DOE EPSCoR Implementation Program DE-FG02-08ER46530 – FINAL REPORT
Title: ***"Materials for Energy Conversion: Materials for Energy Conversion and Storage"***

Lead organization: **The University of New Mexico, Albuquerque, NM 87131**

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Participating National Laboratories: Los Alamos National Labororatoty – LANSCE as facility

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Project Summary

The main objective of this collaborative research project was to identify a formulation and develop a catalyst for electro-oxidation of ethanol. Ethanol is one of the most mass-produced biofuels, and such catalysts will enable the development of Direct Ethanol Fuel Cell technology and through it, will interconnect fuel cells with biofuels.

Several **catalysts for direct electrochemical oxidation of ethanol** have been selected on the principles of rational design from the knowledge built in studying aqueous oxidation of ethanol. The program involved fundamental study of ethanol oxidation in liquid media, and particularly in alkaline solutions. The lessons learned from the heterogeneous catalysis of ethanol thermal oxidation have been applied to the design of an electrocatalyst for direct ethanol fuel cells. The successful chemical compositions are based on PdZn and NiZn allows. The studies reveled the role of the transition metal oxide phase as a co-catalyst and the role of the active support material. To complete the set of materials for ethanol fuel cell, this program also invested in the development of **catalysts for oxygen reduction** that are selective against alcohol oxidation. Non-platinum catalysts based on pyrolyzed macrocycles or similar composites have been studied. This program included also the development of structured supports as an integral part of the catalyst development. A new family of materials has been designed based on mesoporous silica templating with synthetic carbon resulting in hierarchically porous structure. Structure-to-property relationship of catalysis and catalysts has been the center of this program. This have been engaged in both surface and bulk level and pursued with the tools available at the academic institutions and at LANSCE at LANL. The structural studies have been built in interaction with a computational effort on the basis of DFT approach to materials structure and reactivity.

Description of Accomplishments of the NM DOE EPSCoR Implementation Program

An energy-related research consortium, created under this program, brought together scientists from across New Mexico to work on four specific collaborative research projects, building knowledge and contributing to the engineering of materials for energy conversion and storage. This came as an answer to the increased recognition of our need to tap alternative sources to meet our energy needs, as we move away from our dependence on crude oil. Under this program the universities across the State of New Mexico has developed particular strengths in energy related materials research. UNM Center for Emerging Energy Technologies (CEET) was formed at UNM as a research organization with a mission to foster interdisciplinary research in this strategic area of science and engineering. It is a goal of this center to provide for the economic growth of the sate in the area of energy technology and to participate in the training and preparation of the labor force through providing environment of research excellence and pursuit of advanced degree. This center is also charted to provide services to the state of New Mexico as place to grow multi-institutional research. CEET has been the organization that provided home to this program. CEET has also the mission to promote collaborations with the National Laboratories and industry. Several DOE, NSF and DOD programs resulted from the research carried out under the DOE-EPSCoR Implementation award (see list bellow).

This research program contributed to addressing the basic energy science question on what are the fundamental limits and enabling principles for the use and integration of molecular and material structures at atomic level, nano-scale, and macroscopic restrictions that such limitations impose on systems that transfer and transduce energy. This research had an overall objective to contribute to the establishing of the physical limits of resulting power generating processes and efficiency for energy conversion from alternative fuels such as ethanol. Understanding and controlling such energy transfer processes at multiple length scales will have great benefit to technology, resulting in high efficiency conversion of chemical, thermal or solar energy into electrical or chemical energy. The science and engineering targets for this program has been focused on synthesis and understanding of structure-to-property relationships for several classes of materials: catalysts and electroctalysts. New catalysts and catalyst architectures are viewed as key thrusts to address critical technical challenges in many renewable energy fields. Performance and durability of catalysts in biorefinery operations, fuel cells, electrolyzers, and reformers certainly limit the economic viability of many sustainable energy processes and systems. Research among project participants in New Mexico have developed substantial capability in manipulation of catalyst composition, size, dispersion, and nanoscale support structures, as well as the capacity to evaluate catalyst kinetics, performance and durability from lab to bench scale operations. There were two general areas of research supported through this proposal: 1) nanoscale composite catalytic architectures and 2) evaluation of catalysis systems for biofuels (ethanol) processing and reforming.

