Developing Methods for Understanding Chemical Kinetics on Surfaces

Funding proposal
for 2020 SBU/BNL Seed Grant Program

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2020 SBU-BNL SEED GRANT PROGRAM
COVER SHEET

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First Middle Last

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Proposal Title **Developing Methods for Understanding Chemical Kinetics on Surfaces**

Total Budget Requested **$44,250**

BNL Budget Requested ___________________________________

Please list additional collaborators:

Stony Brook University

BROOKHAVEN NATIONAL LABORATORY

managed by Brookhaven Science Associates for the U.S. Department of Energy

Developing Methods for Understanding Chemical Kinetics on Surfaces

PI: Mónica Bugallo, Department of Electrical and Computer Engineering (SBU)
PI: Jorge Anibal Boscoboinik, Center for Functional Nanomaterials (BNL)

1. Introduction

This interdisciplinary proposal aims at developing novel strategies for understanding the kinetics of surface reactions. The Seed funding will result in advances in methodology and data analytics, ultimately leading to an improved mechanistic understanding of heterogeneously catalyzed reactions. The cutting-edge facilities used in this project, coupled with the new methodologies to be developed, will also result in unique capabilities for in-situ studies of surface kinetics in general, attracting the wider user community in the field to adopt these developments.

Heterogeneous catalysts play a significant role in supporting our current lifestyle. They are responsible for a variety of chemical processes in the industry, ranging from cracking of crude oil (to produce chemicals and fuels) to the synthesis of ammonia, with hundreds of other vital processes in between. [1] Many of these reactions have revolutionized the world. For example, the invention of the Haber-Bosch process for ammonia synthesis has resulted in the speedy growth in the human population in the last century.

But what is *catalysis*? Catalysis is a kinetic phenomenon in which a material (the catalyst) changes the mechanism of a chemical reaction, affecting the rate of the reaction and the distribution of products. In "heterogeneous" catalysis, the catalyst is in a phase different from the reactants and products, usually a solid surface. These reactions are, in most cases, complex processes, and the details of their mechanisms are poorly understood. Understanding the mechanisms is essential for improving these processes and developing alternative ones. The field of surface science has contributed tremendously to this aim by providing mechanistic details for some of these reactions.[2] The importance of surface science techniques for understanding how catalysts work was recognized in 2007 with the Nobel prize in Chemistry to Gerhard Ertl for contributions to developing the field and elucidating the mechanism for ammonia synthesis.[3]

Two of the most important techniques in surface science are X-ray photoelectron spectroscopy (XPS) and infrared reflection spectroscopy (IRRAS). XPS is an element-specific quantitative technique that can provide both the relative concentration of chemical elements on the surface (reactants, intermediates, products, spectators, and catalyst) as well as their oxidation state and chemical environment.[4] IRRAS, on the other hand, provides information about the bonding of surface molecules by measuring their vibrational frequencies, and how these change during a reaction. [5]

Elucidating the reaction mechanisms, including the determination of the kinetic parameters, is not trivial. Even simple reactions can have very complex mechanisms. While current surface science methodologies have improved our understanding of heterogeneously catalyzed chemical reactions, new approaches are needed to gain more detailed insights into the kinetics of such processes. An underutilized method for extracting kinetic parameters of the elementary steps of a reaction is modulation

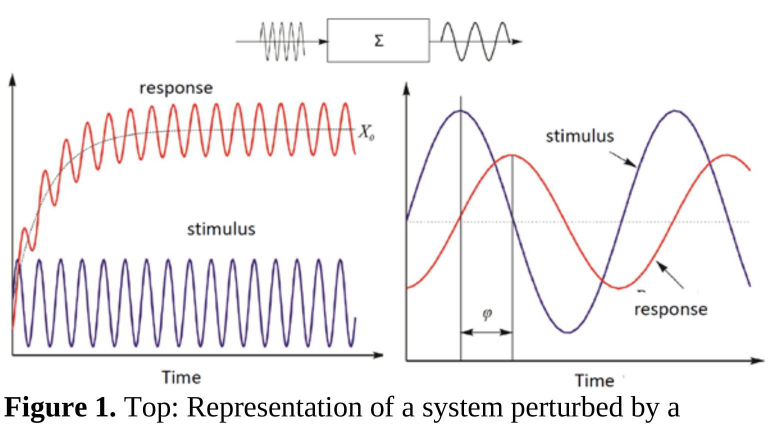

Figure 1. Top: Representation of a system perturbed by a stimulus. Bottom left: Representation of a modulated stimulus and its effect in spectroscopic signal (response). Bottom right: Difference between stimulus and response.

excitation spectroscopy (MES) [6]. In MES, a reaction variable (stimulus), e.g., the concentration of one of the species in a chemical reaction, is varied periodically, while following the response in a spectroscopic signal. This approach is shown schematically in Fig. 1.

