

## CURRICULUM VITAE

### Dionisios (Dion) G. Vlachos

Department of Chemical and Biomolecular Engineering  
Center for Catalytic Science and Technology (CCST)  
Catalysis Center for Energy Innovation (CCEI)  
University of Delaware, Newark, DE 19716-3110

Tel. (302) 831-2830  
Fax (302) 831-2085  
[vlachos@udel.edu](mailto:vlachos@udel.edu)  
<http://www.che.udel.edu/vlachos>

**Date of birth:** 7/11/64

### Education

Ph.D., Chemical Engineering and Materials Science Department, University of Minnesota, 1992; Thesis title: "Structure and Dynamics of Adsorbed Phases and Crystal Surfaces"  
M. S., Chemical Engineering and Materials Science Department, University of Minnesota, 1990; Thesis title: "Step Dynamics for Modeling of Crystal Surfaces"  
Five years diploma, Chemical Engineering Department, National Technical Univ. of Athens, Athens, Greece, 1987

### Current Academic Appointments

Allan and Myra Ferguson Prof. of Chemical and Biomolecular Engineering, Univ. of Delaware, 2016-  
Director, Delaware Energy Institute (UDEI), 2016-  
Director, Catalysis Center for Energy Innovation (CCEI), an Energy Frontier Research Center (EFRC) funded by DOE with \$29.9 M, 2009-2018  
Professor (Joint) of Physics and Astronomy, University of Delaware, 9/1/15-8/31/18  
Affiliated Member, Institute of Chemical Engineering and High Temperature Chemical Processes (ICE-HT) of FORTH (Foundation for Research and Technology, Hellas), Patras, Greece, 2005-  
Affiliated Member, Delaware Environmental Institute (DENIN), University of Delaware, 2014-

### Professional Experience

Elizabeth Inez Kelley Professor of Chemical Engineering, University of Delaware, 2009-2016  
Professor, Chemical Engineering Department, University of Delaware, 2003-09  
Director, Center for Catalytic Science and Technology (CCST), 2008-2011  
George Piercy Distinguished Visiting Professor, Chemical Engineering and Materials Science Department, University of Minnesota, 2007  
Visiting faculty, Thomas Jefferson University and Hospital, 2007  
Associate Professor, Chemical Engineering Department, University of Delaware, 2000-03  
Adjunct Professor, Chemical Engineering Department, University of Massachusetts, 2000-03  
Visiting Fellow, Princeton University, 2000  
Associate Professor, Chemical Engineering Department, University of Massachusetts, 1998-2000  
Assistant Professor, Chemical Engineering Department, University of Massachusetts, 1993-1998  
Research Associate, Army High Performance Computing Research Center, Univ. of Minnesota, 1992-93

### Research Interests

Portable and distributed energy, renewables, fuel and biofuel processing: portable and distributed power generation; multifunctional reactors and devices for H<sub>2</sub> production and electricity; novel catalyst design; alternative and renewable fuels; catalytic combustion, partial oxidation, and reforming; microreactors; thermoelectrics; optimization of chemical processes.  
Surface chemistry: novel microreactors for extraction of kinetics of very fast reactions; prediction of elementary-reaction kinetics through hierarchical multiscale modeling; fuel and biomass process modeling with detailed reaction mechanisms; experimental chemical kinetics (from surface science to high pressure).  
Control thin film and particle microstructure: nucleation and growth of ceramic and metal-composite-based membranes by hydrothermal and supercritical processes; growth of zeolite particles and membranes; template-assisted and capping-agent assisted colloidal growth; bottom-up strategies for patterning of materials.

Multiscale modeling, simulation, and dynamics: kinetic Monte Carlo; molecular dynamics; density functional theory; hybrid, hierarchical, and coarse-grained branches of multiscale modeling; mesoscopic theory; model reduction; computational fluid dynamics; nonlinear dynamics and bifurcation theory.