A particular objective of this research program was to provide fuel cell technology with materials embedding desired chemical functionality and designed for performance based on matching the transport process length-scale with that of the material's structure. As an example, a templated method for non-platinum catalysts synthesis developed at UNM is based on deposition of the precursor (usually a metal chelate complex) on non-carbon dispersed carrier (mono-dispersed, amorphous silica, average particle size of 30-40 nm), followed by pyrolysis of the compound and by chemical extraction (removal) of the carrier. Pyrolysis is then carried out in an inert atmosphere at temperatures from 600° to 800° C. The silica support is then dissolved in KOH solution. The resulting pyropolymer/metal cluster catalyst is a highly dispersed, self-supported nano-composite. This method has produced the most active non-platinum electrocatalysts to date, which have been independently evaluated at LANL. Our effort under this collaborative research program will focus on the development of catalysts with superior stability. A materials-design approach based on the mechanistic lessons learned from the structure-to-property-relations study was applied to address these issues. Investigatations included the effect of transition metal (Co or Fe), chemical derivates of porphyrins and temperature profile during pyrolysis on the operational stability of the catalysts. The research effort will also include development of catalyst materials with hierarchical porosity (in collaboration with Datye and Ward) and polymer-modified catalyst composites for enhanced gas transport through spray pyrolysis and plasma deposition (in collaboration with Weinkauf and Ward).

The most important achievement of the DOE-EPSCoR Implementation Award extension was the clarification of the ethanol electrooxidation reactivity and selectivity and product formation in alkaline and acidic electrolytes. The extension to acidic electrolytes was made based on a specific concern raised by one of the project evaluators. The University of New Mexico team focused on investigations of three specific electrocatalyst classes for ethanol oxidation in both acidic and alkaline media, with an emphasis on establishing and comparing the reaction mechanism for electro-oxidation of ethanol in different pH regimes. This work resulted in synthesis and *ex-situ* characterization of catalysts, as well as electrochemical performance evaluation and *in-situ* electrochemical spectrometry using Fourier Transform Infrared Reflection Adsorption Spectroscopy (FTIRRAS). The catalysts have been evaluated for thermal activity under variable-pH Aqueous Phase Reforming (VpAPR) to differentiate thermal from electrochemical reactions observed. The effect of local pH changes due to the formation of reaction products such as carbonate has been investigated through variable pH thermo and electrochemical experiments and transport control of changes in pH will be determined using fluid modeling coupled with experiments utilizing hierarchical structured supports that provide multimodal porosity. The three classes of catalysts, which were investigated include:

1. Traditional supported Pt-alloy catalysts reflecting state of the art and "benchmarks" such as PtRu and PtSn. Both un-supported (nanostructured) and carbon-supported catalysts will be evaluated and compared. Most of these exist as samples, so the actual work will focus on their electrochemical evaluation and spectroscopy to build structure-to-property relationships.
2. Ternary systems reflecting advanced state of the art ethanol oxidation catalyst as established by BNL (R. Adzic group) and the UNM "equivalent" that replaces Pt with Pd.
   The role of Ru and Rh and the role of SnO_2 and NbO_2 will be compared. Synthetic attempt will be made in scale-up (to gram amounts) of the BNL $PtRhSnO_x/C$ abd UNM $PdRuNbO_x/C$ catalyst (coordinated with BNL).
3. Well-defined nanostructured bimetallic catalysts that will be used to demonstrate reactivity and understand the ternary catalyst systems and catalyst/support interactions for the traditional catalysts. The catalysts selected also reflect the need to shift from Pt-based catalysts for acidic environments to Pd-based catalysts for alkaline environments.