Consider a simple elementary reaction for reactant A converting reversibly to product B as an example to show how this method can aid in extracting kinetic parameters.

$$\mathrm{A} \underset{\mathrm{k_2}}{\overset{\mathrm{k_1}}{\rightleftarrows}} \mathrm{B}$$

Here k_1 is the rate constant for the forward reaction, and k_2 is the rate constant for the reverse reaction. For this ideal reaction, the following equations give the rate law, i.e., how the concentrations of A (C_A) and B (C_B) vary as a function of time, assuming both forward and reverse reactions are of first-order (they change linearly as a function of the concentrations of A and B).

$$\frac{dC_A}{dt} = -k_1 C_A + k_2 C_B \qquad \frac{dC_B}{dt} = k_1 C_A - k_2 C_B$$

Assume now that we measure a spectroscopic signal (it can be the vibrational frequency of the stretching of a bond in the reactant A and a bond in the product B). We introduce then a modulation ω in the pressure of reactant A. The spectroscopic signals for A and B will oscillate at the same frequency as the perturbation, but with a phase lag ϕ in the oscillation. Moreover, the shape of the oscillation in the signals for A and B can also differ. These differences between the spectroscopic signals of A and B contain information about the kinetics of the process. For this simple reaction, there is an exact solution for the previous differential equations:

$$\frac{\overline{C_B}}{\overline{C_A}} = G(i\omega) = \frac{k_1}{k_2}\left[\frac{(1 - \frac{i\omega}{k_2})}{1 + \left(\frac{\omega}{k_2}\right)^2}\right]$$

where *G(iω)* is a transfer function that relates the concentration of A and B, with an imaginary part ***Im*** and a real part ***Re***. The phase lag of B (ϕ) with respect to A, and the amplitude relation (*AR*) for B, can be obtained from the transfer function:

$$tan(\varphi_B - \varphi_A) = -\frac{Im}{Re} = \omega/k_2 \qquad AR = \sqrt{Re^2 + Im^2} = \frac{k_1/k_2}{\sqrt{1 + (\omega/k_2)^2}}$$

Then, getting the phase lag and the amplitude from the experimental measurement allow solving these equations and obtaining the rate constants k_1 and k_2.

Of course, in reality, chemical processes are more much complex, and the resulting set of differential equations rarely have an exact solution.

2. Research Plan

There is a two-fold plan for this project. The **first part** (described in section 2.1) relates to modifying instrumentation at the Center for Functional Nanomaterials (CFN) for implementing pressure modulation capabilities and synchronous or asynchronous data acquisition using XPS, IRRAS, and mass spectrometry. The **second part** (section 2.2) relates to synchronous signal processing or asynchronous data analytics to extract kinetic data from the experimental measurements by solving differential equations for proposed reaction mechanisms, and

Figure 2. Drawing of the instrument with ambient pressure XPS and IRRAS capabilities that will be used for this project.

relating them to the signals in the experimental measurements both in the phase and time domains. The research will also involve approaches to improve the signal-to-noise ratio by filtering components of the signal that do not respond to the same frequency as the stimulus. Comparing filtered to non-filtered spectra will also allow the identification of species spectroscopically evident on the surface but which do not participate in the reaction under study (spectators). Carbon monoxide oxidation ($CO + O_2$) will be used as the initial test reaction on a bare Ru(0001) surface.[7] This reaction has been widely studied for decades, but mechanistic details are still unclear. Other supports and reactions may also be included if time allows.

