Final Technical Report

Sponsoring Agency: Department of Energy

Award no.: DE-FG02-03ER15457

Project Title : Institute for Catalysis in Energy Processes (ICEP)

Institution: Northwestern University

Principal Investigator: Justin M. Notestein (previously, Peter Stair)

Project Period: 09/2006 – 08/2024

Executive Summary

The Institute for Catalysis in Energy Processes (ICEP) was a multi-PI program located at the Northwestern University Center for Catalysis and Surface Science from 2006-2024. Over several renewal cycles and several organizing themes, ICEP addressed fundamental questions in catalysis science. In turn, the scientific questions addressed were directly relevant to the efficient use of the nation's resources to produce fuels and commodity chemicals, harness alternate energy sources for chemical reactions such as light or electricity, reduce emissions and waste, and minimize the impact of our use of plastics. Selective oxidation, (oxidative) dehydrogenation, deNOx, CO_2 reduction, hydrogen release, polymer decomposition / depolymerization, and many other reactions of intense interest to the US Department of Energy were studied in the center. Major ICEP strengths were in catalyst synthesis, in measurements that elucidated catalyst properties, in reaction mechanisms and kinetics, and in predictive theory and modeling. ICEP researchers were often the inventors or developers of materials and methods that were brought to bear on the Institute's catalytic systems. Key characterization tools advanced through this project included resonance Raman and related techniques, sum frequency generation, and X-ray standing wave spectroscopy. Center members relied extensively on computational tools such as density functional theory and microkinetic modeling to fully investigate catalyst structures and catalytic mechanisms. ICEP researchers were early developers of atomic layer deposition (ALD) for catalyst synthesis and were early pioneers of metal organic frameworks for catalysis. ICEP innovations are found in areas of intense research such as single-atom catalysts, catalytic deconstruction of plastics, and catalytic MOFs, to name a few. Research areas initiated by ICEP indirectly led to DOE EFRCs, startup companies, and other achievements.

Over its 18 years of existence, ICEP involved two different PIs (Stair and Notestein) and 24 senior investigators across several academic disciplines at Northwestern University. There were tight collaborations with Argonne National Laboratory, including specialized equipment and experiments permanently located there. The center supported ~400 person-years of effort by graduate students and postdocs, either directly through DOE support or indirectly by leveraging independent support provided to the trainees, e.g. through the NSF GRFP or internal fellowships. The project resulted in 328 manuscripts and numerous conference presentations.

Accomplishments

ICEP was a Basic Energy Sciences project with broad goals in catalysis science that changed over 6 renewals (2 or 3 years each) and a 1-year no-cost extension. Broad goals were to develop atom-precise materials and material interfaces, to characterize these materials with similar precision, and then to use these materials to understand reactions of DOE interest. In this context, all goals and objectives of the project were met.

By our count, ICEP published a total of 328 manuscripts since its inception through the end of its no-cost extension in 2024 under grant number DE-FG02-03ER15457. Manuscripts continue to be published to this day due to the deep roots that ICEP set down in the research enterprise at Northwestern. These manuscripts are broken down approximately as 272 primary research manuscripts on topics that are closely aligned with ICEP themes, 20 articles that are reviews or commentaries, and an additional 16 manuscripts that are less well-aligned with ICEP themes. These latter manuscripts typically use ICEP-derived materials or analytical techniques. Finally, an additional 20 manuscripts were published erroneously under grant DE-FG02-03ER154757 (note the additional '7' inserted in the number). All of those were on core ICEP themes.

Summary of Project Activities

History. The origin of ICEP was the Environmental Molecular Science Institutes (EMSI) program, jointly funded by NSF and DOE/BES Chemical Sciences, beginning in 1998. The EMSI funded at NU and ANL was the *Institute for Environmental Catalysis* (IEC). IEC was a collaborative effort of Northwestern University faculty from the Departments of Chemistry, Physics, Chemical and Biological Engineering, Materials Science and Engineering, and Civil and Environmental Engineering, and Argonne National Laboratory scientists from the Chemistry and Materials Science Divisions.

