Dedicated Beamline Facilities for Catalytic Research: Synchrotron Catalysis Consortium (SCC)

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Project Summary

Synchrotron spectroscopies offer unique advantages over conventional techniques, including higher detection sensitivity and molecular specificity, faster detection rate, and more in-depth information regarding the structural, electronic and catalytic properties under *in-situ* reaction conditions. Despite these advantages, synchrotron techniques are often underutilized or unexplored by the catalysis community due to various perceived and real barriers, which will be addressed in the current proposal. Since its establishment in 2005, the Synchrotron Catalysis Consortium (SCC) has coordinated significant efforts to promote the utilization of cutting-edge catalytic research under *in-situ* conditions. The purpose of the current renewal proposal is **aimed to provide assistance, and to develop new sciences/techniques, for the catalysis community through the following concerted efforts:**

- Coordinating the implementation of a suite of beamlines for catalysis studies at the new NSLS-II synchrotron source
- Providing assistance and coordination for catalysis users at an SSRL catalysis beamline during the initial period of NSLS to NSLS II transition
- Designing *in-situ* reactors for a variety of catalytic and electrocatalytic studies
- Assisting experimental set-up and data analysis by a dedicated research scientist
- Offering training courses and help sessions by the PIs and co-PIs

These tasks will be performed by a consortium consisting of PIs and co-PIs from academic, national, and industrial laboratories. The beamlines and facilities are located in the National Synchrotron Light Source - II (NSLS-II) at Brookhaven National Laboratory that will be operational in September, 2014. The PIs and co-PIs have extensive experience in the areas of catalysis, electrocatalysis and synchrotron techniques. The combined expertise of the team members will continue to create the synergy that is necessary to ensure the success of the dedicated beamline facilities for catalytic research.

Part I: Progress Report

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1. Overview

The Synchrotron Catalysis Consortium (SCC) was funded and established in September, 2005 in the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory. Two dedicated beamlines were open to researchers from the catalysis and electrocatalysis communities in January 2006. Due to the success of the SCC efforts, which led to a significant increase in the number of catalysis users, one additional beamline was made available to SCC in 2008. **The consortium is the first of its kind in the United States, with a mission to promote the utilization of synchrotron techniques for cutting-edge catalytic research under *in-situ* conditions.** Similar types of synchrotron consortium for catalysis currently exist in Europe and Japan. The current consortium represents a critical first step for the catalysis community in the US to remain competitive in catalytic and electrocatalytic research using synchrotron techniques.

Our consortium consists of PIs and co-PIs from academic, national, and industrial laboratories. The PIs and co-PIs have extensive experience in the areas of catalysis, electrocatalysis and synchrotron spectroscopies. During the first decade of its existence the primary goal of the SCC team was to provide assistance and to develop new sciences/techniques to the catalysis community through the following concerted efforts:

1. Dedicated beamtime for catalysis research on three beamlines for *in-situ* X-ray Absorption Fine Structure (XAFS) measurements
2. Dedicated facilities, including state-of-the-art *in-situ* reaction cells, gas-handling systems, and advanced detectors
3. A dedicated research staff with expertise in the application of synchrotron methods to *in situ* catalysis science to assist the experimental set-up and safety training
4. Training courses for graduate students and postdoctoral fellows on XAFS techniques and data analysis
5. Assistance in idea development and proposal-writing for potential XAFS users from the catalysis community
6. Development and test of new hardware/software for catalytic and electrocatalytic research
7. Design and implementation of plans for the transition of SCC operations from NSLS to NSLS-II

During the past funding cycle, the availability of well-maintained, user-friendly and state-of-the-art synchrotron facilities, as provided by SCC, has helped many catalysis and electrocatalysis groups in their efforts to perform cutting-edge beamline research. The SCC also represents a new model for operating synchrotron facilities by providing direct interaction and feedback between funding agencies, beamline scientists, and researchers from academic and national laboratories. As summarized in the Progress Report, such interaction has led to a much more efficient utilization of the synchrotron facilities, which should ultimately benefit the nation as a whole by increasing the return on the investments made in our national laboratory system. The utilization and productivity of the three SCC beamlines by the catalysis community, as

measured by the percentage of beamtime utilization and publications, have increased significantly since the establishment of the consortium. Furthermore, the use of the SCC beamlines is an essential component for many researchers who are currently funded by DOE. This positive impact of SCC on the support of the catalysis science community at NSLS and toward NSLS-II underlies letters of support for this proposal from BNL Directorates included in the Appendix.

2. Description of Progress During Past Funding Period

2.1 Assistance to Catalysis Users

The SCC members have made significant progress in setting up dedicated facilities for the catalysis community on three beamlines, X18A, X18B and X19A. The dedicated SCC beamline staff scientist (Dr. Ned Marinkovic) provided assistance to the catalysis user groups in many ways, including training the users on beamline operation and safety, setting up dedicated reactors and gas-handling systems, and providing experimental assistance when needed.

Since its establishment SCC has helped many catalysis groups, including a large percentage of first-time new catalysis groups who would otherwise not able to start synchrotron research. The catalysis user groups are from academic, industry, and national laboratories. They include Argonne National Lab, BNL, Boston College, Canadian Light Source, Case Western Univ., Colorado State Univ., Columbia Univ., Duracell Technical Center, GE Global, General Motors, Georgia Tech, George Washington Univ., Hunter College, KAIST Korea, Kent State Univ., Lehigh Univ., MIT, Nissan Tech, NJIT, Northeastern Univ., NRL, Ohio State Univ., ORNL, Penn State Univ., PNNL, Rutgers Univ., SUNY Binghamton, Stony Brook Univ., Texas A&M Univ., Univ. Central Florida, Univ. Connecticut, Tufts Univ., Univ. Alberta, UC Berkeley, UC Davis, UC Santa Cruz, Univ. Delaware, Univ. Kansas, Univ. Kentucky, Univ. Illinois, Univ. Madrid, Univ. Maine, Univ. Minnesota, Univ. New Hampshire, Univ. New Mexico, Univ. Puerto Rico, Univ. South Carolina, Univ. Tennessee, Univ. Texas at Austin, Univ. Vermont, Univ. Virginia, United Technologies, Univ. Washington, Univ. Waterloo, Univ. Wisconsin, UOP, UTC Powers, Virginia Tech, Yale Univ., and Yeshiva Univ.

The list below provides a summary of the catalysis groups that utilized the SCC beamlines during the past funding cycle, with most of the research groups sending new students and postdoctoral fellows to be trained by the SCC staff. The list does not include the PIs and co-PIs of the SCC who also sent members of their research groups to each beamline every cycle:

2011:

Beamline X18A:

Xiqian Yu, BNL, Upton, NY (9/1/11-9/5/11)
Minhua Shao, United Technologies, Hartford, CT (3/30/11-4/4/11, /10/27/11-11/1/11)
Eli Stavitski, BNL, Upton, NY (4/21/11-4/22/11, 6/28/11-7/1/11)
Chung Kyung Yoon, KAIST, Korea (11/11/11-11/14/11)
Xiao-Qing Yang, BNL, Upton, NY (1/21/11-1/25/11, 1/28/11-1/31/11, 2/16/11-2/21/11,4/14/11-4/18/11, 6/1/11-6/6/11, 8/8/11-8/15/11, 9/21/11-9/26/11, 10/18/11-10/24/11)
Branko Zugic, Tufts U., Medford, MA (10/5/11-10/10/11)
Ayman Karim, PNNL, Richland, WA (2/4//11-2/7/11)
In Tae Bae, Duracell, Bethel, CT (11/4/11-1/9/11)
Kyung-Wan Nam, BNL, Upton, NY (3/25/11-3/28/11, 6/9/11-6/13/11, 9/8/11-9/12/11)
Adele Wang, BNL, Upton, NY (7/10/11-7/13/11, 8/20/11-8/25/11)

Feng Wang, BNL, Upton, NY (1/25/11-1/28/11
Yanping Zhai, Tufts U., Medford, MA (2/10-11-2/14/11)
Qi Wang, SUNY Binghamton, NY (4/7/11-4/11/11, 4/22/11-4/25/11)

Beamline X18B:
Branko Zugic, Tufts U., Medford, MA (10/27/11-10/31/11)
Lisa Pfefferle, Yale U., New Haven, CT (2/18/11-2/1/11, 6/2/11-6/6/11, 7/22/11-7/25/11, 9/13/11-9/16/11, 11/3/11-11/7/11)
Gary Haller, Yale U., New Haven, CT (6/7/11-6/10/11)
Beatriz Roldan, U. Central Florida, Orlando,FL (3/24/11-3/28/11, 9/1/11-9/5/11, 10/10/11-10/14/11)
Richard Crooks, U. Texas at Austin, Austin, TX (7/8/11-7/13/11, 10/31/11-11/3/11)
Bruce Gates, U. California – Davis, Davis, CA (4/14/11-4/18/11)
Ayman Karim, PNNL, Richland, WA (2/4/11-2/7/11, 6/27/11-7/1/11, 11/1/0/11-11/14/11)
Michael White, BNL, Upton, NY (7/20/11-7/22/11)
Petr Krtil, Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic (4/8/11-4/11/11, 10/14/11-10/17/11)
Robert Rettew, Georgia Tech, Atlanta, GA (2/15/11-2/18/11)
Yanping Zhai, Tufts U., Medford, MA (2/10-11-2/14/11, 8/25/11-8/29/11)
Craig Barnes, U. Tennessee, Knoxville, TN (4/21/11-4/25/11)
Marc Knecht, U. Kentucky, Lexington, KY (6/10/11-6/13/11)
Frank Huggings U. Kentucky, Lexington, KY (8/19/11-8/22/11)
Robert Meulenberg, U. Maine, Orono, ME (7/13/11/7/15/11)
Yuanzhi Tang, Georgia Tech, Atlanta, GA (10/5/11-10/7/11)

Beamline X19A:
Branko Zugic, Tufts U., Medford, MA (10/27/11-10/31/11)
In Tae Bae, Duracell, Bethel, CT (9/4/11-9/7/11)
Kyung-Wan Nam, BNL, Upton, NY (2/4/11-2/7/11, 7/8/11-7/14/11, 10/16/11-10/20/11)
Xiaowei Teng, U.New Hampshire, Durham, NH (10/4/11-10/7/11)
Nagappan Ramaswamy, Nissan Tec, Farmington Hills, MI (3/15/11-3/18/11)
Yanping Zhai, Tufts U., Medford, MA (1/27/11-1/31/11, 6/27/11-7/1/11)
Gary Haller, Yale U., New Haven, CT (4/7/11-4/11/11)
Frank Huggings U. Kentucky, Lexington, KY (11/3/11-11/6/11)

2012:
Beamline X18A:
Xiqian Yu, BNL, Upton, NY (1/19/12-1/25/12, 6/21/12-6/25/12, 10/25/12-10/29/12)
Minhua Shao, United Technologies, Hartford, CT (1/25/12-1/30/12, 6/6/12-6/11/12, 11/14/12-11/19/12)
Eli Stavitski, CLS, Saskatoon, Canada (1/30/12-2/3/12, 6/27/12-7/2/12)
Chung Kyung Yoon, KAIST, Korea (2/3/12, 8/3/12-8/6/12)
Xiao-Qing Yang, BNL, Upton, NY (2/29/12-3/4/12, 3/20/12-3/27/12, 4/26/12-4/29/12, 6/13/12-6/18/12, 7/21/12-7/25/12, 9/26/12-10/1/12)
Branko Zugic, Tufts U., Medford, MA (3/7/12-3/11/12)
Datye Abhaya, U. New Mexico, Albuquerque, NM (3/13/12-3/16/12)
Ayman Karim, PNNL, Richland, WA (3/16/12-3/20/12, 10/16/12-10/19/12)
Natalya Chernova, SUNY Binghamton, Binghamton, NY (3/27/12-4/2/12)
In Tae Bae, Duracell, Bethel, CT (4/4/12-4/6/12)
Jenny Lockard, Rutgers U., New Brunswik, NJ (7/11/12-7/13/12, 10/5/12-10/8/12)
Janos Szanyi, PNNL, Richland, WA (2/14/12-2/17/12)

