#### <u>Suljo Linic</u>

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### Education:

West Chester University, PA, BS Physics (minors: Mathematics, Chemistry)	1998
University of Delaware, DE, Ph.D. Chemical Engineering Adviser: Prof. Mark A. Barteau Thesis Title: From fundamental studies to rational catalyst design: a hybrid experimental/theoretical investigation of ethylene epoxidation	2003
Fritz-Haber Institute der Max Planck Gesellschaft	2003 - 2004

Fritz-Haber Institute der Max Planck Gesellschaft,2003 – 2004Berlin, Postdoctoral fellow in Theory Department,Adviser: Prof. Dr. Matthias Scheffler

#### **Academic Appointments:**

2020 - present	Martin Lewis Perl Professor of Chemical Engineering, University of Michigan, Ann Arbor
2017 – present	Associate Chair, Department of Chemical Engineering, University of Michigan, Ann Arbor
2015 - 2019	Hans Fischer Fellow, Chemistry Department, Technical University, Munich
2014 - present	Professor and 1938 Faculty Scholar Professor of Chemical Engineering and Integrative Systems Design, University of Michigan, Ann Arbor
2010 - 2014	Associate Professor of Chemical Engineering, University of Michigan, Ann Arbor
2004 - 2010	Assistant Professor of Chemical Engineering, University of Michigan, Ann Arbor
2003 - 2004	Postdoctoral Fellow, Fritz-Haber Institute der Max Planck Gesellschaft, Berlin

#### Administrative Appointment:

2010 - present

Director, Energy System Engineering Program, College of Engineering, University of Michigan

#### Honors, Awards, Editorial Work

- Martin Lewis Perl Collegiate Professor of Chemical Engineering, 2020
- Xingda Lectureship, Peking University, Beijing, 2019, awarded to the most accomplished international researchers by Peking University Chemistry Division.

- Integrative Systems + Design Department Excellence Award, College of Engineering, University of Michigan, 2018
- Paul H. Emmett Award in Fundamental Catalysis, North American Catalysis Society, 2017; an international flagship award given biennially to the most influential contributors to the field of chemical catalysis below age 45
- Giuseppe Parravano Memorial Award for Excellence in Catalysis Research, Michigan Catalysis Society, 2016
- Associate Editor, ACS Catalysis, 2014 present
- ACS Catalysis Lectureship for the Advancement of Catalytic Science, American Chemical Society, 2014; awarded annually by the ACS Catalysis journal and the Catalysis Science and Technology Division of the American Chemical Society for groundbreaking research strengthening connections among the various sub-disciplines of catalysis and advancing the field of catalysis as a whole
- Hans Fischer Fellowship, 2015 awarded by the Technical University of Munich for the most accomplished international scholars.
- 1938 Faculty Scholar Professorship, University of Michigan, 2014
- Thiele Lectureship, University of Notre Dame, Department of Chemical Engineering, 2013
- Monroe-Brown Foundation Research Excellence Award, University of Michigan College of Engineering, 2012
- Nanoscale Science and Engineering Forum Young Investigator Award, American Institute of Chemical Engineers, 2011; awarded annually in recognition of outstanding interdisciplinary research in nanoscale science and engineering by an engineer or scientist in the early stages of their professional career (within 10 years of completion of highest degree)
- **1938E Award,** University of Michigan College of Engineering, 2010; awarded annually to one junior faculty member for excellence in research, teaching, and service
- Unilever Award, Colloid and Surface Chemistry Division of American Chemical Society, 2009; awarded annually for significant contributions in colloidal and surface chemistry
- **Camille Dreyfus Teacher-Scholar Award,** Camille and Henry Dreyfus Foundation, 2009; awarded annually to talented young faculty for teaching and research contributions to the field of chemical science
- **DuPont Young Professor Award,** DuPont, 2008, awarded worldwide to ~8 10 young faculty addressing global challenges in food, energy, and protection
- Chemical Engineering Department Excellence Award, College of Engineering, University of Michigan, 2008; awarded annually to a faculty member for excellence in research, teaching, and service
- Frontiers in Chemistry Invitee, 2008, approximately 90 promising early career "rising stars" in chemical sciences (30 from each country: U.S., Germany, and Great Britain) were identified by the American Chemical Society (ACS), the German Chemical Society (GDCh) and the Royal Society of Chemistry (RSC) to participate at the symposium.
- National Science Foundation CAREER Award, 2005
- Max Planck Society postdoctoral fellowship, 2003 2004
- Young Scientist Prize, Council of the International Association of Catalysis Societies, 2004; awarded to the most promising young scientists (under age 35) for exceptional research accomplishments

- University of Delaware Competitive Fellowship Award, 2002; awarded to the most accomplished graduate students at the University for academic and thesis work
- Gordon Research Conference Fellowship, 2002
- Department of Chemical Engineering Teaching Fellowship, 2002, University of Delaware
- Robert L. Pigford Outstanding Teaching Assistant Award, 2001, University of Delaware
- Soros Foundation Fellowship, 1995 1998

# **RESEARCH**

**Research Interests:** Fundamental heterogeneous catalysis, Surface chemistry, Electronic structure calculations, Electro-chemical conversion, Photo-chemical conversion

# Research group

# Past members

- Eranda Nikolla, graduated 5/2009, Associate Professor, Wayne State University
- Siris Laursen, graduated 9/2009, Associate Professor, University of Tennessee
- Neil Schweitzer, graduated 11/2010, Research Assistant Professor, Northwestern University
- Phillip Christopher, graduated 8/2011, Associate Professor, University of California, Santa Barbara
- Marimuthu Andiappan, graduated 5/2013, Assistant Professor, Oklahoma State University
- Hongliang Xin, graduated 6/2013, Assistant Professor, Virginia Tech University
- Adam Holewinski, graduated 1/2014, Assistant Professor, University of Colorado Boulder
- David Ingram, graduated 8/2011, Director of Water Purification Technology, Phillips 66
- Thomas Yeh, graduated 4/2015, Staff Scientist, Johnson Matthey
- Matthew Morabito, graduated 12/2015, Development Engineer, Bryan Research and Engineering
- Brittany Lancaster Farrell, graduated 12/2015, R & D Engineer, Clean Power Research
- Timothy Van Cleve, graduated 12/2015, Postdoctoral Associate, National Renewable Energy Laboratory
- Calvin Boerigter, graduated 9/2016, Business Analyst, Amazon
- Paul Hernley, graduated 1/2017, Lead Engineer, Battery Solutions
- Umar Aslam, graduated 8/2018, Research Scientist, Exxon-Mobil
- Vishal Rao, completed postdoctoral training 1/2019, Assistant Professor, Indian Institute of Technology, Kampur, India
- Joseph Quinn, graduated 12/2019 (DOE-PNNL national laboratory)
- Valentina Omoze Igenegbai, graduated 1/2020, Research Engineer, Phillips 66

# **Current Members**

Steven Chavez Sean Dix John Hemmerling Rawan Almallahi Rachel Elias Jacques Esterhuizen James Wortman Shawn Lu Aarti Mathur Yi Zhang Shiuan-Bai Ann Han-Ting Chen Claire Yin Dongho Lee (Postdoctoral Fellow)

# 100+ Undergraduate Students Supervised in Research Projects

### **Publications in higher impact journals**

- reverse chronological order
- corresponding authorship denoted by \*
- undergraduate students underlined
- graduate students double underlined
  - S. Linic\*, <u>S. Chavez, R. Elias</u>, Flow and Extraction of Energy and Charge Carriers in Hybrid Plasmonic Nanostructures, **Nature Materials**, online publication, 2021: (<u>DOI:</u> <u>10.1038/s41563-020-00858-4</u>)
  - <u>U. Aslam</u>, V.G. Rao, <u>S. Chavez</u>, S. Linic\*, Catalytic conversion of solar to chemical energy on plasmonic metal nanostructures, **Nature Catalysis** 1, 656-665, 2018: (DOI: <u>10.1038/s41929-018-0138-x</u>)
  - <u>U. Aslam, S. Chavez</u>, Linic\* S., Controlling Energy Flow in Multimetallic Nanostructures for Plasmonic Catalysis. Nature Nanotechnology 12, 1000-1005, 2017: (<u>DOI:</u> <u>10.1038/nnano.2017.131</u>)
  - <u>C. Boerigter, R. Campana, M. Morabito</u>, S. Linic\*, Evidence and implications of direct charge excitation as the dominant mechanism in plasmon-mediated photocatalysis, Nature Communications, 7: 10545, 2016: (DOI:10.1038/ncomms10545)
  - S. Linic\*, <u>U. Aslam, C. Boerigter, M. Morabito</u>, Chemical reactions on plasmonic metal nanoparticles induced by hot electrons, **Nature Materials**, 14 (6), 567, 2015: (<u>DOI:</u> <u>10.1038/nmat4281</u>)
  - <u>A. Holewinski</u>, J.C. Idrobo, S. Linic\*, High performance Ag-Co alloy catalysts for electrochemical oxygen reduction, **Nature Chemistry**, 6 (9), 828, 2014: (<u>DOI:</u> <u>10.1038/nchem.2032</u>)
  - <u>M. Andiappan</u>, S. Linic\*, Tuning selectivity in propylene epoxidation by plasmon mediated photo-switching of Cu oxidation state, Science, 339, 1590, 2013: (<u>DOI:</u> <u>10.1126/science.1231631</u>)

- 8. <u>P. Christopher, H. Xin, M. Andiappan</u>, S. Linic\*, Singular characteristics and unique chemical bond activation mechanisms of photocatalytic reactions on plasmonic nanostructures, **Nature Materials**, **11**, 1044, 2012: (<u>DOI: 10.1038/nmat3454</u>)
- S. Linic\*, <u>P. Christopher, D.B. Ingram</u>, Plasmonic-metal nanostructures for efficient conversion of solar to chemical energy, **Nature Materials**, **10**, 911, 2011: (<u>DOI:</u> <u>10.1038/nmat3151</u>)
- <u>P. Christopher, H. Xin</u>, S. Linic\*, Visible-light-enhanced catalytic oxidation reactions on plasmonic silver nanostructures, **Nature Chemistry**, 3, 467, 2011: (<u>DOI:</u> <u>10.1038/nchem.1032</u>)

# **Peer-reviewed publications**

- reverse chronological order
- corresponding authorship denoted by \*
- undergraduate students underlined
- graduate students double underlined

http://scholar.google.com/citations?hl=en&user=99XfGykAAAAJ&view\_op=list\_works)

# Published

- S. Linic\*, <u>S. Chavez, R. Elias</u>, Flow and Extraction of Energy and Charge Carriers in Hybrid Plasmonic Nanostructures, **Nature Materials**, online publication, 2021: (<u>DOI:</u> <u>10.1038/s41563-020-00858-4</u>)
- S. Dix, S. Lu, S. Linic\*, Critical Practices in Rigorously Assessing the Inherent Activity of Nanoparticle Electrocatalysts, ACS Catalysis, 10, 10735–10741, 2020 (DOI: 10.1021/acscatal.0c03028)
- 3. <u>J.A. Esterhuizen</u>, Bryan R. Goldsmith\*, and Suljo Linic\*, Theory-guided Machine Learning Finds Geometric Structure-property Relationships for Chemisorption on Alloys, **Chem**, 1 (11), 3100-3117, 2020, (<u>DOI: 10.1016/j.chempr.2020.09.001</u>)
- J. Hemmerling, J. Quinn, S. Linic, Quantifying Losses and Assessing the Photovoltage Limits in Metal-Insulator-Semiconductor Water Splitting Systems, Advanced Energy Materials, 1903354R3, 2020: (DOI: 10.1002/aenm.201903354)
- J. Quinn, J. Hemmerling, S. Linic\*, Guidelines for Optimizing the Performance of Metal– Insulator–Semiconductor (MIS) Photoelectrocatalytic Systems by Tuning the Insulator Thickness, ACS Energy Letters, 4 (11), pp 2632-2638, 2019: (DOI: 10.1021/acsenergylett.9b01609)
- <u>V.O. Igenegbai, R. Almallahi</u>, R.J. Meyer, S. Linic\*, Oxidative Coupling of Methane over Hybrid Membrane/Catalyst Active Centers: Chemical Requirements for Prolonged Lifetime, ACS Energy Letters, 4 (6), pp 1465-1470, 2019: (<u>DOI:</u> <u>10.1021/acsenergylett.9b01075</u>)

- <u>S. Chavez, V.G. Rao</u>, S. Linic\*, Unearthing the factors governing site specific rates of electronic excitations in multicomponent plasmonic systems and catalysts, Faraday Discussions, 214, 441-453, 2019: (DOI: 10.1039/C8FD00143J)
- S.D. Minteer\*, P. Christopher, S. Linic, Recent Developments in Nitrogen Reduction Catalysts: A Virtual Issue, ACS Energy Letters 4 (1), pp 163-166, 2019: (DOI: 10.1021/acsenergylett.8b02197)
- <u>V.G. Rao, U. Aslam</u>, S. Linic\*, Chemical requirement for extracting energetic charge carriers from plasmonic metal nanoparticles to perform electron-transfer reactions, Journal of American Chemical Society, 141, 647, 2019: (DOI: 10.1021/jacs.8b11949)
- <u>P.A. Hernley</u>, S. Linic\*, Modeling the Impact of Metallic Plasmonic Resonators on the Solar Conversion Efficiencies of Semiconductor Photoelectrodes: When Does Introducing Buried Plasmonic Nanostructures Make Sense?, Journal of Physical Chemistry C, 122(42), pp 24279-24286, 2018: (DOI: 10.1021/acs.jpcc.8b07214)
- 11. <u>U. Aslam, V.G. Rao, S. Chavez</u>, S. Linic\*, Catalytic conversion of solar to chemical energy on plasmonic metal nanostructures, **Nature Catalysis** 1, 656-665, 2018: (DOI: 10.1038/s41929-018-0138-x)
- <u>V.O. Igenegbai</u>, R.J. Meyer, S. Linic\*, In search of membrane-catalyst materials for oxidative coupling of methane: Performance and phase stability studies of gadoliniumdoped barium cerate and the impact of Zr doping, Applied Catalysis B: Environmental, 230. 29-35, 2018: (DOI 10.1016/j.apcab.2018.02.040)
- <u>S. Chavez, U. Aslam</u>, S. Linic\*, Design Principles for Directing Energy and Energetic Charge Flow in Multicomponent Plasmonic Nanostructures. ACS Energy Letters 3 (7), pp 1590-1596, 2018: (DOI: 10.1021/acsenergylett.8b00841)
- 14. S. Linic, Report from the Chemical Sciences and Society Meeting Focusing on Future Challenges in Photocatalysis, ACS Catalysis, 8 (4), pp 3357-3357, 2018: (DOI: 10.1021/acscatal.8b00907)
- G. Kumar, E. Nikolla, S. Linic, J.W. Medlin, M.J. Janik, Multicomponent Catalysts: Limitations and Prospects, ACS Catalysis 8 (4) pp. 3202-3208. 2018: (DOI: 10.1021/acscatal.8b00145)
- J. Quinn, J. Hemmerling, S. Linic\*, Maximizing Solar Water Splitting Performance by Nanoscopic Control of the Charge Carrier Fluxes across Semiconductor-Electrocatalyst Junctions, ACS Catalysis 8 (9) pp 8545-8552, 2018: (DOI: 10.1021/acscatal.8b01929)
- 17. S. Linic, The 2017 Chemical Sciences & Society Summit Report, invited editorial in Chemical and Engineering News 13, 96, 2018: <u>https://cen.acs.org/energy/solar-power/2017-Chemical-Sciences-Society-Summit/96/i13</u>
- <u>U. Aslam, S. Chavez</u>, Linic\* S., Controlling Energy Flow in Multimetallic Nanostructures for Plasmonic Catalysis. **Nature Nanotechnology** 12, 1000-1005, 2017: (<u>DOI:</u> <u>10.1038/nnano.2017.131</u>)
- 19. <u>U. Aslam</u>, S. Linic\*, Addressing challenges and scalability in the synthesis of thin uniform metal shells on large metal nanoparticle cores: Case study of Ag-Pt core-shell nanocubes,

ACS Applied Materials & Interfaces 9 (49), 43127-43132, 2017: (DOI: 10.1021/acsami.7b14474)

