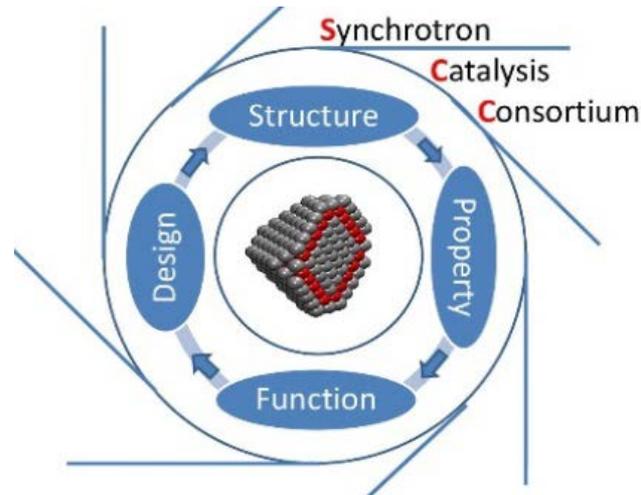


Synchrotron Catalysis Consortium at BNL: Dedicated Beamline Facilities for Catalysis Research



Anatoly Frenkel

Department of Materials Science and Chemical Engineering, SBU

Department of Chemistry, BNL

Synchrotron Catalysis Consortium at BNL

Synchrotron Catalysis Consortium at Brookhaven National Laboratory

Established: 2005 at NSLS with funding from DOE/BES.

Pis: J. Chen (Columbia/BNL), A. Frenkel (Stony Brook U.) and J. Rodriguez (BNL)

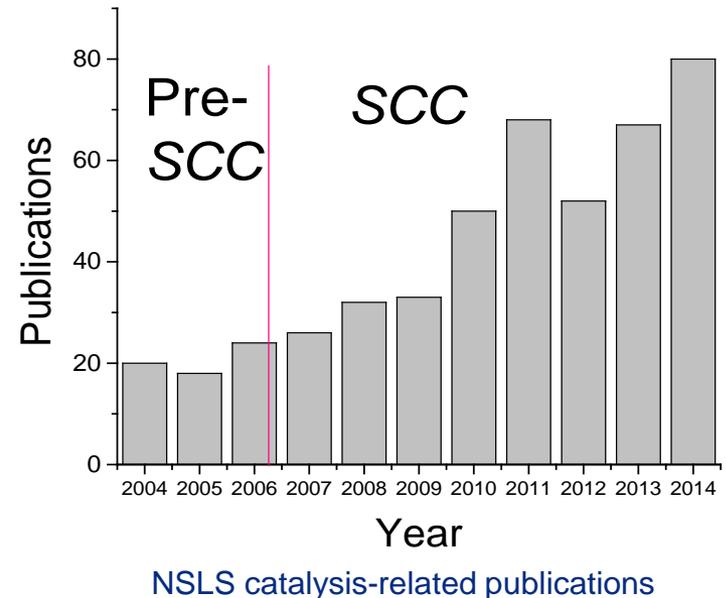
Co-Pis: R. Adzic (BNL), S. Bare (UOP), J. Hanson (BNL), A. Karim (PNNL), S. Overbury, D. Mullins (ORNL)

Mission:

To develop and promote the utilization of synchrotron techniques for catalysis and electrocatalysis research under in-situ reaction conditions

Facilities/Assistance to Catalysis Users:

- Dedicated beamtime on three beamlines,
- Dedicated facilities, *in-situ* reaction cells, gas-handling systems, and advanced detectors
- Dedicated research staff
- Training courses on synchrotron techniques and data analysis
- Assistance in idea development and proposal-writing for potential XAFS users from the catalysis community
- R&D: new hardware/software/methodology for catalytic and electrocatalytic research



Functions and Management of Synchrotron Catalysis Consortium (SCC)

- **Main Functions of SCC:**

- Dedicated beamline on 3 beamlines
- Provide dedicated reactor and gas handling systems
- Dedicated research staff to assist the experimental set-up and safety training
- Organize workshops for experiments and data analysis
- Assistance in idea development and proposal-writing for potential XAFS users from the catalysis community
- Development of new hardware/software for catalytic and electrocatalytic research

- **Management of SCC:**

- Jingguang Chen: Communication with catalysis community; preparation of reports and updates of SCC activities
- Anatoly Frenkel: Overseeing daily operations; Spokesperson for SCC beamline activities
- Ned Marinkovic: Dedicated beamline scientist for SCC
- Other co-PIs are critical part of SCC: R. Adzic, D. Mullins; S. Overbury; J. Rodriguez; S. Bare, J. Hanson, A. Karim