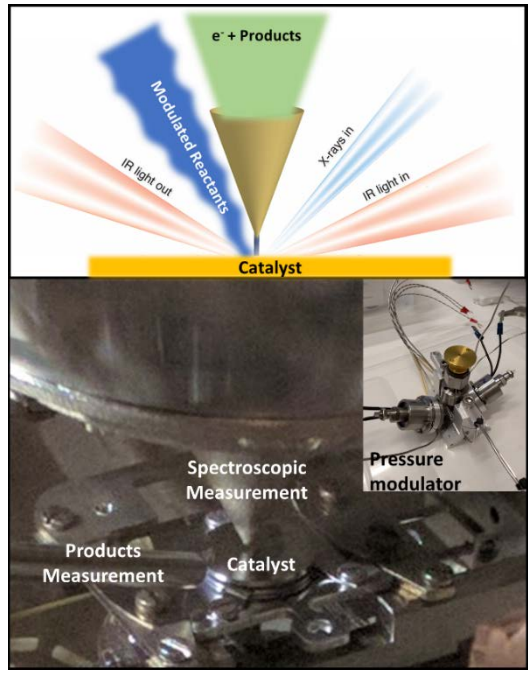

Figure 3. Top: Schematic representing a catalyst surface under study by XPS, IRRAS, and MS, while a reactant pressure is being modulated. Bottom: Photo of a catalyst surface and its surroundings inside of the instrument shown in Fig. 3.

2.1 Instrumentation

Fig. 2 shows a drawing of the experimental system with ambient pressure XPS and IRRAS capabilities at the CFN, which is co-managed by the BNL PI of this proposal. Experiments in this setup will be carried out at pressures varying from ultra-high vacuum conditions (UHV) to elevated pressures. The maximum operating pressures are 25 mbar in the XPS system[8] and 1000 mbar at the IRRAS system[5], taking advantage of a motorized polarizer that allows removing interference from the gas phase species. The sample temperature can be varied between 300 K and 900 K in the XPS system and between 100 K and 800 K in the IRRAS system. Figure 3 (top) shows a schematic of the concept proposed here, where a sample is analyzed with these spectroscopies, while a modulated supply of reactants impinges on the surface. This modulated pressure can supplement gas already present in the chamber during a reaction running in a steady-state. A photo of a typical sample (labeled catalyst) in the instrument is shown at the bottom of Fig. 3. In the current setup, variable precision leak valves are used to introduce gases or vapors of a liquid. However, this does not allow the possibility of introducing pressure modulations. For the proposed experiments, we will use the variable leak valves to achieve steady-state conditions, and a new computer-controlled pressure modulation valve (inset in Fig. 3).

In addition to the pressure modulation, we will develop an interface for data extraction, with timestamps, from the commercial instruments, including a mass spectrometer, electron energy analyzer, and IR detector. XPS and IRRAS data obtained in ultra-high vacuum for a 2D catalyst model system are shown in Fig. 4 as an example of these spectroscopies.

2.2 Signal processing, data analytics, and reaction mechanisms

In addition to the pressure modulation, we will development methods for data extraction from commercial instruments and proper time stamps, including a mass spectrometer, electron energy analyzer, and IR detector. Synchronized data acquisition and postprocessing fusion of time-stamped data will be explored.

The SBU PI is an expert in signal processing and has ample experience in modeling kinetics of chemical reactions using statistical methods.[10-12] For the project proposed here, the initial test reaction will be the oxidation of carbon monoxide ($CO+O_2$),[13-17]. This is arguably the most studied reaction within the surface science literature, and there is extensive material available in the literature. However, there are still conflicting details about the reaction mechanisms. Previously proposed mechanisms will be analyzed in this work using modulation excitation methods. Note that, while modulation excitation was used in combination with other spectroscopies, it has never been implemented for XPS, and there is limited work for IRRAS implementation. Additionally, previous approaches are limited to phase-sensitive detection only and do not explore differences in the shape of modulated signals and modulated system responses, which also carry information related to the reaction kinetics. The possibility of developing methodologies to extract kinetics information from these differences in shapes of modulated responses will be explored as part of this work. One prospect is to develop statistical models that relate the measured spectroscopic signals to the unknown rate constants and time-varying concentrations and to use data-driven methods, such as those from the machine learning literature, to estimate the unknowns of the system.