### **Selected Honors/Awards**

Doumas Lecture, Department of Chemical Engineering, Virginia Tech, 2016  
Philadelphia Catalysis Club Award, 2016  
ICI Distinguished Lecturer, DB Robinson Lectureship Series at the University of Alberta, 2014-2015  
J. D. Lindsay Lecture Series, Chemical Engineering Department, Texas A&M University, Oct. 8, 2014  
R. H. Wilhelm Award in Chemical Reaction Engineering, AIChE Institute Award, 2011  
AAAS Fellow, 2009  
Elizabeth Inez Kelley Professorship of Chemical Engineering, University of Delaware, 2009  
Outstanding Junior Faculty Award, College of Engineering, UMass, 1997  
National Science Foundation Career Award, 1997  
Office of Naval Research Young Investigator Award, 1996  
Outstanding Advisor Service Award, College of Engineering, UMass, 1996 and 1997

### **Editorial Boards/Scientific Advisory Committees**

*Executive Editor, Chemical Engineering Science, 8/1/11-7/31/14*; In 2013, CES broke through into the Top 25 journals in Engineering, Chemical category (ranked #24) edging out AIChE J.

*Editorial Advisory Board Member: Chemical Engineering and Processing: Process Intensification (1/1/17-); ACS Catalysis (11/1/13-10/31/17); Reaction Chemistry & Engineering (7/13/15-7/12/18); Industrial and Engineering Chemistry Research (I&ECR) (1/1/09-12/31/11); Applied Catalysis A: General (4/1/09-3/31/12); Proceedings of The Combustion Institute (ProCI; 2008-2012); The Open Energy and Fuels Journal, Bentham Science Publishers LTD (2007-); Journal of Nano Energy and Power Research (2010-); J. Chem. Eng. & Proc. Tech., OMICS Publishing Group, 2010-2013; Chemical Engineering and Processing: Process Intensification (2016-2019).*

*International Scientific Committee/Board Member: TU Delft Process Technology Institute (2013-); ISCRE 24, Minneapolis, MN, 2016; ISCRE 22, Maastricht, Netherlands, September 2-5, 2012 and NASCRE 3, March 17-20, 2013, Houston; Coarse-graining of many-body systems: Analysis, computations and applications, Applied Math Center, Heraklion, Crete, Greece, [acmac.tem.uoc.gr](http://acmac.tem.uoc.gr), 2010-2011; Int. Symposium Chem. Reaction Engineering (ISCRE) board (2008-2020); Structured Catalysts and Reactors (2009-); International Zeolite Membranes (2007-)*

### **Major Professional Activities, Memberships, and Services**

Council of Fellows, Delaware Environmental Institute (DENIN), 2017-  
Modular Manufacturing Workshop Organizer, Arlington at Ballston, VA January 17/18, 2017.  
ISCRE Vice President (2017-2018), President (2019-20), and Past President (2021-22)  
Director of ORCS and Representative to NACS, 2016  
Representative of Philadelphia Catalysis Club (CCP) in North American Catalysis Society (NACS), 2015-  
International Program Committee Member of the TU Delft Process Technology Institute, 2012-  
Scientific Committee, 23<sup>rd</sup> Int. Symp. Chem. Reaction Eng. (ISCRE 23<sup>rd</sup>), "Tailoring Sustainability through Chemical Reaction Engineering", Central World, Bangkok, Thailand, September 7-10, 2014  
Breakout leader of 'Harnessing DOE's High Performance Computing Expertise to Strengthen the US Chemical Enterprise', a workshop hosted by the Council for Chemical Research (CCR) and DOE, Washington, DC, March 10-11, 2011  
AIChE Executive Board of the National Planning Committee (*EBPC*), 2011-2014  
External Advisory Board, Center for Electrocatalysis, Transport Phenomena, and Materials (CETM), led by Grigori L. Soloveichik of GE, an EFRC, 2010-2012  
Int. Advisory Board, Combustion Energy Frontier Research Center, Univ. of Princeton, led by Ed Law, 2011-2013  
Programming Chair of the Catalysis and Reaction Engineering Division of AIChE, 2008-2013  
Chair, Philadelphia Catalysis Club, 2010-2011  
Chair-elect, Philadelphia Catalysis Club, 2009-2010  
Co-organizer of the Int. Symposium Chem. Reaction Engineering (ISCRE) 21 meeting, 2010  
Co-organizer of the 5th International Zeolite Membrane Meeting (IZMM), May 23-26, 2010 Loutraki, Greece