This program worked on the development of Non-Platinum Group Metal (Non-PGM) catalysts for Oxygen Reduction Reaction (ORR) by UNM, NEU, MSU and UTK in collaboration with LANL as technology validator and BASF and Nissan as industrial partners. UNM has introduced a new method for catalysts synthesis: the Sacrificial Support Method (SSM) that allows fabrication of a controlled porosity self supported catalysts by templating. Non-PGM catalysts were obtained by infiltration of silica particles obtained either by aerosol synthesis or micro-emulsion templating, or commercially available silica particles with defined diameter, with the catalysts precursors. The materials mix is then pyrolyzed under inert atmosphere and the silica particles are dissolved (etched out) with KOH or HF solution. The resulting templated catalysts powder retains hierarchical structure of the silica particles upon which it was synthesized. Such hierarchical structures are advantageous in enhancement of the fuel cell performance since they correspond to the different levels of transport in the corrugated electrode matrixes. We have demonstrated this templating approach on Porphyrins and other ligand-forming compounds are catalyst precursors. A wide variety of materials have been made over the last two years by these methods in which not only the composition but also the microstructure has been varied.

UNM have developed methods for synthesizing monodisperse mesoporous silica particles and silica particles with bimodal porosity by templating of surfactant micelles and nanoemulsion droplet phase (3 issued US patents). The monodispersity of the mesoporous silica particles was achieved by fabricating well-defined equally sized emulsion droplets using a microfluidic approach. The droplets contain the silica precursor/surfactant solution and are suspended in hexadecane as the continuous oil phase. The solvent is then expelled from the droplets, leading to concentration and micellization of the surfactant. At the same time, the silica solidifies around the surfactant structures, forming equally sized mesoporous particles. In a parallel line of research we derived theoretical model for the potential capillary driven flow in expanding porous materials. The results from this research were published in a series of papers listed below. We have published several articles that describe in details the experimental methods for synthesis of the porous particles and their characterization by various methods. Our work includes theoretical analysis of the stability of small micro and nanodroplets against coalescence and model for capillary driven flow in porous materials with expanding shape.

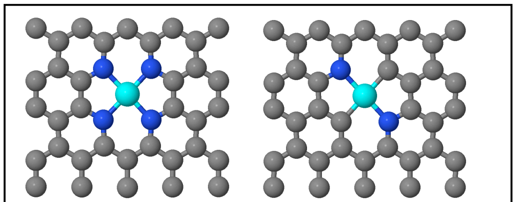

Fig. 1: Model systems for TM-N_x defects in carbon supported ORR electrocatalyst. Left: TM-N_4 defect; right: TM-N_2 (TM= Ni, Co, Fe; x=2, 4).

The main research thrust at NMSU was in using computational materials science methods (Density-Functional-Theory, DFT) to explore mechanistic aspects of the non-PGM electrocatalysts. The main focus was the exploration of nitrogen coordinated transition metals (TM-N_x; TM=Ni, Co, Fe; x=2, 4) defect motif in relation to ORR. The carbon support was integrated in to the computations be embedding the defects into a single carbon sheet (Fig. 1). Computed properties include key indicators for the performance analysis such as adsorption energies for oxygen, peroxide, and other reaction intermediates. The results contributed significantly to the cohesiveness of the program. Here is a list of some of the key results:

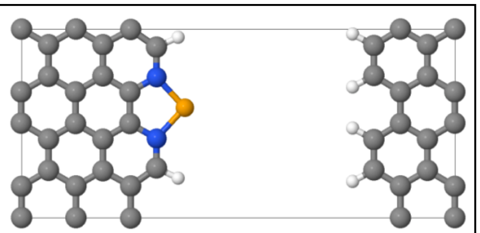

Fig. 2: Model systems for Ni-N2 edge defect in carbon supported ORR electrocatalyst.

In-plane graphitic defects in Ni-N_x are predicted to be inactive for ORR. Thus, ORR occurs only at edge defects. Further computations corroborated that edge Ni-N_2 defects are ORR active. The analysis of the magnetic properties showed that the ORR edge defect is the only defect that carries a magnetic moment. Thus, magnetic measurements such as Moessbauer spectroscopy can be used to evaluate if this defect is indeed present in the electrocatalyst (Kattel et al. 2012).