In 2002 the IEC program was renewed for an additional period of support, and in 2006, DOE/BES programs at NU and ANL were joined with a research focus shifted toward catalytic chemistry relevant to energy. The name of the NU institute was changed to current Institute for Catalysis in Energy Processes (ICEP). From 2006 until 2012, ICEP included efforts in both chemical catalysis and photocatalysis. The NU and ANL programs were reviewed together until 2012. After 2012, the two programs were separated, both administratively and intellectually, and the ICEP effort was focused exclusively on chemical catalysis. In 2015 through its end in 2023 (and no-cost extension through 2024), ICEP subsumed the individual catalysis research programs of several investigators (Kung, Notestein, and T. Marks), creating a centralized home for DOE/BES catalysis research at Northwestern. Expanding the ICEP base enabled an expansion of the science proposed and the scope of collaborative, interdisciplinary activities within ICEP. ICEP was also an effective partner to other DOE BES activities that researchers were a part of, especially EFRCs based at Argonne, Northwestern, and other institutions. ICEP was a key partner in the local Catalysis Club of Chicago and in organizing the North American Catalysis Society Meeting in Chicago (2019). ICEP held internal seminars and underwrote a course on experimental heterogenous catalysis that trained several generations of students at the REACT shared user facility. This ultimately led to a series of rigor and reproducibility workshops and reports led by ICEP member and REACT core facility director Neil Schweitzer. Finally, an international memorandum of understanding was developed with UniCat and UniSysCat, a center of excellence in Berlin on catalysis.

Prof. Peter Stair, Professor of Chemistry at Northwestern, was the PI from the inception through 2018. In 2018, Prof. Justin Notestein, department of Chemical and Biological Engineering, became the co-PI then PI through the end of the center. Additional senior investigators at Northwestern University at project conclusion in 2023 included M. Bedzyk (MatSci), L. Broadbelt (ChemE), O. Farha (Chem), J. Hupp (Chem), H. Kim (Res. Prof. Chem.), H. Kung (ChemE), M. Kung (Res. Prof. ChemE), L. Marks (Chem), T. Marks (Chem), S. Nguyen (Chem), K. Poeppelmeier (Chem), G. Schatz (Chem), N. Schweitzer. (Res. Prof. ChemE), R. Snurr (ChemE), and E. Weitz (Chem). Prof. Stair, Weitz, H. Kung, M. Kung, and L. Marks are now emeritus status. Earlier iterations of ICEP also included as senior personnel M. Delferro (Res. Prof. Chem, before beginning independent role at ANL), D. Ellis (Phys), F. Geiger (Chem), K. Gray (EnvE), M. Hersam (MatSci), W. Sachtler (Chem, deceased), and R. van Duyne (Chem, deceased). At project end, L. Seitz (ChemE), and E. Weiss (Chem), were invited as trial members of the center to prepare for a renewal that was ultimately not allowed.

Themes. ICEP has not been defined by a single research theme during its 18 years of operation, but rather by a collection of research themes. Key reactions have been deNOx catalysis, selective oxidation (e.g. oxidative dehydrogenation of alkanes), and photocatalysis, especially photocatalytic reduction of CO_2. In later years, materials were developed for electrocatalysis applications. Experimental kinetics studies were backed by computational investigations using density functional theory and microkinetic modeling. Paralleling research into these reactions was the development of new synthetic methodologies, including early use of atomic layer deposition (ALD) for catalysis and the development of novel or unique precursors. ICEP was also instrumental in the synthesis of hybrid organic/inorganic materials and metal organic frameworks (MOFs) and their predecessors as catalysts. Finally, ICEP also developed high surface area oxides as unconventional supports for catalysts, especially SrTiO3 and related species, and in later years, lanthanide scandates. In developing these materials, the overarching ICEP goal was to address the inhomogeneity challenge in heterogeneous catalysis. Almost all commercial or research-level catalysts are inhomogeneous, containing unknowably numerous different possible active sites. More precise materials are required to achieve disruptive advances in our understanding and implementation of catalysis and new catalytic processes. The ICEP vision was that we could create catalysts with unique types of active sites in an atomistically controlled fashion so that we can move beyond indirect empiricism to definitive, predictive science.