Organizer of the reaction engineering topical area of the North American Catalysis Society (NACS) Meeting, San Francisco, CA, June 7-12, 2009  
Board of Directors of the Center for Catalytic Science and Technology, 2000-07  
Organizer of the Topical conference on Multiscale Simulation, AIChE meeting, 2005  
International Advisory Committee member of International Conference on “Computational Modeling and Simulation of Materials”, in Simulation of nano-world meeting, Sicily, Italy, May 30-June 4, 2004  
Director of the Catalysis and Reaction Engineering (CRE) Division of the AIChE, 2002-2005  
Secretary: The Catalysis Society of New England (1995-97)

### Consulting/Expert Witness

DuPont, ExxonMobil, Conoco, Praxair, Rohm & Haas, BASF, Engelhard, Celanese, HelBio, Invista

### Overview of Research and Educational Impact

- A total of **>340 refereed publications**, with a total of **>10,700 citations with >1,600 in 2016**, and an **h-index (by ISI) of 57**
- Research funding from recent grants (as the lead principal investigator) in excess of **\$45,000,000**
- Developed **the highest ever thermal efficiency technology of converting chemical energy to electricity** for portable power generation (US Patent No. 7,862,331; employed by the Army Research Lab)
- Developed multiscale **reaction mechanisms** employed by **various companies** (e.g., ConocoPhillips, Praxair, Rohm-Haas (now Dow Chemicals, etc.) for designing chemical processes (e.g., remote conversion of natural gas to syngas to liquids, i.e., compact gas-to-liquid (GTL) technology), new catalysts, and low emissions
- Developed **microtechnology for portable and distributed energy generation and syngas production**, which has been demonstrated among others by Velocys and Oxford Catalysts and HelBio
- Pioneered various **multiscale computational and mathematical** (e.g., hybrid, hierarchical, coarse-grained Monte Carlo) **methods** spearheaded in various divisions of AIChE; introduced the correlative uncertainty quantification in multiscale modeling and atomistic design of catalysts.
- Led strategically the **Catalysis Center of Energy Innovation (CCEI)**, a DOE funded Energy Frontier Research Center (EFRC) since 2009 among >20 investigators and 9 institutions with funding of **\$29.9 million** to **innovate many transformative technologies**, including the first production of renewable aromatics, e.g., para-xylene, the effective one-pot conversion of sugars to furans using homogeneous multifunctional catalysts, and the first introduction of Lewis acid catalysts for the hydrodeoxygenation of furans.
- Developed **the first comprehensive, fundamental mechanisms and kinetic models of biomass derivatives’ transformations in complex media and over multifunctional catalysts** that have led to unprecedented yields of chemicals in his laboratory or by collaborators, transforming the rather empirical field into a science-driven research enterprise.
- *Introduced multiscale modeling and simulation methodologies* along with their application to catalysis, biomass processing, and portable microchemical devices for power generation, nucleation and growth of nanomaterials, and fabrication of and transport in microporous thin films. And their *broad dissemination by creating the first sessions and short courses at the annual AIChE meetings*. Disseminated open-source software and databases (tau-leap, exact stochastic simulation, graph-theoretical KMC, group additivity of furanics, microkinetic models, etc.).
- *Developed and disseminated education material into diverse and interdisciplinary audiences*: Taught various short courses and participated in workshops in applied mathematics, engineering, and chemistry. Created an exchange program of undergraduate, graduate and postdoctoral fellows among CCEI institutions and with the mathematics groups of UMass and UD. Led CCEI training and mentorship opportunities to 59 undergraduate researchers (most of whom went to graduate school) and 5 high school students including students with special needs and from underrepresented groups over the past 7 years. Created four new courses (applied mathematics (2), kinetics (1), and energy principles (1)) at graduate and undergraduate level. Headed software implementation and tutorial development across the undergraduate and graduate curriculum of chemical engineering of UD.