- <u>P. Hernley, S. Chavez, J. Quinn</u>, S. Linic\*, Engineering the Optical and Catalytic Properties of Co-Catalyst/Semiconductor Photocatalysts, ACS Photonics 4 (4), 979-985, 2017: (DOI: <u>10.1021/acsphotonics.7b00047</u>)
- <u>T. Van Cleve, S. Moniri, G. Belok</u>, K. More, S. Linic\*, Nanoscale Engineering of Efficient Oxygen Reduction Electro-Catalysts by Tailoring Local Chemical Environment of Pt Surface Sites, ACS Catalysis, 7, 17, 2017: (DOI: 10.1021/acscatal.6b01565)
- S. Moniri, S. Linic\*, Pitfalls and best practices in measurements of the electrochemical surface area of platinum-based nanostructured electro-catalysts, J. of Catalysis, 345, 1, 2017: (DOI: 10.1016/j.jcat.2016.11.018)
- J.G. Chen\*, C.W. Jones\*, S. Linic\*, V.R. Stamenkovic\*, Best Practices in Pursuit of Topics in Heterogeneous Electrocatalysis, ACS Catalysis 7, 6392-6393, 2017: (DOI: <u>10.1021/acscatal.7b02839</u>)
- 24. <u>U. Aslam</u>, S. Linic\*, Kinetic trapping of immiscible metal atoms into bimetallic nanoparticles through plasmonic visible light-mediated reduction of a bimetallic oxide precursor: Case study of AgPt nanoparticle synthesis, **Chemistry of Materials**, 28(22), 8289, 2016: (DOI:10.1021/acs.chemmater.6b03381)
- 25. <u>C. Boerigter, U. Aslam</u>, S. Linic\*, Mechanism of charge transfer from plasmonic nanostructures to chemically attached materials, **ACS Nano**, 10 (6), 6108, 2016: (<u>DOI:</u> <u>10.1021/acsnano.6b01846</u>)
- <u>B. Lancaster Farrell, V. O.Igenegbai, S. Linic\*</u>, A viewpoint on direct methane conversion to ethane and ethylene using oxidative coupling on solid catalysts, ACS Catalysis, 6 (7), 4340, 2016: (<u>DOI: 10.1021/acscatal.6b01087</u>)
- 27. <u>H. Xin</u>, S Linic\*, Analyzing relationships between surface perturbations and local chemical reactivity of metal sites: alkali promotion of O2 dissociation on Ag (111), **Journal of Chemical Physics**, 144, 234704, 2016: (<u>DOI:10.1063/1.4953906</u>)
- <u>C. Boerigter, R. Campana, M. Morabito</u>, S. Linic\*, Evidence and implications of direct charge excitation as the dominant mechanism in plasmon-mediated photocatalysis, Nature Communications, 7, 2016: (<u>DOI:10.1038/ncomms10545</u>)
- <u>B. Lancaster Farrell</u>, S. Linic\*, Oxidative coupling of methane over mixed oxide catalysts designed for solid oxide membrane reactors, Catalysis Science and Technology, 6, 4370, 2016: (DOI: 10.1039/c5cy01622c)
- <u>B. Lancaster Farrell</u>, S. Linic\*, Direct electrochemical oxidation of ethanol on SOFCs: Improved carbon tolerance of Ni anode by alloying, Applied Catalysis B: Environmental, 183, 386, 2016: (DOI: 10.1016/j.apcatb.2015.11.002)
- <u>T. Van Cleve, E. Gibara</u>, S. Linic\*, Electrochemical oxygen reduction reaction on Ag nanoparticles of different shapes, ChemCatChem, 8 (1), 256, 2016: (DOI: <u>10.1002/cctc.201500899</u>)
- 32. S. Chang, P. Fornasiero, T.B. Gunnoe, C.W. Jones, S. Linic, R.M. Williams, H. Zhao, ACS Catalysis and the scope of papers sought in three catalysis subdisciplines: biocatalysis and

enzymology, molecular catalysis for organic synthesis, and heterogeneous photocatalysis, **ACS Catalysis**, 6 (7), 4782, 2016: (<u>DOI:10.1021/acscatal.6b01749</u>)

- S. Linic\*, <u>U. Aslam, C. Boerigter, M. Morabito</u>, Chemical reactions on plasmonic metal nanoparticles induced by hot electrons, **Nature Materials**, 14 (6), 567, 2015: (<u>DOI:</u> <u>10.1038/nmat4281</u>)
- <u>T.M. Yeh, R.L. Hockstad</u>, S Linic\*, PE Savage\*, Hydrothermal decarboxylation of unsaturated fatty acids over PtSnx/C catalysts, Fuel, 156, 219, 2015: (DOI: 10.1016/j.fuel.2015.04.039)
- <u>A. Holewinski</u>, J.C. Idrobo, S. Linic\*, High performance Ag-Co alloy catalysts for electrochemical oxygen reduction, **Nature Chemistry**, 6 (9), 828, 2014: (<u>DOI:</u> <u>10.1038/nchem.2032</u>)
- <u>T. Yeh</u>, S. Linic\*, P.E. Savage\*, Deactivation of Pt catalysts during hydrothermal decarboxlation of butyric acid, ACS Sustainable Chemistry and Engineering, 2(10), 2399, 2014: (DOI: 10.1021/sc500423b)
- S. Linic\*, <u>P. Christopher, H. Xin, A. Marimuthu</u>, Catalytic and photocatalytic transformations on metal nanoparticles with targeted geometric and plasmonic properties, Accounts of Chemical Research, 46 (8), 1890, 2013: (<u>DOI: 10.1021/ar3002393</u>)
- <u>M. Andiappan</u>, S. Linic\*, Tuning selectivity in propylene epoxidation by plasmon mediated photo-switching of Cu oxidation state, Science, 339, 1590, 2013: (DOI: <u>10.1126/science.1231631</u>)
- <u>A. Holewinski, H. Xin, E. Nikolla, S. Linic\*</u>, Identifying optimal active sites for heterogeneous catalysis by metal alloys based on molecular descriptors and electronic structure engineering, **Current Opinion in Chemical Engineering**, 2 (3), 312, 2013: (DOI: 10.1016/j.coche.2013.04.006)
- <u>T.M. Yeh</u>, J.G. Dickinson, A. Franck, S. Linic\*, L.T. Thompson\*, P.E. Savage\*, Hydrothermal catalytic production of fuels and chemicals from aquatic biomass Journal of Chemical Technology and Biotechnology 88 (1), 13, 2013: (DOI: 10.1002.jctb.3933)
- 41. <u>P. Christopher, H. Xin, M. Andiappan</u>, S. Linic\*, Singular characteristics and unique chemical bond activation mechanisms of photocatalytic reactions on plasmonic nanostructures, **Nature Materials**, **11**, 1044, 2012: (<u>DOI: 10.1038/nmat3454</u>)
- 42. <u>A. Holewinski</u>, S. Linic\*, Elementary mechanisms in electrocatalysis: revisiting the ORR Tafel slope, **Journal of Electrochemical Society**, 159, H864, 2012: (DOI: 10.1149.2.022211jes)
- M. Andiappan, P. Christopher, S. Linic\*, Design of plasmonic platforms for selective molecular sensing based on surface enhanced Raman spectroscopy, Journal of Physical Chemistry C, 116, 9824, 2012: (DOI: 10.1021/jp301443y)
- 44. <u>H. Xin, A. Holewinski, N. Schweitzer, E. Nikolla</u>, S. Linic\*, Electronic structure engineering in heterogeneous catalysis: identifying novel alloy catalysts based on rapid screening for materials with desired electronic properties, **Topics in Catalysis**, 55, 376, 2012: (DOI: 10.1007/s11244-012-9794-2)

- 45. <u>H. Xin, A. Holewinski</u>, S. Linic\*, Predictive structure-reactivity models for rapid screening of Pt-based multimetallic electrocatalysts for the oxygen reduction reaction, **ACS Catalysis**, 2, 12, 2012: (<u>DOI: 10.1021/cs200462f</u>)
- S. Linic\*, <u>P. Christopher, D.B. Ingram</u>, Plasmonic-metal nanostructures for efficient conversion of solar to chemical energy, **Nature Materials**, **10**, 911, 2011: (<u>DOI:</u> <u>10.1038/nmat3151</u>)
- 47. <u>P. Christopher, H. Xin</u>, S. Linic\*, Visible-light-enhanced catalytic oxidation reactions on plasmonic silver nanostructures, **Nature Chemistry**, 3, 467, 2011: (<u>DOI:</u> <u>10.1038/nchem.1032</u>)
- <u>D. B. Ingram, P. Christopher</u>, <u>J. Bauer</u>, S. Linic\*, Predictive model for the design of plasmonic metal/semiconductor composite photocatalysts, ACS Catalysis., 1, 1441, 2011: (<u>DOI: 10.1021/cs200320h</u>)
- <u>D. B. Ingram</u>, S. Linic\*, Water splitting on composite plasmonic-metal/semiconductor photo-electrodes: evidence for selective plasmon-induced formation of charge carriers near the semiconductor surface, **Journal of the American Chemical Society**, 133, 5202, 2011: (DOI: 10.1021/ja200086g)
- 50. <u>N. Schweitzer</u>, J. Schaidle, E. Obiefune, X. Pan\*, S. Linic\*, L. Thompson\*, High activity carbide supported catalysts for water gas shift, **Journal of the American Chemical Society**, 133, 2378, 2011: (<u>DOI: 10.1021/ja110705a</u>)
- 51. S. Linic\*, <u>P. Christopher</u>, Overcoming limitation for the design of selective heterogeneous catalysts by manipulating shape and size of catalytic particles: Expoxidation reactions on silver (Ag), **ChemCatChem**, 2, 1061, 2010: (<u>DOI: 10.1002/cctc.201000163</u>)
- 52. <u>H. Xin</u>, S. Linic\*, Exceptions to the d-band Model of Chemisorption on Metal Surfaces: The Dominant Role of Repulsion between Adsorbate States and Metal d-states, **Journal** of Chemical Physics, 132, 221101, 2010: (DOI: 10.1063/1.3437609) Selected for 2010 Editors' Choice list highlighting "notable JCP articles published in 2010 that present ground-breaking research"
- <u>P. Christopher, D.B. Ingram,</u> S. Linic\*, Enhancing photo-chemical activity of semiconductor nanoparticles with optically active Ag nano-structures: Photo-chemistry mediated by Ag surface plasmons, **Journal of Physical Chemistry C**, 114, 9173, 2010: (<u>DOI: 10.1021/jp101633u</u>)
- <u>H. Xin, N. Schweitzer, E. Nikolla</u>, Suljo Linic\*, Developing relationships between the local chemical reactivity of alloy catalysts and physical Characteristics of Constituent Metal Elements, Journal of Chemical Physics, 132, 111101, 2010: (DOI: 10.1063/1.3336015)
- 55. <u>P. Christopher</u>, S. Linic\*, Shape and size specific chemistry of Ag nanostructures in catalytic ethylene epoxidation, **ChemCatChem**, 78, 2, 2010: (<u>DOI:</u> <u>10.1002/cctc.200900231</u>)
- 56. <u>N. Schweitzer, H. Xin, E. Nikolla</u>, Suljo Linic\*, Establishing relationships between the geometric structure and chemical reactivity of alloy catalysts based on their measured electronic structure, **Topic in Catalysis**, 53, 348, 2010: (<u>DOI: 10.1007/s11244-010-9448-1</u>)

- 57. <u>E. Nikolla</u>, J. Schwank, S. Linic\*, Direct electrochemical oxidation of hydrocarbon fuels on SOFCs: improved carbon tolerance of Ni alloy anodes, **Journal of Electrochemical Society**, 156(11), B1312, 2009: (<u>DOI: 10.1149/1.3208060</u>)
- <u>D. Ingram</u>, S. Linic\*, First-principles analysis of the activity of transition and noble metals in the direct utilization of hydrocarbon fuels at solid oxide fuel cell operating conditions, Journal of Electrochemical Society, 156(12), B1457, 2009: (DOI: 10.1149/1.3240101)
- 59. <u>S. Laursen</u>, S. Linic\*, Geometric and electronic characteristics of active sites on TiO2supported Au nano-catalysts: insights from first principles, **Physical Chemistry Chemical Physics**, 11, 11006, 2009: (DOI: 10.1039/b912641d)
- 60. <u>S. Laursen</u>, S. Linic, Strong chemical interactions between Au and off-stoichiometric defects on TiO<sub>2</sub> as a possible source of chemical activity of nano-sized Au adsorbed on the oxide, **Journal of Physical Chemistry C**, 113, 6689–6693, 2009: (<u>DOI:</u> 10.1021/jp810603u)
- 61. <u>E. Nikolla</u>, J. Schwank, and S. Linic\*, Measuring and relating the electronic structures of non-model supported catalytic materials to their performance, **Journal of the American Chemical Society**, 131 (7), 2747, 2009: (<u>DOI: 10.1021/ja809291e</u>)
- 62. <u>E. Nikolla</u>, J. Schwank, and S. Linic\*, Comparative study of the kinetics of methane steam reforming on supported Ni and Sn/Ni alloy catalysts: the impact of the formation of Ni alloy on chemistry, **Journal of Catalysis**, 263, 220, 2009: (<u>DOI:</u> <u>10.1016/j.jcat.2009.02.006</u>)
- J. Carlson, F. Henke, S. Linic\*, M. Scheffler\*, Two-step mechanism for low temperature oxidation of vacancies in graphene, Physical Review Letters, 102, 166104, 2009: (DOI: 10.1103/PhysRevLett.102.166104)
- 64. <u>P. Christopher</u>, S. Linic\*, Engineering selectivity in heterogeneous catalysis: Ag nanowires as selective ethylene epoxidation catalysts, **Journal of the American Chemical Society**, 130, 34, 11264, 2008: (DOI: 10.1021/ja803818k)
- <u>E. Nikolla</u>, J. Schwank, and S. Linic\*, Hydrocarbon steam reforming on Ni alloys at solid oxide fuel cell operating conditions, Catalysis Today, 136, 243, 2008: (<u>DOI:</u> <u>10.1016/j.cattod.2008.03.028</u>)
- <u>E. Nikolla</u>, J. Schwank, S. Linic\*, Promotion of the long-term stability of reforming Ni catalysts by surface alloying, Journal of Catalysis, 250(1), 85, 2007: (<u>DOI:</u> <u>10.1016/j.jcat.2007.04.020</u>)
- 67. <u>J. Mukherjee</u>, S. Linic\*, First principles investigations of electrochemical oxidation of hydrogen at solid oxide fuel cell operating conditions, **Journal of the Electrochemical Society**, 154(9), B919, 2007: (DOI: 10.1149/1.2752983)
- 68. <u>E. Nikolla, A. Holewinski</u>, J. Schwank, S. Linic\*, Controlling carbon surface chemistry by alloying: carbon tolerant reforming catalyst, **Journal of the American Chemical Society**, 128(35); 11354, 2006: (<u>DOI: 10.1021/ja0638298</u>)
- <u>S. Laursen</u>, S. Linic\*, Oxidation catalysis by oxide-supported Au nanostructures: the role of supports and the effect of external conditions, **Physical Review Letters**, 97 (2), 026101, 2006: (DOI: 10.1103/PhysRevLett.97.026101)

- M. Enever, S. Linic, <u>K. Uffalussy</u>, J.M. Vohs and M.A. Barteau\*, Synthesis, structure and reactions of stable oxametallacycles from styrene oxide on Ag(111), Journal of Physical Chemistry B, 109, 2227, 2005: (<u>DOI: 10.1021/jp048939k</u>)
- S. Linic\*, M.A. Barteau\*, On the mechanism of Cs promotion in ethylene epoxidation on Ag, Journal of the American Chemical Society, 126, 8086, 2004: (DOI: 10.1021/ja048462q)
- S. Linic, H. Piao, K. Adib, M.A. Barteau\*, Ethylene epoxidation on Ag: identification of the crucial surface intermediate by experimental and theoretical investigation of its electronic structure, Angewandte Chemie International Edition, 43, 2918, 2004: (DOI: <u>10.1002/anie.200353584</u>)
- 73. S. Linic, J. Jankowiak, M.A. Barteau<sup>\*</sup>, Selectivity driven design of bimetallic ethylene epoxidation catalysts from first principles, **Journal of Catalysis (Priority Communication)**, 224, 489, 2004: (DOI: 10.1016/j.jcat.2004.03.007)
- 74. S. Linic, M.A. Barteau<sup>\*</sup>, Construction of a reaction coordinate and a microkinetic model for ethylene epoxidation on silver from DFT calculations and surface science experiments, **Journal of Catalysis**, 214, 200, 2003: (DOI: 10.1016/S0021-9517(02)00156-2)
- 75. S. Linic\*, M.A. Barteau\*, Control of ethylene epoxidation selectivity by surface oxametallacycle, **Journal of the American Chemical Society**, 125, 4034, 2003: (DOI: 10.1021/ja029076g)
- 76. S. Linic, M.A. Barteau\*, Formation of a stable surface oxametallacycle that produces ethylene oxide, Journal of the American Chemical Society, 124, 310, 2002: (DOI: 10.1021/ja0118136)
- 77. S. Linic, J.W. Medlin, M.A. Barteau, Synthesis of oxametallacycles from 2-iodoethanol on Ag (111) and the structure dependence of their reactivity, Langmuir, 18, 5197, 2002: (DOI: 10.1021/la011783k)

#### **Invited book chapters and publications:**

- 1. <u>E. Nikolla</u>, S. Linic\*, From Molecular Insights to Novel Catalysts," Chapter 13 in Model Systems in Catalysis: Single Crystals to Supported Enzyme Mimics, ed by R. Rioux, Springer, pp. 275-292, 2010.
- 2. S. Linic\*, M.A. Barteau\*, "*Heterogeneous Catalysis of Alkene Epoxidation*," *Chapter* 14.11.6 in the Handbook of Heterogeneous Catalysis, 2<sup>™</sup> edition, volume 7, G. Ertl, H. Knözinger, F. Schüth, J. Weitkamp (eds.), Wiley-VCH, pp. 3448-3464, 2008.