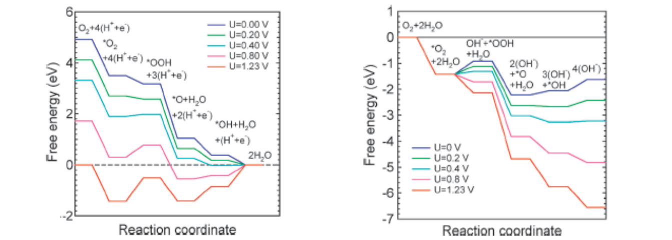

Fig. 3: Free-energy diagrams for Co-N_2 model electrocatalyst. Left: acidic medium (pH=1); right: alkaline medium (pH=14).

In-plane graphitic defects in Co-N_x are ORR active. Free-energy diagram were computed for cases with and without applied potential. The results show that formation energies of the defects are exothermic, hence they are predicted to be thermodynamically stable, which contrasts to the corresponding metal free defects which are thermodynamically unstable (Kattel et al., 2011) and if present in the ORR electrocatalyst need to be kinetically stabilized. Therefore the transition metal stabilizes nitrogen defects. The Co-N_4 defects are predicted to be most stable which suggests that they remain thermodynamically favorable up to high potentials (U~1.5 V) which encompasses the voltage range expected to occur in fuel cells (Kattel et al., 2013). The analysis of the interactions of Co-N_x defects shows that ORR occurs on Co-N_4 via a 2x2e process and requires a distinct second site for the reduction of peroxide. In contrast, ORR occurs on Co-N_2 defects as a single site 2x2e process. Finally the free-energy diagrams (Fig. 3) provide a rational for the observed increased performance of Co-N_x catalysts in alkaline conditions as compared to acidic conditions: Under alkaline conditions ORR is a downhill process while in acidic medium several uphill processes occur. Thus, Co-N_x is predicted to perform better in alkaline medium as compared to acidic medium, consistent with experimental observations (Kattel et al., 2013).

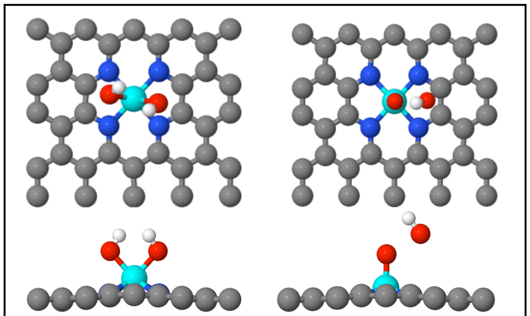

Fig. 3: Peroxide O-O splitting on Fe-N_4 defect motif. Left column: top view and side view of H_2O_2; right column: top view and side view of OOH.

The corresponding graphitic Fe-N_x family of defect motifs is overall predicted to behave similar to the Co-Nx family with one important difference: For Fe-N_4 defect ORR is predicted to occur as a 2x2e process on a single site. This difference is attributed to the O-O bond scission of peroxide (Fig. 4), which did not occur on the Co-N_4 defect motif. As for the Co-N_x defect we find downhill processes at potentials relevant for ORR under alkaline conditions.

In essence DFT computations continue to provide new insights for the understanding of mechanistic aspects of fuel cells. The computations provide detailed insights into the thermochemistry of ORR for a wide range of TM-N_x (TM=Ni, Co, Fe; x=2, 4) defects and enables us to assess catalyst behavior under alkaline and acidic conditions. In particular the results provide a rational for the experimentally reported order of increased ORR performance: Ni < Co < Fe as well as the observation that the catalysts are more ORR active in alkaline media.

This work resulted in numerous publictaions and several issued US patents. A large number of graduate and undergraduate students were supported and exposed to the work through internships. This resulted in several cases of graduate recruitment and career advancement in all involved faculty.

