of North America. Deadline for Nomination: January 31, 2009.
- Nominations should describe the specific work for which the nominee should be recognized.

- Nominations should consist of complete curriculum vitae with letters of support for the nominee.

Letters of nomination and supporting documentation must be sent by January 31, 2009 as a single PDF document to:

Manuela Serban  
President – Catalysis Club of Chicago  
UOP  
50 E Algonquin Rd.  
Des Plaines, IL 60017  
847-391-2144  
Manuela.Serban@uop.com

## Notes from the Michigan Catalysis Society

### Meeting Schedule

The beginning of the fall season also marks the start of the monthly dinner meeting series of the Michigan Catalysis Society. The 2008-2009 MCS season officially began on October 14th with a visit by current NACS Ciapetta Lecturer Dr. Robert Farrauto from BASF Corporation. His excellent lecture on "Catalysis for the 21st Century: Convergence of Energy and the Environment" covered many diverse topics, including automobile emissions control catalysts, biomass to energy conversion, and fuel cells. On November 12th we welcomed Professor Israel Wachs from Lehigh University, who discussed his research on operando molecular spectroscopy for establishing catalytic molecular/electronic structure-performance relationships. The final presentation of the calendar year took place on December 9th when Professor Charles Campbell from the University of Washington lectured on the thermodynamics and kinetics of chemical reactions in catalysis.

The new year should provide equally interesting talks as the MCS will host John Yates from the University of Virginia on February 3rd, Peter Crozier from Arizona State University on March 3rd, and Jingguang Chen from the University of Delaware on April 7th. The 2008-09 season will come to a close in May at the 31st Annual Spring Symposium of the Michigan Catalysis Society. This year's Symposium will be held at the University of



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# Clubs & Societies News

Michigan and will feature an invited keynote lecture from the winner of the 2009 Michigan Catalysis Society Giuseppe Parravano Memorial Award for Excellence in Catalysis Research (to be announced in February). Recent winners of this award include Professor Bruce Gates, University of California-Davis in 2005 and Professor Alexis Bell, University of California-Berkeley in 2007. Awards will also be given to recognize the outstanding student oral and poster presentations at the meeting.

## 2009 Giuseppe Parravano Award Nominations

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Nominations are invited for the 2009 Michigan Catalysis Society Giuseppe Parravano Memorial Award for Excellence in Catalysis Research. The award is given biennially in odd numbered years to an individual from North America to formally recognize outstanding contributions to catalytic science and technology. The award consists of a medal and prize of \$500 and is sponsored by the Memorial Trust Fund for Professor Giuseppe Parravano, which has been established at the Department of Chemical Engineering, The University of Michigan. The recipient of the award is selected by a committee that is appointed by the officers of the Michigan Catalysis Society and includes one representative of the Parravano family.

Nominations must include the following:

- Name, occupational address, phone, fax, and e-mail of the nominator
- Name, occupational address, phone, fax, and e-mail of the nominee
- Nominee's curriculum vitae and bibliography of significant publications
- A proposed citation - limit to 1 or 2 sentences
- A narrative statement describing the Nominee's award qualifications
- One confidential letter of support requested by the nominator

An email of intent to nominate would be appreci-

ated. Letters of nomination and supporting documentation must be received by January 16, 2009, and should be sent to:

Paul Fanson

Toyota Motor Engineering & Manufacturing, North America

1555 Woodridge Road

Ann Arbor, MI 48105

(734) 995-5138 (phone)

(734) 995-0002 (fax)

paul.fanson@tema.toyota.com

## NAM22 Status

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Plans are under way for the Michigan Catalysis Society to host the 22nd NAM in Detroit, Michigan in 2011. Galen Fisher, NACS Representative and Chair of NAM22, presented a status report to the NACS Board of Directors in August. The date and location have been finalized, with the meeting to be held on June 5-10, 2011 in the Marriott Hotel at the Detroit Renaissance Center, home of the General Motors World Headquarters. The next task will be to establish the Committee chairs and start the more detailed activities of each group. We will be drawing mainly from MCS members at the auto companies, Dow Chemical, local universities, catalyst suppliers, and other catalytic scientists in nearby areas.

## Western States Catalysis Club

2009 Western States Catalysis Club Meeting on April 3rd in Golden, Colorado. Keynote speaker is Bob Furruto, Ciapetta lecturer. Additional information coming soon. Contact: Ryan Richards at rrichard@mines.edu.



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