# Patents

- 1. UM 4082: Highly Selective Catalysts for Epoxidation of Ethylene to Form Ethylene Oxide. US Patent No. 7,820,840
- 2. UM 4414: Nanostructures for Photo-Catalytic Applications. US Patent Application No. 12/800,294

3. UM 4719: Plasmon Driven Chemical Reaction. Provisional Patent Application No. 61/346,771

#### **Invited and Keynote Lectures at Meetings and Workshops**

reverse chronological order

- 1. 4<sup>a</sup> International Congress of Chemists and Technologists of Bosnia and Herzegovina, "Electrochemistry on metal alloys," Sarajevo, Bosnia and Herzegovina, October 2020 (postponed until 2021).
- 2. Bridging the Gap: Nano Meets Quantum workshop by the Munich-based Center for NanoScience (CeNS), "Hybrid plasmonic: what governs energy and charge movement" Venice International University (VIU), Venice, Italy, September 2020.
- Politecnico di Milano and Boreskov Institute of Catalysis International ChemReactor Conference, "Oxidative coupling of methane over membrane/catalysts reacting systems," Milan, Italy, September 2020
- 4. Gordon Research Conference on Catalysis, "Metal-insulator-semiconductor material platforms as water spiting photocatalysts," Colby-Sawyer College, New London, NH, June 2020
- 5. American Institute of Chemical Engineers National Meeting, "Electronic Structure Engineering in Heterogeneous Catalysis: From Simple Analytical to Machine Learnt Models of Chemisorption on Alloys," Orlando, FL, November 2019
- 6. American Chemical Society Fall National Meeting, "Electronic Structure Engineering in Heterogeneous Catalysis: from Simple Analytical to Machine Learnt Models of Chemisorption on Alloys," ACS Catalysis Lectureship for the Advancement of Catalytic Science: Symposium in Honor of Maria Flytzani-Stephanopoulos and Charles Sykes, San Diego, CA, August 2019
- American Chemical Society Spring National Meeting, "Direct Methane Conversion to Ethylene and Ethane by Oxidative Coupling in Membrane/Catalysts Reacting Systems," Orlando, FL, April 2019
- 8. American Chemical Society Spring National Meeting, "Maximizing Efficiencies of Photocatalytic Water Splitting by Engineering Interfaces in Multi-component Photocatalysts," Orlando, FL, April 2019
- American Chemical Society Spring National Meeting, "Nanoscale Engineering of Efficient Oxygen Reduction Electrocatalysts by Tailoring the Local Chemical Environment to Pt Surface Sites," Orlando, FL, March 2019
- 10. Chemistry As Innovating Science (CHAINS) Conference, "Photocatalysis on plasmonic metal nanostructures," Veldhoven, Netherlands, December 2018
- 11. Materials Research Society Annual Meeting, "Controlling Energy Flow in Plasmonic Photocatalysis Through the Design of Hybrid Plasmonic Nanostructures for Selective Catalysis," Boston, MA, November 2018

- 12. American Institute of Chemical Engineers National Meeting, "Maximizing Efficiencies of Photocatalytic Water Splitting By Engineering Interfaces in Multi-Component Photocatalysts," Pittsburgh, PA, October 2018
- American Chemical Society Fall National Meeting, "Controlling energy flow in plasmonic photocatalysis through the design of hybrid plasmonic nanostructures," Boston, MA, August 2018
- 14. American Chemical Society Fall National Meeting, "Nanoscale engineering of efficient oxygen reduction electrocatalysts by tailoring the local chemical environment of Pt surface sites," Boston, MA, August 2018
- 15. Electrochemical Society Spring National Meeting, "Nanoscale Engineering of Efficient Oxygen Reduction Electrocatalysts by Tailoring the Local Chemical Environment of Pt Sites," Seattle, WA, May 2018
- 16. Electrochemical Society Spring National Meeting, "Controlling Energy Flow in Plasmonic Photocatalysis through the Design of Hybrid Plasmonic Nanostructures," Seattle, WA, May 2018
- 17. Electrochemical Society Spring National Meeting, "Maximizing Efficiencies of Photocatalytic Water Splitting by Engineering Interfaces in Multi-Component Photocatalysts," Seattle, WA, May 2018
- 18. American Chemical Society Spring National Meeting, "Nanoscale engineering of Efficient Oxygen Reduction Electrocatalysts by Tailoring the Local Chemical Environment of Pt Surface Sites," Finding Our Place at the Bottom: A Symposium in Memory of Richard Feynman, New Orleans, LA, March 2018
- 19. American Chemical Society Spring National Meeting, "Controlling energy flow in plasmonic photocatalysis through the design of hybrid plasmonic nanostructures," New Orleans, LA, March 2018
- 20. MOLIM workshop "Molecules in Motion: Multiscale Modelling From Quantum Effects to Material Properties" at the Nanoscale Graz University of Technology, Institute of Experimental Physics, "Controlling Energy Flow in Plasmonic Catalysis," Graz, Austria, February 2018
- 21. Workshop on Fundamentals of Catalysis, "Analysis of the mechanism of electrochemical oxygen reduction and development of Ag- and Pt-alloy catalysts for low temperature fuel cells," Munich, Germany, November 2017
- 22. American Institute of Chemical Engineers National Meeting, celebrating Prof. Israel Wachs' AIChE R. H. Wilhelm Award in Chemical Reaction Engineering, "Analysis of the mechanism of electrochemical oxygen reduction and development of Ag- and Pt-alloy catalysts for low temperature fuel cells," Minneapolis, MN, November 2017
- 23. CS3 Summit at Dalian (China), "The CO2 problem and potential catalytic solutions," Dalian, China, September 2017
- 24. American Chemical Society Fall National Meeting, "Analysis of the mechanism of electrochemical oxygen reduction and development of Ag- and Pt-alloy catalysts for low temperature fuel cells," Washington, DC, August 2017

- 25. Emmett Award Lecture, Biannual meeting North American Catalysis Society, "Catalysis on plasmonic nanostructures," Denver, CO, July 2017
- 26. Gordon Research Conference on Plasmon Energy Transfer, "Photocatalysis on plasmonic metal nanostructures," The Chinese University of Hong Kong, Hong Kong, July 2017
- 27. Materials Research Society Annual Meeting, "Photocatalysis on plasmonic metal nanostructures: known knowns and known unknowns about hot electron distribution," Phoenix, AZ, April 2017
- 28. Materials Research Society Annual Meeting, "Analysis of the mechanism of electrochemical oxygen reduction and development of Ag- and Pt-alloy catalysts for low temperature fuel cells," Phoenix, AZ, April 2017
- 29. Pittcon Conference of Analytical Chemistry NH, "Photocatalysis on plasmonic metal nanostructures," Chicago, IL, March 2017
- 30. 4th Thomas Young Centre TOUCAN Energy Materials Workshop, "Analysis of the mechanism of electrochemical oxygen reduction and development of Ag- and Pt-alloy catalysts for low temperature fuel cells," King's College London, December 2016
- 31. U.S. Department of Energy Conference on Scientific Opportunities for Ultrafast Hard Xrays at High Repetition Rate: An Energy Upgrade of LCLS-II "Catalysis on metals," Stanford Linear Accelerator Center (SLAC), Stanford University, Menlo Park, CA, September 2016
- 32. Gordon Research Conference on Catalysis, "Analysis of the mechanism of electrochemical oxygen reduction and development of Ag- and Pt-alloy catalysts for low temperature fuel cells," Colby-Sawyer, NH, June 2016
- 33. U.S. Department of Energy Basic Energy Sciences Contractor's Meeting, "Analysis of the mechanism of electrochemical oxygen reduction and development of Ag- and Pt-alloy catalysts for low temperature fuel cells," Washington, MI, June 2016
- 34. Michigan Catalysis Society Annual Symposium, "Analysis of the mechanism of electrochemical oxygen reduction and development of Ag- and Pt-alloy catalysts for low temperature fuel cells," Midland, MI, May 2016
- 35. American Chemical Society Spring National Meeting, "Analysis of the mechanism of electrochemical oxygen reduction and development of Ag- and Pt-alloy catalysts for low temperature fuel cells," San Diego, CA, March 2016
- 36. American Chemical Society Spring National Meeting, "Photochemical reactions on plasmonic metal nanostructures," San Diego, CA, March 2016
- 37. American Chemical Society Pacific-Chem meeting, "Photochemical reactions on plasmonic metal nanostructures," Honolulu, HI, December 2015
- 38. American Chemical Society Pacific-Chem meeting, "Electrochemical ORR on metal alloys," Honolulu, HI, December 2015
- 39. Symposium on Photonics at Boston University, "Photochemical reactions on plasmonic metal nanostructures: known knowns and known unknowns about hot carrier distribution," Boston, MA, December 2015

- 40. American Vacuum Society Annual Meeting, "Photo-chemical reactions on plasmonic metal nanoparticles," San Jose, CA, October 2015
- 41. North American Catalysis Society Meeting, "Photochemical reaction on plasmonic metal nanoparticles," Pittsburgh, PA, June 2015
- 42. Southwest Catalysis Society Annual Meeting, "Analysis of the Mechanism of Electrochemical Oxygen Reduction and Development of Ag- and Pt-alloy Catalysts for Low Temperature Fuel Cells," Houston, TX, April 2015
- 43. Materials Research Society Annual Meeting, "Photo-chemical reactions on plasmonic metal nanoparticles," San Francisco, CA, April 2015
- 44. American Chemical Society Spring National Meeting, "Analysis of the Mechanism of Electrochemical Oxygen Reduction and Development of Ag- and Pt-alloy Catalysts for Low Temperature Fuel Cells," celebration of Prof. Jingguang Chen's ACS Olah award, Denver, CO, March 2015
- 45. American Chemical Society Spring National Meeting, "Conversion of solar into chemical energy on plasmonic metal nanostructures," Denver, CO, March 2015
- 46. American Chemical Society annual meeting, "Microscopic mechanisms of plasmonmediated charge transfer in adsorbates on metal nanoparticles and its chemical consequences," Denver, CO, March 2015
- 47. Gordon Research Conference on Reactions on Surfaces, "Chemical reaction on plasmonic metal nanoparticles induced by energetic electrons," Ventura, CA, February 2015
- 48. Material Research Society Annual Meeting, "Plasmonic metal nanoparticles in the conversion of solar to chemical energy," Boston, MA, November 2014
- 49. DIET 14: Dynamics, Interactions and Electronic Transitions at Surfaces "Chemical reaction on plasmonic metal nanoparticles induced by energetic electrons," San Jose, CA, October 2014
- 50. American Chemical Society Fall National Meeting, "Controlling electron- and phonondriven chemical transformations on metals," award lecture celebrating Suljo Linic's ACS catalysis lectureship award, San Francisco, CA, August 2014
- 51. American Chemical Society Fall National Meeting, "Photo-chemical reactions on plasmonic metal nanostructures," San Francisco, CA, (award lecture celebrating Suljo Linic's ACS catalysis lectureship award), August 2014
- 52. Gordon Research Conference on Plasmonics, "Chemical reaction on plasmonic metal nanoparticles induced by energetic electrons," Keene, NH, July 2014
- 53. C1P Catalysis from first principles workshop, "Using molecular understanding of electrochemical oxygen reduction reaction to design novel alloy electro-catalysts," Ulm, Germany, May 2014
- 54. Philadelphia Catalysis Society Annual Meeting, "Analysis of the Mechanism of Electrochemical Oxygen Reduction and Development of Ag- and Pt-alloy Catalysts for Low Temperature Fuel Cells," Philadelphia, PA, May 2014

- 55. American Chemical Society Spring National Meeting, "Molecular mechanism of electrochemical oxygen reduction reaction," Dallas, TX, March 2014
- 56. American Chemical Society Spring National Meeting, "Conversion of solar into chemical energy on plasmonic metal nanostructures," Dallas, TX, March 2014
- 57. American Chemical Society Spring National Meeting, "Modelling molecular processes taking place on optically excited plasmonic metal nanoparticles," Dallas, TX, March 2014
- 58. American Physical Society Spring National Meeting, "Conversion of solar into chemical energy on plasmonic metal nanostructures," Denver, CO, March 2014
- American Chemical Society Fall National Meeting, "Developing molecular mechanism for oxygen reduction reaction and using it to design Pt-free electro-catalysts," Indianapolis, IN, August 2013
- 60. American Chemical Society Fall National Meeting, "Catalysis on optically excited plasmonic nano-particles of noble metals (Ag)," Indianapolis, IN, August 2013
- American Chemical Society Fall National Meeting, "Theoretical models for molecular processes taking place on optically excited plasmonic metal nanoparticles," Indianapolis, IN, August 2013
- 62. American Chemical Society Fall National Meeting, "Designing catalysts based on their electronic structure fingerprints: Predictive structure-performance models for metal alloy catalysts," Indianapolis, IN, August 2013
- 63. American Chemical Society Colloids and Surface Science Meeting, "Photochemistry on metals," Riverside, CA, June 2013
- 64. Workshop on catalysis on plasmonic metals, "Catalysis on optically excited plasmonic nano-particles of noble metals (Ag)," Rice University, Houston, TX, June 2013
- 65. U.S. Department of Energy Contractors' meeting, "Catalysis on optically excited plasmonic nano-particles of noble metals (Ag)," Annapolis, MD, June 2013
- 66. Institute for Pure and Applied Mathematic workshop, "Design of targeted nanostructures for efficient and environmentally friendly catalysis and photo-catalysis," Los Angeles, CA, May 2013
- 67. American Chemical Society Spring National Meeting, "Developing molecular mechanism for oxygen reduction reaction and using it to design Pt-free electro-catalysts," New Orleans, LA, April 2013
- 68. American Chemical Society Spring National Meeting, "Catalysis on optically excited plasmonic nano-particles of noble metals (Ag)," New Orleans, LA, April 2013
- 69. International Congress on Nano Meta Materials (NANOMETA) organized by European Physics Society, "Chemical transformation on optically excited plasmonic nanoparticles," Seefeld, Austria, January 2013
- 70. Symposia celebrating 60<sup>th</sup> birthday of Prof. Jens. K. Norskov at Stanford University, "Photo-reaction on plasmonic metal nanostructures," Stanford, CA, September 2012

- 71. Danish Technical University, 2012 Summer School, "Computational Heterogeneous Catalysis: Surface Chemistry of Alloys," Lungby, Denmark, August 2012
- 72. Workshop on Heterogeneous Catalysis, Surface Science and Energy Research, "Direct photo-catalysis on optically excited plasmonic metal nanostructures," Georg-August University of Göttingen, Göttingen, Germany, July 2012
- 73. 7th Chemical Engineering Conference for Collaborative Research in Eastern Mediterranean Countries (EMCC7), "Photo-catalysis on Plasmonic Metal/Semiconductor Composites: H2O splitting using visible light," Corfu, Greece, April 2012
- 74. Catalysis Club of Chicago, "Designing catalysts based on their spectroscopic fingerprints: Relationships between measured local geometric and electronic structure of alloy catalysts and their chemical reactivity," Chicago, IL, January 2012
- 75. Entretiens Jacques Cartier Colloquium on 21st Century Catalysis Science and Applications, "Design of Targeted Nanostructures for Efficient and Environmentally Friendly Catalysis and Photocatalysis," Ottawa, Canada, November 2011
- 76. National Science Foundation Nanoscale Science and Engineering Grantee Conference, "Plasmonic nanostructures in photochemistry," Washington, DC, November 2011
- 77. American Institute of Chemical Engineers National Meeting, "Design of energy efficient and environmentally friendly nanomaterials for catalysis and photo-catalytic solar fuel production," Nanoscience and Engineering Forum Young Investigator Award lecture, Minneapolis, MN, October 2011
- American Chemical Society Fall National Meeting, "Photo-catalysis on plasmonic metallic nanostructures and plasmonic nanostructure/semiconductor composites," Denver, CO, August 2011
- 79. American Chemical Society Fall National Meeting, "Improving carbon tolerance of Ni heterogeneous (electro)catalysts by alloying: catalysts design guided by first principles calculations," Denver, CO, August 2011
- 80. American Chemical Society Fall National Meeting, "Designing catalysts based on their spectroscopic fingerprints: relationships between measured local geometric and electronic structure of alloy catalysts and their chemical reactivity," Denver, CO, August 2011
- 81. C1P Network of Excellence in Computational Catalysis, "Development of predictive structure-performance relationships for rational design of multi-component catalytic materials," Copenhagen, Denmark, May 2011
- 82. Workshop on New Trends of Computational Chemistry in Industry Applications, "Development of predictive structure-performance relationships for rational design of multi-component catalytic materials," Barcelona, Spain, May 2011
- 83. Workshop on Materials Design in Chemical Compound Space, Institute for Pure and Applied Mathematics at UCLA, "Using electronic structure descriptors to identify new catalysts," Los Angeles, CA, May 2011
- 84. Symposium on Catalysis Science at the Dawn of the Twenty-First Century, "Exploiting Nanotechnology for Heterogeneous Catalysis: Shaped Metallic Nanostructures as