Beamline X18B:
Branko Zugic, Tufts U., Medford, MA (2/1/12-2/6/12, 7/18/12-7/23/12, 10/3/12-10/8/12)
Jenny Lockard, Rutgers U., New Brunswik, NJ (2/21/12-2/24/12)
Lisa Pfefferle, Yale U., New Haven, CT (3/1/12-3/5/12, 7/13/12-7/16/12)
Beatriz Roldan, U. Central Florida, Orlando,FL (3/8/12-3/12/12)
Richard Crooks, U. Texas at Austin, Austin, TX (3/20/12-3/23/12, 6/28/12-7/2/12, 10/11/12-10/16/12)
Bruce Gates, U. California – Davis, Davis, CA (4/11/12-4/15/12)
Rui Si, BNL, Upton, NY (4/23/12-4/27/12, 11/16/12-11/21/12)
Robert Davis, U. Virginia, Charlottesville, VA (11/2/12-11/5/12)
Ayman Karim, PNNL, Richland, WA (10/16/12-10/19/12)
Faisal Alamgir, Georgia Tech, Atlanta, GA (2/22/12-2/26/12)
Petr Krtil, Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic (4/19/12-4/22/12)

Beamline X19A:
Branko Zugic, Tufts U., Medford, MA (2/12/12-2/6/12, 7/19/12-7/23/12)
Chris Keturakis, Lehigh U., Lehigh, PA (2/23/12-2/27/12, 6/7/12-6/11/12, 10/17/12-10/22/12)
In Tae Bae, Duracell, Bethel, CT (9/25/12-9/28/12)
Kyung-Wan Nam, BNL, Upton, NY (2/19/13-2/21/13)
Ayman Karim, PNNL, Richland, WA (10/31/12-11/2/12)
Craig Barnes, U. Tennessee, Knoxville, TN (6/28/12-7/2/12)

2013:
Beamline X18A:
Xiqian Yu, BNL, Upton, NY (1/17/13-1/21/13, 6/7/13-6/11/13)
Minhua Shao, United Technologies, Hartford, CT (4/5/13-4/8/13)
Eli Stavitski, CLS, Saskatoon, Canada (4/16/13-4/19/13)
Chung Kyung Yoon, KAIST, Korea (3/29/13-4/1/13)
Xiao-Qing Yang, BNL, Upton, NY (1/21/13-1/22/13, 3/1/13-3/4/13, 4/22/13-4/26/13, 6/6/13-6/7/13,7/8/13/-7/13/13, 9/14/13-9//17/13, 10/18/13-10/21/13)
Ayman Karim, PNNL, Richland, WA (1/29/13-2/4/13, 11/15/13-11/18/13)
Natalya Chernova, SUNY Binghamton, Binghamton, NY (5/31/13-6/6/13)
In Tae Bae, Duracell, Bethel, CT (10/4/13-10/6/13)
Jenny Lockard, Rutgers U., New Brunswik, NJ (2/18/13-2/22/13, 5/29/13-5/31/13, 11/8/13-11/12/13)
Janos Szanyi, PNNL, Richland, WA (2/14/13-2/18/13)
Feng Wang, BNL, Upton, NY (2/21/13-2/25/13, 4/26/13-4/30/13, 7/15/13/7/19//13,9/24/13/-927/13, 10/25/13-10/28/13)
Qi Wang, SUNY Binghamton, NY (7/13/13/-7/15/13, 10/12/13-10/16/13, 11/22/13-11/26/13)
Kyung-Wan Nam, BNL, Upton, NY (9/27/13-9/30/13)
Carlos Cabrera, U. Puerto Rico, San Juan, Puerto Rico (1/22/13/1/25/13)
Steven Suib, U. Connecticut, Storrs, CT (11/12/13-11/15/13)

Beamline X18B:
Lisa Pfefferle, Yale U., New Haven, CT (3/15/13-3/18/13)
Beatriz Roldan, U. Central Florida, Orlando, FL (3/4/13-3/11/13)
Richard Crooks, U. Texas at Austin, Austin, TX (3/29/13-4/1/13, 7/19/13-7/22/13, 10/21/13-10/25/13)
Rui Si, BNL, Upton, NY (8/8/13-8/12/13, 11/22/13-11/27/13)
Robert Davis, U. Virginia, Charlottesville, VA (3/22/13-3/25/13)
Ayman Karim, PNNL, Richland, WA (4/24/13-4/26/13, 6/14/13-6/19/13, 11/15/13-11/18/13)
Michael White, BNL, Upton, NY (4/16/13-4/19/13)
Faisal Alamgir, Georgia Tech, Atlanta, GA (2/22/13-2/26/13, 7/16/13-7/19/13)
Michael Morrill, Georgia Tech, Atlanta GA (3/26/13 – 3/28/13, 11/11/13-11/15/13)

Petr Krtil, Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic (4/19/13-4/22/13)
Qi Wang, SUNY Binghamton, NY (4/24/13-4/30/13, 7/22/13-7/26/13)
Branko Zugic, Tufts U., Medford, MA (6/20/13-6/24/13)
Xiaowei Teng, U. New Hampshire, Durham, NH (6/25/13-6/27/13, 9/30/13-10/4/13)
Feng Jiao, University of Delaware, Newark, DE (11/6/2013-11/11/2013)

Beamline X19A:
Branko Zugic, Tufts, Medford, MA (1/18/13-1/22/13, 6/21/13-6/24/13)
Chris Keturakis, Lehigh University, Lehigh, PA (2/7/13-2/12/13)
Kyung-Wan Nam, BNL, Upton, NY (2/19/13-2/21/13, 8/20/13-8-23/13)
Ayman Karim, PNNL, Richland, WA (4/22/13-4/24/13, 6/12/13-6/14/13, 11/12/13-11/15/13)
Richard Crooks, Univ. Texas at Austin, Austin, TX (4/3/13-4/4/13, 6/7/19/13-7/21/13)
Lisa Pfefferle, Yale, New Haven, CT (2/1/13-2/4/13)
Qingying Jia, Northeastern Univ., Boston, MA (4/26/13-4/29/13)
Qi Wang, SUNY Binghamton, NY (10/14/13-10/18/13)
Faisal Alamgir, Georgia Tech, Atlanta, GA (11/15/13-11/18/13)
Charles Spanjers, Penn State U., University Park, PA (8/14/13-8/16/13)

2.2 Maintenance and Upgrading of Dedicated SCC Facilities for Catalysis Users

One of the critical facilities for catalysis users, especially new users, is the availability of dedicated and user-friendly gas-handling systems. The SCC staff member, Dr. Marinkovic, collected input from the SCC team and the users on the most efficient configuration of the gas handling systems and specifications for the residual gas analyzer. Two identical systems (see example in Fig. 1), consisting of four mass flow controllers (MFC), two gas purifier systems for carrier gas (oxygen and moisture traps, providing O_2 and H_2O levels below 5 ppm), and two residual gas analyzers (RGAs, i.e. quadrupole mass spectrometers) have been assembled and mounted permanently in the hutches of the X18B and X19A beamlines. An additional gas-handling system was constructed for the SCC operations in beamline X18A and is now in use.

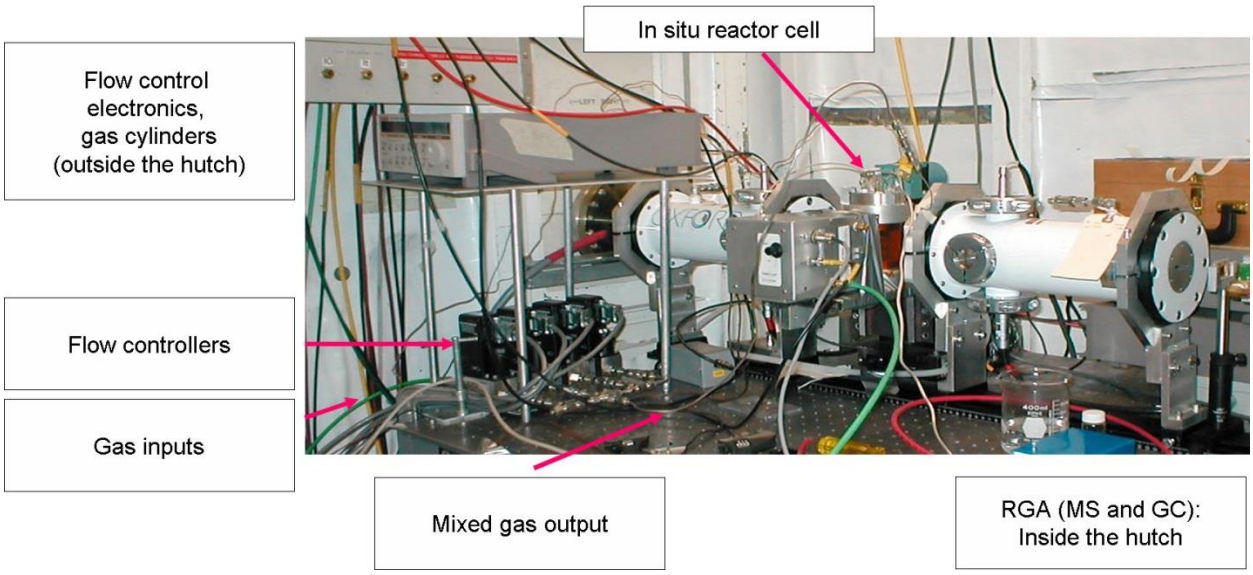

Figure 1: Configuration of the *in-situ* XAFS experiment in X18B hutch

Based on the input from the catalysis and electrocatalysis users, the SCC team also built several types of dedicated reactors that allowed *in-situ* measurements for both heterogeneous catalysis and electrocatalysis studies. The availability of versatile gas-handling systems and a variety of *in-situ* reactors have been extremely valuable to attract new synchrotron users who had not previously had access and expertise in synchrotron research.

2.3 Development of New instrumentation for Catalysis Research

The SCC team has led the development efforts on commissioning, testing and operating new techniques tailored to catalysis and electrocatalysis research, which have been utilized by catalysis users over a wide range of research topics [1-15]. In the earlier funding cycles, such examples include the commission of QEXAFS monochromators on X18B and X18A beamlines, development and installation of combined XAFS/XRD and XAFS/DRIFTS instrument at X18A beamline. All these techniques were successfully integrated into *in-situ* catalysis and electrocatalysis research programs of SCC users. Below are two recent examples of facilities developed by SCC members during the past funding cycle.

***2.3.1 Combined XAS/Raman instrument*:** Complex reactions, such as iron and chromium oxide catalyzed water gas shift reaction, or Mars-van-Krevelen mechanism of CO oxidation, make a good case for the development and application of multi-technique experimental tools. In this funding cycle, we have developed a new methodology for *in-situ* studies based on combining X-ray absorption spectroscopy (XAS), XRD and Raman spectroscopy measurements in the same catalytic experiment. The use of these methods is clearly advantageous for composite catalytic systems such as metal oxide catalysts.

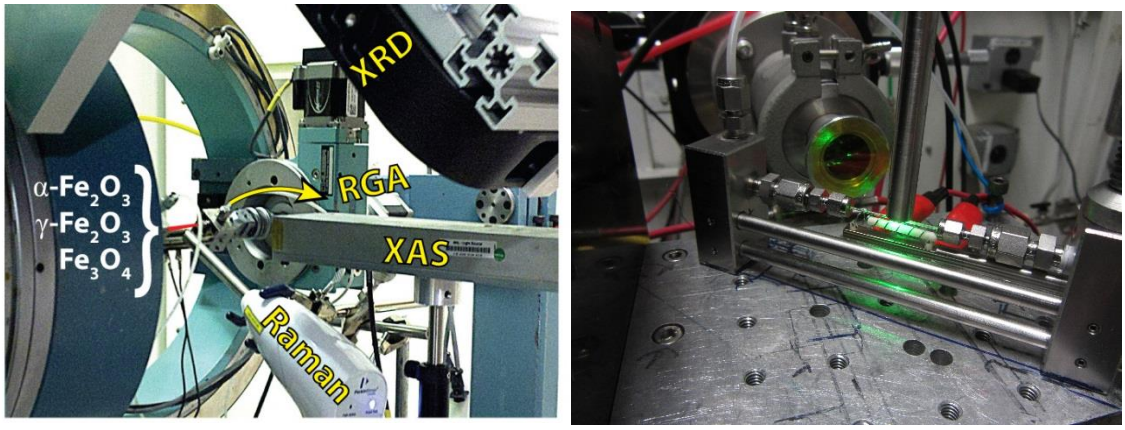

Figure 2. Combined XAFS-XRD-Raman-MS setup at the X18A beamline (a) and combined XAFS-Raman-MS setup at the X19A beamline (b).

For example, in Fe_2O_3 catalyst the transformation of phases cannot be identified by extended X-ray Absorption Fine Structure (EXAFS), but XRD and Raman spectra show clear distinctions between the phases. Similarly in 3% Cr_2O_3/ Fe_2O_3, chromium oxide species could not be detected by XRD but give rise to broad vibrational bands in the Raman spectrum. We assembled an operando setup that consisted of a Perkin Elmer Raman spectrometer, XAFS and XRD detectors, as well as the SCC-built gas input and output systems at the X18A beamline (Fig. 2 a) [16]. The studies provide new information about the oxidation state, local atomic

structure, crystal structure in the bulk and in the surface, before, during and after WGS reaction (Fig. 3). A different type of setup (Fig. 2b) was built using a Bay Spec Raman spectrometer with a fiber optic probe and filters that enable high temperature studies. With this setup, the SCC group was the first to successfully perform the high temperature (300 °C) *in-situ* study of CO oxidation reaction [17].