### Scientific and Professional Societies

American Institute of Chemical Engineers (AIChE); American Chemical Society (ACS); The Combustion Institute; Materials Research Society (MRS); The North American Catalysis Society (NACS); Society for Industrial and Applied Mathematics (SIAM)

**Graduate and Postdoctoral Advisors**

L. D. Schmidt, Ph.D. thesis and postdoctoral advisor, Dept. Chem. Eng. & Mat. Sci., Univ. of Minnesota.

R. Aris, Ph.D. thesis and postdoctoral advisor, Dept. Chem. Eng. & Mat. Sci., Univ. of Minnesota. Deceased.

K. F. Jensen, M. S. thesis advisor, Dept. Chem. Eng., M.I.T.

## RESEARCH PUBLICATIONS, TEXTBOOKS, AND PATENTS

### Textbooks

An introduction to multiscale analysis for well-mixed, chemical and biological reacting systems (in preparation).

### Patents, Patent Applications, Disclosures

1. Catalytic Microcombustors for Compact Power or Heat Generation, US Patent No. 7,862,331.
2. P. J. Dauenhauer, C. L. Williams, W. Fan, C.-C. Chang, D. G. Vlachos, and R. F. Lobo, Production Of Para-Xylene By Catalytically Reacting 2,5-Dimethylfuran And Ethylene In A Solvent. U.S. Non-Provisional Patent Application 14/230,903 (filed on 3/31/2014).
3. D. S. Park, C. Krumm, M. Koehle, K. Joseph, D. G. Vlachos, R. F. Lobo, and P. J. Dauenhauer, Methods of Forming Aromatic and Linear Chain Containing Compounds. U.S. Provisional Patent Application 62/252,200 (filed on 11/6/2015).

### Editorial Reviews

1. Review of Handbook of Nanophase Materials Edited by Avery N. Goldstein (The Dow Chemical Company). Dekker: New York. 1997, *J. Am. Chem. Soc.* **120(18)**, 4556-4556 1998. 10.1021/ja9756026 S0002-7863(97)05602-3.
2. D. G. Vlachos, Plastics from Renewable Sources, *J. Chem. Eng. Process Technol.* **3(4)**, 1000e108 (2012).

### In the News

Several articles highlighted as cover art of journals; see <http://www.efrc.udel.edu/facultypubs.html>

**Top cited article in 2011-2012 in Carbohydrate Research** [S. Caratzoulas and D. G. Vlachos, Converting fructose to 5-hydroxymethylfurfural: A quantum mechanics/molecular mechanics study of the mechanism and energetics, *Carb. Res.* **346**, 664–672 (2011)].

Chemical Engineering News, Nov. 19<sup>th</sup> Issue, 2012; Commentary on biofuels production

**Most Cited Author of Chemical Engineering Science in 2011**, for the article ‘The roles of catalysis and reaction engineering in overcoming the energy and the environment crisis’.

The para-xylene work published in *ACS Catal.* **2**, 935-939 (2012) was highlighted in Chem. Eng. News and The Catalyst Review, May 2012 pg. 9.

Our pyrolysis paper in *Energy Env. Sci.* **5**, 5414-5424 (2012) was highlighted in *Nature Chemistry* **4**, 68-69 (2012) and in Chemical Engineering Progress (CEP) in March 2012, pages 9 & 10:  
<http://www.iche.org/uploadedFiles/CEP/Issues/2012-03/031206.pdf>

Biofuels digest:<http://biofuelsdigest.com/bdigest/2012/01/26/return-of-the-pyromaniac/>, January 2012.