Selective Catalysts and for Characterization of Surface Chemical Reactions," Lyon, France, November 2010

- 85. Catalysis Society of New York, "Design of materials for energy conversion from first principles: metallic nanoparticles of targeted shapes as highly selective catalysts, photocatalysts, and platforms for chemical characterization," Rutherford, NJ, October 2010
- 86. American Chemical Society Fall National Meeting, "Enhancing Photo-chemical activity of semiconductor nanoparticles with optically active metallic nano-structures: Photo-chemistry mediated by surface plasmons," Boston, MA, August 2010
- 87. American Chemical Society Spring National Meeting, "Well defined, highly uniform, targeted nano-structures as highly selective heterogeneous catalysts, photo-catalysts and characterization tools," Symposium organized in honor Prof. Christopher W. Jones, 2010 recipient of the Ipatieff Prize, San Francisco, CA, March 2010
- American Vacuum Society Annual Meeting, "Catalysis on supported metal nano-clusters," San Jose, CA, November 2009
- 89. American Chemical Society Unilever Award Lecture, "Well defined, highly uniform, targeted nano-structures as highly selective heterogeneous catalysts, photo-catalysts and characterization tools," American Chemical Society Division of Colloids and Surface Science Meeting, New York, NY, June 2009
- 90. American Chemical Society Division of Colloids and Surface Science Meeting, "Measuring the electronic structure of metal alloys and relating it to their performance," New York, NY, June 2009
- Philadelphia Catalysis Society Annual Symposium, "Targeted metallic nanostructures as heterogeneous catalysis, electro-catalysts, and platforms for chemical characterization," Newark, DE, May 2009
- 92. American Chemical Society Spring National Meeting, "Measuring the electronic structure of metal alloys and relating it to their performance," Symposium of the convergence between theory and experiment in surface chemistry and heterogeneous catalysis; organized by Prof. John Yates in honor of Prof. Jens Norskov, 2009 recipient of the Gabor A. Somorjai Award for Creative Research in Catalysis, Salt Lake City, UT, April 2009
- 93. Transatlantic Frontiers in Chemistry Symposium, "Catalysis at nano length scales," Manchester, England, August 2008
- 94. International Symposium on Creation and Control of Advanced Selective Catalysis Celebrating the 50th Anniversary of Catalysis Society of Japan, "(Electro)catalyst design guided by molecular insights: controlling carbon poisoning of Ni (electro)catalysts by alloying," Kyoto, Japan, July 2008
- 95. Gordon Research Conference on Catalysis, "Design of heterogeneous (Electro)catalysts guided by molecular insights," Colby-Sawyer, NH, June 2008
- 96. U.S. Department of Energy National Energy Technology Laboratory symposium, "Hybrid theoretical/experimental studies aimed at the development of carbon- and sulfur-tolerant reforming catalysts," Pittsburgh, PA, April 2008

- 97. American Chemical Society Spring National Meeting, "Controlling carbon chemistry on Ni surfaces by alloying: First principles approaches toward carbon-tolerant alloy catalysts and electrocatalysts," New Orleans, LA, April 2008
- 98. American Chemical Society Fall National Meeting, "Controlling carbon chemistry on Ni surfaces by the surface alloying: An *ab-initio* approach towards carbon-tolerant alloy catalysts for chemical energy conversion," Boston, MA, August 2007
- 99. American Chemical Society Division of Colloids and Surface Science Meeting, "Surface chemistry of carbon on Ni and Ni-alloys: carbon-tolerant hydrocarbon reforming catalysts from molecular insights," Newark, DE, June 2007
- 100. American Chemical Society Division of Colloids and Surface Science, "Heterogeneous catalysis by gold: DFT and *ab initio* thermodynamic investigations of Au oxidation state and the role of oxide supports," Boulder, CO, June 2006
- 101. Delphi Automotive Company, "Ethylene epoxidation on Au: First-principles design of more selective catalysts," Flint, MI, April 2005
- 102. Michigan Catalysis Society, "Ethylene epoxidation on Au: First-principles design of more selective catalysts," Livonia, MI, November 2004
- 103.Ford Motor Company, "First principles approaches to hydrogen economy and sustainability," Dearborn, MI, October 2004
- 104.  $\Psi_{\kappa}$  network of excellence workshop on novel materials from first principles, "Selectivity in Heterogeneous Ethylene Epoxidation on Ag: From Fundamental Studies to Rational Catalyst Design," workshop organized by Jens K. Norskov, Matthias Scheffler, and Juergen Hafner, Copenhagen, Denmark, June 2004
- 105. Max Planck Society Meeting, "Ethylene epoxidation on Au: First-principles design of more selective catalysts," Straslund, Germany, February 2004

#### **Invited Lectures at Universities**

reverse chronological order

- 1. University of Oklahoma, Department of Chemical Engineering, "Electrochemical oxygen reduction: kinetic analysis and the development of Ag- and Pt-alloy catalysts for low temperature fuel cells," Norman, OK, March 2020
- Princeton University, Department of Chemical and Biological Engineering, "Plasmonic chemistry and catalysis: opportunities for selective and sustainable chemical conversion," Princeton, NJ, March 2020
- 3. Pennsylvania State University, Department of Chemical Engineering, "Electrochemical oxygen reduction: kinetic analysis and the development of Ag- and Pt-alloy catalysts for low temperature fuel cells," University Park, PA, February 2020
- 4. University of Pennsylvania, Department of Chemistry, "Electrochemical oxygen reduction: kinetic analysis and the development of Ag- and Pt-alloy catalysts for low temperature fuel cells," Philadelphia, PA, February 2020

- Boston College, Chemistry Department, "Electrochemical oxygen reduction: kinetic analysis and the development of Ag- and Pt-alloy catalysts for low temperature fuel cells," Boston, MA, January 2020
- 6. University of Pennsylvania, Department of Chemical Engineering, "Plasmonic catalysis," Philadelphia, PA, October 2019
- XINGDA Lecture, Peking University, Chemistry Division, "Plasmonic chemistry and catalysis: opportunities for selective and sustainable chemical conversion," September 2019
- Tufts University, Department of Chemistry, "Electrochemical oxygen reduction: kinetic analysis and the development of Ag- and Pt-alloy catalysts for low temperature fuel cells," Boston, MA, February 2019
- 9. University of South Carolina, Department of Chemical Engineering, "Engineering metal/insulator/co-catalysts systems for photocatalytic water splitting," Columbia, SC, January 2019
- 10. Dutch Institute for Renewable Energy Conversion (DIFFER), "Electrochemical oxygen reduction: kinetic analysis and the development of Ag- and Pt-alloy catalysts for low temperature fuel cells," Eindhoven, Netherlands, December 2018
- 11. University of Pennsylvania, Department of Chemical Engineering, "Selectivity in plasmonic catalysis: controlling the energy flow at molecular scales," Philadelphia, PA, May 2018
- 12. U.S. Congressional Hearing Capitol Hill, "Energy challenges and solutions," Washington, DC, August 2018
- Mason Lecture, Stanford University, Department of Chemical Engineering, "Selectivity in plasmonic catalysis: Controlling the energy flow at molecular scales," Stanford, CA, May 2018
- 14. Johns Hopkins University, Department of Chemical and Biomolecular Engineering, "Catalysis on plasmonic metal nanoparticles: opportunities for highly selective chemical conversion," Baltimore, MD, April 2018
- 15. D.B. Robinson Lecture, University of Alberta, Department of Chemical and Materials Engineering, "Catalysis on plasmonic metal nanoparticles: opportunities for highly selective chemical conversion," Edmonton, Alberta, Canada, April 2018
- 16. Harvard University, Integrated Mesoscale Architecture for Sustainable Catalysis (IMASC), "Catalysis on plasmonic metal nanoparticles: opportunities for highly selective chemical conversion," Cambridge, MA, February 2018
- 17. University of Rochester, Hajim School of Engineering and Applied Sciences, Department of Chemical Engineering, "Catalysis on plasmonic metal nanoparticles: Opportunities for highly selective chemical conversion," Rochester, NY, January 2018
- 18. Tulane University, Department of Chemical and Biomolecular Engineering, "Photochemical reactions on plasmonic metal nanostructures," New Orleans, LA, December 2017

- Dumas Lecture, Virginia Polytechnic Institute and State University, Department of Chemical Engineering, "Photo-chemical reactions on plasmonic metal nanostructures," Blacksburg, VA, November 2017
- 20. Yale University, Department of Chemistry, "Electrochemical Oxygen Reduction: Kinetic analysis and the development of Ag- and Pt-alloy catalysts for low temperature fuel cells," New Haven, CT, January 2017
- 21. Carnegie Mellon University, Department of Chemical Engineering, "Electrochemical Oxygen Reduction: Kinetic analysis and the development of Ag- and Pt-alloy catalysts for low temperature fuel cells," Pittsburgh, PA, January 2017
- 22. University of Minnesota, Department of Chemistry, "Photo-chemical reactions on plasmonic metal nanostructures," Minneapolis, MN, November 2016
- 23. Tianjin University, Department of Chemical Engineering, "Photo-chemical reactions on plasmonic metal nanostructures," Tianjin, CA, September 2016
- 24. ExxonMobil, "Oxidative coupling of methane," Clinton, NJ, September 2016
- 25. Rutgers University, Department of Chemical Engineering, "Photo-chemical reactions on plasmonic metal nanostructures," New Brunswick, NJ, April 2016
- 26. Technical University, Department of Chemistry, "Design of targeted nanostructures for efficient and environmentally friendly catalysis and photo-catalysis," Munich, Germany, January 2016
- 27. ExxonMobil, "Oxidative coupling of methane," Clinton, NJ, December 2015
- 28. Iowa State University, Department of Chemical Engineering, "Electrochemical Oxygen Reduction: Kinetic analysis and the development of Ag- and Pt-alloy catalysts for low temperature fuel cells," Ames, IA, November 2015
- 29. University of Washington, Nanoscience and Technology Institute, "Photo-chemical reactions on plasmonic metal nanostructures," Seattle, WA, October 2015
- 30. SABIC Corp., "Reactions on metals," Houston, TX, April 2015
- 31. University of California, Berkeley, Department of Chemical Engineering, "Electrochemical Oxygen Reduction: Kinetic analysis and the development of Ag- and Ptalloy catalysts for low temperature fuel cells," Berkeley, CA, March 2015
- 32. McGill University, Department of Chemistry, "Photo-chemical reactions on plasmonic metal nanostructures," Montreal, Canada, March 2015
- 33. Technical University, Department of Chemistry, "Electro-catalysis of oxygen reduction reaction (ORR)," Munich, Germany, January 2015
- 34. University of California, Riverside, Department of Materials Science, "Design of targeted nanostructures for efficient and environmentally friendly catalysis and photo-catalysis," Riverside, CA, December 2014
- 35. University of Pittsburgh, Department of Chemistry, "Design of targeted nanostructures for efficient and environmentally friendly catalysis and photo-catalysis," Pittsburgh, PA, November 2014

- 36. University of Toronto, Department of Chemical Engineering, "Design of targeted nanostructures for efficient and environmentally friendly catalysis and photo-catalysis," Toronto, Canada, January 2014
- 37. Bowling Green State University, Department of Chemistry, "Design of targeted nanostructures for efficient and environmentally friendly catalysis and photo-catalysis," Bowling Green, OH, January 2014
- ExxonMobil, "Relating Experimental to Theoretical Studies in Heterogeneous Catalysis," Clinton, NJ, December 2013
- 39. Vanderbilt University, Department of Chemical Engineering, "Design of targeted nanostructures for efficient and environmentally friendly catalysis and photo-catalysis," Nashville, TN, December 2013
- 40. Georgia Tech University, Department of Chemical Engineering, "Design of targeted nanostructures for efficient and environmentally friendly catalysis and photo-catalysis," Atlanta, GA, November 2013
- 41. Thiel Lectureship, Notre Dame University, Department of Chemical Engineering, "Design of targeted nanostructures for efficient and environmentally friendly catalysis and photocatalysis," South Bend, IN, September 2013
- 42. National Renewable Energy Laboratory, "Developing molecular mechanism for oxygen reduction reaction and using it to design Pt-free electro-catalysts," Golden, CO, April 2013
- 43. National Energy Technology Laboratory, "Catalysis of Fuel Cells," Pittsburgh, PA, February 2013
- 44. University of Colorado, Department of Chemical Engineering, "Catalysis on optically excited plasmonic nano-particles of noble metals (Ag)," Boulder, CO, January 2013
- 45. Columbia University, Department of Chemical Engineering, "Catalysis on optically excited plasmonic nano-particles of noble metals (Ag)," New York, NY, January 2013
- 46. University of Pittsburgh, Department of Chemical Engineering, "Nano-scale solutions in catalysis and photo-catalysis," Pittsburgh, PA, October 2012
- 47. Rensselaer Polytechnic Institute, Department of Chemical and Biological Engineering, "Designing Efficient Heterogeneous (Photo)Catalysis by Controlling the Size, Shape, and Optical Properties of Metal Nanoparticles," Troy, NY, October 2012
- 48. University of Pittsburgh, Department of Chemical Engineering, "Nano-scale solutions in catalysis and photo-catalysis," Pittsburgh, PA, October 2012
- 49. University of Southern Florida, Department of Chemical Engineering, "Nano-scale solutions in catalysis and photo-catalysis," Tampa, FL, October 2012
- 50. Wayne State University, Department of Chemical Engineering, "Nano-scale solutions in catalysis and photo-catalysis," Detroit, MI, November 2011
- 51. Duke University, Department of Chemistry, "Nano-scale solutions in catalysis and photocatalysis," Durham, NC, November 2011

- 52. Ohio State University, Department of Chemical Engineering, "Nano-scale solutions in catalysis and photo-catalysis," Columbus, OH, April 2011
- 53. University of Alabama, Department of Chemical Engineering, "Nano-scale solutions in catalysis and photo-catalysis," Tuscaloosa, AL, April 2011
- 54. University of California, Department of Chemical Engineering, "Nano-scale solutions in catalysis and photo-catalysis: materials for efficient conversion of solar to chemical energy," Santa Barbara, CA, March 2011
- 55. Stanford University, Department of Chemical Engineering, "Nano-scale solutions in catalysis and photo-catalysis: materials for efficient conversion of solar to chemical energy," Stanford, CA, February 2011
- 56. University of Washington, Center for Nanotechnology, "Nano-scale solutions in catalysis and photo-catalysis: materials for efficient conversion of solar to chemical energy," Seattle, WA, January 2011
- 57. Washington University in St. Louis, "Nano-scale solutions in catalysis and photocatalysis," St. Louis, MO, December 2010
- 58. University of Toledo, Department of Chemical Engineering, "Nano-scale solutions in catalysis and photo-catalysis: materials for efficient conversion of solar to chemical energy," Toledo, OH, October 2010
- 59. University of Delaware, Department of Chemical Engineering, "Design of materials for energy conversion from first principles: metallic nanoparticles of targeted shapes as highly selective catalysts, photo-catalysts, and platforms for chemical characterization," Newark, DE, May 2010
- 60. Pennsylvania State University, Department of Chemical Engineering, "Nano-scale solutions in catalysis and photo-catalysis: materials for efficient conversion of solar to chemical energy," State College, PA, September 2010
- 61. Massachusetts Institute of Technology, Department of Chemical Engineering, "Design of materials for energy conversion from first principles: metallic nanoparticles of targeted shapes as highly selective catalysis and photo-catalysts," Cambridge, MA, March 2010
- 62. Technical University of Denmark, Department of Physics, "Design of materials for energy conversion from first principles: metallic nanoparticles of targeted shapes as highly selective catalysis and photo-catalysts," Lyngby, Denmark, January 2010
- 63. University of Wisconsin, Department of Chemical and Biological Engineering, "Molecular approaches to heterogeneous catalysis," Madison, WI, November 2009
- 64. Lindsay Lectureship, Texas A&M University, Department of Chemical Engineering, "Design of heterogeneous (electro)catalysts guided by molecular insights," College Station, TX, November 2008
- 65. The City College of New York, Department of Chemical Engineering, "Design of heterogeneous (electro)catalysts guided by molecular insights," New York, NY, February 2008