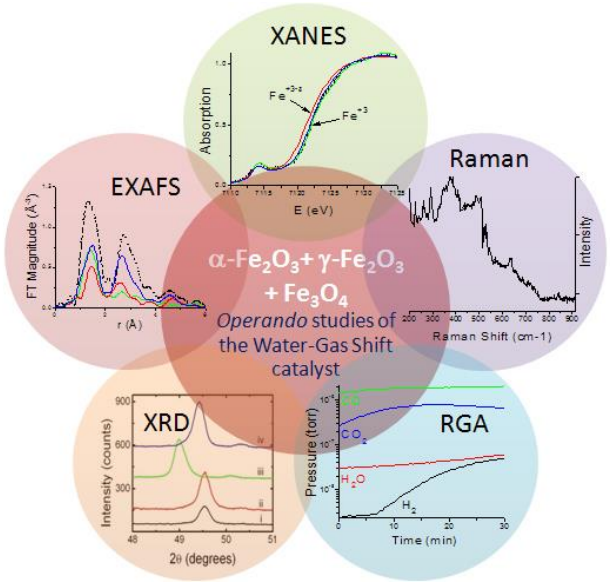

Figure 3. Results obtained by multiple techniques investigating catalytically active phases in the Water-Gas Shift reaction.

2.3.2 Correlative, in-situ XAS/TEM studies of catalytic mechanisms in a portable micro-reactor: During 6 months in 2012, the SCC supported a visiting undergraduate student, Philipp Baumann, who came to perform a senior project for his thesis. He was supervised by Frenkel. With his prior experience at the Swiss Light Source's beamline SuperXAS, Philipp brought to the SCC a much needed experience in designing equipment for third generation synchrotrons. During his stay, he designed, implemented and tested a remote control system for a gas manifold built for an environmental reaction cell. This reaction cell will be used for catalysis processes for combined, *in-situ* investigations as described in the following sections. His contributions to the instrument development at the SCC warranted his co-authorship in two articles that acknowledged the SCC funding [17, 18].

The SCC team members have been collaborating with the Center for Functional Nanomaterials (CFN) to pursue a new approach in *in-situ* methodology. The new method, proposed by Frenkel and Stach (CFN), will utilize a portable micro-reaction cell for experiments in heterogeneous (gas and solid phases) catalysis. Such cell will be compatible with both XAS and TEM instruments, where the same catalyst will be investigated in the same cell under identical reaction conditions by both techniques. Preliminary results were obtained in 2011 using the cell developed by Hummingbird, Inc., for TEM imaging and XAS spectroscopy studies of a model Au/TiO_2 nanoparticle system. In addition, Raman spectroscopy data obtained in the same cell demonstrated excellent sensitivity to catalytic transformations that occur in oxide supports. In 2012-2013, we have assembled with the help of a visiting undergraduate student Ph. Baumann

and a staff at the CFN, the working system that consisted of an automated gas supply manifold with several mass flow controllers and gas analysis system (mass spectrometer). The SCC team has already collected time-resolved XAS data in the course of catalytic reaction using this cell in the micro-focusing beamline X27A and FEI Titan TEM. The SCC PIs (Frenkel and Chen) are collaborators on the Early Science proposal to use the SRX beamline of NSLS-II where this cell will be used for studying bimetallic (Pt/Ni) hydrogenation catalysts.

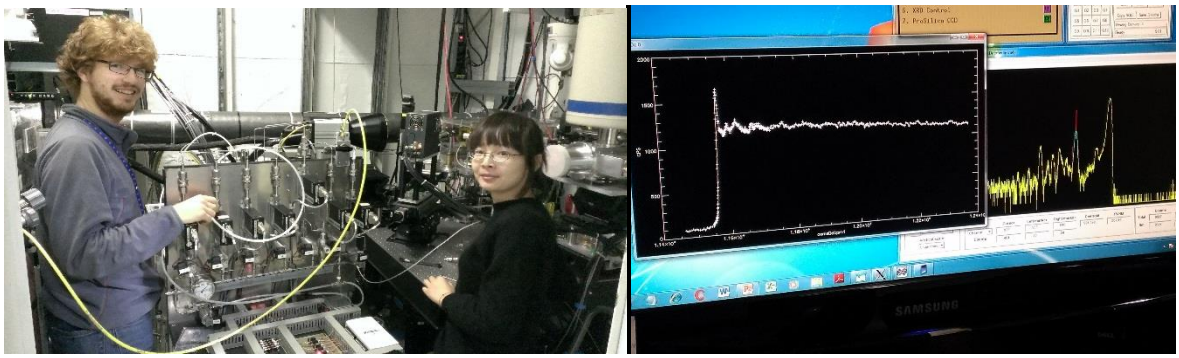

Figure 4. Ph. Baumann (SCC visiting student) and Y. Li (a postdoc working with Frenkel) at the micro-focusing beamline X27A with the operando micro-cell XAS setup. The screen shot of the first micro-XAS scan at Pt L_3 edge of 1nm Pt/SiO_2 nanocatalyst measured in-situ conditions is shown in the right.

2.4 Workshops, On-Site Help and Training Courses Offered by SCC

In order to promote the utilization of synchrotron facilities in the catalysis and electrocatalysis communities, it is critical to train graduate students, postdoctoral fellows, and research staff on data collection and data analysis. The SCC PIs and staff have provided training to all new catalysis users working on the SCC beamlines. For example, Frenkel gave on-site help 2-3 days a week, and consulted visiting groups on issues ranging from XAFS data analysis to planning of *in-situ* experiments. Marinkovic was always present to provide assistance to catalysis users during their experiments. In addition, SCC members have organized several training courses and workshops, **which were over-subscribed and received very positive feedback**. Many of the SCC catalysis users attended one of the training courses. Below is a brief description of three short courses.

XAFS Short Course: Introduction to the Experiment, Data Analysis and Modeling, NSLS, Nov. 3-5, 2011

This short course in X-ray absorption fine-structure (XAFS) spectroscopy was geared toward beginners with overall familiarity with other structural techniques who have read basic literature about XAFS but needed hands-on practice. The course included beamline demonstrations, lectures by experts in the field, tutorials, and data analysis sessions. Emphasis was made on applications of XAFS, both in the near-edge and extended energy regions, to typical problems in nanocatalysis, environmental and materials sciences, and structural biology. The course was oversubscribed by a factor of two, and 32 registered participants were selected on the basis of their project descriptions and diversity of research interests. In addition, about 30 auditors attended lectures and data analysis sessions.

Below we will provide a detailed schedule to illustrate the course structure and the connection between teaching and hands-on experience. The first two days of the course began with morning lectures on “Overview of XAS techniques and applications” (Frenkel, Yeshiva University), “Introduction to XAS theory” (Ravel, NIST), “Components of XAS experiment” (Khalid, NSLS), “Sample preparation” (Pandya, SAIC, Inc), “Introduction to data analysis: LCF and PCA” (Wang, SCC and University of Delaware), "Introduction to data analysis: FEFF fitting" (Ravel), "Application of XAS to nanocatalysis" (Frenkel), "Application of XAS to Physics and Materials Science", (Sterbinsky, NIST), "Application of XAS to Environmental science and biology", (Farquhar, Case Western University) and "XAFS and complementary techniques", (Marinkovic, SCC and University of Delaware). On the first day the participants were divided into two parallel sessions and participated in hands-on beamline experiments led by several instructors, with NSLS beamlines X23A2, X11B, X3B, X18B and X19A designated for the course.

Beamline projects varied between different instructors, and participants were divided into groups led by instructors with research interests that best matched their own. While the half of the class was at the beamlines, the second half was in a seminar room for training in XAFS data processing and analysis software led by Frenkel. The two parts of the course switched places after two hours: the first part came back from the beamlines for data analysis training, and the second part went to the experimental floor for beamline training. On Friday, after the morning and afternoon lectures, participants gathered in the large auditorium and participated in an analysis session with the data they collected at the beamlines. Data analysis instructors were Frenkel, Ravel, Wang, Khalid, Marinkovic, Sterbinsky, Farquhar, and Pandya. During the data analysis session, participants were trained in using the XAFS analysis package IFEFFIT. On Saturday, the course participants continued analyzing the data they collected during the workshop.

XANES Short Course: Theory, Analysis, Applications NSLS, Nov. 8-10, 2012

This short course in X-ray absorption near-edge structure (XANES) spectroscopy was geared toward beginners with overall familiarity with XAFS but needed advanced training in theory, analysis and various problem solving methods. Among the most advanced methods used in this field today are the data modeling and analysis with FEFF9, investigations of valence band structure and spin-selective transition by RIXS, investigation of adsorbate binding by HERFD and other modifications of XANES methods. The course consisted of lectures that covered the XANES fundamentals, described recent developments in theory and data analysis, and specific application of XANES to research problems. One of the main attraction of the course to local and visiting participants was the presence of expert XANES theorists and code developers: Joshua Kas (U. Washington), Pieter Glatzel (ESRF), Bruce Ravel (NIST). Other course instructors were Frenkel, Balasubramanian (Argonne), Alamgir (Georgia Tech), Bare (UOP and SCC co-PI), and Kelly (UOP).

A Short Course: In-Situ Methods of X-ray Absorption Spectroscopy NSLS, Oct. 24-26, 2013

The short course in X-ray absorption spectroscopy methods focused on techniques and applications of XAS to characterization of functional nanomaterials at work. Examples included catalytic materials and catalysis mechanisms, electrochemistry, fuel cells and battery research, but also included other materials, devices and processes where such

methods prove useful. The focus was on those techniques, currently used at the NSLS and other synchrotrons, that will also be available at the NSLS-II in the first few years after the start of its operations in 2014. Instructors discussed unique characteristics of NSLS-II beamlines (e.g., improved time, space and energy resolution) and the new opportunities for studying nanomaterials at work that emerge. The course format included an "idea development" session on the last day of the workshop, where instructors will help new users plan their synchrotron research using in situ and operando methods. The course Instructors were: Attenkofer (BNL), Khalid (BNL), Balasubramanian (ANL), Alamgir (Georgia Tech), Wang (Binghamton U.), Frenkel (Yeshiva U.), Porosoff (Columbia U.), Karim (PNNL), Golovchak (Austin Peay State U.), Nam (BNL), Marinkovic (U. Delaware), Koenig (PSI), Rodriguez (BNL) .

2.5 Coordination of Catalysis Efforts at NSLS-II

The SCC team has actively participated in the planning stage of NSLS-II to try to ensure that catalysis interests and needs are addressed during planning for beamlines at the NSLS-II facility. Due to its uniquely high brightness, flux, and spectral resolution of the NSLS-II source, the new synchrotron source can offer significant improvement in instrument capabilities for research in the areas of catalysis. To exploit the new NSLS-II capabilities, the SCC team organized workshops as early as 2008, participated in beamline development workshops in 2010, and acted as a coordinated team in supporting beamline proposals to NSLS-II in 2010 through 2012.