List of Publictaions Resulting from the NM DOE EPSCoR Implementation Program - 54

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T.S. Olson, B. Blizanac, S.Pylypenko, B. Piela, J.R. Davy, P. Zelenay and P. Atanassov, Electrochemical Evaluation of Porous Non-Platinum Oxygen Reduction Catalysts for Polymer Electrolyte Fuel Cells, *Fuel Cells*, 9 (2009) 547-553

E. Switzer, T.S. Olson, A. K. Datye, P. Atanassov, M.R. Hibbs and C.J. Cornelius Templated Pt-Sn Electrocatalysts for Ethanol, Methanol and CO Oxidation in Alkaline Media, *Electrochimica Acta* 54 (2009) 989-995

Intellectual Property Resulting from the NM DOE EPSCoR Implementation Program

Filed Provisional Patent Applications - 6

P. Atanassov, B. Halevi, A. Datye, C. Leclerc, B. Roy, PdZn Intermetallic Alloy Catalysts for Alcohol Oxidation, Water Gas Shift, Reverse Water Gas Shift, Methane Oxidation, and Ethanol Synthesis, *Provisional Application* 61/623,726 filed on April 13, 2012 (UNM 2012-089)

A. Serov, U. Martinez, P. Atanassov, Promotion Effect of Oxides in Oxidation of Fuels for Fuel Cell Applications, *Provisional Application* 61/608,718 filed on March 9, 2012 PCT/US13/30151 (UNM 2012-083)

A. Serov, B. Halevi, U. Martinez, M. Padilla, A. Falase, M. Visitacion, K. Artyushkova, P. Atanassov, Silver-based Catalyst for Effective Oxidation of Organic and Inorganic Fuels, *Provisional Application* 61/538,184 filed on September 23, 2011 (UNM 2012-021)

W. Patterson, P. Atanassov, A. Serov, C. Walker, Hierarchically Structured Carbonaceous Materials Derived from Microemulssion Templating, *Provisional Application* 61/535,408 filed with the USPTMO on September 16, 2011 (UNM 2012-016)

B. Kiefer, S. Kattel, P. Atanassov, Material Template for High-Density Data Storage, *Provisional Application* 61/516,068 filed on March 29, 2011 (UNM 2011-066)

2012-089-01 PDZN Intermetallic Alloy Catalysts for Alcohol Oxidation, Water Gas Shift, Reverse Water Gas Shift, Methane Oxidation, and Ethanol Synthesis 61/623,726 Provisional Filed4/13/2012 United States.

US Patents Filed at Different stages of Prosecution – 5

W. Patterson, P. Atanassov, K. Artyushkova, B. Halevi, M. Robson, A. Serov, C. Walker, Structured Cathode Catalysts for Fuel Cell Application Derived from Metal-Nitrogen-Carbon Precursors, Using Hierarchically Structured Silica as a Sacrificial Support, *US Patent Application* 12/55974 filed with the USPTMO on September 17, 2012 (UNM 2012-015)

B. Halevi, C. Lau, M. Robson, A. Serov, B. Kiefer, A. Datye, P. Atanassov, Biomimetic Inspired Structured Mixed Oxides for Oxygen Electro-Reduction, *US Patent Application* 13/270,854 filed on October 11, 2011 (UNM 2010-124)

B. Halevi, T. Olson, S. Pylypenko, A. Datye, P. Atanassov, U. Martinez, Binary Metallic Allows for Electro-Oxidation in alkaline Media and Method of Making the Same, *US Patent Application* 13/178,420 filed on July 7, 2011 PCT/US/11/43241 (UNM 2010-113)

S. Pylypenko, N. Carroll, P. Atanassov, D.N.Petsev, Fabrication of Monidispersed Oxide Particles with Bimodal Porosity Derived from Simultaneous Templating with Microemulsion Droplets and Surfactant Micelles, *US Patent Application* 13/161,302 filed on June 15, 2011 (UNM 2009-142)

2011-038-02 Synthesis of Pd particles by alcohols-assisted photoreduction for use in supported catalysts, 13/344,462 Utility Filed 1/5/2012 United States Datye Abhaya.