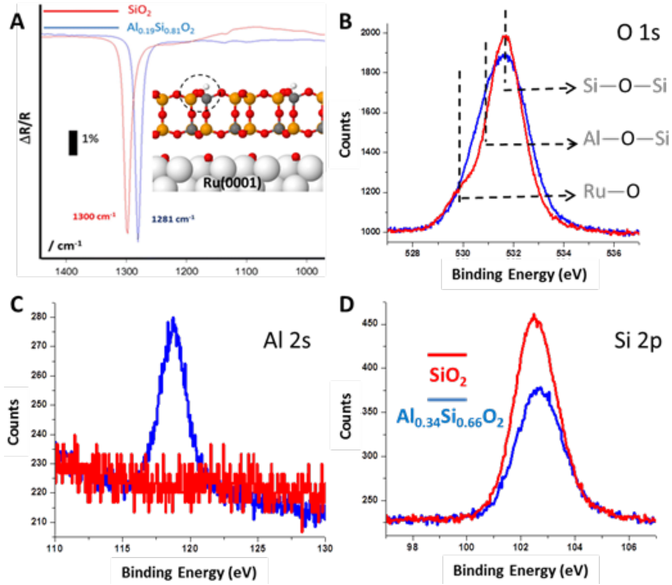

Figure 4. A. IRRA spectra of silicate and aluminosilicate hexagonal bilayer structures on Ru(0001) showing the characteristic phonon vibration associated with the interlayer T-O-T linkage in an aluminosilicate film (T=Si or Al). **B-D**. XPS core level spectra of O 1s, Al 2s and Si 2p regions respectively for silicate and aluminosilicate bilayer frameworks.

3. Project Management, Timeline, and Future Funding

The experimental work will be carried out at the CFN at BNL, by modifying a system currently operating at the BNL PI's lab. Given the different areas of expertise required in this project, funding is requested for two Ph.D. students at 50% effort each. This approach is more practical than have a single student working in parallel on both efforts, since a student that already has experience with surface science instrumentation will be more efficient on the instrument development and reaction experiments. Meanwhile, a second student with expertise in signal processing and data analytics will be more suited for that part of the project. Both PIs have current students, whose schedules can be adjusted to dedicate 50% of their time to the proposed project. Both efforts will start in parallel in July 2020 and extend for the duration of the funding (1.5 years at the requested budget).

The student doing experimental work will be supervised by Boscoboinik while the student working on the signal processing and reaction modeling will be supervised by Bugallo. To accomplish the proposed research project, the PIs and students will hold biweekly meetings. Results from this collaborative research will be disseminated in peer-reviewed journals and at presentations at conferences. After establishing this SBU-BNL SEED proposal research, results will be included in NSF and DOE proposals (Bugallo, SBU) and DOE proposals (Boscoboinik, BNL). On the instrument development side, the data obtained from this project can set the basis for facility upgrade proposals at BNL. The new methodologies developed will also contribute to participation in research centers like Energy Frontier Research Centers (EFRC) and Energy Research Hubs. For example, part of the data obtained from small funding on zeolite model systems resulted in the current participation of the BNL PI in two EFRCs. This project is well-aligned with the missions of SBU and BNL, especially given that the CFN is a user facility whose purpose is to provide cutting-edge instrumentation and methods to the nanoscience user communities. This interdisciplinary proposal will leverage the expertise of the SBU PI in signal processing and mathematical methods for modeling chemical reactions, and the expertise of the BNL PI in surface science instrumentation and heterogeneous catalysis. This interaction will open new avenues for time-resolved surface science spectroscopies. This can have transformative consequences in the understanding of elementary steps in heterogeneously catalyzed reaction mechanisms.

References

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Budget Justification
SBU-BNL RESEARCH INITIATIVES
SEED GRANTS 2020

Proposal title: Developing Methods for Understanding Chemical Kinetics on Surfaces

Proposal budget

The proposed budget is summarized in the following table.

	Amount
Students	
Two graduates student with 50% effort (One Electrical Engineering student and one Materials Science and Chemical Engineering student)	$37,500
Total Salary and Wages	**$37,500**
Fringe Benefits	
Graduate student (18%)	$6,750
Total Fringe	**$6,750**
Total Cost	**$44,250**

The justification of the budget is as follows:

- All the funds will be used to support two graduate students (one in Electrical Engineering one in Materials Science and Chemical Engineering) during the period of the award (18 months) at 50% effort. One of the students will do experimental work under the supervision of A. Boscoboinik, and the second student will develop signal processing algorithms for detection and estimation under the supervision of M. Bugallo. A more detailed description of the students' activities is included in section 3 of the main body of the proposal. Current students with experience relevant to the proposed project will spend 50% of their time toward the work described in this proposal.
- All materials necessary for the experimental part of this project are already available at BNL or included within the scope of the CFN's operating budget.

- The fringe benefit rate is 18% for the graduate student salary.