Finally, this work on developing new, atomically-precise catalytic materials was complemented by the development of state-of-the-art characterization tools. This included pioneering work in resonance, surface-enhanced, and tip-enhanced Raman spectroscopy, or rRaman, SERS, and TERS, respectively. ICEP researchers in earlier years were active in developing sum frequency generation (SFG) to interrogate catalytically relevant surfaces. Special tools were built at Argonne National Laboratory and especially at the Advanced Photon Source. Beyond conventional use of X-ray absorption spectroscopy, ICEP researchers also developed X-ray standing wave (XSW) spectroscopy to gain atomic-level information about the structure and electronics of supported metal and metal oxide catalysts. Finally, ICEP established the user facility called the Reactor Engineering and Catalyst Testing (REACT) core facility at Northwestern, the first of its kind in the United States. In later years, this substantially broadened the impact of catalysis science principles on other fields and technologies, such as carbon capture, atmospheric water harvesting and surface characterization of biological or biomedical materials. This center was also the vector for workshops and best practices in rigor and reproducibility in catalysis, which eventually became a series of independent DOE-supported meetings and publications.

Over many years, these efforts have been tightly aligned with the Grand Challenges identified in the 2007 DOE workshop report "Basic Research Needs: Catalysis for Energy" and the Priority Research Directions identified in the 2017 DOE workshop "Basic Research Needs for Catalysis Science". As mentioned above ICEP was responsible for at least 328 manuscripts. It is impossible to describe each of these here, but several of particular note are described below. These are not necessarily the highest cited works or those appearing in the highest 'impact' journals, but they speak to themes that would persist throughout the life of ICEP. Manuscript numbers refer to the list included following this narrative. The invention and patent report is handled separately. No databases were developed directly from ICEP support.

In 2009, four of the manuscripts published by ICEP researchers were notable for representing recurring themes and serve here as introductions to classes of major research accomplishments. Manuscript 10 by Christensen et. al. (NU PIs Stair, Poeppelmeier, Hersam, and Marks) reported on "Controlled Growth of Platinum Nanoparticles on Strontium Titanate Nanocubes by Atomic Layer Deposition" This work leveraged the extensive knowledge of $SrTiO_3$ materials to create high surface area supports for Pt. $SrTiO_3$ has lattice parameters close to those of Pt and other noble metals, such that nanoparticles deposited on these surfaces are small and stable, with well-defined Wulff shapes of their own (**Figure 1**). The deposition of active catalyst sites by ALD would become a recurring theme for the center, as would the use of $SrTiO_3$ as a stable surface, useful both for characterization and to stabilize sites during reaction. See for example, a follow up manuscript in 2010 in *Nature Materials* (manuscript 28). The latter property would make these materials useful as catalysts for polyolefin depolymerization, which would underpin the iCOUP EFRC and at least one spinoff startup company not directly tied to ICEP. ALD as a synthesis tool will be used repeatedly throughout the lifetime of ICEP. See for example manuscript 34, 68, 75, 95, 215, 223, and many others. New precursors were developed for ALD as manuscripts 132 and 145, and the details of ALD were analyzed in many manuscripts such as 128 and 140. Surface enhanced Raman spectroscopy was used to interrogate ALD synthesis mechanisms and ALD was used to create oxide overcoats on SERS-active surfaces for interrogation of other chemistries, e.g. manuscript 140.