To meet the diverse research needs in catalysis and energy research, the SCC team has proposed to combine several dedicated and shared facilities at the NSLS-II as summarized below. A total of nine proposals were submitted to the NSLS-II evaluation team. In order to assure a coherence of the individual proposals, the SCC team prepared an appendix that was attached to all nine proposals. The appendix clearly stated the needs for a suite of beamlines in the new facility. The SCC team members were active participants in the individual proposals and presented or attended the oral presentations to the evaluation team. **These concerted efforts have led to the approval of six catalysis-related beamlines.** Both the number of proposals and the success rate demonstrate the critical contributions of the SCC team to ensure the catalysis presence in the NSLS-II facilities. Current and future activities are devoted to developing a detailed plan of support and operation of catalysis research activities at these beamlines, such as Partner User Proposals at the QAS and TES beamlines. In addition, an Early Science proposal was submitted to a Project beamline SRX. More discussion will be provided in the Proposed Research section on the path forward for the implementation of these beamlines in NSLS-II. Below is the list of the six approved proposals and SCC participants. Beamlines on insertion devices (undulators or damping wigglers) are underscored:

1) Project beamline: The X-ray powder diffraction (XPD) beamline (Active members include Rodriguez from SCC)
2) NEXT beamline: The inner shell spectroscopy (ISS) beamline (BAT members include Rodriguez from SCC)
3) NEXT beamline: The photoemission microscopy facility (ESM) beamline (Proposed BAT members include Chen, Hulbert, Rodriguez from SCC)
4) NxtGen beamline: The quick absorption and scattering (QAS) beamline (Spokesperson: Frenkel; Proposed BAT members include Chen, Adzic, Bare, Hanson, Rodriguez from SCC)

5) NxtGen beamline: The powder diffraction beamline (IXD) for *in-situ* studies (BAT members include Hanson, Rodriguez from SCC)
6) NxtGen beamline: The tender X-ray spectroscopy (TES) beamline (Proposed BAT members include Bare, Chen,. Frenkel, Rodriguez from SCC)

3. Publications Utilizing SCC Facilities during Past Funding Cycle:

Publications of catalysis users at the SCC beamlines are listed below. The numbers of publications during the past six years (2008 – 2013) are compared to those of the three years prior to SCC (2003 – 2005) to illustrate the significant impact of SCC on research productivity:

Pre-SCC: 2003: **9**, 2004: **20**, 2005: **19**,
After SCC: 2008: **33**, 2009: **50**, 2010: **68,** 2011: **52**, 2012: **67**, 2013: **80**

Publication List:

2011:

L Yang, New Materials for Intermediate-Temperature Solid Oxide Fuel Cells to be Powered by Carbon- and Sulfur-Containing Fuels, Ph.D. Thesis. Georgia Institute of Technology, Atlanta (2011).

S Ehrlich, J Hanson, A Lopez Camara, L Barrio, M Estrella, G Zhou, R Si, S Khalid, Q Wang, Combined XRD and XAS, *Nucl. Instrum. Meth. A*, **649**(1), 213-215 (2011).

N Marinkovic, Q Wang, L Barrio, S Ehrlich, S Khalid, C Cooper, A Frenkel, Combined in situ X-ray Absorption and Diffuse Reflectance Infrared Spectroscopy: An Attractive Tool for Catalytic Investigations, *Nucl. Instrum. Meth. A*, **649**(1), 204-206 (2011).

N Marinkovic, Q Wang, A Frenkel, In Situ Diffuse Reflectance IR Spectroscopy and X-ray Absorption Spectroscopy for Fast Catalytic Processes, *J. Synch. Rad.*, **18**, 447-455 (2011).

H Lei, H Ryu, A Frenkel, C Petrovic, Anisotropy in BaFe2Se3 single crystals with double chains of FeSe tetrahedra, *Phys. Rev. B: Condens. Matter*, **84**, 214511 (2011).

H Shin, K Nam, W Chang, B Cho, W Yoon, X Yang, K Chung, Comparative Studies on C-coated and Uncoated LiFePO4 Cycling at Various Rates and Temperatures using Synchrotron Based in situ X-ray Diffraction, *Electrochim. Acta*, **56**, 1182-1189 (2011).

X Wang, Investigation of the Structural Changes in Li1-xFePO4 upon Charging by Synchrotron Radiation Techniques, *J Mater. Chem.*, **21**, 11406 (2011).

Y Zhou, X Wang, H Lee, K Nam, X Yang, O Haas, Electrochemical Investigation of Li–Al Anodes in Oligo (ethylene glycol) Dimethyl ether/LiPF6, *J Appl. Electrochem.*, **41**, 271 (2011).

L Yang, Y Choi, W Qin, H Chen, K Blinn, M Liu, P Liu, J Bai, T Tyson, M Liu, Promotion of Water-mediated Carbon Removal by Nanostructured Barium Oxide/nickel Interfaces, *Nat. Commun.*, **2**, 357 (2011).

M Song, S Park, F Alamgir, J Cho, M Liu, Nanostructured Electrodes for Lithium-ion and Lithium-air Batteries: The Latest Developments, Challenges, and Perspectives, *Mat. Sci. Eng. R*, **72**(11), 203-252 (2011).

Z Xu, C Jing, J Hao, C Christodoulatos, G Korfiatis, F Li, X Meng, Effect of Bonding Interactions between Arsenate and Silver Nanofilm on Surface-Enhanced Raman Scattering Sensitivity, *J. Phys. Chem. C*, **325-329**, 116 (2011).

S Cheng, R Rettew, M Sauerbrey, F Alamgir, Architecture-Dependent Surface Chemistry for Pt Monolayers on Carbon-Supported Au, *ACS Appl. Mater.*, **3**(10), 3948-3956 (2011).

S Zhang, C Pelligra, G Keskar, P Majewski, F Ren, L Pfefferle, C Osuji, Liquid Crystalline Order and Magnetocrystalline Anisotropy in Magnetically Doped Semiconducting ZnO Nanowires, *ACS Nano*, **5**(10), 8357-8364 (2011).

D Konopka, M Li, K Artyushkova, N Marinkovic, K Sasaki, R Adzic, T Ward, P Atanassov, Platinum Supported on NbRuyOz as Electrocatalyst for Ethanol Oxidation in Acid and Alkaline Fuel Cells, *J. Phys. Chem. C*, **115**, 3043–3056 (2011).

S Lee, C Zoican Loebick, L Pfefferle, G Haller, High-Temperature Stability of Cobalt Grafted on Low-Loading Incorporated Mo-MCM-41 Catalyst for Synthesis of Single-Walled Carbon Nanotubes, *J. Phys. Chem. C*, **115**, 1014–1024 (2011).

S Bare, S Kelly, F Vila, D Boldingh, E Karapetrova, J Kas, G Mickelson, F Modica, N Yang, J Rehr, Experimental (XAS, STEM, TPR, and XPS) and Theoretical (DFT) Characterization of Supported Rhenium Catalysts, *J. Phys. Chem. C*, **115**(13), 5740–5755 (2011).

C Aydin, J Lu, M Shirai, N Browning, B Gates, Ir6 Clusters Compartmentalized in the Supercages of Zeolite NaY: Direct Imaging of a Catalyst with Abrerration-Corrected Scanning Transmission Electron Microscopy, *ACS Catal*., **1**, 1613-1620 (2011).

V Schwartz, A Campos, A Egbebi, J Spivey, S Overbury, EXAFS and FT-IR Characterization of Mn and Li Promoted Titania-Supported Rh Catalysts for CO Hydrogenation, *ACS Catal*., **1**, 1298-1306 (2011).

M Shao, B Merzougui, K Shoemaker, L Stolar, L Protsailo, Z Mellinger, I Hsu, J Chen, Tungsten Carbide Modified High Surface Area Carbon as Fuel Cell Catalyst Support, *J. Power Sources*, **196**(18), 7426-7434 (2011).

B Roldan Cuenya, M Alcantara-Ortigoza, L Ono, F Behafarid, S Mostafa, J Croy, K Paredis, G Shafai, T Rahman, et. al., Thermodynamic Properties of Pt Nanoparticles: Size, Shape, Support, and Adsorbate Effects, *Phys. Rev. B: Condens. Matter*, **84**, 245438 (2011).

C Aydin, J Lu, A Liang, C Chen, N Browning, B Gates, Tracking Iridium Atoms with Electron Microscopy: First Steps of Metal Nanocluster Formation in One-Dimensional Zeolite Channels, *Nano Lett*., **11**, 5537-5541 (2011).

W Alley, I Hamdemir, Q Wang, A Frenkel, L Li, J Yang, L Menard, R Nuzzo, S Ozkar, et al., Industrial Ziegler-Type Hydrogenation Catalysts Made from Co(neodecanoate)2 or Ni(2-ethylhexanoate)2 and AlEt3: Evidence for Nanoclusters and Sub-Nanocluster or Larger Ziegler-Nanocluster Based Catalysis, *Langmuir*, **27**(10), 6279-6294 (2011).

E Carino, R Crooks, Characterization of Pt@Cu Core@Shell Dendrimer-Encapsulated Nanoparticles Synthesized by Cu Underpotential Deposition, *Langmuir*, **27**, 4227-4235 (2011).

B Cheney, J Lauterbach, J Chen, Reverse Micelle Synthesis and Characterization of Supported Pt/Ni Bimetallic Catalysts on gamma-Al2O3, *Appl. Catal. A*, **394**(1-2), 41-47 (2011).

R Rettew, Near-Surface Study of Structure-Property Relationships in Electrochemically Fabricated Multi-Component Catalysts, Ph.D. Thesis. Georgia Institute of Technology, Atlanta (2011).

S Mehraeen, A Kulkarni, M Chi, B Reed, N Okamoto, N Browning, B Gates, Triosmium Clusters on a Support: Determination of Structure by X-ray Absorption Spectroscopy and High-Resolution Microscopy, *Chem. Eur. J*., **17**(3), 1000-1008 (2011).

V Petrykin, K Macounova, J Franc, O Shlyakhtin, M Klementova, S Mukerjee, p Krtil, Zn-Doped RuO2 Electrocatalyts for Selective Oxygen Evolution: Relationship Between Local Structure and Electrocatalytic Behavior in Chloride Containing Media, *Chem. Mater*., **23**, 200-207 (2011).

H Shou, R Davis, Reactivity and in situ X-ray Absorption Spectroscopy of Rb-promoted Mo2C/MgO Catalysts for Higher Alcohol Synthesis, *J. Catal*., **282**(1), 83-93 (2011).

V Parvulescu, V Parvulescu, D Ciuparu, C Hardacre, H Garcia, High-surface Thermally Stable Mesoporous Gallium Phosphates Constituted by Nanoparticles as Primary Building Blocks, *J. Catal*., **278**(1), 111-122 (2011).

K Paredis, L Ono, F Behafarid, Z Zhang, J Yang, A Frenkel, B Roldan Cuenya, Evolution of the Structure and Chemical State of Pd Nanoparticles During the in Situ Catalytic Reduction of NO with H2, *J. Am. Chem. Soc*., **133**(34), 13455-13464 (2011).

K Paredis, L Ono, S Mostafa, L Li, Z Zhang, J Yang, L Barrio, A Frenkel, B Roldan Cuenya, Structure, Chemical Composition, And Reactivity Correlations during the In Situ Oxidation of 2-Propanol, *J. Am. Chem. Soc*., **133**(17), 6728–6735 (2011).

W O'Grady, D Roeper, P Natishan, Structure of Chlorine K-Edge XANES Spectra During the Breakdown of Passive Oxide Films on Aluminum, *J. Phys. Chem. C*, **115**, 25298-25303 (2011).

J Gao, M Lowe, Y Kiya, H Abruna, Effects of Liquid Electrolytes on the Charge-Discharge Performance of Rechargeable Lithium/Sulfur Batteries: Electrochemical and in-Situ X-ray Absorption Spectroscopic Studies, *J. Phys. Chem. C*, **115**(50), 25132-25137 (2011).

L Zhang, G Liang, A Ignatov, M Croft, X Xiong, I Hung, Y Huang, X Hu, W Zhang, Y Peng, Effect of Vanadium Incorporation on Electrochemical Performance of LiFePO(4) for Lithium-Ion Batteries, *J. Phys. Chem. C*, **115**(27), 13520-13527 (2011).

K Sasaki, K Kuttiyiel, D Su, R Adzic, Platinum Monolayer on IrFe Core–Shell Nanoparticle Electrocatalysts for the Oxygen Reduction Reaction, *Electrocatal*., **2**(2), 134-140 (2011).

J Bauer, D Mullins, M Li, Z Wu, E Payzant, S Overbury, S Dai, Synthesis of Silica Supported AuCu Nanoparticle Catalysts and the Effects of Pretreatment Conditions for the CO Oxidation Reaction, *Phys. Chem. Chem. Phys*., **13**, 2571-2581 (2011).

W Lonergan, X Xing, R Zheng, S Qi, B Huang, J Chen, Low-temperature 1,3-butadiene Hydrogenation over Supported Pt/3d/gamma-Al2O3 Bimetallic Catalysts, *Catal. Today*, **160**(1), 61-69 (2011).

S Bak, K Nam, C Lee, K Kim, H Jung, X Yang, K Kim, Spinel LiMn2O4/reduced Graphene Oxide Hybrid for High Rate Lithium Ion Batteries, *J Mater. Chem*., **21**(43), 17309 (2011).

M Goesten, J Juan-Alcaniz, E Ramos-Fernandez, K Gupta, E Stavitski, H van Bekkum, J Gascon, F Kapteijn, Sulfation of Metal–organic Frameworks: Opportunities for Acid Catalysis and Proton Conductivity, *J. Catal*., **281**, 177-187 (2011).

V Boppana, H Schmidt, F Jiao, D Doren, R Lobo, Structure Analysis and Photocatalytic Properties of Spinel Zinc Gallium Oxonitrides, *Chem. Eur. J*., **17**, 12417-12428 (2011).