List of current funding held by the PIs

Jorge Anibal Boscoboinik (BNL)
* DOE EFRC: IMASC. FY19-FY23: $120,000. No overlap.
* DOE EFRC: CCEI. FY19-FY23: $12,000. No overlap.
*SBIR Subcontract. FY20-FY-21: $10,000. Testing of a new pulsing valve (potentially useful for the proposed project).
*ACS PRF Grant. FY21-22: $110,000. Complementary work on hydrocarbon chemistry using gas pulsing techniques.

Mónica Bugallo (SBU):
*NSF: CIF: Small: Advancing Adaptive Importance Sampling for Signal Processing. 6/2016-8/2020: $498,493 (PI)
*NSF: Education, Guidance, Advancement, and Learning in Technology and Engineering (EGALITE). 1/2017-12/2020: $698,666 (PI)
*NSF: E3: Excellence in Engineering Education - A Workshops Series for School Administrators. 8/2018-7/2021. $99,781(PI)
*NSF: Strategies: Engineering Academy: Educating Engineers of the Future. 5/2019-4/2022. $1,193,776 (PI)
*NSF: The State University of New York (SUNY) LSAMP: Meeting the grand challenge of preparing students for successful transition into STEM majors and beyond. 10/2016-9/2021. $3,999,961 (co-PI)

Mónica F. Bugallo

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(a) Professional Preparation

Institution	Location	Major/Area	Degree & Year
Universidade da Coruña	Spain	Computer Science & Engineering	B.S. 1996
Universidade da Coruña	Spain	Computer Science & Engineering	M.S. 1998
Universidade da Coruña	Spain	Signal Processing & Communications	Ph.D. 2001

(b) Appointments

Aug. 2019 – present	• Associate Dean for Diversity & Outreach College of Engineering & Applied Sciences Stony Brook University (SBU), Stony Brook, NY
Aug. 2017 – present	• Professor Department of Electrical & Computer Engineering, Area: Signal Processing Stony Brook University (SBU), Stony Brook, NY
Sept. 2016 – present	• Faculty Director of Women In Science and Engineering (WISE) Honors College of Engineering & Applied Sciences Stony Brook University (SBU), Stony Brook, NY
Aug. 2010 – Jul. 2017	• Associate Professor Department of Electrical & Computer Engineering, Area: Signal Processing Stony Brook University (SBU), Stony Brook, NY
2012 2012 – present	• Chair of Excellence Adjunct Faculty Department of Signal Theory & Communications Universidad Carlos III de Madrid, Spain
Sept. 2004 – Jul. 2010	• Assistant Professor Department of Electrical & Computer Engineering, Area: Signal Processing Stony Brook University (SBU), Stony Brook, NY
Jan. 2002 – Aug. 2004	• Lecturer Department of Electrical & Computer Engineering, Area: Signal Processing Stony Brook University (SBU), Stony Brook, NY
1996 – 2001	• Research Associate Department of Electronics & Systems Universidade da Coruña (Spain)

(c) Products

Authored and co-authored two book chapters and more than 190 journal and refereed conference papers.

- **Products related to the proposed project**

1. Y. El-Laham, V. Elvira, and M. F. Bugallo, "Robust covariance adaptation in adaptive importance sampling," Signal Processing Letters, vol. 25, July 2018.
2. D. Luengo, L. Martino, V. Elvira, M. F. Bugallo, "Efficient linear fusion of partial estimators," Digital Signal Processing, vol. 78, July 2018.
3. M. F. Bugallo, V. Elvira, L. Martino, D. Luengo, J. Míguez, and P. M. Djurić, "Adaptive importance sampling: The past, the present, and the future," IEE Signal Processing Magazine, vol. 34, July 2017.

4. I. Urteaga, M. F. Bugallo, and P. M. Djurić, "Sequential Monte Carlo for inference of latent ARMA time-series with innovations correlated in time," EURASIP Journal on Advances in Signal Processing, vol. 17:84, December 2017.
5. M. F. Bugallo, L. Martino, and J. Corander, "Adaptive importance sampling in signal processing," Digital Signal Processing, vol. 47, December 2015.