XAFS Short Courses at BNL

2005



2009



2013



2006



2010



2014



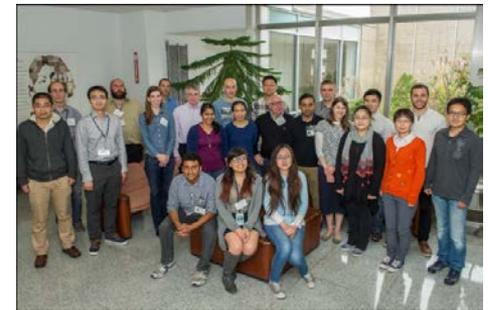
2007



2011



2015



2008



2012



Impact (2005-2014):

Research groups supported: **75**

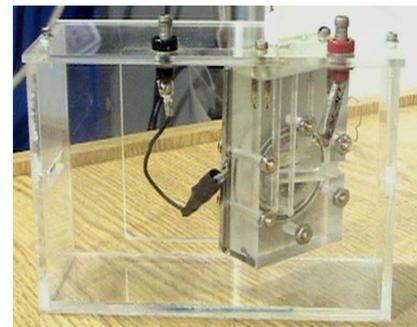
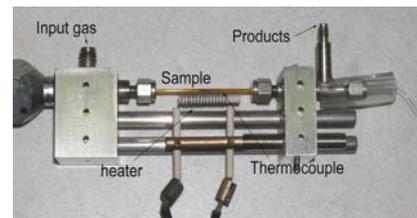
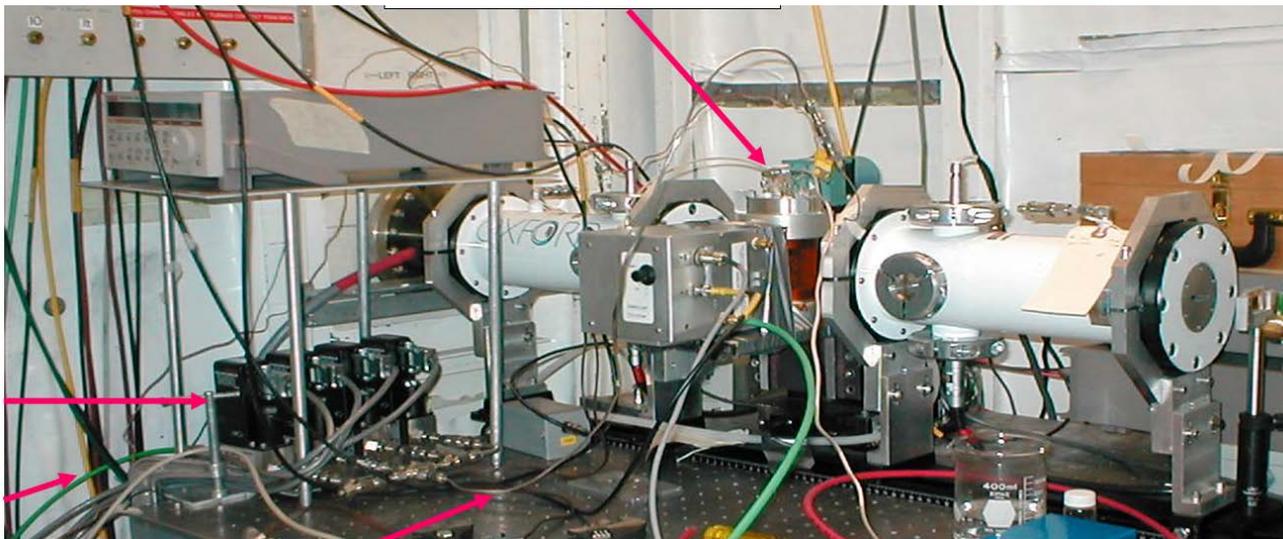
Total beamline users: **>2,000**

Publications: **432**

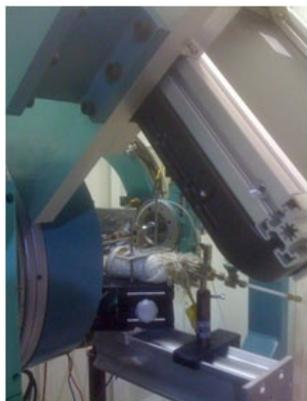
Short course participants: **371**

Combining Techniques for Catalysis Research

<http://you.stonybrook.edu/scc2>



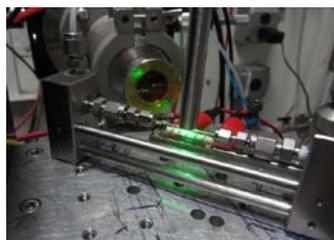
AIF, J. A. Rodriguez, J. G. Chen,
Perspective, ACS Catalysis 2012, 2,
2269