- 66. University of Colorado, "Design of heterogeneous (electro)catalysts guided by molecular insights," Boulder, CO, January 2008
- 67. Colorado School of Mines, "Design of heterogeneous (electro)catalysts guided by molecular insights," Golden, CO, January 2008
- 68. Purdue University, "Ab-initio approach to heterogeneous catalysis," West Lafayette, IN, October 2005
- 69. Michigan Catalysis Society Annual Symposium, "From surface chemistry to novel heterogeneous catalysts," Ann Arbor, MI, April 2005
- 70. University of Michigan, Department of Chemical Engineering, "Ethylene epoxidation on Au: First-principles design of more selective catalysts," Ann Arbor, MI, 2004
- 71. Case Western Reserve University, Department of Chemical Engineering, "Ethylene epoxidation on Au: First-principles design of more selective catalysts," Cleveland, OH, 2003
- 72. University of California, Los Angeles, Department of Chemical Engineering, "Ethylene epoxidation on Au: First-principles design of more selective catalysts," Los Angeles, CA, 2003
- 73. Fritz Haber Institute, "Ethylene epoxidation on Au: First-principles design of more selective catalysts," Berlin, Germany, September 2003

#### **Recent non-invited Conference Presentations (2004-present)**

presenter underlined reverse chronological order

- 1. <u>Jacques Esterhuizen</u>, Bryan R. Goldsmith, Suljo Linic, "Theory-Guided, Interpretable Machine Learning Finds Predictive Geometric Structure-Property Relationships for Chemisorption on Alloys," American Institute of Chemical Engineers National Meeting, online, November 2020
- 2. <u>Steven Chavez</u>, Umar Aslam, Vishal Govind Rao, Suljo Linic, "Designing Hybrid Plasmonic Nanostructures for Photocatalysis," American Institute of Chemical Engineers National Meeting, online, November 2020
- <u>Steven Chavez</u>, Suljo Linic, "Factors Governing Charge Carrier Generation and Extraction in Hybrid Plasmonic Systems," American Institute of Chemical Engineers National Meeting, online, November 2020
- 4. John Hemmerling, Joseph Quinn, Suljo Linic, "Nanoscopic Control of the Interfaces to Optimize Metal-Insulator-Semiconductor Systems for Solar Water Splitting," American Institute of Chemical Engineers National Meeting, Orlando, FL, November 2019
- <u>Steven Chavez</u>, Suljo Linic, "Factors Governing Site Specific Rates of Electronic Excitations in Multicomponent Plasmonic Materials," American Institute of Chemical Engineers National Meeting, Orlando, FL, November 2019

- Joseph Quinn, John Hemmerling, Suljo Linic, "Maximizing the Efficiencies of Metal-Insulator-Semiconductor (MIS) Photoelectrodes by Controlling the Flux of Charge Carriers with Interfacial Design," American Institute of Chemical Engineers National Meeting, Orlando, FL, November 2019
- 7. <u>Valentina Omoze Igenegbai, Randall J. Meyer,</u> Suljo Linic, "Enhancing Selectivity in Oxidative Coupling of Methane Using Catalytic Solid Oxide Membrane Reactors," American Institute of Chemical Engineers National Meeting, Orlando, FL, November 2019
- 8. <u>Sean Dix</u>, Suljo Linic, "Operando Surface Enhanced Raman Spectroscopy Study of the Oxygen Reduction Reaction on a Non-Model Pt Catalyst," American Institute of Chemical Engineers National Meeting, Orlando, FL, November 2019
- 9. <u>Valentina Omoze Igenegbai, Randall J. Meyer, Suljo Linic, "Enhancing Selectivity in</u> Oxidative Coupling of Methane Using Catalytic Solid Oxide Membrane Reactors," University of Michigan Chemical Engineering Graduate Symposium, Ann Arbor, MI, September 2019
- <u>Valentina Omoze Igenegbai</u>, Rawan Almallahi, Randall J. Meyer, Suljo Linic, "Investigating Solid Oxide Membrane/Catalyst Reacting Systems for Direct Methane Conversion to Ethylene and Ethane by Oxidative Coupling," North American Catalysis Society Meeting, Chicago, IL, June 2019
- 11. Joseph Quinn, John Hemmerling, Suljo Linic, "Interfacial Design of Metal-Insulator-Semiconductor (MIS) Structurs for Photoelectrochemical Water Splitting, North American Catalysis Society Meeting, Chicago, IL, June 2019
- 12. <u>Sean Dix</u>, Suljo Linic, "Using in-Situ Surface Enhanced Raman Spectroscopy for Studying the Oxygen Reduction Reaction Mechanism on Platinum," North American Catalysis Society Meeting, Chicago, IL, June 2019
- 13. <u>Steven Chavez</u>, Suljo Linic, "Factors Governing Site Specific Rates of Electronic Excitations in Multicomponent Plasmonic Photocatalysts," North American Catalysis Society Meeting, Chicago, IL, June 2019
- 14. John Hemmerling, Joseph Quinn, Suljo Linic, "Understanding the Role of the Insulator in Optimizing Metal-Insulator-Semiconductor Systems for Solar Water Splitting," North American Catalysis Society Meeting, Chicago, IL, June 2019
- 15. <u>Rawan Almallahi</u>, Valentina Omoze Igenegbai, Suljo Linic, "Developing Solid-Oxide Membrane Reactors for Thermoneutral Propane Dehydrogenation," North American Catalysis Society Meeting, Chicago, IL, June 2019
- 16. <u>Valentina Omoze Igenegbai</u>, Randall J. Meyer, Suljo Linic, "Investigating Solid Oxide Membrance Reactors for Direct Methane Conversion to Ethylene and Ethane by Oxidative Coupling," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, November 2018
- 17. <u>Valentina Omoze Igenegbai</u>, Randall J. Meyer, Suljo Linic, "Performance and Phase Stability Studies of Gadolinium-Doped Barium Cerate in Oxidative Coupling of Methane and the Impact of Zr Doping," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, October 2018

- <u>Steven Chavez</u>, Umar Aslam, Suljo Linic, "Elucidating Mechanisms of Plasmon Decay in Multimetallic Nanostructures for the Rational Design of Plasmonic Photocatalysts," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, October 2018
- <u>Steven Chavez</u>, Umar Aslam, Suljo Linic, "Elucidating Mechanisms of Plasmon Decay in Multimetallic Nanostructures for the Rational Design of Plasmonic Photocatalysts," University of Michigan Chemical Engineering Graduate Symposium, Ann Arbor, MI, September 2018
- 20. <u>Valentina Omoze Igenegbai</u>, Suljo Linic, "Direct Methane Conversion to Ethylene by Oxidative Coupling in Packed Bed and Membrane Reactors," American Institute of Chemical Engineers National Meeting, Minneapolis, MN, November 2017
- <u>Steven Chavez</u>, Umar Aslam, Suljo Linic, "Mechanism and Design Principles for Directing Energy Flow in Multicomponent Plasmonic Systems," American Institute of Chemical Engineers National Meeting, Minneapolis, MN, November 2017
- 22. <u>Umar Aslam</u>, Steven Chavez, Suljo Linic, "Controlling Energy Flow in Plasmonic Photocatalysis through the Design of Hybrid Plasmonic Nanostructures," American Institute of Chemical Engineers National Meeting, Minneapolis, MN, November 2017
- 23. <u>Joseph Quinn</u>, Suljo Linic, "Engineering the Interface to Improve the Efficiencies of Insulator-Protected Semiconductors for Photoelectrochemical Cells," American Institute of Chemical Engineers National Meeting, Minneapolis, MN, October 2017
- 24. <u>Umar Aslam</u>, Suljo Linic, "Synthesis of Bimetallic Alloy Nanoparticles through the Visible-Light Mediated Reduction of a Bimetallic Oxide Precursor: Case Study of Ag-Pt Nanoparticle Synthesis," American Institute of Chemical Engineers National Meeting, Minneapolis, MN, October 2017
- 25. <u>Umar Aslam</u>, Suljo Linic, "Engineering energy flow in plasmonic catalysis through the design of multicomponent nanostructures," Michigan Catalysis Society Symposium, Ann Arbor, MI, May 2017
- 26. <u>Umar Aslam</u>, Steven Chavez, Suljo Linic, "Engineering plasmonic nanostructures to direct energy flow to catalytically active sites," University of Michigan Chemical Engineering Graduate Symposium, Ann Arbor, May 2017
- 27. <u>Steven Chavez</u>, Umar Aslam, Suljo Linic, "Mechanism and Design Principles for Directing Energy Flow in Multicomponent Plasmonic Nanoparticles," University of Michigan Chemical Engineering Graduate Symposium, Ann Arbor, May 2017
- 28. <u>Brittany Lancaster Farrell</u>, Valentina Omoze Igenegbai, Suljo Linic, "Direct methane conversion to ethylene and ethane by oxidative coupling in packed bed and membrane reactors," University of Michigan Chemical Engineering Graduate Symposium, Ann Arbor, MI, May 2017
- Paul Hernley, <u>Steven Chavez</u>, Joseph Quinn, Suljo Linic, "Impact of Combining Metal Nanoparticle Catalysts and Semiconductor Photoelectrodes on Photocatalytic Performance," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2016

- Calvin Boerigter, Umar Aslam, <u>Suljo Linic</u>, "Photochemical Reactions on Plasmonic Metal Nanoparticles: Mechanism of Charge Extraction from Nanoparticles to Adsorbates," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2016
- Joseph Quinn, Paul Hernley, Steven Chavez, Suljo Linic, "Modeling the Sensitivity of Design Parameters for Photo-Electrochemical Cells Containing a Semiconductor Absorber and Metal Photocatalysts," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2016
- 32. <u>Steven Chavez</u>, Paul Hernley, Joseph Quinn, Suljo Linic, "Understanding the Mechanisms and Key Parameters That Influence the Performance of Composite Semiconductor/Electrocatalyst Photoelectrodes," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2016
- 33. <u>Timothy Van Cleve</u>, Saman Moniri, Hongliang Xin, Suljo Linic, "Enhancing Oxygen Reduction Activity on Pt Monolayer Electrocatalysts through Selective Tuning of Ligand and Lattice Effects," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2016
- 34. <u>Steven Chavez</u>, Paul Hernley, Joseph Quinn, Suljo Linic, "Embedded Electrocatalyst/Semiconductor Scheme for Improved Solar Fuel Generation Systems," Society of Hispanic Professional Engineers National Conference, Seattle, WA, November 2016
- 35. <u>Calvin Boerigter</u>, Suljo Linic, "Engineering Highly Efficient Charge Transfer from Plasmonic Nanostructures to Chemically Attached Materials," University of Michigan Chemical Engineering Symposium, Ann Arbor, MI, May 2016
- 36. <u>Saman Moniri</u>, Timothy Van Cleve, Suljo Linic, "Atomistic Engineering of Efficient Oxygen Reduction Electro-Catalysts by Tailoring Local Chemical Environment on Pt Surface Sites," University of Michigan Chemical Engineering Symposium, Ann Arbor, MI, May 2016
- <u>Paul Hernley</u>, Suljo Linic, "Enhancement Mechanisms by Metal Co-Catalysts and Plasmonic Nanoparticles in the Photo-Electrochemical Activity of Semiconductors," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2015
- Brittany Lancaster, Suljo Linic, "Methane Conversion to Ethane and Ethylene Using Packed Bed and Solid Oxide Membrane Reactors," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2015
- Matthew Morabito, <u>Suljo Linic</u>, "First Principles Modeling of Plasmon-Mediated Charge Transfer Mechanisms for Photo-Catalytic Rate Enhancement," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2015
- <u>Calvin Boerigter</u>, Robert Campana, Matthew Morabito, Suljo Linic, "Using SERS to shed light on the mechanism of photocatalytic enhancement in plasmonic nanoparticle systems," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2015

- 41. <u>Timothy Van Cleve</u>, Saman Moniri, Gabrielle Belok, Hongliang Xin, Suljo Linic, "Development of Multi-Metallic Pt Alloy Electrocatalysts for the Oxygen Reduction Reaction in PEM Fuel Cells," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2015
- 42. Adam Holewinski, <u>Timothy Van Cleve</u>, Suljo Linic, "Kinetic Analysis of Electrochemical Oxygen Reduction and Development of Novel Catalysts for Low Temperature Fuel Cells," North American Catalysis Society Meeting, Pittsburgh, PA, June 2015
- 43. <u>Timothy Van Cleve</u>, Gabrielle Belok, Hongliang Xin, Suljo Linic, "Development of Novel Pt Monolayer Electrocatalysts for Oxygen Reduction in PEM Fuel Cells," North American Catalysis Society Meeting, Pittsburgh, PA, June 2015
- 44. <u>Timothy Van Cleve</u>, Gabrielle Belok, Hongliang Xin, Suljo Linic, "Development of Novel Pt Monolayer Electrocatalysts for Oxygen Reduction in PEM Fuel Cells," Michigan Catalysis Society Spring Symposium, Detroit, MI, May 2015
- 45. <u>Brittany Lancaster</u>, Suljo Linic, "Methane Conversion to Ethane and Ethylene Using Packed Bed and Solid Oxide Membrane Reactors," Michigan Catalysis Society Spring Symposium, Detroit, MI, May 2015
- 46. <u>Paul Hernley</u>, "Understanding Enhancements of Photo-Electrochemical Hydrogen Evolution on Silicon by Co-Catalysts and Plasmonic Nanoparticles, University of Michigan Chemical Engineering Graduate Symposium, Ann Arbor, MI, May 2015
- 47. <u>Brittany Lancaster</u>, Suljo Linic, "Methane Conversion to Ethane and Ethylene Using Solid Oxide Membrane Reactors," American Institute of Chemical Engineers National Meeting, Atlanta, GA, November 2014
- 48. <u>Calvin Boerigter</u>, Suljo Linic, "Using Surface-Enhanced Raman Spectroscopy to Probe and Understand the Mechanism of Electron-Mediated Chemical Reactions on Plasmonic Nanoparticle Catalysts," American Institute of Chemical Engineers National Meeting, Atlanta, GA, November 2014
- 49. <u>Matthew Morabito</u>, Hongliang Xin, Suljo Linic, "First Principles Modeling of Surface Plasmon Dynamics and Mechanism for Photo-Catalytic Rate Enhancement," American Institute of Chemical Engineers National Meeting, Atlanta, GA, November 2014
- 50. <u>Timothy Van Cleve</u>, Gaby Belok, Hongliang Xin, Suljo Linic, "Development of Novel Pt Monolayer Electrocatalysts for Oxygen Reduction in PEM Fuel Cells," American Institute of Chemical Engineers National Meeting, Atlanta, GA, November 2014
- 51. <u>Timothy Van Cleve</u>, Gaby Belok, Suljo Linic, "Development of Novel Pt Monolayer Electrocatalysts for Oxygen Reduction in PEM Fuel Cells," American Chemical Society National Meeting, San Francisco, CA, August 2014
- 52. <u>Hongliang Xin</u>, Adam Holewinski, Eranda Nikolla, Suljo Linic, "Identifying Optimal Alloys for Heterogeneous Catalysis via Molecular Descriptors and Electronic Structure Engineering," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2013