- **Other significant products**

6. M. F. Bugallo and A. M. Kelly, "Engineering outreach: Yesterday, today, and tomorrow," IEEE Signal Processing Magazine, vol. 34, May 2017.
7. V. Elvira, L. Martino, D. Luengo, and M. F. Bugallo, "Improving population Monte Carlo: Alternative weighting and resampling schemes," Signal Processing, vol. 131, February 2017.
8. J. P. Beaudeau, M. F. Bugallo, and P. M. Djurić, "RSSI-based multi-target tracking by cooperative agents using fusion of cross-target information," IEEE Transactions on Signal Processing, vol. 63, October 2015.
9. M. F. Bugallo, A. M. Kelly, and M. Ha, "Impact of a university-based electrical and computer engineering summer program for high school students," International Journal of Engineering Education, vol. 31, January 2015.
10. M. F. Bugallo and P. M. Djurić, "Statistical signal processing models and methods for cancer stem formation and evolution," Handbook on Bio- and Neuro-Informatics. By N. Kasabov and D. Mandić (Eds.), Springer, 2014.

(d) Synergistic Activities

Dr. Bugallo research interests are in the area of statistical signal processing with applications to different fields including communications, sensor networks, astronomy or biology. Her recent research also focuses on engineering education and on making engineering available to broader and diverse audiences.

1. She is the Chair of the EURASIP Theoretical and Methodological Trends in Signal Processing Technical Area Committee, the vice-Chair (Chair elect) of the IEEE Signal Processing Theory and Methods (SPTM) Technical Committee, and a member of the IEEE Women in Signal Processing Subcommittee. She was the past Chair of the IEEE Signal Processing Society Education Committee. She is Senior Associate Editor of the IEEE Signal Processing Letters and Associate Editor of the IEEE Transactions on Signal Processing and the EURASIP Digital Signal Processing.
2. Professional recognition for research, teaching and service includes the Ada Byron Professional Career Award from the Galician Computer Engineering Society (2019), the SUNY Chancellor's Award for Excellence in Teaching (2017), the Higher Education Resource Services (HERS) Clare Boothe Luce (CBL) Scholarship Award (2017), the National Science Foundation (NSF) Career Award (2010-2016), the IEEE Athanasios Papoulis Award Long Island Chapter (2011), and the IEEE Outstanding Young Engineer Award Long Island Chapter (2009).
3. She was the general co-Chair of the 2019 EUSIPCO and 2014 IEEE SAM Workshop (both in A Coruña, Spain); Financial Co-Chair of the 2019 IEEE CAMSAP Workshop (Guadeloupe, France); Publications Co-Chair of the 2020 IEEE ICASSP Conference (Barcelona, Spain); and Chair for Educational Activities of the 2021 IEEE ICASSP Conference (Toronto, Canada).
4. As Faculty Director of WISE Honors, she created a formal four-year undergraduate curriculum designed to promote academics, research, service and leadership. She is also the faculty advisor of the Society of Women Engineers (SWE) and mentor of students on engineering career paths.
5. She is the director of the Engineering Summer Camps and Engineering Teaching Laboratories at Stony Brook University, offered to middle and high school students. She has also created engineering professional development opportunities for school counselors, teachers and school administrators.

Jorge **Anibal** Boscoboinik
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Education

01.24.2011 – 09.30.2013	**Post-Doc./A. von Humboldt Fellow.** Fritz-Haber Institute of the Max-Planck Society. Berlin, Germany.
09.01.2005 – 12.19.2010	**PhD Chemistry**. University of Wisconsin Milwaukee. Milwaukee, United States.
03.01.2000 – 06.17.2005	**Licenciado en Química**. Universidad Nacional de San Luis. San Luis, Argentina.
03.01.2000 – 07.10.2003	**Analista Químico**. Universidad Nacional de San Luis. San Luis, Argentina.

Employment

10.01.2018 – current	**Materials Scientist.** Center for Functional Nanomaterials. Brookhaven National Laboratory. Upton, NY, United States.
10.01.2015 – 09.30.2018	**Associate Materials Scientist.** Center for Functional Nanomaterials. Brookhaven National Laboratory. Upton, NY, United States.
10.07.2013 – 09.30.2015	**Assistant Materials Scientist.** Center for Functional Nanomaterials. Brookhaven National Laboratory. Upton, NY, United States.
08.15.2005 – 01.15.2011	**Teaching and Research Assistant**. University of Wisconsin Milwaukee. Milwaukee, WI, United States.
02.01.2005 – 07.31.2005	**Quality and Development Analyst**. Kimberly Clark Corp. Buenos Aires, Argentina.