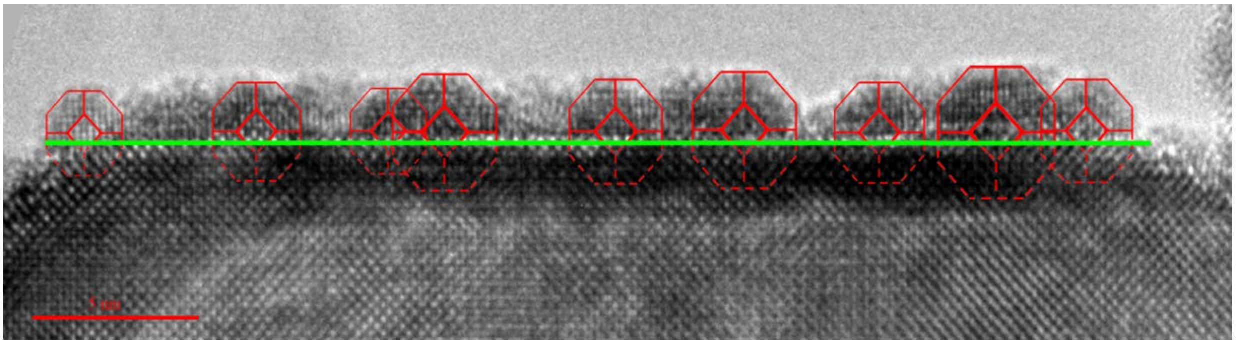

Figure 1. image of Pt nanoparticles epitaxed on $SrTiO_3$ nanocuboids. The nanoparticles have self-similar shapes and the same active sizes exposed.

H. Feng et. al. (NU PI Stair) published work on "Catalytic Nanoliths" (Manuscript 11), which used catalysts deposited on anodic aluminum oxide disks as catalytic reactors (**Figure 2**). These structured catalysts allow for true single-pass, ultra-low contact time catalytic measurements, while still being sufficiently high surface area to observe product formation with standard tools (ie GC and process MS). This tool was not extensively utilized but likely has potential as a platform for high fidelity catalytic data collection. Many manuscripts from ICEP addressed selective oxidation catalysis, especially oxidative dehydrogenation over supported vanadia and copper oxides, including 29, 32, 75, 97, 133, 165, 218, 275, 284, and 288.

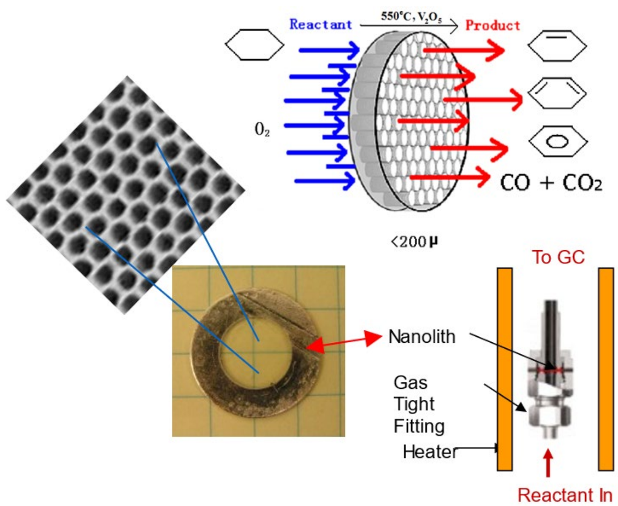

Figure 2. Catalytic nanolith reactors based on the 1D channels of anodic aluminum oxide disks are ideal platforms for examining selective oxidation catalysis and similar reactions under true single-pass conditions. Active sites are readily deposited inside the channels using atomic layer deposition.

ZX Feng et. al. (NU PI Bedzyk) published in 2009 on "Direct Atomic-Scale Observation of Redox-Induced Cation Dynamics in an Oxide-Supported Monolayer Catalyst: WO_x/α-Fe_2O_3 (0001)." (Manuscript 12). This is the first of many manuscripts in ICEP on the use of XSW to interrogate supported metal oxides relevant to catalysis. The XSW technique locates surface atoms with respect to an underlying crystalline oxide in all three directions. This can be used to understand surface reconstructions, or to understand the structure of supported catalysts deliberately synthesized. Later developments would add the capability to carry out measurements in reactive environments for in situ XSW, and to add oxidation state sensitivity for XWS-XPS. Manuscripts 207 and 225 are other key works in this area, addressing these additional capabilities. See **Figure 3**. This technique was a unique tool for interrogation of heterogeneous catalysts developed by ICEP. Manuscript 27 by Buchbinder et. al. (NU PIs Weitz and Geiger) describes the use of sum frequency generation (SFG) to interrogate the organization of organic monolayers on oxide surfaces. This work would eventually be discontinued from the center but would be supported separately by the NSF and other agencies. As with the above manuscript, this is another one of the unique ICEP tools for interrogating the inorganic and organic components interacting at the surfaces of catalytic materials. Under reaction conditions.