- 53. <u>Hongliang Xin</u>, Suljo Linic, "First-principles Modeling of Energetic Electron Assisted Chemical Bond Breaking on Plasmonic Metal Surfaces," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2013
- <u>Brittany Lancaster</u>, Suljo Linic, "Direct Conversion of Oxygenated Fuels to Power Using Solid Oxide Fuel Cells," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2013
- 55. <u>Timothy Van Cleve</u>, Emily Gibara, Suljo Linic, "Dependence of Oxygen Reduction Activity on Ag Nanoparticles," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2013
- 56. <u>Hongliang Xin</u>, Suljo Linic, "Ab Initio Studies of Electron-Driven Photocatalytic Reactions on Plasmonic Metal Nanoparticles," 23rd North American Catalysis Society Meeting, Louisville, KY, June 2013
- 57. <u>Brittany Lancaster</u>, Suljo Linic, "Direct conversion of oxygenated fuels to power using solid oxide fuel cells," Blue/Green Seminar, Lansing, MI, November 2012
- 58. <u>Brittany Lancaster</u>, Suljo Linic, "Direct conversion of oxygenated fuels to power using solid oxide fuel cells," Engineering Graduate Symposium, Ann Arbor, MI, November 2012
- 59. <u>Timothy Van Cleve</u>, Suljo Linic, "Shape dependence of oxygen reduction activity on Ag nanoparticles," UM Engineering Graduate Symposium, Ann Arbor, MI, November 2012
- <u>Timothy Van Cleve</u>, Suljo Linic, "Shape dependence of oxygen reduction activity on Ag nanoparticles," Blue/Green Seminar Student Poster Session, East Lansing, MI, November 2012
- 61. <u>Brittany Lancaster</u>, Suljo Linic, "Direct conversion of oxygenated fuels to power using solid oxide fuel cells," Blue/Green Seminar, Lansing, MI, November 2012
- 62. <u>Hongliang Xin</u>, Suljo Linic, "Development of Predictive Structure-Reactivity Relationships for Multimetallic Catalyst Design," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, November 2012
- 63. Marimuthu Andiappan, Hongliang Xin, Phillip Christopher and <u>Suljo Linic</u>, "Optically Excited Plasmonic Metal Nanostructures as Selective Direct Propylene and Ethylene Epoxidation Catalysts," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, November 2012
- 64. <u>Marimuthu Andiappan</u>, Suljo Linic "Surface plasmon mediated highly selective epoxidation of propene over Cu catalyst," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, October-November 2012
- 65. Marimuthu Andiappan, Hongliang Xin, Phillip Christopher, <u>Suljo Linic</u>, "Optically excited plasmonic metal nanostructures as selective direct propylene and ethylene epoxidation catalysts," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, October-November 2012
- 66. <u>Matthew Morabito</u>, Hongliang Xin, Suljo Linic, "Establishing the Connection Between the Geometric and Electronic Structure of Oxygen Species on Ag Surfaces: First-Principles DFT and Monte Carlo Studies," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, October 2012

- 67. <u>Thomas Yeh</u>, Suljo Linic, Phillip Savage, "Pt/C and PtSn/C deactivation in decarboxylation of butyric acid," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, October 2012
- 68. <u>Adam Holewinski</u>, Suljo Linic, "Revisiting the Tafel Slope: Understanding ORR Kinetics Through Microkinetic Modeling," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, October 2012
- 69. <u>Adam Holewinski</u>, Suljo Linic, "Pt-free electrocatalysts for efficient oxygen reduction in alkaline fuel cells: Experimental and computational insights," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, October 2012
- Hongliang Xin, Marimuthu Andiappan, Phillip Christopher, <u>Suljo Linic</u>, "Ab Initio Studies of Electron-Driven Photo-Reactions on Surfaces of Plasmonic Metal Nanoparticles," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, October 2012
- David B. Ingram, <u>Suljo Linic</u>, "Solar Water Splitting on Plasmonic-Metal/Semiconductor Composites," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, October 2012
- 72. <u>Phillip Christopher</u>, Suljo Linic, Matthew Kale, "Well-Controlled Nanosynthesis Approaches for Optimized (Photo)Catalytic Materials," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, October 2012
- 73. <u>Michelle Przybylek</u>, Suljo Linic, "Towards Kinetic Studies of Composite Plasmonic-Metal/Semiconductor Photocatalysts for Water Splitting," American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, October 2012
- 74. <u>Phillip Christopher</u>, Hongliang Xin, Suljo Linic, "Catalytic applications of nanotechnology: (Photo)catalyst design and mechanistic analysis," American Chemical Society Fall National Meeting, Philadelphia, PA, August 2012
- 75. <u>Adam Holewinski</u>, and Suljo Linic, "Understanding and optimizing the kinetic behavior of the oxygen reduction reaction," American Chemical Society Fall National Meeting, Philadelphia, PA, August 2012
- 76. <u>Marimuthu Andiappan</u>, Hongliang Xin, Phillip Christopher, Suljo Linic, "Direct photocatalysis on optically excited plasmonic metal nanostructures of coinage metals," American Chemical Society Fall National Meeting, Philadelphia, PA, August 2012
- 77. Hongliang Xin, Eranda Nikolla, Adam Holewinski, <u>Suljo Linic</u>, "Designing catalysts based on their electronic structure fingerprints: predictive structure-performance models for metal alloys," International Congress on Catalysis, Munich, Germany, July 2012
- 78. <u>Adam Holewinski</u>, Hongliang Xin, and Suljo Linic, "Understanding the kinetic behavior of the oxygen reduction reaction for rapid catalyst screening," Michigan Catalysis Society Spring Symposium. Midland, MI, May 2012
- 79. Marimuthu Andiappan, <u>Suljo Linic</u>, "Design of selective propylene epoxidation catalysts: Heterogeneous catalysis on optically excited plasmonic metal nanostructures," American Chemical Society Spring National Meeting, San Diego, CA, March 2012

- 80. <u>Phillip Christopher</u>, Suljo Linic, "Utilizing molecular insights to guide shape- and sizecontrolled synthesis of Ag nanostructures for catalytic ethylene epoxidation," American Chemical Society Spring National Meeting, San Diego, CA, March 2012
- <u>Phillip Christopher</u>, Hongliang Xin and Suljo Linic, "Visible light driven photo-catalytic oxidation reactions on plasmonic nanostructures," American Chemical Society Spring National Meeting, San Diego, CA, March 2012
- 82. <u>Hongliang Xin</u>, Suljo Linic, "Understanding of environment-dependent mechanisms of alkali promotion in heterogeneous catalysis using first-principles based Monte Carlo simulation," American Institute of Chemical Engineers National Meeting, Minneapolis, MN, October 2011
- 83. <u>Hongliang Xin</u>, Phillip Christopher, Suljo Linic, "Energetic electron induced chemical reactions on metal surfaces: first-principles based electron scattering model," American Institute of Chemical Engineers National Meeting, Minneapolis, MN, October 2011
- 84. <u>Marimuthu Andiappan</u>, Phillip Christopher, Suljo Linic, "Surface plasmon-enhanced selective molecular sensing using unique silver nanoaggregates," American Institute of Chemical Engineers National Meeting, Minneapolis, MN, October 2011
- 85. David B. Ingram, <u>Suljo Linic</u>, "Composite plasmonic metal/semiconductor photoelectrodes for overall water splitting," American Institute of Chemical Engineers National Meeting, Minneapolis, MN, October 2011
- 86. <u>Phillip Christopher</u>, Hongliang Xin, Suljo Linic, "Plasmonic nanostructures as platforms for efficient coupling of visible light and thermal energy to drive chemical transformations," American Institute of Chemical Engineers National Meeting, Minneapolis, MN, October 2011
- 87. <u>Adam Holewinski</u>, Suljo Linic, "Pt-free electrocatalysts for efficient oxygen reduction in alkaline fuel cells: experimental and computational insights," American Institute of Chemical Engineers National Meeting, Minneapolis, MN, October 2011
- 88. <u>Hongliang Xin</u>, Suljo Linic "Development of predictive models for screening multimetallic electrocatalysts," American Institute of Chemical Engineers National Meeting, Minneapolis, MN, October 2011
- 89. <u>Phillip Christopher</u>, Suljo Linic, "Shape- and size-specific chemistry of Ag nanostructures in catalytic ethylene epoxidation," American Institute of Chemical Engineers National Meeting, Minneapolis, MN, October 2011
- 90. <u>Marimuthu Andiappan</u>, Jianwen Zhang, Suljo Linic, "Visible light enhanced selective propylene epoxidation over copper based catalyst," American Institute of Chemical Engineers National Meeting, Minneapolis, MN, October 2011
- 91. <u>Hongliang Xin</u>, Suljo Linic, "Exceptions to the d-Band Model of Chemisorption On Metal Surfaces: The Role of Repulsion Between Adsorbate States and Metal d-States," 22nd North American Catalysis Society Meeting, Detroit, MI, June 2011

- 92. <u>Adam Holewinski</u>, Suljo Linic, "Oxygen Reduction on Metals in Acidic and Basic Media: Insights toward design of Pt-free electrocatalysts," 22nd North American Catalysis Society Meeting, Detroit, MI, June 2011
- 93. <u>Phillip Christopher</u>, Hongliang Xin, Suljo Linic, "Multiple Stimuli Driven Catalysis: Catalytic Processes at Lower Temperatures Driven by Solar and Thermal Energy," 22nd North American Catalysis Society Meeting, Detroit, MI, June 2011
- 94. <u>David B. Ingram</u>, Suljo Linic, "Novel Composite Photocatalysts for Visible Light Water Splitting," 22nd North American Catalysis Society Meeting, Detroit, MI, June 2011
- 95. Eranda Nikolla, <u>Suljo Linic</u>, "Improving carbon tolerance of Ni electro(catalysts) by alloying," American Chemical Society Annual Meeting, Anaheim, CA, March 2011
- 96. David B. Ingram, <u>Suljo Linic</u>, "Visible light semiconductor photocatalysis enhanced by Ag nanoparticle plasmon resonance," American Chemical Society Annual Meeting, Anaheim, CA, March 2011
- 97. Phillip Christopher, <u>Suljo Linic</u>, "Optically active metallic nanostructures as platforms for efficient coupling of thermal and photonic stimuli for energy efficient chemical conversion," American Chemical Society Annual Meeting, Anaheim, CA, March 2011
- 98. <u>Hongliang Xin</u>, Suljo Linic, "Exceptions to the *d*-Band Model of Chemisorption On Metal Surfaces: The Dominant Role of Repulsion Between Adsorbate States and Metal *d*-States," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2010
- 99. Hongliang Xin, <u>Suljo Linic</u>, "Developing Relationships Between the Local Geometric Structure and Chemical Reactivity of Alloy Catalysts Based On Their Measured Electronic Structure," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2010
- 100. <u>Hongliang Xin</u>, Suljo Linic, "First-Principles Investigation of the Environment-Dependent Mechanisms of Alkali Promotion in Heterogeneous Catalysis," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2010
- 101. <u>Phillip Christopher</u>, Suljo Linic, "Size and shape specific chemistry of uniform, welldefined Ag nanoparticles of different shapes in catalytic ethylene epoxidation," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2010
- 102. <u>Phillip Christopher</u>, Suljo Linic, "Optically active metallic nano-structures for efficient coupling of thermal and photonic stimuli for energy efficient chemical conversion," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2010
- 103. Phillip Christopher, David B. Ingram, <u>Suljo Linic</u>, "Exploiting recent advancement in the field of nanotechnology in heterogeneous catalysis: shaped metallic nanostructures as selective catalysts, photo-catalysts and platform for the characterization of surface chemical reactions," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2010
- 104. <u>David B. Ingram</u>, Phillip Christopher, Suljo Linic, "Visible light semiconductor photocatalysis enhanced by Ag nanoparticle plasmon resonance," American Institute of

Chemical Engineers National Meeting, Salt Lake City, UT, November 2010

- 105. <u>Adam Holewinski</u>, Suljo Linic, "Comparative Studies of Oxygen Reduction on Metals in Acidic and Basic Media: Experimental and Computational Insights," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2010,
- 106. <u>Siris Laursen</u>, Suljo Linic, "The Support Effect in Heterogeneous Catalysis by Oxide Supported Gold (Au): A Combined Experimental and Theoretical Investigation," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2010
- 107. Neil M. Schweitzer, <u>Joshua Schaidle</u>, Suljo Linic and Levi Thompson, "Strong Interactions Between Molybdenum Carbide and Metal Catalysts: The Source of Enhanced Dispersion and Catalytic Activity," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2010
- 108. <u>Eranda Nikolla</u>, Suljo Linic, "Improving Carbon-Tolerance of Ni Reforming Catalysts and Electro-Catalysts by Surface Alloying and the Impact of Alloying on the Surface Chemistry," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2010
- 109. <u>Hongliang Xin</u>, Suljo Linic, "First-Principles Investigation of Alkali Promotion Mechanism in Oxidation Reactions Over Ag(111) Surfaces," American Institute of Chemical Engineers National Meeting, Nashville, TN, November 2009
- 110. <u>Phillip Christopher</u>, Suljo Linic, "Targeted, Well-Defined, and Uniform Ag Nanostructures as Highly Selective Olefin Epoxidation Catalysts," American Institute of Chemical Engineers National Meeting, Nashville, TN, November 2009
- 111. <u>Siris Laursen</u>, Suljo Linic, "Investigation of the Catalytically Active Site in Oxidation Catalysis by Gold: Insights from First Principles," American Institute of Chemical Engineers National Meeting, Nashville, TN, November 2009
- 112. <u>Eranda Nikolla</u>, Johannes Schwank, Suljo Linic, "Improving Long-Term Stability of Reforming Catalysts and Electro-Catalysts: from First Principles Studies to Novel Alloy Catalysts," American Institute of Chemical Engineers National Meeting, Nashville, TN, November 2009
- 113. <u>David B. Ingram</u>, Adam Holewinski, Suljo Linic, "First-Principles Analysis of the Activity of Transition and Noble Metals in the Direct Utilization of Hydrocarbon Fuels at Solid Oxide Fuel Cell Operating Conditions," American Institute of Chemical Engineers National Meeting, Nashville, TN, November 2009
- 114. Phillip Christopher, David B. Ingram, <u>Suljo Linic</u>, "Exploiting the Optical Properties of Well-Defined Nano-Structures for Photo-Catalytic Applications," American Institute of Chemical Engineers National Meeting, Nashville, TN, November 2009
- 115. <u>Suljo Linic</u>, Hongliang Xin, Neil Schweitzer, Eranda Nikolla, "Measuring and Relating the Electronic Structure of Alloys to Their Chemical and Catalytic Performance," American Institute of Chemical Engineers National Meeting, Nashville, TN, November 2009

- 116. <u>Neil M. Schweitzer</u>, Suljo Linic, Levi Thompson, "An Investigation of the Nature of Active Sites on Pt/Mo2C Water-Gas Shift Catalysts," American Institute of Chemical Engineers National Meeting, Nashville, TN, November 2009
- 117. <u>Siris Laursen</u>, Suljo Linic, "The Effect of the Gold–Oxide Interface on the Catalytic Chemistry of Au," 21st National Annual Meeting of the North American Catalysis Society, San Francisco, CA, June 2009
- 118. <u>Phillip Christopher</u>, Suljo Linic "The effect of Ag particle shape and surface structure on ethylene epoxidation selectivity," 21st North American Catalysis Society Meeting, San Francisco, CA, June 2009
- 119. <u>Hongliang Xin</u>, Suljo Linic, "Adsorbate-adsorbate Interactions on Metal Surfaces: First-Principles Studies of Alkali Promotion in Chemical Reactions over Ag(111)," 21st North American Catalysis Society Meeting, San Francisco, CA, June 2009
- 120. Eranda Nikolla, Neil Schweitzer, Hongliang Xin, <u>Suljo Linic</u>, "Measuring the electronic structure of metal alloys and relating it to their performance," 21st North American Catalysis Society Meeting, San Francisco, CA, June 2009
- 121. <u>David B. Ingram</u>, Suljo Linic, "Exploiting the optical properties of well-defined nanostructures for photo-catalytic applications," Michigan Catalysis Society Annual Symposium, University of Michigan, Ann Arbor, MI, May 2009
- 122. Phillip Christopher, <u>Suljo Linic</u>, "Well-defined metallic nano-structures as highly selective heterogeneous catalysts," American Chemical Society Annual Meeting, Salt Lake City, UT, April 2009
- 123. <u>David B. Ingram</u>, Suljo Linic, "First Principles Studies of Electrochemical Reactions at Solid Oxide Fuel Cell (SOFC) Electrodes," American Institute of Chemical Engineers National Meeting, Philadelphia, PA, November 2008
- 124. <u>Siris Laursen</u>, Suljo Linic, "Relating the Electronic Structure of the Oxide Support to the Chemical Activity of Au/oxide Catalysts: A First Principles Study," American Institute of Chemical Engineers National Meeting, Philadelphia, PA, November 2008
- 125. <u>Neil M. Schweitzer</u>, Suljo Linic, Levi Thompson, "Platinum Supported on Molybdenum Carbide for the Water-Gas Shift Reaction, a Theoretical and Experimental Study," American Institute of Chemical Engineers National Meeting, Philadelphia, PA, November 2008
- 126. Eranda Nikolla, <u>Suljo Linic</u>, "Predicting Catalytic Activity from Measured Electronic Structure of Supported Catalytic Materials: Supported Ni Versus Ni Alloys," American Institute of Chemical Engineers National Meeting, Philadelphia, PA, November 2008
- 127. Eranda Nikolla, <u>Suljo Linic</u>, "Improving Long-Term Stability of SOFC Anodes: First Principles Approaches toward Carbon-Tolerant Alloy Electrocatalysts," American Institute of Chemical Engineers National Meeting, Philadelphia, PA, November 2008
- 128. Hongliang Xin, <u>Suljo Linic</u>, "Adsorbate-Adsorbate Interactions in Heterogeneous Catalysis: Frist Principle DFT and Statistical Mechanics Studies of Impact of Alkalis on Oxidation Reactions," American Institute of Chemical Engineers National Meeting, Philadelphia, PA, November 2008