Issued US Patents - 4

D.N. Petsev, A. Ortiz, N. Carroll, P. Atanassov, S. Pylypenko, Monodispersed Particles Fabricated by Microfluidic Device, *US Patent Number* 9,260, 311, February 16, 2016 (UNM 2009-142-DIV)

D.N. Petsev, A. Ortiz, N. Carroll, P. Atanassov, S. Pylypenko, Monodispersed Particles Fabricated by Microfluidic Device, *US Patent Number* 8,911, 864, December 16, 2014 (UNM 2009-142)

S. Pylypenko, N. Carroll, P. Atanassov, D.N. Petsev, Microparticles with Hierarchical Porosity, *US Patent Number* 8,334,014, December 18, 2012 (UNM 2008-089 CIP)

A. Datye, E. Switzer, P. Atanassov, S. Pylypenko, T. Olson, D. Konopka, T. Ward, Spray Pyrolysis Synthesis of Mesoporous NbRuOx as Electrocatalyst Support for Fuel Cells, *US Patent Number* 8,333,94, December 18, 2012 (UNM 2006-094)

List of Personnel Working of the NM DOE EPSCoR Implementation Program:

Total of 19 graduate students and 19 undergraduate students involved/graduated;
Total of 9 postdoctoral fellows trained and 9 research faculty/scientists involved;
Total of 9 participating tenured/tenure track faculty members from 4 NM universities.

UNM Graduate Students – 8

Daniel Konopka **Prof. T.L. Ward**	Research Assistant, IGERT Project: *Novel Supports for Electrocatalysts for Fuel Cells*	PhD	ChE	Started Fall 2006 Graduated Fall 210
Bayo Falase	Research Assistant, IGERT Project: *Glycerol Fuel Cells*	PhD	ChE	Started Spring 2009 Graduated Fall 2011
Michael Robson	Research Assistant (PSM) Project: *Cathode Catalysis for Alkaline Membrane Fuel Cells*	PhD	NSMS	Started Fall 2009 Graduated Fall 2012
Ulises Martinez **Prof. A. Datye**	Research Assistant, NSF-GRF Project: *Ethanol Oxidation Catalysts for Fuel Cells*	PhD	ChE	Started Summer 2009 Graduated Fall 2012
Sarah Stariha	Research Assistant Project: *Design of Membrane Electrode Assemblies*	PhD	ChE	Started Fall 2012 Graduated Spring 2016
Nalin Andersen	Research Assistant *Complex Oxide Catalysts*	MS	NSMS	Started Summer 2012, Project: Graduated Fall 2013
Sadia Kabir **Prof. B. Kiefer**	Research Assistant Project: *DFT of Non-PGM Catalysts*	MS	ChE	Started Fall 2012, Graduated Fall 2013
Aaron Roy **Prof. T.L. Ward**	Research Assistant Project: *Synthesis of Non-carbon Supports*	MS	ChE	Started Fall 2011, Graduated Fall 2013

NMSU Gradute Students - 3

Shyam Kattel (New Mexico State University, Department of Physics)
Fulltime support, 01/2010 – 07/2012. Graduated with PhD in 08/2012

Joe Peterson (New Mexico State University, Department of Physics)
Part time support, Graduated with PhD in 05/2013

Manjita Shresta (New Mexico State University, Department of Physics)
Fulltime support, MS degree: 05/2013

NMSU Graduate Students - 6

Srikanth Challa, "Fabricating through-Hole Anodic Aluminum Oxide on Aluminum for Gold Electrodeposition", MS thesis, completed in fall 2013

Erynn J. Swigonski, "In-situ Reflectance Spectroscopy for Ethanol Oxidation in Alkaline Media on Palladium Based Electrocatalysts", MS thesis, completed in fall 2011

Chandra Guntakandla, "Simultaneous Chromatographic Detection and Quantitation of Carbonate and Acetate Ions in the Electro-Oxidation of Ethanol in Alkaline Media on Palladium Based Electrodes", MS thesis, completed in summer 2013

Venkat Devireddy, "Electrochemical Studies of Ethanol Oxidation in Alkaline Media on Palladium Electrode", MS thesis, completed in fall 2013

Zhiyang Liu, "Simultaneous Analysis of Carbonate and Acetate in the Oxidation Mixture of Ethanol by Ion Chromatography", MS thesis, completed in fall 2013

Cassandra Marrs, "Ion Chromatographic Analysis of Carbonate and Acetate in the Oxidation Mixture of Ethanol", MS thesis, completed in fall 2014