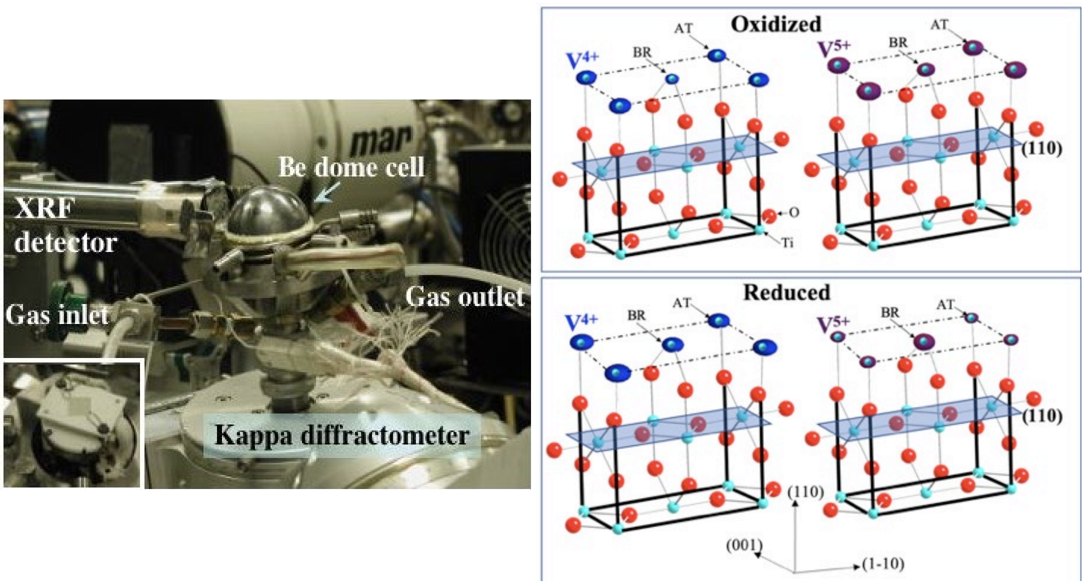

Figure 3. (left) Temperature controlled gas reaction sample cell for in situ XPS-XSW at ICEP-controlled station at the APS. (bottom) For sub-monolayer VOx on a-TiO2 (110), XSW-XPS gives 3D atomic maps for V^{4+} (left) and V^{5+} (right) referenced to the ball and stick model of the substrate after oxidation and reduction. V unequally occupies bridge (BR) and atop (AT) sites with occupation fractions indicated by the size of the V "ball".

A final manuscript of note in 2009 (Manuscript 22) was on "A Catalytically Active, Permanently Microporous MOF with Metalloporphyrin Struts" by NU PIs Farha, Hupp, and Nguyen. While now common, this was one of the very first reports of catalysis by a metal organic framework. This work built off prior work in ICEP's predecessor center on catalysis by 'molecular squares' which were supramolecules that researchers today would recognize as a finite set of MOF nodes and linkers. Pioneering work on MOF catalysis, both discovery / synthesis and interrogation, via tools both experimental and computational (e.g. manuscript 180, **Figure 4**), would continue to be a significant focus of ICEP over the following years (e.g. manuscripts 59, 72, 97, 152, 202, and others). While not developed directly under ICEP support, the QMOF database followed from the groundwork set up in ICEP. The QMOF database, https://github.com/Andrew-S-Rosen/QMOF, includes more than 20,000 DFT-optimized MOF structures ideal for machine learning based discovery of new catalysts.