S Qi, B Cheney, R Zheng, W Lonergan, W Yu, J Chen, The Effects of Oxide Supports on the Low Temperature Hydrogenation Activity of Acetone over Pt/Ni Bimetallic Catalysts on SiO2, gamma-Al2O3 and TiO2, *Appl. Catal. A*, **393**, 44-49 (2011).

W Lonergan, T Wang, D Vlachos, J Chen, Effect of Oxide Support Surface Area on Hydrogenation Activity: Pt/Ni Bimetallic Catalysts Supported on Low and High Surface Area Al2O3 and ZrO2 , *Appl. Catal. A*, **408**, 87-95 (2011).

D Nguyen-Thanh, A Frenkel, J Wang, S O'Brien, D Akins, Cobalt–polypyrrole–carbon black (Co–PPY–CB) Electrocatalysts for the Oxygen Reduction Reaction (ORR) in Fuel Cells: Composition and Kinetic Activity, *Appl. Catal. B*, **105**(1-2), 50-60 (2011).

S Khalid, S Ehrlich, A Lenhard, B Clay, Hard X-rays QEXAFS Instrumentation with Scan Range 20 to 4000 eV, *Nucl. Instrum. Meth. A*, **649**, 64-66 (2011).

N Shiju, A Alberts, S Khalid, D Brown, G Rothenberg, Mesoporous Silica with Site-Isolated Amine and Phosphotungstic Acid Groups: A Solid Catalyst with Tunable Antagonistic Functions for One-Pot Tandem Reactions, *Angew. Chem. Int. Ed*., **50**, 9615–9619 (2011).

X Teng, W Du, D Su, Q Wang, A Frenkel, Promotional Effects of Bismuth on the Formation of Platinum−Bismuth Nanowires Network and the Electrocatalytic Activity toward Ethanol Oxidation, *Cryst. Growth Des*., **11**(2), 594 (2011).

A Frenkel, Q Wang, N Marinkovic, J Chen, L Barrio, R Si, A Lopez Camara, A Estella, J Rodriquez, J Hanson, Combining X-ray Absorption and X-ray Diffraction Techniques for in Situ Studies of Chemical Transformations in Heterogeneous Catalysis:Advantages and Limitations , *J. Phys. Chem. C*, **115**, 17884-17890 (2011).

K Sasaki, K Kuttiyiel, L Barrio, D Su, A Frenkel, N Marinkovic, D Mahajan, R Adzic, Carbon-Supported IrNi Core-Shell Nanoparticles: Synthesis, Characterization, and Catalytic Activity, *J. Phys. Chem. C*, **115**(20), 9894-9902 (2011).

J Mohandas, M Gnanamani, G Jacobs, W Ma, Y Ji, S Khalid, B Davis, Fischer-Tropsch Synthesis: Characterization and Reaction Testing of Cobalt Carbide, *ACS Catal*., **1**(11), 1581–1588 (2011).

W Du, Q Wang, C LaScala, L Zhang, D Su, A Frenkel, V Mathur, X Teng, Ternary PtSnRh–SnO2 Nanoclusters: Synthesis and Electroactivity for Ethanol Oxidation Fuel Cell Reaction, *J Mater. Chem*., **21**, 8887-8892 (2011).

W Ma, G Jacobs, Y Ji, T Bhatelia, D Bukur, S Khalid, B Davis, Fischer-Tropsch Synthesis: Influence of CO Conversion on Selectivities, H2/CO Usage Ratios, and Catalyst Stability for a 0.27% Ru 25%Co/Al2O3 using a Slurry Phase Reactor, *Top. Catal*., **54**, 757-767 (2011).

W Du, Q Wang, D Saxner, N Deskins, D Su, J Krzanowski, A Frenkel, X Teng, Highly Active Iridium/Iridium–Tin/Tin Oxide Heterogeneous Nanoparticles as Alternative Electrocatalysts for the Ethanol Oxidation Reaction, *J. Am. Chem. Soc*., **133**(38), 15172-15183 (2011).

2012:

A Patlolla, E Carino, S Ehrlich, E Stavitski, A Frenkel, Application of Operando XAS, XRD, and Raman Spectroscopy for Phase Speciation in Water Gas Shift Reaction Catalysts, *ACS Catal*., **2**, 2216-2223 (2012).

M Humbert, B Smith, Q Wang, S Ehrlich, M Shao, Synthesis and Characterization of Palladium–Platinum Core–Shell Electrocatalysts for Oxygen Reduction, *Electrocatal*., **3**(3-4), 298-303 (2012).

S Kim, K Nam, D Seo, J Hong, H Kim, H Gwon, K Kang, Energy Storage in Composites of a Redox Couple Host and a Lithium Ion Host, *Nano Today*, **7**(3), 168 (2012).

Z He, M Yang, X Wang, Z Zhao, A Duan, Effect of the Transition Metal oxide Supports on Hydrogen Production from Bio-Ethanol Reforming, *Catal. Today*, **194**, 2-8 (2012).

Z He, X Wang, Y Pu, Z Qian, Fundamental Understanding of the Role of Potassium on the Activity of Pt/CeO2 for the Hydrogen Production from Ethanol, *Int. J. Hydrogen Energ*., **37**(15), 11132-11140 (2012).

J Dong, X Yu, Y Sun, L Liu, X Yang, X Huang, Triplite LiFeSO4F as Cathode Material for Li-ion Batteries, *J. Power Sources*, **244**, 716-720 (2012).

H Zhou, S Upreti, N Chernova, R Zhang, M Whittingham, Pyrophosphates-Novel Cathode Materials For Lithium Batteries, Ph.D. Thesis. State University of New York at Binghamton, Binghamton (2012).

R Zhang, X Yu, K Nam, C Ling, T Arthur, W Song, A Knapp, S Ehrlich, X Yang, M Matsui, α-MnO2 as a Cathode Material for Rechargeable Mg Batteries, *Electrochem. Commun*., **23**, 110-113 (2012).

G Nolis, F Omenya, R Zhang, B Fang, S Upreti, N Chernova, F Wang, J Graetz, Y Hu, et. al., Structure, Defects and Thermal Stability of Delithiated Olivine Phosphates, *J Mater. Chem*., **22**, 20482-20489 (2012).

R. Korobko, A. Patlolla, E. Wachtel, H. Tuller, A. I. Frenkel, I. Lubomirsky, Giant electrostriction in Gd-doped ceria, *Adv. Materials* **24**, 5857-5861 (2012).

G Jacobs, W Ma, P Gao, B Todic, T Bhatelia, D Bukur, S Khalid, B Davis, Fischer-Tropsch Synthesis: Differences Observed in Local Atomic Structure and Selectivity with Pd Compared to Typical Promoters (Pt, Re, Ru) of Co/Al2O3 Catalysts, *Top. Catal*., **55**, 811-817 (2012).

X Wang, N Li, C Liu, L Pfefferle, G Haller, One-Step Synthesis of a Pt–Co–SWCNT Hybrid Material from a Pt–Co–MCM-41 Catalyst, *J. Mater. Chem*., **22**, 25083-25092 (2012).

F Behafarid, L Ono, S Mostafa, J Croy, G Shafai, S Hong, T Rahman, S Bare, B Roldan Cuenya, Electronic Properties and Charge Transfer Phenomena in Pt Nanoparticles on γ-Al2O3: Size, Shape, Support, and Adsorbate Effects, *Phys. Chem. Chem. Phys*., **14**, 11766-11779 (2012).

F Cardenas-Lizana, S Gomez-Quero, G Jacobs, Y Ji, B Davis, L Kiwi-Minsker, M Keane, Alumina Supported Au-Ni: Surface Synergism in the Gas Phase Hydrogenation of Nitro-Compounds, *J. Phys. Chem. C*, **116**(20), 11166-11180 (2012).

C Liu, S Lee, D Su, Z Zhang, L Pfefferle, G Haller, Synthesis and Characterization of Nanocomposites with Strong Interfacial Interaction: Sulfated ZrO2 Nanoparticles Supported on Multiwalled Carbon Nanotubes, *J. Phys. Chem. C*, **116**(41), 21742-21752 (2012).

R Coppage, J Slocik, B Briggs, A Frenkel, R Naik, M Knecht, Determining Peptide Sequence Effects That Control the Size, Structure, and Function of Nanoparticles, *ACS Nano*, **2**, 1625-1636 (2012).

C Aydin, A Kulkarni, M Chi, N D. Browning, B C. Gates, Atomically Resolved Site-Isolated Catalyst on MgO: Mononuclear Osmium Dicarbonyls formed from Os3(CO)12, *J. Phys. Chem. Letts*., **3**(14), 1865−1871 (2012).

E Bayram, J Lu, C Aydin, A Uzun, N Browning, B Gates, R Finke, Mononuclear Zeolite-Supported Iridium: Kinetic, Spectroscopic, Electron Microscopic, and Size-Selective Poisoning Evidence for an Atomically Dispersed True Catalyst at 22 °C, ACS Catal., 2, 1947-1957 (2012).

X Wang, N Li, Z Zhang, C Wang, L Pfefferle, G Haller, High-Yield Hydrogen Production from Aqueous Phase Reforming over Single-Walled Carbon Nanotube Supported Catalysts, *ACS Catal*., **2**(7), 1480-1486 (2012).

H Shou, D Ferrari, D Barton, C Jones, R Davis, Influence of Passivation on the Reactivity of Unpromoted and Rb-Promoted Mo2C Nanoparticles for CO Hydrogenation, *ACS Catal*., **2**(7), 1408–1416 (2012).

J Kwak, R Tonkyn, D Tran, D Mei, S Cho, L Kovarik, J Lee, C Peden, J Szanyi, Size-Dependent Catalytic Performance of CuO on γ-Al2O3: NO Reduction Versus NH3 Oxidation, *ACS Catal*., **2**(7), 1432-1440 (2012).

J Lu, C Aydin, A Liang, C Chen, N Browning, B Gates, Site-Isolated Molecular Iridium Complex Catalyst Supported in the 1- Dimensional Channels of Zeolite HSSZ-53: Characterization by Spectroscopy and Aberration-Corrected Scanning Transmission Electron Microscopy, *ACS Catal*., **2**(6), 1002-1012 (2012).

A Karim, C Howard, B Roberts, L Kovarik, L Zhang, D King, Y Wang, In Situ X-ray Absorption Fine Structure Studies on the Effect of pH on Pt Electronic Density during Aqueous Phase Reforming of Glycerol, *ACS Catal.*, **2**, 2387–2394 (2012).

E Carino, H Kim, G Henkelman, R Crooks, Site-Selective Cu Deposition on Pt Dendrimer-Encapsulated Nanoparticles: Correlation of Theory and Experiment, *J. Am. Chem. Soc*., **134**, 4153-4162 (2012).

M.Li, N.Marinkovic, K.Sasaki, In situ characterization of ternary Pt-Rh-SnO2/C catalysts for ethanol electrooxidation", *Electrocatalysis* **3**, 376-385 (2012).

V Myers, A Frenkel, R Crooks, In Situ Structural Characterization of Platinum Dendrimer-Encapsulated Oxygen Reduction Electrocatalysts, *Langmuir*, **28**, 1596-1603 (2012).

R Zheng, M Porosoff, J Weiner, S Lu, Y Zhu, J Chen, Controlling Hydrogenation of C O and C C Bonds in Cinnamaldehyde Using Silica Supported Co-Pt and Cu-Pt Bimetallic Catalysts, *Appl. Catal. A*, **419-420**, 126-132 (2012).

C Shi, Y Ji, U Graham, G Jacobs, M Crocker, Z Zhang, Y Wang, T Toops, NOx Storage and Reduction Properties of Model Ceria-based Lean NOx Trap Catalysts, *Appl. Catal. B*, **119-120**, 183-196 (2012).

W Yan, R Vasic, A Frenkel, B Koel, Intraparticle Reduction of Arsenite (As(III)) by Nanoscale Zerovalent Iron (nZVI) Investigated with In Situ X-ray Absorption Spectroscopy, *Environ. Sci. Tech*., **46**, 7018-7026 (2012).

G Landrot, M Ginder-Vogel, K Livi, J Fitts, D Sparks, Chromium(III) Oxidation by Three Poorly-Crystalline Manganese(IV) Oxides. 1. Chromium(III)-Oxidizing Capacity, *Environ. Sci. Tech*., **46**, 11594-11600 (2012).

V. Lyahovitskaya, Y. Feldman, I. Zon, A. Yoffe, A. I. Frenkel Strain- arranged structure in amorphous films *J. Mater. Research* **27**, 2819-2828 (2012).