**Combined
XAFS/XRD**



**Combined
XAFS/DRIFTS**



**Combined
XAFS/Raman**



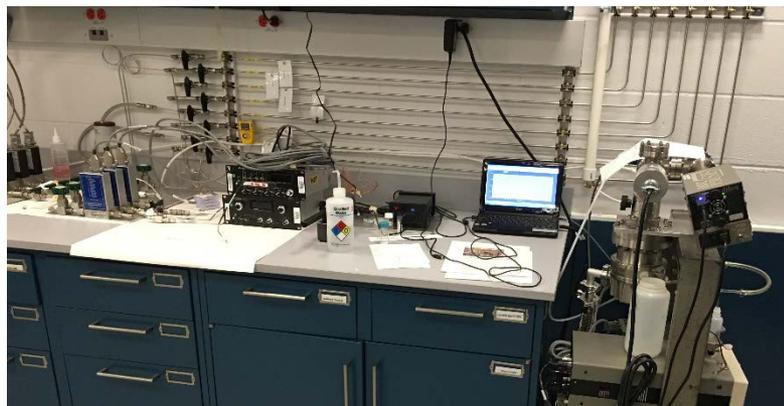
Quick EXAFS

***In situ* reactors**

Staging laboratory for in situ/operando experiments (BNL Chemistry)



Vapor delivery



Gas lines, MFCs, reaction cell, RGA



Glovebox
MBraun



Raman Spectroscopy
Bay Spec ($\lambda = 532 \text{ nm}$)

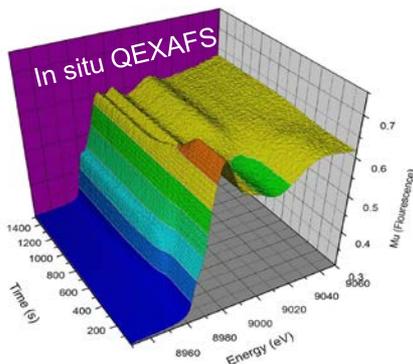


DRIFTS
Nicolet & Harrick

Summary: Synchrotron Catalysis Consortium: 2005-2016

Science:

- Development of advanced in situ techniques.



ACS Catalysis

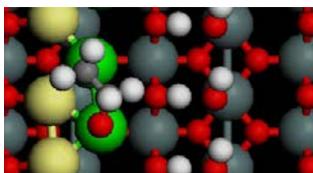
Perspective

pubs.acs.org/acscatalysis

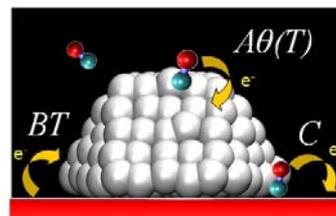
Synchrotron Techniques for In Situ Catalytic Studies: Capabilities, Challenges, and Opportunities

Anatoly I. Frenkel,^{*,†} Jose A. Rodriguez,^{*,‡} and Jingguang G. Chen^{*,§,||}

- Investigation of active phases and mechanisms of catalysis and rational design of new catalysts.



Electrocatalysts for C-C bond splitting



Catalyst-Support-Adsorbate interactions

SCC Current and Future

- Growing the synchrotron catalysis community and strengthening US catalysis science.
- Transitioning to NSLS-II, will have new capabilities for fast & operando techniques



SCC will partner at NSLS-II beamlines ISS, QAS & TES from 2017.

Comparative in Operando Studies in Heterogeneous Catalysis: Atomic and Electronic Structural Features in the Hydrogenation of Ethylene over Supported Pd and Pt Catalysts

Ulrich Jung,[†] Annika Elsen,[†] Yuanyuan Li,[‡] Jeremy G. Smith,[†] Matthew W. Small,[†] Eric A. Stach,[#] Anatoly I. Frenkel,^{*,‡} and Ralph G. Nuzzo^{*,†}

Synchrotron Techniques for In Situ Catalytic Studies: Capabilities, Challenges, and Opportunities

Anatoly I. Frenkel,^{*,†} Jose A. Rodriguez,^{*,‡} and Jingguang G. Chen^{*,§,||}



Critical review: Effects of complex interactions on structure and dynamics of supported metal catalysts