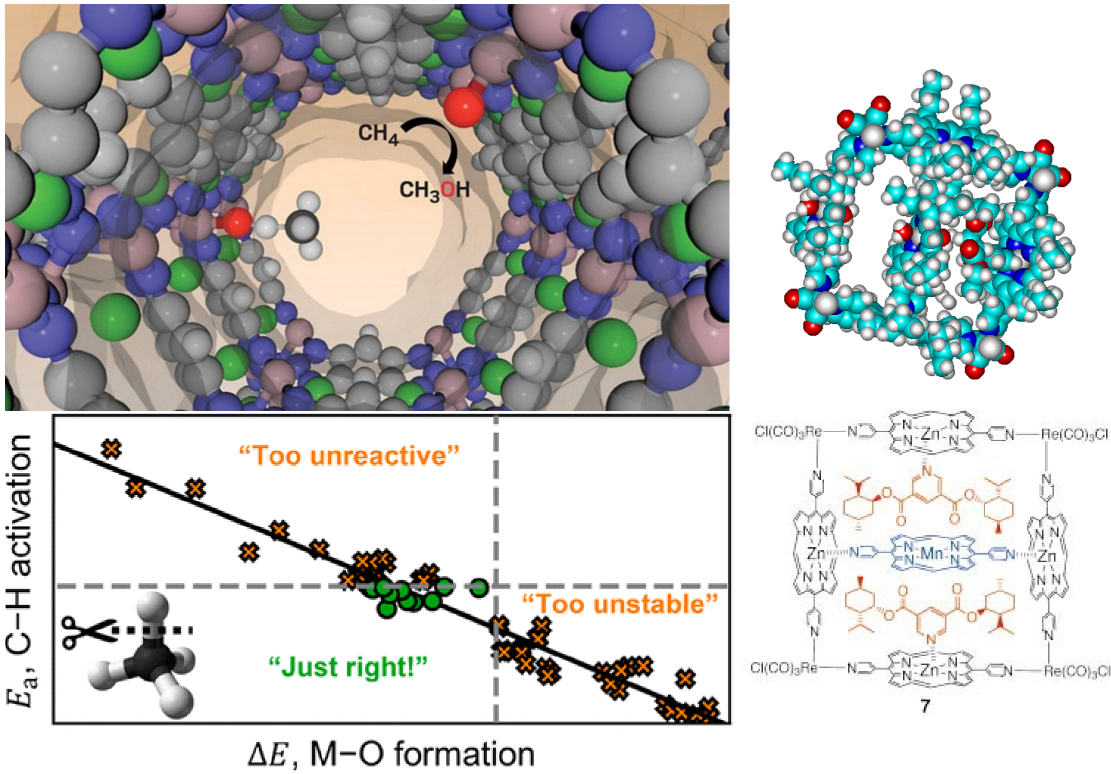

Figure 4. Computational discovery of catalytically active metal organic frameworks (MOFs), left, was a major research area at the conclusion of ICEP, building off pioneering work developing some of the first examples of this class. That work included the first synthesis and testing of precursors to MOFs (at right), consisting of enzyme mimics known as molecular squares developed in 2001 during the predecessor grant of ICEP.

In addition to the broad themes discussed in the previous paragraph, three combinations of innovations in both materials and catalysis science are of special note. First is the manuscript by Ding et. al. (NU PIs L. Marks and Stair) on "Identification of active sites in CO oxidation and water-gas shift over supported Pt catalysts" published in *Science* in 2015 (manuscript 106). In this work, atomic layer deposition or low-temperature grafting was used to introduce Pt precursors into a mesoporous ZSM-5 material or an Al-doped mesoporous silica. Through controlled synthesis, Pt could be deposited as single atoms or as small nanoparticles. The existence of single atoms was confirmed through microscopy and through CO DRIFTS (**Figure 5**). At this point in history, 'single-atom' catalysts were gaining attention, but were not yet as popular as now. Then, as now, was much speculation that these catalysts were exceptionally active, but much evidence was indirect or not appreciated to be extremely support dependent. The primary finding of this work was to show that cationic Pt single atoms on these supports were catalytically inert for CO oxidation or water-gas shift, and that all activity in these reactions – on these supports – could be ascribed to small nanoparticles. Emblematic of the general approach in ICEP was that well-defined syntheses allowed relatively simple tools, here CO DRIFTS, to give broad insights into structure function relationships across a broader swath of materials.