P.T. Do, A.J. Foster, J.G. Chen and R.F. Lobo, "Bimetallic Effects in the Hydrodeoxygenation of meta-Cresol on Al2O3 Supported Pt-Ni and Pt-Co Catalysts", *Green Chemistry*, **14**, 1388-1397 (2012).

W. Yu, M.D. Porosoff and J.G. Chen, "Review of Pt-based Bimetallic Catalysis: From Model Surfaces to Supported Catalysts", *Chemical Reviews*, **112**, 5780-5817 (2012).

J Matos, L Ono, F Behafarid, J Croy, S Mostafa, A DeLaRiva, A Datye, A Frenkel, B Roldan Cuenya, In Situ Coarsening Study of Inverse Micelle-prepared Pt Nanoparticles Supported on c-Al2O3: Pretreatment and Environmental Effects, *Phys. Chem. Chem. Phys*., **14**, 11457-11467 (2012).

L Barrio, G Zhou, I Gonzalez, M Estrella, J Hanson, J Rodriguez, R Navarro, J Fierro, In Situ Characterization of Pt Catalysts Supported on Ceria Modified TiO2 for the WGS Reaction: Influence of Ceria Loading, *Phys. Chem. Chem. Phys*., **14**, 2192-2202 (2012).

E Erickson, M Thorum, R Vasic, N Marinkovic, A Frenkel, A Gewirth, R Nuzzo, In Situ Electrochemical X-ray Absorption Spectroscopy of Oxygen Reduction Electrocatalysis with High Oxygen Flux, *J. Am. Chem. Soc*., **134**, 197-200 (2012).

K Yih, I Hamdemir, J Mondloch, E Bayram, S Özkar, R Vasić, A Frenkel, O Anderson, R Finke, Synthesis and Characterization of [Ir(1,5-Cyclooctadiene)(μ-H)]4: A Tetrametallic Ir4H4-Core, Coordinatively Unsaturated Cluster, *Inorg. Chem*., **51**, 3186-3193 (2012).

W Xu, R Si, S Senanayake, J Llorca, H Idriss, D Stacchiola, J Hanson, J Rodriquez, In Situ Studies of CeO2-supported Pt, Ru, and Pt–Ru Alloy Catalysts for the Water–gas Shift Reaction: Active Phases and Reaction Intermediates , *J. Catal*., **291**, 117-126 (2012).

L Zhang, G Liang, G Peng, Y Huang, L Wang, L Qie, M Croft, A Ignatov, J Goodenough, Insight Into Fe-Incorporation in Li3V2(PO4)3/C Cathode Material Batteries and Energy Storage , *J. Electrochem. Soc*., **159**, A1573-A1578 (2012).

M Lowe, In-Operando Studies of Next-Generation Electrochemical Energy Storage Systems, Ph.D. Thesis. Cornell University, Ithaca (2012).

J Kwak, D Kim, J Szanyi, S Cho, C Peden, Enhanced High Temperature Performance of MgAl2O4-Supported Pt-BaO Lean NOx Trap Catalysts, *Top. Catal*., **55**(1-2), 70-77 (2012).

K Huang, K Sasaki, R Adzic, Y Xing, Increasing Pt Oxygen Reduction Reaction Activity and Durability with a Carbon-doped TiO2 Nanocoating Catalyst Support, *J Mater. Chem*., **22**, 16824-16832 (2012).

H Liang, J Raitano, G He, A Akey, I Herman, L Zhang, S Chan, Aqueous Co-precipitation of Pd-doped Cerium Oxide Nanoparticles: Chemistry, Structure, and Particle Growth, *J. Mater. Sci*., **47**(1), 299-307 (2012).

S Kundu, J Ciston, S Senanayake, D Arena, E Fujita, D Stacchiola, L Barrio, R Navarro, J Fierro, J Rodriguez, Exploring the Structural and Electronic Properties of Pt/Ceria-Modified TiO2 and Its Photocatalytic Activity for Water Splitting under Visible Light, *J. Phys. Chem. C*, **116**(26), 14062-14070 (2012).

L Zhang, G Liang, G Peng, F Zou, Y Huang, M Croft, A Ignatov, Significantly Improved Electrochemical Performance in Li3V2(PO4)3/C Promoted by SiO2 Coating for Lithium-Ion Batteries, *J. Phys. Chem. C*, **116**(23), 12401-12408 (2012).

X Yang, Z Wu, M Moses-Debusk, D Mullins, S Mahurin, R Geiger, M Kidder, C Narula, Heterometal Incorporation in Metal-Exchanged Zeolites Enables Low-Temperature Catalytic Activity of NOx Reduction, *J. Phys. Chem. C*, **116**, 23322-23331 (2012).

R Si, J Tao, J Evans, J Park, L Barrio, J Hanson, Y Zhu, J Hrbek, J Rodriguez, Effect of Ceria on Gold−Titania Catalysts for the Water−Gas Shift Reaction: Fundamental Studies for Au/CeOx/TiO2(110) and Au/CeOx/ TiO2 Powders, *J. Phys. Chem. C*, **116**, 23547-23555 (2012).

M Yeager, W Du, R Si, D Su, N Marinkovic, X Teng, Highly Efficient K0.15MnO2 Birnessite Nanosheets for Stable Pseudocapacitive Cathodes, *J. Phys. Chem. C*, **116**(38), 20173-20181 (2012).

M Small, S Sanchez, N Marinkovic, A Frenkel, R Nuzzo, Influence of Adsorbates on the Electronic Structure, Bond Strain, and Thermal Properties of an Alumina-Supported Pt Catalyst, *ACS Nano*, **6**(6), 5583-5595 (2012).

J Landon, E Demeter, N İnoğlu, C Keturakis, I Wachs, R Vasić, A Frenkel, J Kitchin, Spectroscopic Characterization of Mixed Fe−Ni Oxide Electrocatalysts for the Oxygen Evolution Reaction in Alkaline Electrolytes, *ACS Catal*., **2**, 1793-1801 (2012).

H. Lei, H. Ryu, V. Ivanovski, J. B. Warren, A. I. Frenkel, B. Cekic, W.-G. Yin, C. Petrovic Structure and physical properties of new layered iron oxychalcogenide BaFe_2OSe_2 *Phys. Rev. B* **86**, 195133 (2012)

H. Ryu, H. Lei, A. I. Frenkel, C. Petrovic Local structural disorder-induced superconductivity in K(x)Fe(2-y)Se(2) materials *Phys. Rev. B* **85**, 224515 (2012)

H Karan, K Sasaki, K Kuttiyiel, C Farberow, M Mavrikakis, R Adzic, Catalytic Activity of Platinum Monolayer on Iridium and Rhenium, *ACS Catal*., **2**, 817-824 (2012).

J Shearer, P Callan, C Masitas, C Grapperhaus, Influence of Sequential Thiolate Oxidation on a Nitrile Hydratase Mimic Probed by Multiedge X-ray Absorption Spectroscopy, *Inorg. Chem*., **51**(11), 6032-3045 (2012).

A. I. Frenkel, J. A. Rodriguez, J. G. Chen Synchrotron techniques for in situ catalytic studies: Capabilities, challenges and opportunities. Invited Perspective Article, *ACS Catal.* **2**, 2269-2280 (2012).

S Tupy, A Karim, C Bagia, W Deng, Y Huang, D Vlachos, J Chen, Correlating Ethylene Glycol Reforming Activity with In Situ EXAFS Detection of Ni Segregation in Supported NiPt Bimetallic Catalysts, *ACS Catal*., **2**, 2290–2296 (2012).

M Song, S Cheng, H Chen, W Qin, K Nam, S Xu, X Yang, A Bongiorno, J Lee, et al., Anomalous Pseudocapacitive Behavior of a Nanostructured, Mixed-Valent Manganese Oxide Film for Electrical Energy Storage, *Nano Lett*., **12**(7), 3483-3490 (2012).[premier]

S Bo, F Wang, Y Janssen, D Zeng, K Nam, W Xu, L Du, J Graetz, X Yang, Y Zhu et al., Degradation and (de)lithiation processes in the high capacity battery material, *J Mater. Chem*., **22**, 8799 (2012).

J Hong, X Wang, Q Wang, F Omenya, N Chernova, M Whittingham, J Graetz, Structure and Electrochemistry of Vanadium-Modified LiFePO4, *J. Phys. Chem. C*, **116**(39), 20787-20793 (2012).

X Yu, Q Wang, Y Zhou, H Li, X Yang, K Nam, S Ehrlich, S Khalid, Y Meng, High Rate Delithiation Behaviour of LiFePO4 Studied by Qiuck X-ray Absorption Spectroscopy, *Chem. Commun*., **48**, 11537–11539 (2012).

A Frenkel, R Vasic, B Dukesz, D Li, M Chen, L Zhang, T Fujita, Thermal Properties of Nanoporous Gold, *Phys. Rev. B: Condens. Matter*, **85**, 195419 (2012).

R Si, J Raitano, N Yi, L Zhang, S Chan, M Flytzani-Stephanopoulos, Structure Sensitivity of the Low-temperature Water-gas Shift Reaction on Cu–CeO2 Catalysts, *Catal. Today*, **180**, 68-80 (2012). [97015]

K Kuttiyiel, K Sasaki, Y Choi, D Su, P Liu, R Adzic, Bimetallic IrNi Core Platinum Monolayer Shell Electrocatalysts for the Oxygen Reduction Reaction, *Energy Environ. Sci*., **5**(1), 5297-5304 (2012).

K Sasaki, H Naohara, Y Choi, Y Cai, W Chen, P Liu, R Adzic, Highly Stable Pt Monolayer on PdAu Nanoparticle Electrocatalysts for the Oxygen Reduction Reaction, *Nat. Commun*., **3**, 1115 (2012).

W Chen, K Sasaki, C Ma, A Frenkel, N Marinkovic, J Muckerman, Y Zhu, R Adzic, Hydrogen-Evolution Catalysts Based on Non-Noble Metal Nickel–, *Angew. Chem. Int. Ed*., **51**, 6131-6135 (2012).

L Yadgarov, R Rosentsveig, G Leitus, A Albu-Yaron, A Moshkovich, V Perfilyev, R Vasic, A Frenkel, A Enyashin, et al., Controlled Doping of MS2 (M=W, Mo) Nanotubes and Fullerene-like Nanoparticles, *Angew. Chem. Int. Ed*., **51**(5), 1148-1151 (2012).

A. Patlolla, J Zunino, III, A Frenkel, Z Iqbal, Thermochromism in Polydiacetylene-metal Oxide Nanocomposites, *J Mater. Chem.*, **22**, 7028-7035 (2012).

2013:

M Herklotz, F Scheiba, M Hinterstein, K Nikolowski, M Knapp, A Dippel, L Giebeler, J Eckert, H Ehrenberg, Advances in in Situ Powder Diffraction of Battery Materials: a Case Study of the New Beamline P02.1 at DESY, Hamburg, *J. Appl. Cryst.*, **46**(4), 1117-1127 (2013).

B Wen, N Chernova, R Zhang, Q Wang, F Omenya, J Fang, M Stanley Whittingham, Layered Molybdenum (Oxy)Pyrophosphate as Cathode for Lithium-Ion Batteries, *Chem. Mater.*, **25**(17), 3513-3521 (2013).

M Goesten, E Stavitski, E Pidko, C Gucuyener, B Boshuizen, S Ehrlich, E Hensen, F Kapteijn, J Gascon, The Molecular Pathway to ZIF-7 Microrods Revealed by In Situ Time-Resolved Small- and Wide-Angle X-Ray Scattering, Quick-Scanning Extended X-Ray Absorption Spectroscopy, and DFT Calculations, *Chem. Eur. J.*, **19**(24), 7809-7816 (2013).

J Sun, A Karim, H Zhang, L Kovarik, X Li, A Hensley, J McEwen, Y Wang, Carbon-Supported Bimetallic Pd–Fe Catalysts for Vapor-Phase Hydrodeoxygenation of Guaiacol, *J. Catal.*, **306**, 47-57 (2013).

J Xiao, X Yu, J Zheng, Y Zhou, F Gao, X Chen, J Bai, X Yang, J Zhang, Interplay Between Two-Phase and Solid Solution Reactions in High Voltage Spinel Cathode Material for Lithium Ion Batteries, *J. Power Sources*, **242**, 736-741 (2013).

X Yu, H Pan, W Wan, C Ma, J Bai, Q Meng, S Ehrlich, Y Hu, X Yang, A Size-Dependent Sodium Storage Mechanism in Li4Ti5O12 Investigated by a Novel Characterization Technique Combining in Situ X-ray Diffraction and Chemical Sodiation, *Nano Lett.*, **13**(10), 4721-4727 (2013).