- 129. <u>David B. Ingram</u>, Suljo Linic, "First Principles Studies of Electrochemical Reactions at Solid Oxide Fuel Cell (SOFC) Electrodes," American Institute of Chemical Engineers National Meeting, Philadelphia, PA, November 2008
- 130. <u>Phillip Christopher</u>, Suljo Linic, "Engineering Selectivity in Heterogeneous Catalysis: The Impact of Ag Surface Structure on Ethylene Epoxidation Selectivity," American Institute of Chemical Engineers National Meeting, Philadelphia, PA, November 2008
- 131. David B. Ingram, <u>Suljo Linic</u>, "Electrochemistry from first principles: Studies of electrochemical oxidation reactions at solid oxide fuel cells (SOFCs)," International Congress on Catalysis, Seoul, Korea, July 2008
- 132. <u>Phillip Christopher</u>, Suljo Linic, "Engineering Selectivity In Heterogeneous Catalysis: The Impact of Ag Surface Structure on Ethylene Epoxidation Selectivity," Michigan Catalysis Society Annual Symposium, Midland, MI, May 2008
- 133. <u>Eranda Nikolla</u>, Johannes Schwank, Suljo Linic, "Carbon-tolerant reforming alloy catalysts," American Chemical Society Annual Meeting, New Orleans, LA, April 2008
- 134. <u>Siris Laursen</u>, Suljo Linic, "Surface chemistry of gold nanostructures deposited on oxides: Oxide-specific O2 interactions with supported gold and the oxidation state of gold," American Chemical Society Annual Meeting, New Orleans, LA, April 2008
- 135. <u>Eranda Nikolla</u>, Johannes Schwank, Suljo Linic, "Carbon-tolerant reforming alloy catalysts," American Chemical Society Annual Meeting, New Orleans, LA, April 2008
- 136. <u>Siris Laursen</u>, Suljo Linic "Catalysis at nano-scales: impact of oxide support and external conditions on Au/oxide model systems," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2007
- 137. <u>Eranda Nikolla</u>, Suljo Linic, "From molecular studies to novel carbon-tolerant hydrocarbon reforming alloy catalysts," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2007
- 138. Joydeep Mukherjee, David B. Ingram, <u>Suljo Linic</u>, "First Principles Studies of Electrochemical Reactions at Solid Oxide Fuel Cell (Sofc) Anodes," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2007
- 139. Hongliang Xin and <u>Suljo Linic</u>, "Adsorbate-adsorbate Interactions on Surfaces: First Principles Studies of Alkali Promotion in Chemical Reaction on Surfaces," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2007
- 140. Eranda Nikolla, <u>Suljo Linic</u>, "Rational design of heterogeneous catalysts," American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2007
- 141. <u>Eranda Nikolla</u>, Suljo Linic, "From molecular studies to novel carbon-tolerant hydrocarbon reforming alloy catalysts," American Chemical Society Annual Meeting, Boston, MA, August 2007
- 142. Joydeep Mukherjee, Suljo Linic, "First Principles Studies of Electrochemical Reactions at Solid Oxide Fuel Cell (Sofc) Anodes," American Chemical Society Annual Meeting, Boston, MA, August 2007

- 143. Siris Laursen and <u>Suljo Linic</u> "Catalysis at nano-scales: impact of oxide support and external conditions on Au/oxide model systems," American Chemical Society Annual Meeting, Boston, MA, August 2007
- 144. <u>Siris Laursen</u>, Suljo Linic, "Surface chemistry of gold nano-structures deposited on oxides: oxide-specific O<sub>2</sub> interactions with supported gold," Michigan Catalysis Society Symposium, Dearborn, MI, May 2007
- 145. <u>Eranda Nikolla</u>, Suljo Linic, "Controlling carbon surface chemistry on Ni by alloying: Carbon-tolerant hydrocarbon reforming alloy catalysts," American Chemical Society Annual Meeting, Chicago, IL, March 2007
- 146. Siris Laursen, <u>Suljo Linic</u>, "Catalysis at nano-scales: impact of oxide support and external conditions on Au/oxide model systems," American Chemical Society Annual Meeting, Chicago, IL, March 2007
- 147. Joydeep Mukherjee, Suljo Linic, "First Principles Studies of Electrochemical Reactions at Solid Oxide Fuel Cell (Sofc) Anodes," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2006
- 148. Jeb Adams, <u>Suljo Linic</u>, "Alkali-Promotion in Heterogeneous Catalysis: Dft Studies of the Pressure- and Temperature-Dependant Impact of Alkalis on Oxidation Reactions," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2006
- 149. <u>Eranda Nikolla</u>, Johannes Schwank, Suljo Linic, "Hybrid Theoretical/Experimental Studies Aimed at the Development of Carbon-Tolerant Reforming Alloy Catalysts," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2006
- 150. Eranda Nikolla, Johannes Schwank, <u>Suljo Linic</u>, "Molecular Insight into Carbon Poisoning of Ni Surfaces: Dft-Guided Formulation of Carbon-Tolerant Steam Reforming Catalysts," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2006
- 151. Siris Laursen, <u>Suljo Linic</u>, "Heterogeneous Catalysis by Gold: Oxide-Specific O2 Interactions with Supported Gold," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2006
- 152. Joydeep Mukherjee, <u>Suljo Linic</u>, "First Principles and Kinetic Monte Carlo Investigations of Pd-Based Metallic Membranes for Hydrogen Separation," American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2006
- 153. Eranda Nikolla, <u>Suljo Linic</u>, "Hybrid theoretical/experimental studies aimed at the development of carbon- and sulfur-tolerant reforming catalysts," U.S. Department of Energy National Energy Techonology Laboratory symposium, Philadelphia, PA, September 2006
- 154. Eranda Nikolla, Johannes Schwank, <u>Suljo Linic</u>, "Hybrid theoretical/experimental studies aimed at the development of carbon-tolerant reforming catalysts," ACS Colloids and Surface Science Meeting, Boulder, CO, June 2006

- 155. Joydeep Mukherjee, <u>Suljo Linic</u>, "Pd-based membranes for hydrogen separation: from atomistic understanding to rational design," U.S. Department of Energy National Energy Technology Laboratory workshop," Pittsburgh, PA, May 2006
- 156. Siris Laursen, P. Larkowski, <u>Suljo Linic</u>, "Heterogeneous catalysis by Au: DFT investigations of O<sub>2</sub> interactions with oxide supported Au materials," American Institute of Chemical Engineers National Meeting, Cincinnati, OH, November 2005
- 157. J. Adams, <u>Suljo Linic</u>, "Alkali-Promotion in Heterogeneous Catalysis: DFT Study of the Impact of Alkalis on a Number of Elementary Dissociation Surface Reactions," American Institute of Chemical Engineers National Meeting, Cincinnati, OH, November 2005
- 158. <u>Eranda Nikolla</u>, Johannes Schwank, Suljo Linic, "First-principles design of carbon-tolerant reforming catalysis," American Institute of Chemical Engineers National Meeting, Cincinnati, OH, November 2005
- 159. <u>Suljo Linic</u>, Mark A. Barteau, "Cs Additives in Heterogeneous Catalyst: Proposed Mechanism of Cs-Promotion in Ethylene Epoxidation on Silver," North American Catalysis Society Meeting, Philadelphia, PA, May 2005
- 160. <u>Suljo Linic</u>, Mark A. Barteau, "Bimetallic catalysts for ethylene epoxidation designed from first principles," American Chemical Society Annual Meeting, San Diego, CA, March 2005
- 161. <u>Suljo Linic</u>, J. Carlson, Mattias Scheffler, "Carbon Nano-Materials as Efficient Heterogeneous Catalysts: Fundamental Studies of the Mechanism of Oxidative Dehydrogenation of Ethyl Benzene," American Institute of Chemical Engineers National Meeting, Austin, TX, November 2004
- 162. <u>Suljo Linic</u>, Mark A. Barteau, "Bimetallic catalysts for ethylene epoxidation designed from first principles," American Institute of Chemical Engineers National Meeting, Austin, TX, November 2004
- 163. <u>Suljo Linic</u>, Mark A. Barteau, "Ethylene epoxidation on Ag: From fundamental studies to novel catalyst formulation," 13<sup>th</sup> Congress on Catalysis, Paris, France, July 2004

# <u>Research Proposals Funded (in reverse chronological order)</u> <u>Sponsored Research</u>

- 1) DOE-BES, "Title: Experimental and modelling studies of the role of chemical promoters in heterogeneous catalysis," \$570,000, 9/2020 8/2023, **PI: S. Linic**
- DOE-BES, "Title: Operando atomistic characterization of structural, physical, and chemical characteristics of semiconductor/metal interfaces on functioning hybrid photocatalysts," \$550,000, 9/2020 – 8/2023, PI: S. Linic
- DOD-MURI, "Title: Plasma-Driven Solution Electrochemistry", co-PIs; Peter Bruggeman, Rene Frontiera, Uwe Kortshagen (U of Minnesota), George Schatz (Northwestern U), S. Linic and M. Kuschner (U of Michigan), 6.25 Million, Linic share \$1.1 Million, 6/2020 – 5/2025

- 4) National Science Foundation, (Division of Chemistry, CHE-Catalysis), "Controlling the energy flow in multi-component plasmonic structures for selective catalysis," \$447,000, 9/2018 8/2021. PI: S. Linic
- National Science Foundation, (CBET-Catalysis), "Maximizing efficiency in solar water splitting by engineering interfaces in hybrid photo-catalysts," \$330,000, 9/2018 – 8/2021.
   PI: S. Linic
- 6) National Science Foundation, DMREF Collaborative Research: Multiscale computational design of electrocatalytic cascade reactions, my share: \$80,000, 9/2018 8/2019, **PI: S. Linic**
- 7) ExxonMobil Corporation, "Development of methane upgrading technologies," \$360,000, 6/2018 6/2021, **PI: S. Linic**
- 8) DOE, RAPID manufacturing, "Thermo-neutral Propane Dehydrogenation via a Solid Oxide Membrane Reactor," \$900,000, 1/2018 12/2020, **PI: S. Linic**
- 9) ExxonMobil Corporation, "Development of methane upgrading technologies," \$190,000, 9/2017 9/2018, **PI: S. Linic**
- 10) National Science Foundation, INFEWS N/P/H2O: Photo-thermal ammonia synthesis of plasmonic metal nanoparticles, \$40,000, 2017 2020, PI: S. Linic
- 11) National Science Foundation, "Ammonia synthesis on plasmonic materials," \$300,000, 2017
   2020, PI: S. Linic
- 12) DOE-BES, "Development of physically transparent, predictive structure-performance relationships for rational design of multi-component catalytic materials," \$510,000, 9/2017 8/2020, PI: S. Linic
- ExxonMobil Corporation, "Heterogeneous catalytic processes for chemical upgrading of methane," \$186,000, 10/2015 – 9/2017, PI: S. Linic
- 14) National Science Foundation, DMREF Collaborative Research: Multiscale computational design of electrocatalytic cascade reactions, 9/2014 8/2018, Total 1.6 Million (with Michael Janik (Penn State), Will Medlin (U of Colorado), Eranda Nikolla (Wayne State), my share: \$400,000, PI: S. Linic
- 15) National Science Foundation, (Division of Chemistry, CHE-Catalysis), "Heterogeneous Catalysis on Plasmonic Metallic Nanostructures: Selective Catalytic Conversion at Lower Temperatures co-Driven by Solar and Thermal Energy," \$420,000, 9/2014 – 8/2017. PI: S. Linic
- 16) National Science Foundation, "Studies of the impact of plasmonic metal nano-particles on co-catalysts/semiconductor photocatalysts in the solar water splitting," \$362,000, 2014 – 2017, PI: S. Linic
- 17) DOE-BES, "Development of physically transparent, predictive structure-performance relationships for rational design of multi-component catalytic materials," \$460,000, 9/2014 8/2017, PI: S. Linic
- 18) National Science Foundation, "Designing Efficient Platinum-Free Electrocatalysts for Oxygen Reduction Reaction," \$41,000, 2012, **PI: S. Linic**

- 19) National Science Foundation, "Exploiting links between nano-technology and heterogeneous catalysis: Shaped silver nano-particles as selective catalysts for partial oxidation of olefins to form chiral and nonchiral epoxides," \$41,000, 2012, **PI: S. Linic**
- 20) DOE-BES, "Development of physically transparent, predictive structure-performance relationships for rational design of multi-component catalytic materials," \$510,000, 9/2011 8/2014, PI: S. Linic
- 21) National Science Foundation, (Division of Chemistry, CHE-Catalysis), "Heterogeneous Catalysis on Plasmonic Metallic Nanostructures: Selective Catalytic Conversion at Lower Temperatures co-Driven by Solar and Thermal Energy," \$300,000, 9/2011 – 8/2014. PI: S. Linic
- 22) National Science Foundation, "Designing Efficient Platinum-Free Electrocatalysts for Oxygen Reduction Reaction," \$41,000, 9/2011 8/2014. **PI: S. Linic**
- 23) NSF-CBET, "Designing Efficient Platinum-Free Electrocatalysts for Oxygen Reduction Reaction," \$285,000, 9/2011 8/2014. PI: S. Linic
- 24) ACS-PRF, "From first principles studies to novel electro-catalysts for oxygen reduction reaction: design, synthesis and testing," \$100,000, 9/2011 8/2014. **PI: S. Linic**
- 25) DOE-BES, "Acquisition of a state-of-the-art multiple laser line Raman spectrometer," \$250,000, 10/2011 9/2012, PI: S. Linic
- 26) Sandia National Laboratory, "Development of first principle methodology to study electrocatalytic reactions at metal/electrolyte interfaces," **PI: S. Linic (fellowship for Matt Morabito)**, \$50,000 per year over a period of five years
- 27) National Science Foundation, NSF-CBET, "First-principles studies of heterogeneous electrochemistry: Electrochemical oxidation reactions over solid oxide fuel cell (SOFC) metal/electrolyte anodes," \$30,000, 9/2010 9/2011, **PI: S. Linic**
- 28) NSF-CBET: "Exploiting Links Between Nano-Technology and Heterogeneous Catalysis: Shaped Silver Nano-Particles as Selective Catalysts for Partial Oxidation of Olefins to Form Chiral and Non-Chiral Epoxides," \$300,000, 9/2010 – 8/2013, PI: S. Linic
- 29) National Science Foundation, "EFRI-HyBi: The Science and Engineering of Microalgae Hydrothermal Processing," co-PI S. Linic, PI: P. Savage, total 2 Mil (my share: ~ \$300,000), 9/2009 9/2013
- 30) National Science Foundation, NSF-CBET, "First-principles studies of heterogeneous electrochemistry: Electrochemical oxidation reactions over solid oxide fuel cell (SOFC) metal/electrolyte anodes," \$30,000, 9/2008 9/2011, **PI: S. Linic**
- 31) Dreyfus Foundation, Camille Dreyfus Teacher-Scholar Award, "Targeted metallic nanostructures as heterogeneous catalysis, electro-catalysts, and platforms for chemical characterization" \$75,000, 9/2009, **PI: S. Linic**
- 32) DARPA, "Development of sulfur-tolerant catalysts and electro-catalysts," \$500,000, co-PI
   S. Linic, PI: Andrew Tadd, total \$1.5 mil (my share: \$300,000), 4/2009
- 33) U.S. Department of Energy (Basic Energy Science division), "Adsorbate-adsorbate Interactions on Metal Surface, \$450,000, 9/2008 8/2011, **PI: S. Linic**