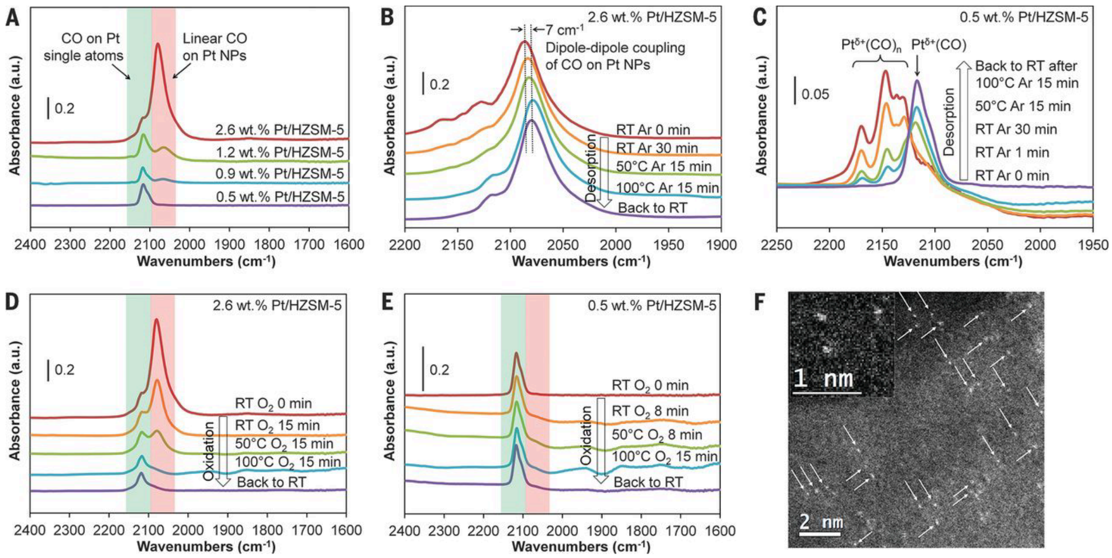

Figure 5. CO DRIFTS used to identify Pt single atoms and nanoparticles synthesized on H-ZSM5 and Al-doped silica. From manuscript 106.

Another area of research involved the synthesis of isolated Mo dioxo species on carbon surfaces. Lohr et. al. (NU PIs T. Marks and Stair) found that a molecular complex could be grafted onto activated carbon and related surfaces (reduced graphene oxide, carbon nanohorns, carbon nanotubes, etc). See manuscript 131, 175, 263, 279, and 291. This catalyst was imaged with atomic resolution with collaborators in Japan, as reported in reference 210. This catalyst was, over time, shown to be capable of carrying out several different reactions, chief among them being the acceptorless dehydrogenation of alcohols to give H_2 and aldehyde (manuscript 145, **Figure 6**) As reported in 2017, this could be considered as an early report of alcohols as "liquid organic hydrogen carriers". These materials are also capable of polyethylene terephthalate deconstruction (manuscript 190). This spurned a wave of research into other catalysts and catalyst systems capable of polymer deconstruction or depolymerization. These include the formal hydrogenolysis via reverse hydrooxygenation by a metal triflate and then hydrogenation of the transient olefin by a support metal in the same reactor. Another system was discovered by Mason et. al. (NU PI T. Marks, manuscript 237) for polyolefin hydrogenolysis using supported cationic zirconium catalysts, which, under other conditions, are also exceptional arene hydrogenation catalysts or olefin polymerization catalysts.

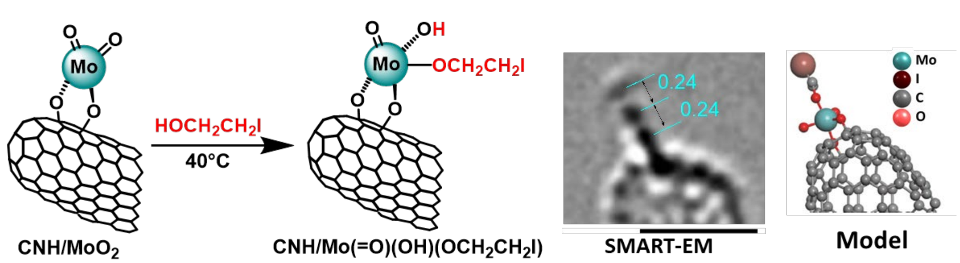

Figure 6. C/MoO_2 (supported on carbon nanohorns) and the reaction with ICH_2CH_2OH. On right is a representative SMART-EM image and a simulation of an isolated 2-iodoethanol addition complex. From manuscript 210. These catalysts were demonstrated to be proficient at PET deconstruction, alcohol dehydrogenation, transfer oxidation, and other reactions.