J Ding, Y Zhou, Q Sun, X Yu, X Yang, Z Fu, Electrochemical Properties of P2-phase Na0.74CoO2 Compounds as Cathode Material for Rechargeable Sodium-ion Batteries, *Electrochim. Acta*, **87**, 388-393 (2013).

Y Chen, J Zhang, J Li, J Lockard, Monitoring the Activation of a Flexible Metal–Organic Framework Using Structurally Sensitive Spectroscopy Techniques, *J. Phys. Chem. C*, **117**(39), 20068-20077 (2013).

A Peela, W Zheng, I Lee, A Karim, D Vlachos, Core-Shell Nanocatalyst Design by Combining High Throughput Experiments and First Principles Simulations, *ChemCat.Chem*, **5**(12), 3712 – 3718 (2013).

Y Wang, X Yu, S Xu, J Bai, R Xiao, Y Hu, H Li, X Yang, L Chen, X Huang, A Zero-Strain Layered Metal Oxide as the Negative Electrode for Long-Life Sodium-Ion Batteries, *Nat. Commun.*, **4**, 2365 (2013).

M Shao, J Odell, M Hunbert, T Yu, Y Xia, Electrocatalysis on Shape-Controlled Palladium Nanocrystals: Oxygen Reduction Reaction and Formic Acid Oxidation, *J. Phys. Chem. C*, **117**(8), 4172-4180 (2013).

M Sina, K Nam, D Su, N Pereira, X Yang, G Amatucci, F Cosandey, Structural Phase Transformation and Fe Valence Evolution in FeOxF2-x/C Nanocomposite Electrodes During Lithiation and De-lithiation Processes, *J. Mater. Chem. A*, **1**(38), 11629-11640 (2013).

K Karthikeyan, K Nam, E Hu, X Yang, Y Lee, Preparation and Cyclic Performance of Li1.2(Fe0.16Mn0.32Ni0.32)O2 Layered Cathode Material by the Mixed Hydroxide Method, *Bull. Korean Chem. Soc.*, **34**(7), 1995 (2013).

S Azoz, J Jiang, G Keskar, C McEnally, A Alkas, F Ren, N Marinkovic, G Haller, S Ismail-Beigi, L Pfefferle, Mechanism for Strong Binding of CdSe Quantum Dots to Multiwall Carbon Nanotubes for Solar Energy Harvesting, *Nanoscale*, **5**, 6893-6900 (2013).

A Frenkel, M Small, J Smith, R Nuzzo, K Kvashnina, M Tromp, An in Situ Study of Bond Strains in 1 nm Pt Catalysts and Their Sensitivities to Cluster−Support and Cluster−Adsorbate Interactions, *J. Phys. Chem. C*, **117**(44), 23286-23294 (2013).

Y Amit, H Eshet, A Faust, A Patllola, E Rabani, U Banin, A Frenkel, Unraveling the Impurity Location and Binding in Heavily Doped Semiconductor Nanocrystals: The Case of Cu in InAs Nanocrystals, *J. Phys. Chem. C*, **117**(26), 13688-13696 (2013).

L Li, M Morrill, H Shou, D Barton, D Ferrari, R Davis, P Agrawal, C Jones, D Sholl, On the Relationship between Mo K-Edge Energies and DFT Computed Partial Charges, *J. Phys. Chem. C*, **117**(6), 2769-2773 (2013).

F Fang, E Iyyamperumal, M Chi, G Keskar, M Majewska, F Ren, C Liu, G Haller, L Pfefferle, Templated One-Step Catalytic Fabrication of Uniform Diameter MgxBy Nanostructures, *J. Mater. Chem. C*, **1**, 2568-2576 (2013).

I Perelshtein, E Ruderman, N Perkas, T Tzanov, J Beddow, E Joyce, T Mason, M Blanes, K Moll´a, et al., Chitosan and Chitosan–ZnO-Based Complex Nanoparticles: Formation, Characterization, and Antibacterial Activity, *J. Mater. Chem. B*, **1**(14), 1968-1976 (2013).

L Merte, M Ahmadi, F Behafarid, L Ono, E Lira, J Matos, L Li, J Yang, B Roldan Cuenya, Correlating Catalytic Methanol Oxidation with the Structure and Oxidation State of Size-Selected Pt Nanoparticles, *ACS Catal.*, **3**(7), 1460-1468 (2013).

L Wang, S Zhang, Y Zhu, A Patlolla, J Shan, H Yoshida, S Takeda, A Frenkel, F Tao, Catalysis and In Situ Studies of Rh1/Co3O4 Nanorods in Reduction of NO with H2, *ACS Catal.*, **3**(5), 1011-1019 (2013).

M Morrill, N Thao, H Shou, R Davis, D Barton, D Ferrari, P Agrawal, C Jones, Origins of Unusual Alcohol Selectivities over Mixed MgAl Oxide-Supported K/MoS2 Catalysts for Higher Alcohol Synthesis from Syngas, *ACS Catal.*, **3**(7), 1665-1675 (2013).

T Ramírez Reina, W Xu, S Ivanova, M Ángel Centeno, J Hanson, J Rodriguez, J Antonio Odriozola, In Situ Characterization of Iron-Promoted Ceria–Alumina Gold Catalysts During the Water-Gas Shift Reaction, *Catal. Today*, **205**, 41-48 (2013).

V Petrykin, K Macounová, M Okube, S Mukerjee, P Krtil, Local Structure of Co Doped RuO2 Nanocrystalline Electrocatalytic Materials for Chlorine and Oxygen Evolution, *Catal. Today*, **202**, 63-69 (2013).

H Wang, L Wei, F Ren, Q Wang, L Pfefferle, G Haller, Y Chen, Chiral-Selective CoSO4/SiO2 Catalyst for (9,8) Single-Walled Carbon Nanotube Growth, *ACS Nano*, **7**(1), 614-626 (2013).

R Anderson, L Zhang, J Loussaert, A Frenkel, G Henkelman, R Crooks, An Experimental and Theoretical Investigation of the Inversion of Pd@Pt Core@Shell Dendrimer-Encapsulated Nanoparticles, *ACS Nano*, **7**(10), 9345-9353 (2013).

W Chen, C Wang, K Saski, N Marinkovic, W Xu, J Muckerman, Y Zhu, R Adzic, Highly Active and Durable Nanostructured Molybdenum Carbide Eelectrocatalysts for Hydrogen Production, *Energy Environ. Sci.*, **6**, 943-951 (2013).

W Chen, S Iyer, S Iyer, K Sasaki, C Wang, Y Zhu, J Muckerman, E Fujita, Biomass-Derived Electrocatalytic Composites for Hydrogen Evolution, *Energy Environ. Sci.*, **6**, 1818-1826 (2013).

D Yancey, S Chill, L Zhang, A Frenkel, G Henkelman, R Crooks, A Theoretical and Experimental Examination of Systematic Ligand-Induced Disorder in Au Dendrimer-Encapsulated Nanoparticles, *Chem. Sci.*, **4**, 2912-2921 (2013).

M Zhu, B Puls, C Frandsen, J Kubicki, H Zhang, G Waychunas, In Situ Structural Characterization of Ferric Iron Dimers in Aqueous Solutions: Identification of μ-Oxo Species, *Inorg. Chem.*, **52**(12), 6788-6797 (2013).

A Frenkel, Q Wang, S Sanchez, M Small, R Nuzzo, Short Range Order in Bimetallic Nanoalloys: An Extended X-Ray Absorption Fine Structure Study, *J. Chem. Phys.*, **138**(6), 064202 (2013).

X Wang, N Li, L Pfefferle, G Haller, Metal Nanoparticles Inside Multi-Walled Carbon Nanotubes: A simple Method of Preparation and of Microscopic Image Analysis, *Microporous Mesoporous Mater.*, **176**, 139-144 (2013).

A Kossoy, Q Wang, R Korobko, V Grover, Y Feldman, E Wachtel, A Tyagi, A Frenkel, I Lubomirsky, Evolution of the Local Structure at the Phase Transition in CeO2-Gd2O3 Solid Solutions, *Phys. Rev. B: Condens. Matter*, **87**(5), 054101 (2013).S Khabuanchalad, J Wittayakun, R Lobo-Lapidus, S Stoll, R Britt, B Gates, Formation of MgO-Supported Manganese Carbonyl Complexes by Chemisorption of Mn(CO)5CH3, *Langmuir*, **29**(21), 6279-6286 (2013).

K Amakawa, L Sun, C Guo, M Hvecker, P Kube, I Wachs, S Lwin, A Frenkel, A Patlolla, et al., How Strain Affects the Reactivity of Surface Metal Oxide Catalysts**, *Angew. Chem. Int. Ed.*, **52**(51), 13553-13557 (2013).

H Chen, Q Hao, O Zivkovic, G Hautier, L Du, Y Tang, Y Hu, X Ma, C Grey, G Ceder, Sidorenkite (Na3MnPO4CO3): A New Intercalation Cathode Material for Na-Ion Batteries, *Chem. Mater.*, **25**(14), 2777-2786 (2013).

S Garcia, R Anderson, H Celio, N Dahl, A Dolocan, J Zhou, S Humphrey, Microwave Synthesis of Au–Rh Core–Shell Nanoparticles and Implications of the Shell Thickness in Hydrogenation Catalysis, *Chem. Commun.*, **49**, 4241-4243 (2013).

H Shou, L Li, D Ferrari, D Sholl, R Davis, Use of Infrared Spectroscopy and Density Functional Theory to Study the Influence of Rubidium on Alumina-Supported Molybdenum Carbide Catalyst for Higher Alcohol Synthesis from Syngas, *J. Catal.*, **299**, 150-161 (2013).

H Wang, F Ren, C Liu, R Si, D Yu, L Pfefferle, G Haller, Y Chen, CoSO4/SiO2 Catalyst for Selective Synthesis of (9, 8) Single-Walled Carbon Nanotubes: Effect of Catalyst Calcination, *J. Catal.*, **300**, 91-101 (2013).

M Li, D Cullen, K Sasaki, N Marinkovic, K More, R Adzic, Ternary Electrocatalysts for Oxidizing Ethanol to Carbon Dioxide: Making Ir Capable of Splitting C–C Bond, *J. Am. Chem. Soc.*, **135**(1), 132-141 (2013).

Q Jia, D Ramaker, J Ziegelbauer, N Ramaswamy, A Halder, S Mukerjee, Fundamental Aspects of ad-Metal Dissolution and Contamination in Low and Medium Temperature Fuel Cell Electrocatalysis: A Cu Based Case Study Using In Situ Electrochemical X-ray Absorption Spectroscopy , *J. Phys. Chem. C*, **117**(9), 4585-4596 (2013).

A Gaur, B Shrivastava, S Khalid, Study of XAFS Spectroscopic Methods of Speciation Using Mixtures of Cu(I) and Cu(II) Chlorides, *J Phys.: Conf. Ser.*, **430**, 012045 (2013).

H Liu, K Schonberger, C Peng, J Ferguson, E Desormeaux, P Meyerhofer, H Luckenbach, G Korshin, Effects of Blending of Desalinated and Conventionally Treated Surface Water on Iron Corrosion and its Release From Corroding Surfaces and Pre-Existing Scales, *Water Res.*, **47**, 3817-3826 (2013).

P Cordeiro, P Guillo, C Spanjers, J Chang, M Lipschutz, M Fasulo, R Rioux, T Tilley, Titanium–Germoxy Precursor Route to Germanium-Modified Epoxidation Catalysts with Enhanced Activity, *ACS Catal.*, **3**, 2269-2279 (2013).

R Guzman-Blas, D Suazo-Davila, C Valez, C Molina, C Daza, D Stacchiola, K Sasaki, S Senanayake, A Johnston-Peck, et al., EDTA-Ce(III) Modified Pt Vulcan XC-72 Catalyst Synthesis for Methanol Oxidation in Acid Solution, *Electrocatal.*, **4** (Online), 1-12 (2013).

J Vecchietti, S Collins, W Xu, L Barrio, D Stacchiola, M Calatayud, F Tielens, J José Delgado, A Bonivardi, Surface Reduction Mechanism of Cerium−Gallium Mixed Oxides with Enhanced Redox Properties, *J. Phys. Chem. C*, **117**(17), 8822-8831 (2013).

W Kang, C Spanjers, R Rioux, J Hoefelmeyer, Synthesis of Brookite TiO2 Nanorods with Isolated Co(II) Surface Sites and Photocatalytic Degradation of 5,8-dihydroxy-1,4-Naphthoquinone Dye, *J. Mater. Chem. A*, **1**, 7717-7728 (2013).