NMSU Undergraduate students - 3

Lesa Blandin
Cassandra Y. Lazos
Stephen Smith

UNM Undergraduate Students - 14

Claudia Narvaez	Research Assistant	Senior	Chem. Engin.	Fall 2008 – Sumer 2009
Pablo De La Iglesia	Research Assistant	Senior	Chem. Engin.	Spring 2009 – Summer 2010
Candace Walker	Research Assistant		Chem. Engin.	Spring 2010 – Fall 2013
Kristen Garcia	Research Assistant-IMSD		Chem. Engin.	Spring 2010 – Fall 2013
Dharma Voisine	Research Assistant	Junior	Chem. Engin.	Fall 2010 – Summer 2011
Cameron Harrison	Research Assistant	Junior	Chem. Engin.	Fall 2010 – Summer 2011
Santiago Carbonell	Research Assistant	Senior	Chem. Engin.	Spring 2011 – Summer 2011
Corey Rosenthal	Research Assistant	Sophomore	Chem. Engin.	Spring 2011 – Summer 2011
Monica Padilla	Research Assistant	Junior	Chem. Engin.	Spring 2011 – Fall 2013
Sergio Omar Garcia	Research Assistant	Sophomore	Chem. Engin.	Spring 2010 – Fall 201
Michelle Visitacion	Research Assistant	Senior	Chem. Engin.	Summer 2011 – Fall 2012
Mayat Smolnik	Research Assistant	Senior	Chem. Engin.	Spring 2012 – Fall 2013
Edward Jameson	Research Assistant	Senior	Chem. Engin.	Spring 2012 – Summer 2013
Alex Mirabal,	Research Assistant	Senior	Chem. Engin.	Spring 2013–Spring 2014

UNM Postdoctoral Fellows - 5

Svitlana Pylypenko (PhD UNM) **Asst. Prof. Colorado School of Mines, Golden, CO** Fall 2006-Fall 2009

Tim Olson (PhD UNM) **NREL, Golden, CO** Fall 2008-Fall 2009

Wendy Patterson (PhD UNM) **Res. Assoc. Regensburg University, Regensburg, Germany** Fall 2009-Fall 2011

Barr Halevi (PhD University of Pennsylvania) **President and CTO of Pajarito Powder LLC** Spring 2009-2012

Ulises Martinez (PhD Univ. of New Mexico) **Postdoc at LANL, MPA-11** Spring 2013-Fall 2013

UNM Research Faculty / Summer Sabbatical Visiting Faculty - 4

Boris Kiefer (PhD University of Stuttgart) **Assoc. Prof. NMSU, on sabbatical visit** Summer 2009-Summer 2012

Kateryna Artyushkova (PhD Kent State), **Research Associate Professor, Associate Director of CEET** Since 2006

Alexey Serov (PhD University of Bern), **Research Associate Professor** Since 2010

Ivana Mtanovic-Gonzalez (PhD University of Zagreb), **Research Assistant Professor** Since 2013

Tenured Faculty Investigators - 9

Principal Investigator: **Plamen Atanassov**, Professor of Chemical & Nuclear Engineering, Director of UNM Center for Emerging Energy Technologies

Co-Principal Investigator: **Abhaya Datye**, Professor of Chemical & Nuclear Engineering,
Director of UNM Center for Micro-Engineered Materials

Participating Faculty: **Tim Ward**, Professor, Chemical & Nuclear Engineering, UNM
Dimiter Petsev, Professor of Chemical & Nuclear Engineering, UNM

Co-Principal Investigator: **Boris Kiefer,** Professor of Physics, NMSU
Heinz Nakotte, Professor of Physics, NMSU and LANL LANSCE
Igor Sevostianov, Professor of Mechanical Engineering, NMSU

Co-Principal Investigator: **Corey Leclerc**, Professor of Petroleum & Chemical Engineering, NMT

Co-Principal Investigator: **Juchao Yan**, Professor of Chemistry, ENMU

List of Follow on Support Resulting from the NM DOE EPSCoR Implementation Program

- **NSF – Major Research Instrumentation** (MRI) 01/10/09-03/31/11
  Title: "*X-Ray Photoelectron Spectroscopy Surface Characterization Facility*" Amount: $360,000
  This project requests an upgrade of the UNM XPS instrument with a state-of-the- art new tool.