- 34) Sandia National Laboratory, "Development of first principle methodology to study electrocatalytic reactions at metal/electrolyte interfaces," **PI: S. Linic (fellowship for Matt Morabito)**, \$50,000 per year over a period of five years
- 35) ONR, "Degradation of SOFC cathodes by impurity gases in air feed," \$201,000, 5/2008 5/2010; **PI: S. Linic**
- 36) DuPont Young Professor award, "Direct electrochemical conversion of chemical energy of biofuels to electricity," \$75,000, 9/2008 9/2011, **PI: S. Linic**
- 37) National Science Foundation, NSF-CBET, "First-principles studies of heterogeneous electrochemistry: Electrochemical oxidation reactions over solid oxide fuel cell (SOFC) metal/electrolyte anodes," \$300,000, 9/2008 9/2011, **PI: S. Linic**
- 38) NSF-CAREER, "Hybrid theoretical/experimental studies of metal/metal-oxide interface chemistry: The role of oxide support in Au/oxide catalytic activity," \$400,000, 9/2006 8/2011, **PI: S. Linic**
- 39) DOE-NETL, Phase II: "Development of sulfur and carbon tolerant reforming alloy catalysts aided by fundamental atomistic insights," \$140,000, 6/2006 12/2008, **PI: S. Linic**
- 40) DOE-BES, "Investigations of alkali promotion in heterogeneous catalysis: First principles DFT and ab-initio atomistic thermodynamics studies of Cs promotion in oxidation reactions over Ag," \$450,000, 9/2005 8/2008; **PI: S. Linic**
- 41) DOE-NETL, "First-principle investigation of H2 separation using Pd-based metallic membranes," \$50,000, 9/2005 9/2006, **PI: S. Linic**
- 42) DOE-NETL, "Development of sulfur and carbon tolerant reforming alloy catalysts aided by fundamental atomistic insights," \$141,508, 6/2006 7/2007, **PI: S. Linic**
- 43) ACS-PRF, "Theoretical and Experimental Investigations of Propylene Epoxidation on TiO2 supported Gold Nano-particles," \$35,000, 6/2004 5/2006, **PI: Suljo Linic**
- 44) DOD-Army, "Development of sulfur and carbon tolerant solid oxide fuel cells" phase III, Co-Pi: S. Linic, PI: J. Schwank, Approximately \$1,690,000, 6/06 12/08. (my share: \$155,000)
- 45) DOE, "Energy Storage and Distributed Energy Generation Initiative at the UM Transportation Energy Center (TEC)," Co-Pi: S. Linic, PI: J. Schwank, ~\$1,000,000 starting 2/07 12/08. (my resources: ~ \$70,000)
- 46) Rackham school of graduate studies "Towards rational discovery of novel SOFC electrodes," \$15,000, 4/05 4/50, PI: **S. Linic**
- U.S. Department of Energy, Basic Energy Science Division Equipment Grant, Acquisition of a PC cluster for quantum calculations, \$65,000 (\$30,000 cost share), 9/06 9/07, PI: S. Linic
- 48) UM Dean's Equipment Grant, Acquisition of a Scanning Tunneling Microscope (STM), \$95,000, PI: S. Linic

### **Research proposals pending**

- 49) DOE, "In-situ atomistic characterization of structural, physical and chemical characteristics of semiconductor/metal interfaces on functioning hybrid photocatalysts," PI: S. Linic, \$600,000, 9/2020 8/2023 (submitted 2020)
- 50) DOE-BES, "Experimental and modelling studies of the role of chemical promoters in heterogeneous catalysis," **PI: S. Linic**, \$570,788, 9/2020 8/2023 (submitted 2020)
- 51) NSF-CBET, "Collaborative Research: EAGER: Machine Learning-aided Discovery of Synthesizable Active and Stable Heterogeneous Catalysts," PI: S. Linic, Co-PIs: B.R. Goldsmith, N. Singh, E. Nikolla, \$225,000, (Linic share = \$75,000), 1/2020 12/2020 (submitted 2019)
- 52) ARO, "Plasma-Driven Solution Electrochemistry," **Co-PIs: Linic, Kushner, Schatz, Kortshagen, Frontiera, PI: Bruggeman**, \$6,250,000, (Linic share = \$1,300,000), 5/2020 4/2025 (submitted 2019)

### **Student Funding from External Sources**

- 53) Sean Dix: NSF-GRFP, "Alkaline Electrocatalyst Design for Improved Hydrogen Fuel Cells," \$132,000, 9/2017 9/2020
- 54) Rawan Almallahi: NSF-GRFP, "Membrane Reactors for Oxidative Coupling of Methane," \$138,000, 9/2017 8/2020
- 55) Steven Chavez: Ford Foundation, Predoctoral Fellowship. \$72,000, 9/2015 9/2018
- 56) Steven Chavez, NSF-GRFP, "Investigation of Acetic Acid Oxidation via Noble Catalysts for the Electrochemical Stabilization of Bio-oil," \$138,000, 9/2015 9/2018
- 57) John Hemmerling, DoD-NDSEG, "Plasmonic catalysts for water splitting, \$153,600, 9/2017 - 9/2021

# Funded Proposals for shared cyber infrastructure resources

- 58) National Science Foundation Cyber-infrastructure Partnership, "MRAC: DFT studies of metal/oxide interface chemistry: Investigations of H2/O2 interactions at Au/TiO2, and H2 oxidation at Ni/ZrO2 interfaces," 4/2005 – 3/2007, 95,000 CPU hours of computing time at San Diego Computing Site, PI: S. Linic
- 59) National Science Foundation Cyber-infrastructure Partnership, "Development grant: Pdbased metallic membrane for H2 separation: First principles studies of separation mechanisms aimed at knowledge-based rational formulations of improved materials," 1/2005 – 12/2005, 10,000 CPU hours of computing time at San Diego Computing Site, PI: S. Linic
- 60) National Science Foundation Cyber-infrastructure Partnership, "MRAC: DFT studies of metal/oxide interface chemistry: Investigations of H2/O2 interactions at Au/TiO2, and H2 oxidation at Ni/ZrO2 interfaces," 9/2005 – 3/2006, 100,000 CPU hours of computing time at San Diego Computing Site, **PI: S. Linic**

- 61) National Science Foundation Cyber-infrastructure Partnership, "MRAC: DFT studies of metal/oxide interface chemistry: Investigations of H2/O2 interactions at Au/TiO2, and H2 oxidation at Ni/ZrO2 interfaces," 4/2005 – 3/2007, 150,000 CPU hours of computing time at San Diego Computing Site, **PI: S. Linic**
- 62) U.S. Department of Energy Cyber-infrastructure, "Pd-based metallic membrane for H2 separation: First principles studies of separation mechanisms aimed at knowledge-based rational formulations of improved materials," 20,000 CPU hours from Pittsburgh Supercomputing Center, **PI: S. Linic**

# **TEACHING**

# Courses taught

Seminars in Energy Technologies (CEE 565/ESE 501) Fluid Mechanics (ChE 341) Chemical Reaction Engineering (ChE 344) *Ab initio* Electronic Structure Calculations in Engineering (ChE 696) Graduate Reaction Engineering (ChE 528) Energy Conversion Systems (ChE 696/ESENG 505/MECHENG 571) Fuel Cells and Fuel Processors (ChE 696) Molecular Foundation for Heterogeneous Catalysis and Electro-catalysis (ChE 696) Research Project in Energy Systems Engineering (ESENG 503);

# **Graduate Elective Courses Developed**

#### CHE 496/696: Molecular foundation for heterogeneous catalysis and electro-catalysis

The course addressed numerous topics including:

- 1) Chemical bonding on metal surfaces
- 2) Various experimental tools used to study chemical transformations on surfaces at molecular level
- 3) Various theoretical tools used to study chemical interactions on surfaces

The material was discussed through a number of examples addressing contemporary issues related to the fields of energy and environment. These examples focused on the chemistry of fuel cells, chemistry of alloys, chemistry on nano-sized catalytic materials, characterization of these materials, relationships between the electronic structure of a material and its (electro)catalytic activity, etc.

We also discussed strategies that can be utilized to employ molecular insights to identify optimal electro(catalysts) for different electro(chemical) processes. For example, we developed a molecular foundation for a number of important phenomena including Sabatier's principle, Bronsted-Evans-Polanyi (BEP) relationships, volcano curves, and many others.

# CHE 496/696: Ab initio Electronic Structure Calculations in Engineering

This course described various methods of solving the governing equation of quantum mechanics (Schrödinger equation) with a particular emphasis on Density Functional Theory (DFT). Furthermore, it was illustrated how to utilize the electronic structure calculations to develop atomistic insights into elementary processes which govern the performance of heterogeneous catalysts, fuel cell electrodes, chemical sensors, etc. We also discussed different methodologies that allow us to use the atomistic insights obtained in the DFT calculations to draw conclusions about macroscopic observables such as catalytic activity and selectivity.

### CHE 696/ESE505: Energy Conversion Systems

The course focused on discussing electrochemical energy conversion systems. We emphasized fundamental framework for the analysis and development of energy conversion systems.

# **SERVICE**

### **External Professional Activities**

reverse chronological order

- 1. Invited Member, National Science Foundation, enabling task team charged with developing Transformative Advances in Materials Engineering through Development of Novel Approaches to Electron Microscopy, September 2020
- 2. Reviewer, U.S. Department of Energy Solar Photosynthesis Panel; July 2020
- 3. Reviewer, U.S. Department of Energy Basic Energy Sciences (DOE-BES); April 2020
- Invited Member, U.S. Department of Energy Basic Energy Sciences (DOE-BES) task team charged with developing a long-term plan for basic research on artificial photosynthesis, August 2019
- Reviewer, U.S. Department of Energy SLAC-Stanford center on catalysis; Palo Alto, CA, May 2019
- 6. Testified in front of U.S. Congress on the state of national energy and sustainability research, September 2018
- 7. Chair, U.S. American Chemical Society/National Science Foundation delegation, 2017 Chemical Sciences and Society (CS3) Summit, Dalian, China; tasked with the development of a long-term strategy in the field of photo-catalysts and photonics along with the teams from the UK, China, Germany and Japan; Dalian, China, 2017
- 8. Associate Editor, ACS Catalysis, 2014 present
- 9. Member, Organizing Committee, 2020 International Congress on Catalysis; Worked with multiple colleagues on putting together an application for the hosting of the meeting; application positively reviewed; meeting to take place in San Diego in 2020.
- Invited Member, U.S. Department of Energy Basic Energy Sciences (DOE-BES) task team charged with developing a long-term plan for basic research in the development of high energy electron source at Stanford Linear Accelerator Center (SLAC) National Accelerator Laboratory, Stanford University, Menlo Park, CA, September 2016

- 11. Invited Member, U.S. Department of Energy task team charged with developing a longterm plan for basic research in the development of material characterization infrastructure, June 2016
- 12. Member, Scientific Committee, 24<sup>th</sup> International Symposium on Chemical Reaction Engineering (ISCRE 24), to be held in Minneapolis on June 12 15, 2016
- 13. Workshop participant, topic: the future of hydrocarbon feedstock, National Academies, March 2016
- 14. Reviewer, U.S. Department of Energy Energy Frontier Research Center (DOE-EFRC) program; reviewed three EFRC centers in DC, February 2016
- Reviewer, National Science Foundation (NSF); reviewed 28 proposals at the NSF panel, February 2016
- 16. On-site U.S. Department of Energy reviewer: surface science and computational catalysis program at the Stanford Linear Accelerator Center (SLAC) National Accelerator Laboratory, Stanford University, Menlo Park, CA, August 2013
- 17. Member, Selection Committee, *AICHE Journal*, 2010 2011; committee charged to select new Editor-in-Chief
- 18. Coordinator, Kokes Student Travel Award for June 2011 North American Catalysis Society meeting in Detroit, MI; Obtained funding for the award from the National Science Foundation and the U.S. Department of Energy, selected awardees among 204 applicants, and coordinated the process.
- 19. Editorial Advisory Board, ACS Catalysis, 2010 present
- 20. Editorial Advisory Board, AIChE Journal, 2010 present
- 21. Elected board member, American Institute of Chemical Engineers, Division 20 (Catalysis and Reaction Engineering)
- 22. Chair, Michigan Catalysis Society, 2009 2010
- 23. On-site reviewer for the surface science, nanoscience, and catalysis programs at Pacific Northwest National Laboratory (PNNL), Richland, Washington, March 2009
- 24. President, Michigan Catalysis Society, 2008 2009
- 25. Invited Member, DOE task team charged to develop long-term plan for the basic energy research; along with four other faculty members drafted a document describing the grand challenges in basic energy research, August 2007
- Programming Chair, American Institute of Chemical Engineers, Division 20c, 2007 2008
- 27. Vice-president, Michigan Catalysis Society, 2007 2008
- Programming Vice-Chair, American Institute of Chemical Engineers, Division 20c, 2006 – 2007
- 29. Treasurer, Michigan Catalysis Society, 2006 2007
- 30. National Meetings Sessions (chair and co-chair)
  - Photo and Electro-Catalysis, Bi-annual Meeting of North American Catalysis Society, Louisville, KY, June 2013
  - Computational Catalysis (2 sessions), American Institute of Chemical Engineers National Meeting, Pittsburgh, PA, October 2012
  - Fundamental Catalysis, American Institute of Chemical Engineers National Meeting, Minneapolis, MN, October 2011
  - Computational Catalysis, Bi-annual Meeting of North American Catalysis Society, Detroit, MI, June 2011

- Electro- and Photo-catalysis (2 sessions), American Institute of Chemical Engineers National Meeting, Minneapolis, MN, November 2010
- Computational Catalysis (2 sessions), American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2010
- Rational Catalyst Design (2 sessions), American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2010
- Electro-catalysis, American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2010
- Computational Catalysis (2 sessions), American Institute of Chemical Engineers National Meeting, Nashville, TN, November 2009
- Rational Catalyst Design (2 sessions), American Institute of Chemical Engineers National Meeting, Nashville, TN, November 2009
- Electrocatalysis, American Institute of Chemical Engineers National Meeting, Nashville, TN, November 2009
- Fundamental Catalysis, 21st National Annual Meeting: North American Catalysis Society, San Francisco, CA, June 2009
- Fundamental Catalysis, 21st National Annual Meeting: North American Catalysis Society, San Francisco, CA, June 2009
- Computational Catalysis (2 sessions), American Institute of Chemical Engineers National Meeting, Philadelphia, PA, November 2008
- Computational Catalysis (organizer of the entire symposium on the topic 4 different sessions), American Chemical Society Annual Meeting, New Orleans, LA, April 2008
- Computational Catalysis (2 sessions), American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2007
- Fundamentals of Electro-catalysis, American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2007
- Catalyst Deactivation, American Institute of Chemical Engineers National Meeting, Salt Lake City, UT, November 2007
- Computational Catalysis (2 sessions), American Institute of Chemical Engineers National Meeting, San Francisco, CA, November 2006
- Fundamentals of Surface Reactivity from *Ab Initio* Modeling, American Institute of Chemical Engineers National Meeting, Cincinnati, OH, November 2005
- Rational Catalyst Design, American Institute of Chemical Engineers National Meeting, Cincinnati, OH, November 2005
- Catalyst Poisoning, American Institute of Chemical Engineers National Meeting, Cincinnati, OH, November 2005
- 31. Regular reviewer for Nature Materials, Journal of the American Chemical Society, Physical Review Letters, Surface Science, Journal of Physical Chemistry B and C, Journal of Catalysis, Physical Review B, Angewandte Chemie, and many others.
- 32. Regular proposal reviewer for NSF, ACS-PRF, Army, ONR, and DOE.
- 33. Member of proposal review panels for:
  - i. NSF-CTS, 2008, ~30 large proposals reviewed
  - ii. NSF-CTS, 2006, ~30 large proposals reviewed
  - iii. DOE-BES, 2006, ~20 large proposals reviewed
  - iv. NSF-Career-Chemistry, ~ 12 proposals

### **Internal Professional Activities:**

reverse chronological order

- 1. Member, Faculty Search Committee, 2019
- 2. Chair, Internal Review Committee, 2017 2018
- 3. Chair, Space Committee, 2017 2018
- 4. Chair, Faculty Search Committee, 2015 2018
- 5. Member, University Energy Institute Evaluation Committee, 2017 2018
- 6. Member, Launch Committee (Bryan Goldsmith), 2017 2018
- 7. Member, Launch Committee (Andrej Lenert), 2017 2018
- 8. Director, Energy Systems Engineering Program, 2010 present; College of Engineering Masters program, currently over 200 student advisees enrolled
- 9. Multiple PhD thesis committees in Chemical Engineering and other departments
- 10. Member, (UM) Chemical Engineering Advisory Committee (CHEAC), 2011 2014
- 11. Member, University Search Committee; formed to identify potential hires in the field of energy
- 12. Member, College of Engineering Nominating Committee, 2009
- 13. Member, Faculty Search Committee, 2007 2009
- Member, College of Engineering Faculty Search Committee, area: distributed power, 2007 – 2008
- 15. Member, UM Department of Chemical Engineering Strategic Planning Committee, 2007
- 16. Member, College Battery Task Team; 2006 2007; established by the Dean to define the direction the College should follow in expanding its research efforts in the field of energy storage and delivery
- 17. Member, Graduate Program Committee, 2005 present; handle graduate program, developed Teaching Fellowship Program
- 18. Chair and co-chair, Graduate Student Recruiting Committee, 2005 present
  - a. Review applications for graduate program, make admission decisions
  - b. Planned and organized events for the graduate student recruiting weekend, 2006 present
- Faculty Advisor, American Institute of Chemical Engineers Undergraduate Chapter, 2004 2009

# **Memberships**

American Institute of Chemical Engineers (AIChE) American Chemical Society (ACS) North American Catalysis Society (NACS) Tau Beta Pi National Engineering Honor Society Phi Eta Sigma National Honor Society