Research Interests:

1. Surface Science Methods
2. Chemistry in Confined Spaces
3. Two-dimensional porous nanomaterials

Teaching:

2015 - 2019

Course: Advanced Synchrotron Techniques and Electron Spectroscopy of Materials. *Taught at Stony Brook University, Yale University, Columbia University, and online to various universities abroad.*

Students an postdocs

Past postdocs: Dr. JianQiang Zhong, Dr. John Kestell. Past Ph.D. Students: Dr. Nusnin Akter, Dr. Mengen Wang. Present Ph.D. students: Zubin Darbari, Chen Zhou, Yixin Xu, Angela Norton. Present Postdocs: Matheus Dorneles de Mello.

Selected Publications (10 out of 82)

1. M. Wang, C. Zhou, N. Akter, W.T. Tysoe, **J.A. Boscoboinik***, D. Lu. Mechanism of the Accelerated Water Formation Reaction under Interfacial Confinement. *ACS Catal.* ***2020***, accepted, DOI: 10.1021/acscatal.9b05289.

2. M. Karatok, K. Duanmu, C.R. O'Connor, **J.A. Boscoboinik**, P. Sautet, R.J. Madix, C. Friend. Tuning reactivity layer-by-layer: Formic Acid Activation on Ag/Pd(111). *Chem. Sci.,* **2020**, DOI: 10.1039/D0SC01461C.
3. J. Fu, J. Lym, W. Zheng, K. Alexopoulos, A.V. Mironenko, N. Li, **J.A. Boscoboinik**, D. Su, R.T. Weber, D.G. Vlachos. C–O bond activation using ultralow loading of noble metal catalysts on moderately reducible oxides. *Nat. Catal.* **2020**, 152, 084705, DOI: 10.1038/s41929-020-0445-x.
4. X. Sun, W. Zhu, D. Wu, C. Li, J. Wang, Y. Zhu, X. Chen, **J.A. Boscoboinik**, R. Sharma, G. Zhou. Surface-reaction induced structural oscillations in the subsurface. *Nat. Commun.* **2020**, DOI: 10.1038/s41467-019-14167-1.
5. J.A. Boscoboinik*: Chemistry in confined space through the eyes of surface science—2D porous materials. *J. Phys.: Condens. Matter* **2019**, 31, 063001, DOI: 10.1088/1361-648X/aaf2ce.
6. J.-Q. Zhong,M. Wang, N. Akter, J.D. Kestell, T. Niu, A.M. Boscoboinik, T. Kim, D.J. Stacchiola, Q. Wu, D. Lu, **J.A. Boscoboinik***: Ionization-Facilitated Formation of Two-Dimensional (Alumino)silicate-Noble Gas Clathrate Compounds. *Adv. Funct. Mater.* **2019.** DOI:10.1002/adfm.201806583.
7. J.-Q. Zhong, M. Wang, W.H. Hoffmann, M.A. van Spronsen, D. Lu, **J.A. Boscoboinik***: Synchrotron-based ambient pressure X-ray photoelectron spectroscopy of hydrogen and helium. *Appl. Phys. Lett.* **2018**, 112, 091602, DOI: 10.1063/1.5022479.
8. J.-Q. Zhong, M. Wang, N. Akter, J.D. Kestell, A.M. Boscoboinik, T. Kim, D. J. Stacchiola, D. Lu, **J. A. Boscoboinik***: Immobilization of single argon atoms in nano-cages of two-dimensional zeolite model systems. *Nat. Commun.* **2017**. DOI: 10.1038/ncomms16118.
9. J.D. Kestell, K. Mudiyanselage, X. Ye, C.-Y. Nam, D. Stacchiola, J. Sadowski, **J.A. Boscoboinik***: Stand-alone polarization-modulation infrared reflection absorption spectroscopy instrument optimized for the study of catalytic processes at elevated pressures. *Rev. Sci. Inst.*, **2017**, 88, 105109, DOI: 10.1063/1.5007024.
10. J.D. Kestell, J.-Q. Zhong, M. Shete, I. Waluyo, J.T. Sadowski, D. J. Stacchiola, M. Tsapatsis, **J.A. Boscoboinik*:** Studying Two-Dimensional Zeolites with the Tools of Surface Science: MFI Nanosheets on Au(111). *Catal. Today,* **2016**, DOI: 10.1016/j.cattod.2016.07.015.

Awards, Fellowships, etc.