- **DOE – EERE Fuel Cell Technology Program** (University Research Initiative) 03/1/10-06/30/15
  Title: "*Novel Non Pt Group Metal Electrocatalysts for PEMFC*" (S. Mukerjee, NEU, PI) UNM Amount: $970,000
  This Subcontract is a part of a NEU-lead collaborative program with P. Atanassov as the PI of the UNM sub-contract.

- **DOE – EERE Fuel Cell Technology Program** (Business Research Initiative) 03/1/10-02/28/13
  Title: "*Development of Micro-structural Mitigation Strategies for PEMFC*" (S. Wessel, BPS, PI) UNM Amount: $900,000
  This Subcontract is a part of a Ballard-lead collaborative program with P. Atanassov as the PI of the UNM sub-contract.

- **DOE – EERE Hydrogen Storage Program** (NREL Hydrogen Storage Center) 03/1/10-02/28/13
  Title: "*Development of Nano-structured Materials for Hydrogen Storage*" (T. Gannett, NREL, PI) Amount: $50,000
  This subcontract is a part of a NREL-lead collaborative program in hydrogen storage by spill-over.

- **Sandia National Laboratories** (LDRD Sub-contract) 01/24/11-09/30/13
  Title: "*Cathode Catalysts for Anion Exchange Membrane Fuel Cells*" Amount: $195,000
  This is a subcontract to the Sandia NL in the area AEMFC

- **DOE – EERE Fuel Cell Technology Program** (Incubator Program) 06/01/15-05/31/17
  Title: "*Development of non-PGM Catalysts for HOR in Alkaline Media*" (A. Serov, UNM, PI) Amount: $1,000,000
  UNM-lead collaborative program with LANL, Pajarito Powder Co., IRD (nor WII Fuel Cells)

- **DOE – EERE Fuel Cell Technology Program** (Incubator Program) 06/01/15-05/31/17
  Title: "*High Performance PGM-free MEA through Control of Interfacial Process*" (K. Ayers, PI) Amount: $120,000
  This subcontract is a part of a Proton-on-Site-lead collaborative program with P. Atanassov as the UNM Co-PI.

- **DOE – EERE Fuel Cell Technology Program** (Incubator Program) 06/01/15-05/31/17
  Title: "*Innovative Non-PGM Catalysts for CHP Relevant PEMFC*" (S. Mukerjee, NEU, PI) Amount: $160,000
  This subcontract is a part of a NEU-lead program with Advent LLC, FC Energy & PPC P. Atanassov as the UNM Co-PI.

- **Bill & Melinda Gates Foundation** 11/12/15-11/30/17
  Title: "*Efficient Microbial Bio-electrochemical Systems*" Amount: $450,000
  UNM-led contract with sub-award to Bristol Robotics Lab (UK) in MFC for sanitation

- **DOE – EERE Fuel Cell Technology Program** (originally awarded to IIT) 06/01/16-05/31/19
  Title: "*Corrosion-resistant non-carbon support materials for PEFCs*" (V. Ramani, PI) Amount: $853,000
  This is subcontract to Washington University-led program with UNM and Nissan Technical Center North America.

- **DOE – ARPA-E** (awarded to Pajarito Powder Co.) 10/01/16-09/30/19
  Title: "*Precious Metal Free Regenerative Hydrogen Electrode*" (B. Halevi, PI) Amount: $640,000
  This is subcontract to Pajarito Powder Co-led program with UNM, NEU and Proton-on-Site as subcontracts.

- **DOD – ARO SBIR Phase II** (awarded to CFDRC.) 10/01/16-09/30/18
  Title: *"Pulsed Voltammetry Tools for Advanced Analysis of PENFC"* (P. Atanassov, Co-PI) Amount: $100,000

Note: all currently active awards are highlighted in "maroon" font