

Chair

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SOUTHWEST CATALYSIS SOCIETY

SEMINAR BY PROF. WACHS

Thursday, September 17

Engineering Building 1: 4726 Calhoun Rd., Building #579

University of Houston, Houston, TX

The SWCS officers and I welcome you to this year's first SWCS Seminar by Prof. Israel Wachs from Lehigh University, **Thursday evening, September 17, 2015**, at the University of Houston. Here is the agenda for the event,

5:30 PM, Registration & networking 6:00 PM, Buffet Dinner 7:00 PM, Prof. Wachs' Seminar 8:30 PM, Adjourn

The registration fee this event is \$20 for regular members, and free to students and postdocs. You can pre-register and/or make payment using credit cards following this link, <u>https://www.eventbrite.com/e/southwest-catalysis-society-dinner-event-prof-wachs-tickets-18522710927</u>

Alternatively if you prefer to pay using paypal account, you can preregister and make pre-payment here <u>https://www.paypal.com/cgi-</u> <u>bin/webscr?cmd=_s-xclick&hosted_button_id=UGPJ4MRNCWCKA</u>

We do have onsite registration. We will be able to accept credit cards (Visa, MasterCard, Discover, and American Express) for the registration fee or corporate donations. Credit card receipts will be sent via e-mail, so please be prepared to input your e-mail address into our system when you pay. But note, that checks are faster (especially if you have them ready to go). We will also continue to accept cash.



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NACS Representative

Mike Reynolds Shell International Exploration and Production 3333 Highway 6 South Houston, TX 77082 mike.reynolds@shell.com The reception is to be held in the "Commons" on the 1st floor of **Engineering Building 1:** 4726 Calhoun Rd., Building #579. Direction to the parking garage, the reception and presentation room is at the end of this announcement.

Look forward to seeing you at the dinner event.

Teng Xu

Chair, Southwest Catalysis Society



Heterogeneous Catalysis Research in the 21st Century: Application of *Operando* Molecular Spectroscopy to CH₄ Activation and Other Reactions

Israel E. Wachs *Operando* Molecular Spectroscopy & Catalysis Laboratory Department of Chemical & Biomolecular Engineering Lehigh University Bethlehem, PA 18015 USA



The *operando* molecular spectroscopy methodology is rapidly making significant inroads into the fundamental understanding of heterogeneous catalysts for many applications. *Operando* spectroscopy refers to the simultaneous collection of catalyst spectroscopic information (catalytic active sites, surface reaction intermediates and bulk structure) and online analysis of reactants and products (kinetics and selectivity). These unprecedented molecular and electronic insights are allowing for establishment of catalyst structure-activity/selectivity relationships and guiding the rational design of advanced catalysts.

The presentation will primarily focus on application of *operando* molecular spectroscopy studies to methane activation reactions. For CH₄ activation to aromatic liquids by supported Mo/ZSM-5 catalysts, four distinct surface MoO_x sites on the ZSM-5 support have been identified with the $(O=)_2Mo(-O-Al)_2$ being the most active catalytic site. For CH₄ activation to C_2H_4/C_2H_6 by supported Na₂WO₄/SiO₂ catalysts, several catalytic active sites are also found to be present reflecting the complexity of this catalyst system for oxidative coupling of methane (OCM). Several other examples of operando molecular spectroscopy will also be highlighted (e.g., olefin metathesis by supported ReOx/Al₂O₃, ethylene polymerization by supported CrOx/SiO₂, high temperature water-gas shift for H₂ production by CrOx-FeOx and selective catalytic reduction of NO with NH₃ by supported VOx-WOx/TiO₂).

Bio for Prof. Wachs

EDUCATION: Israel E. Wachs received his undergraduate education at The City College of The City University of New York where he graduated with a B.E. (ChE) in June, 1973. He continued his graduate ChE education at Stanford University under the mentorship of Professor Robert J. Madix in the area of surface science, and graduated with a PhD (ChE) in 1978.

INDUSTRIAL YEARS (1977-1986): Israel joined Exxon Research & Engineering Company in their Corporate Research Labs towards the end of 1977. At Exxon, he was involved with many different catalytic technologies over the years (selective oxidation, solid acid catalysis, synthesis of synthetic fuels, hydrodesulfurization (HDS) and hydrocarbon conversion). One of his inventions on the selective oxidation of o-xylene to phthalic anhydride by promoted supported V_2O_5/TiO_2 catalysts became the leading international industrial catalyst for this technology and is still used around the world. He received an Exxon Research Award for his inventions on the synthesis of synthetic fuels. Israel was also selected to be an Exxon Fellow for the spring semester of 1986 at California Institute of Technology (CalTech). He departed Exxon for academia at the end of 1986.

<u>ACADEMIC YEARS (1987-present)</u>: Israel joined the Chemical Engineering Department of Lehigh University in January 1987. At Lehigh, he has taught many different courses over the years: Heterogeneous Catalysis, Advanced Heterogeneous Catalysis, Environmental Catalysis, Reactor Engineering, Surface and Interface Analysis of Functional Materials, Fluid Mechanics, Unit Operations, Air Pollution Control, Energy, Opportunities for Student Innovation (research course) and Professional Development. He set up a world-class catalysis research laboratory focusing on mixed metal oxide catalytic materials and their characterization under reaction conditions



(*in situ* and *operando* molecular spectroscopy). These studies have established the foundation for the molecular/electronic structure – activity/selectivity relationships that are developing a unified model of mixed metal oxide catalysts and guiding their rational design.

The current focus of the Wachs catalysis group is to develop catalyst characterization techniques under reaction conditions, referred to as *operando* spectroscopy in the recent literature, and apply them to determine how high profile catalytic systems actually function. The term *operando* spectroscopy implies that the catalyst characterization information is being conducted <u>simultaneously</u> with online product analysis to allow for establishing direct structure-activity/selectivity relationships. Along these lines, the Wachs group has developed instrumentation that can simultaneously obtain Raman, IR, UV-vis and TPSR spectroscopic information and product analysis with an online mass spectrometer/GC system. This cutting-edge instrument is allowing the Wachs catalysis research group to rapidly develop fundamental molecular/electronic structure – catalytic activity/selectivity relationships for many different catalytic materials and reactions (conversion of CH₄ liquids (GTL), conversion of CH₄ to C₂ hydrocarbons, solids for CO₂ capture, selective hydrocarbon oxidation, selective catalytic reduction of NO by NH₃, high temperature water-gas shift, photocatalytic splitting of water H₂ fuel, olefin metathesis, ethylene polymerization, hydrocarbon conversion with solid acid catalysts, enzyme catalysis, rational catalyst design, etc.).



Direction to the parking garage, Commons, and presentation room.



- **1) Parking garage:** 4400 University Drive, Houston, TX 77204
- Engineering Building 1: 4726 Calhoun Rd., Building #579 Commons (1st floor): Reception and Dinner
- **3) L2D2 Lecture Hall:** Building #580, Presentation
 - walking path from parking garage