10.18.2016	Visiting Professor. Universidad Nacional de San Luis. San Luis, Argentina.
11.08.2012	A.T. Kearney Fellowship for the Falling Walls Conference. Talk Presented at Falling Walls Lab: *"Breaking the Wall of The thinnest clay".*
03.14.2011	Humboldt Fellowship for Post-Doctoral Researchers for project: "*Synthesis and nano-scale characterization of ordered thin film zeolites by surface science techniques*".

Recent Invited Talks

12.12.2019	*"Looking at Silicates Through the Eyes of Surface Science: A Story of Struggle, Incompatibility, Compromise, Hope, ... and Curiosities". **Center for Functional Nanomaterials** Colloquium series, Brookhaven National Laboratory, Upton, NY.*
07.03.2019	*"Surface Science Model Systems for Zeolites (and other interesting things found along the way)". **University of Oslo**, Oslo, Norway.*

06.25.2019	*"Exploring Confinement Effects in Supported Nanoporous Silicates". **Fritz-Haber Institute of the Max-Planck Society**, Berlin, Germany.*
04.01.2019	*"Two-dimensional (alumino)silicate-noble gas clathrates formation mechanism". **Spring ACS National Meeting**, Orlando, FL.*
11.09.2018	*"Confinement Effects in Two Dimensional Silicates". **University of Wisconsin Milwaukee**, Milwaukee WI.*
11.02.2018	*"Research Opportunities using Two-Dimensional Silicates". **SBU Materials Science Colloquium**, Stony Brook, NY.*
10.15.2018	*"Ultra-thin two-dimensional crystalline nanoporous coatings as cathode protection layers". **Photocathode Physics for Photoinjectors** 2018, Santa Fe, NM.*
09.19.2018	*"Ambient Pressure XPS Studies of Two-Dimensional Zeolite Models". **IOS Beamline SAC review**, NSLS-II, BNL.*
06.07.2018	*"Confinement of Noble Gas Atoms in Two-dimensional Zeolite Models". **San Luis VI conference**, Santa Fe, Argentina.*
05.08.2018	*"Exploring 2D-Nanoporous Materials with Operando Tools at BNL". **BNL Science Council Meeting**, BNL.*
03.18.2018	*"Two-dimensional models for surface science studies of zeolites". **ACS Spring National Meeting**, New Orleans, LA.*
12.13.2017	*"Exploring Nanomaterials with AP-XPS". **AP-XPS Workshop**, Shanghai, China.*
11.07.2017	*"Ambient Pressure XPS at Brookhaven National Laboratory and First Studies on 2D-Zeolite Model Systems". **British Petroleum Workshop**, IL, USA.*
10.03.2017	*"Exploring 2D-Nanoporous Materials with Ambient Pressure Photoelectron Spectroscopy". **ALS User's Meeting**, Berkeley, CA, USA.*
08.07.2017	*"Surface Science Studies of Nanoporous Materials: Zeolite Model Systems and Zeolite Nanosheets". **GREEN-NIMS**, Tsukuba, Japan.*
08.03.2017	*"2D-Zeolites, their study with surface science tools, and some potential applications". **L'Oreal Japan**, Tokyo, Japan.*
08.01.2017	*"Understanding Nanoporous Materials with the Tools of Surface Science". **NGO NIMS Workshop**, Tsukuba, Japan.*
04.02.2017	*"Looking at zeolites through the eyes of surface science". 253rd **ACS National Meeting** in San Francisco, CA, USA.*
04.21.2017	*"Surface Science Techniques for the Study of Two-Dimensional Nanoporous Materials".* **University of Delaware**, DE, USA.

Synergistic Activities

• Reviewer for: J. Am. Chem. Soc., Angew. Chem., Rev. Sci. Inst., Catal. Lett., J. Phys. Chem. C., Catal. Today., J. Phys. Chem. Lett., Top. Catal., Micropor. Mesopor. Mater., Surf. Sci., Physica A, ACS Catal., Nat. Commun., etc.
• Founder of the Surface Science Network in 2009. An initiative aiming to create an interactive community among people that work in fields related to surface science. Website: www.surfacesciencenetwork.com
• General organizer of the San Luis International Conference and Summer School on Surface Science and Heterogeneous Catalysis. www.surfacecatalysis.org
• Regular organizer of symposia related to heterogeneous catalysis and ambient pressure surface science methods at American Chemical Society National Meetings.
• Co-organizer of workshops at the CFN-NSLS-II users' meeting in 2015 and 2018.
• Guest Editor, Special Issue in Springer journal "Topics in Catalysis", in 2019.