As a final example, Yan et. al. (NU PIs Notestein and Stair) published work in *Science* in 2021 on "Tandem In_2O_3-Pt/Al_2O_3 catalyst for coupling of propane dehydrogenation to selective H_2 combustion," listed as manuscript 290. In this work atomic layer deposition was used to add In_2O_3 on top of a typical Pt/Al_2O_3 catalyst (**Figure 7**). In_2O_3 is a known selective hydrogen combustion catalyst, while Pt-based catalysts are known to be proficient at propane (nonoxidative) dehydrogenation. Combined, these materials allowed for a new mode of tandem catalysis equivalent to oxidative dehydrogenation. Key to the performance of the material was the creation of extensive interface between the metal and the metal oxide during the ALD process. Control materials with physical mixing or deposition of Pt on In_2O_3 failed to create enough of these critical interfaces. Structurally related oxide 'overcoated' catalysts are also discussed in manuscripts 159, 170, 187, 215, 223, and 254, among other manuscripts. These catalysts show SMSI-like effects that improve CO_2 hydrogenation rates, stabilize a variety of catalysts against sintering under harsh conditions such as dry reforming, or create new acid sites at oxide-oxide interfaces. These types of materials became a hallmark of ICEP in its later years.

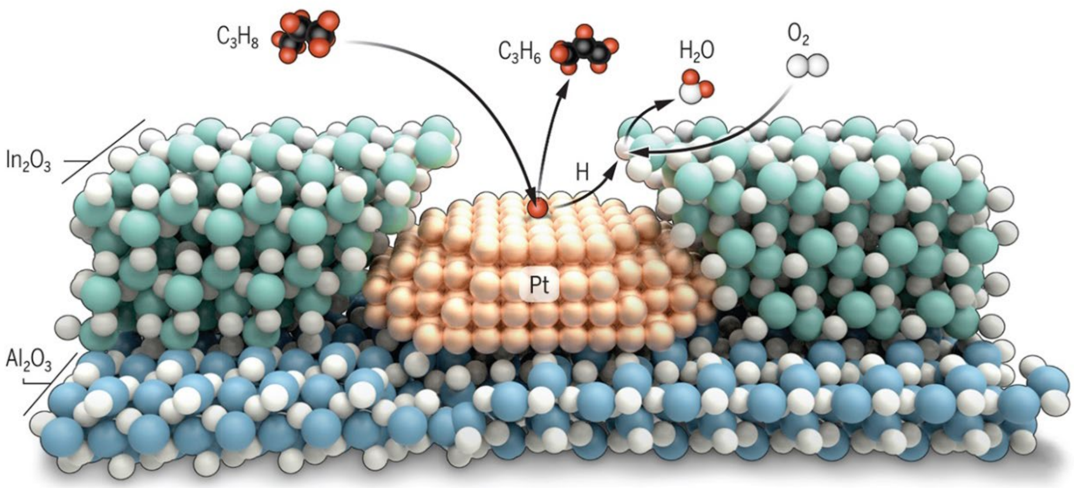

Figure 7. Structure of a In_2O_3-Pt/Al_2O_3 overcoated catalyst. Because of extensive oxide-metal interface, hydrogen atoms from propane dehydrogenation of Pt quickly migrated to the In_2O_3 surface for selective combustion. The extensive oxygen storage capacity and fast kinetics of the oxide also kept the Pt surface O-free, resulting in high selectivity to propylene, rather than combustion.

Products Developed

a. Manuscripts on DE-FG02-03ER15457 (272)

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