Anatoly I. Frenkel, Michael W. Cason, Annika Elsen, Ulrich Jung, Matthew W. Small, Ralph G. Nuzzo, Fernando D. Vila, John J. Rehr, Eric A. Stach, and Judith C. Yang



ANNUAL REVIEWS
A NONPROFIT SCIENTIFIC PUBLISHER

Modeling the Structure and Composition of Nanoparticles by Extended X-Ray Absorption Fine-Structure Spectroscopy

Anatoly I. Frenkel, Aaron Yevick, Chana Cooper, and Relja Vasic

new science opportunities

Journal of
Synchrotron
Radiation

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X-ray spectroscopy for chemical and energy sciences: the case of heterogeneous catalysis

Anatoly I. Frenkel^{*,*} and Jeroen A. van Bokhoven^{b,c,*}

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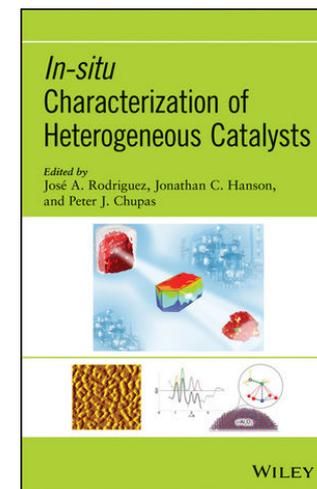
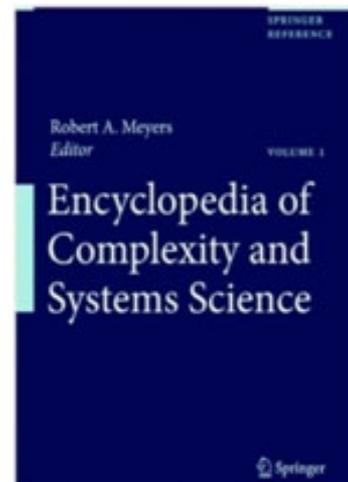
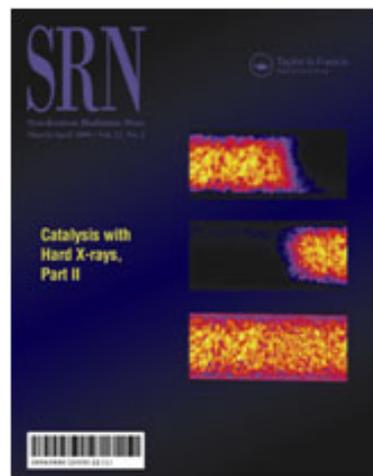
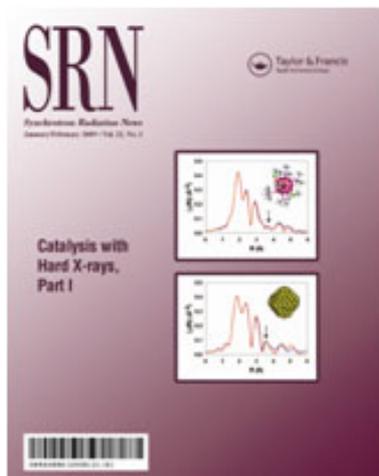
Cite this: *Chem. Soc. Rev.*, 2012, **41**, 8163–8178

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CRITICAL REVIEW

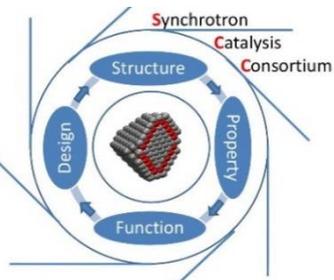
Applications of extended X-ray absorption fine-structure spectroscopy to studies of bimetallic nanoparticle catalysts[†]

Anatoly I. Frenkel^{*}



Acknowledgements:

PIs & collaborators of the SCC
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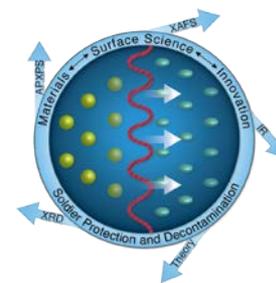


Raman, DRIFTS,
Staging lab:
BNL Chem.

XAFS experiments:
BL 2-2 @ SSRL
9BM @APS

XRD experiments:
XPD @ NSLS2
17BM @APS

Q. Wang, A. Plonka (SBU)
R. Chapleski, D. Troya, C. Sharp, J. Morris (VT)
W. Guo, C. Hill, D. Musaev (Emory)
S. Senanayake (BNL)
W. Gordon, A. Balboa (ECBC)
M. Mitchell (Kennesaw)



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