Y Qiao, X Hu, Y Liu, G Liang, M Croft, Y Huang, Surface Modification of MoOxSy on Porous TiO2 Nanospheres as an Anode Material with Highly Reversible and Ultra-Fast Lithium Storage Properties, *J. Mater. Chem. A*, **1**(47), 15128-15134 (2013).

R Guzmán-Blas, C Menéndez, C Vélez, E Fachini, A Johnston-Peck, S Senanayake, D Stacchiola, K Sasaki, C Cabrera, Vulcan/Pt/Ce Catalysts Prepared by Impregnation Using EDTA for Direct Methanol Fuel Cell, Direct Ethanol Fuel Cell, and Polymer Electrolyte Membrane Fuel Cell, *SGRE*, **4**, 1-9 (2013).

T Wang, W Lonergan, J Chen, Selection of Oxide Supports to Anchor Desirable Bimetallic Structures for Ethanol Reforming and 1,3-Butadiene Hydrogenation, *Chinese J Catal*, **34**(11), 2009-2017 (2013).

L Zhang, G Liang, G Peng, Y Jiang, H Fang, Y Huang, M Croft, A Ignatov, Evolution of Electrochemical Performance in Li3V2(PO4)3/C Composites Caused by Cation Incorporation, *Electrochim. Acta*, **108**, 182-190 (2013).

H Fang, G Liang, L Zhao, T Wallace, H Arava, L Zhang, A Ignatov, M Croft, Electrochemical Properties of Cathode Material LiFePO4 with Ti Substitution, *J. Electrochem. Soc.*, **160**(5), A3148-A3152 (2013).

M Trahan, Q Jia, S Mukerjee, E Plichta, M Hendrickson, K Abraham, Cobalt Phthalocyanine Catalyzed Lithium-Air Batteries, *J. Electrochem. Soc.*, **160**(9), A1577-A1586 (2013).

M Moses-DeBusk, M Yoon, L Allard, D Mullins, Z Wu, X Yang, G Veith, G Malcolm Stocks, C Narula, CO Oxidation on Supported Single Pt Atoms: Experimental and ab Initio Density Functional Studies of CO Interaction with Pt Atom on θ-Al2O3(010) Surface, *J. Am. Chem. Soc.*, **135**(34), 12634-12645 (2013).

H Wang, W Zhou, J Liu, R Si, G Sun, M Zhong, H Su, H Zhao, J Rodriguez, et al., Platinum-Modulated Cobalt Nanocatalysts for Low-Temperature Aqueous-Phase Fischer−Tropsch Synthesis, *J. Am. Chem. Soc.*, **135**(10), 4149-4158 (2013).

C Tian, S Chai, D Mullins, X Zhu, A Binder, Y Guo, S Dai, Heterostructured BaSO4–SiO2 Mesoporous Materials as New Supports for Gold Nanoparticles in Low-Temperature CO Oxidation, *Chem. Commun.*, **49**, 3464-3466 (2013).

A Frenkel, S Khalid, J Hanson, M Nachtegaal, QEXAFS in catalysis research: Principles,Data Analysis and Applications, *In-Situ characterization of hetrogenious catalysis*, p. 23-48, John Wiley and Sons, Hoboken (2013).

K Nam, S Bak, E Hu, X Yu, Y Zhou, X Wang, L Wu, Y Zhu, K Chung, X Yang, Combining In Situ Synchrotron X-Ray Diffraction and Absorption Techniques with Transmission Electron Microscopy to Study the Origin of Thermal Instability in Overcharged Cathode Materials for Lithium-Ion Batteries, *Adv. Func. Mater.*, **23**(8), 1047-1063 (2013).

A Frenkel, J Hanson, Combined X-ray Diffraction and Absorption Spectroscopy in Catalysis Research: Techniques and Applications, *In situ characterziation of heterogeneous catalysts*, p. 345-369, Wiley, Hoboken (2013).

Y Hu, Z Liu, K Nam, O Borkiewicz, J Cheng, X Hua, M Dunstan, X Yu, K Wiaderek, et al., Origin of Additional Capacities in Metal Oxide Lithium-Ion Battery Electrodes, *Nat. Mater.*, **12**(12), 1130-1136 (2013).

M Shao, B Smith, S Guerrero, L Protsailo, D Su, K Kaneko, J Odell, M Humbert, K Sasaki, et al., Core–Shell Catalysts Consisting of Nanoporous Cores for Oxygen Reduction Reaction, *Phys. Chem. Chem. Phys.*, **15**, 15078-15090 (2013).

A Patlolla, P Baumann, W Xu, S Senanayake, J Rodriguez, A Frenkel, Characterization of Metal-Oxide Catalysts in Operando Conditions by Combining X-Ray Absorption and Raman Spectroscopies in the Same Experiment , *Top. Catal.*, **56**(11), 896-904 (2013).

A Kugbacka, R Si, P Michorczyk, A Martínez-Arias, W Xu, J Hanson, J Rodriguez, M Fernández-García, Tungsten as an Interface Agent Leading to Highly Active and Stable Copper–Ceria Water Gas Shift Catalyst, *Appl. Catal. B*, **132-133**, 423-432 (2013).

S Bak, K Nam, W Chang, X Yu, E Hu, S Hwang, E Stach, K Kim, K Chung, X Yang, Correlating Structural Changes and Gas Evolution during the Thermal Decomposition of Charged LixNi0.8Co0.15Al0.05O2 Cathode Materials, *Chem. Mater.*, **25**(3), 337-351 (2013).

K Nam, S Bak, E Hu, X Yu, Y Zhou, X Wang, L Wu, Y Zhu, K Chung, X Yang, Combining In Situ Synchrotron X-Ray Diffraction and Absorption Techniques with Transmission Electron Microscopy to Study the Origin of Thermal Instability in Overcharged Cathode Materials for Lithium-Ion Batteries, *Adv. Func. Mater.*, **23**(8), 1047-1063 (2013).

M Yeager, W Du, Q Wang, N Deskins, M Sullivan, B Bishop, D Su, W Xu, S Senanayake, et al., Pseudocapacitive Hausmannite Nanoparticles with (101) Facets: Synthesis, Characterization, and Charge-Transfer Mechanism, *ChemSusChem*, **6**(10), 1983-1992 (2013).

V Rico Pérez, M Ángeles Velasco Beltrán, Q He, Q Wang, C Salinas Martínez de Lecea, A Bueno López, Preparation of Ceria-Supported Rhodium Oxide Sub-Nanoparticles with Improved Catalytic Activity for CO Oxidation, *Catal. Commun.*, **33**, 47-50 (2013).

J Rodriguez, J Hanson, D Stacchiola, S Senanayake, In Situ/Operando Studies for the Production of Hydrogen Through the Water-gas Shift on Metal Oxide Catalys, *Phys. Chem. Chem. Phys.*, **15**(29), 12004-12025 (2013).

F Behafarid, B Roldan Cuenya, Towards the Understanding of Sintering Phenomena at the Nanoscale: Geometric and Environmental Effects, *Top. Catal.*, **56**, 1542-1559 (2013).

K Kuttiyiel, K Sasaki, D Su, M Vukmirovic, N Marinkovic, R Adzic, Pt Monolayer on Au-stabilized PdNi Core–Shell Nanoparticles for Oxygen Reduction Reaction, *Electrochim. Acta*, **110**, 267-272 (2013).

X Teng, Anodic Catalyst Design for the Ethanol Oxidation Fuel Cell Reactions, *Materials and Processes for Energy: Communicating Current Research and Technological Developments*, p. 473-784, Formatex Research Center, Badajoz (2013).

J Bauer, D Mullins, Y Oyola, S Overbury, S Dai, Structure Activity Relationships of Silica Supported AuCu and AuCuPd Alloy Catalysts for the Oxidation of CO, *Catal. Lett.*, **143**(9), 926-935 (2013).

M Porosoff, J Chen, Trends in the Catalytic Reduction of CO2 by Hydrogen Over Supported Monometallic and Bimetallic Catalysts, *J. Catal.*, **301**, 30-37 (2013).

S Zhang, J Shan, Y Zhu, A Frenkel, A Patlolla, W Huang, S Yoon, L Wang, J Yoshida, et al., WGS Catalysis and In Situ Studies of CoO1−x, PtCon/Co3O4, and PtmCom′/CoO1−x Nanorod Catalysts, *J. Am. Chem. Soc.*, **135**(22), 8283-8293 (2013).

N Ramaswamy, U Tylus, Q Jia, S Mukerjee, Activity Descriptor Identification for Oxygen Reduction on Nonprecious Electrocatalysts: Linking Surface Science to Coordination Chemistry, *J. Am. Chem. Soc.*, **135**(41), 15443-15449 (2013).

Y. Amit, A. Faust, O. Milo, E. Rabani, A. Frenkel, U. Banin, How to dope a semiconductor nanocrystal, *ECS Trans*. **58**, 127-133 (2013).

G. M. Veith, A. R. Lupini, L. Baggetto, J. F. Browning, J. K. Keum, A. Villa, L. Prati, A. B. Papandrew, G. A. Goenaga, D. R. Mullins, S. E. Bullock and N. J. Dudney, "Evidence for the Formation of Nitrogen-Rich Platinum and Palladium Nitride Nanoparticles", *Chem. Mater*., **25** (2013) 4936.

D. Vlachos, V. Choudhary, S. Mushrif, C. Ho, A. Anderko, V. Nikolakis, N. Marinković, A. Frenkel, S. Sandler, "Insights into the Interplay of Lewis and Brønsted Acid Catalysts in Glucose and Fructose Conversion to 5-(Hydroxymethyl)furfural and Levulinic Acid in Aqueous Media", *J.Am.Chem.Soc*. **135** (2013) 3997.

2014:

H Mistry, F Behafarid, E Zhou, L Ono, L Zhang, B Cuenya, Shape-Dependent Catalytic Oxidation of 2-Butanol over Pt Nanoparticles Supported on γ-Al2O3, *ACS Catal.*, **4**, 109-115 (2014).

Wang, J.; Ji, Y.; Jacobs, G.; Jones, S.; Kim, D.-J.; Crocker, M., "Effect of aging on NO_X reduction in coupled LNT-SCR systems," *Appl. Catal. B: Environmental* **148-149** (2014) 51-61.

P Kayser, M Martínez-Lope, J Alonso, M Retuerto, M Croft, A Retuerto, M Fernández-Díaz, Crystal and Magnetic Structure of Sr2MIrO6 (M = Ca, Mg) Double Perovskites – A Neutron Diffraction Study, *Eur. J. Inorg. Chem.*, **2014**(1), 178-185 (2014).

F Ren, S Kanaan, M Majewska, G Keskar, S Azoz, H Wang, X Wang, G Haller, Y Chen, L Pfefferle, Increase in the Yield of (and Selective Synthesis of Large-Diameter) Single-Walled Carbon Nanotubes Through Water-Assisted Ethanol Pyrolysis, *J. Catal.*, **309**, 419-427 (2014).

R Guzman-Blas, D Suazo-Davila, C Valez, C Molina, C Daza, D Stacchiola, K Sasaki, S Senanayake, A Johnston-Peck, et al., EDTA-Ce(III) Modified Pt Vulcan XC-72 Catalyst Synthesis for Methanol Oxidation in Acid Solution, *Electrocatal.*, **5**(1), 50-61 (2014).

Jermwongratanachai, T.; Jacobs, G.; Shafer, W.D.; Pendyala, V.R.R.; Ma, W.; Gnanamani, M.K.; Hopps, S.; Thomas, G.A.; Kitiyanan, B.; Khalid, S.; Davis, B.H., "Fischer-Tropsch synthesis: TPR and XANES analysis of the impact of oxidation-reduction (OR) cycles on the reducibility of Co/alumina catalysts with different promoters (Pt, Ru, Re, Ag, Au, Rh, Ir)," *Catal. Today, published online*.

Yang, J.; Jacobs, G.; Jermwongratanachai, T.; Pendyala, V.R.R.; Ma, W.; Chen, D.; Holmen, A.; Davis, B.H., "Fischer-Tropsch synthesis: impact of activation by H_2 or CO on methane selectivity," *Catal. Let., published online*.

Azzam, K.; Jacobs, G.; Ma, W.; Davis, B.H. "Effect of cobalt particle size on the catalyst intrinsic activity for Fischer-Tropsch synthesis," *Catal. Lett., published online*.

Jermwongratanachai, T.; Jacobs, G.; Shafer, W.D.; Ma, W.; Pendyala, V.R.R.; Davis, B.H.; Kitiyanan, B.; Khalid, S.; Cronauer, D.C.; Kropf, A.J.; Marshall, C.L., "Fischer-Tropsch synthesis: oxidation of a fraction of cobalt crystallites in research catalysts at the onset of FT at partial pressures mimicking 50% CO conversion," *Topics Catal., published online*.