In the Movers and Shakers, Catalyst Review by the Catalyst Group (September 2011),  
[http://www.catalystgrp.com/php/tcgr\\_catalystreview.php](http://www.catalystgrp.com/php/tcgr_catalystreview.php)

Technology Review, published by MIT, March 19<sup>th</sup>, 2010, commentary of Dion Vlachos  
Increasing Yield from Gasification, A new process can make more fuel from biomass.  
<http://www.technologyreview.com/energy/24838/page1/>

Chemistry World, April 25<sup>th</sup>, 2010.

New strategy yields best ever catalyst for ammonia decomposition  
<http://www.rsc.org/chemistryworld/News/2010/April/25041001.asp>

Pacific Northwest National Labs, Chemical & Materials Sciences Division Research Highlights, October 2010.  
Getting the Catalysts You Really Need  
<http://www.pnl.gov/science/highlights/highlight.asp?id=828>

Catalysis and Reactors for Decentralized Fuel and Biofuel Processing: A Perspective, *The Catalyst Review Newsletter*, January 2009.

Papers [36, 53] have appeared as paper of the month in Chem. Eng. Progress

### Invited Papers

1. P. Aghalayam, Y. K. Park, and D. G. Vlachos, "Partial oxidation of light alkanes in short contact time microreactors," *Catalysis* **15**, Spivey, J. J., ed., pp. 98-137 (2000).
2. A. Chatterjee, M. A. Snyder, and D. G. Vlachos, "Mesoscopic modeling of chemical reactivity", *ISCRE Issue of Chem. Eng. Sci.* **59**, 5559–5567 (2004).
3. D. G. Vlachos, "A review of multiscale analysis: Examples from systems biology, materials engineering, and other fluid-surface interacting systems", *Adv. Chem. Eng.* **30**, 1-61 (2005).
4. D. G. Vlachos, "Molecular modeling for non-equilibrium chemical processes", in *Encyclopedia of Chemical Processing*, Ed. Lee, S., Decker Encyclopedia of Chemical Processing, Taylor & Francis, New York, pg. 1717-1726 (2006).
5. A. Chatterjee and D. G. Vlachos, "An overview of spatial microscopic and accelerated kinetic Monte Carlo methods", *J. Comput.-Aided Mater. Des.* **14(2)**, 253-308 (2007).

### Ranked 1<sup>st</sup> in citations on 4/12/13 among all papers published in 2007 in the journal

6. D. G. Vlachos, *Microreaction Engineering: Processes, Detailed design and Modeling*, in *Microfabricated Power Generation Devices*, ed. P. I. Barton and A. Mitsos, Wiley-VCH, Berlin (2009), p. 179-198.
7. N. Kaisare, G. D. Stefanidis, and D. G. Vlachos, *Transport Phenomena in Microscale Reacting Flows*, in *Handbook of Micro Reactors: Fundamentals, Operations and Catalysts*, V. Hessel et al., Editors. Wiley-VCH, Berlin (2009), p. 283-302.
8. D. G. Vlachos and S. Caratzoulas, The roles of catalysis and reaction engineering in overcoming the energy and the environment crisis, *Chem. Eng. Sci.* **65**, 18–29 (2010), invited as a plenary talk at the ICSRE 20<sup>th</sup> meeting.
9. D. G. Vlachos, J. G. Chen, R. J. Gorte, G. W. Huber, and M. Tsapatsis, Catalysis Center for Energy Innovation for Biomass Processing: Research Strategies and Goals, *Cat. Letters* **140**, 77–84 (2010).
10. G. Mpourmpakis and D. G. Vlachos, Computational-based catalyst design for thermochemical transformations, *MRS Bulletin* **36**, 211-215 (2011).
11. M. Saliccioli, M. Stamatakis, S. Caratzoulas, and D. G. Vlachos, A review of multiscale modeling of catalytic reactions: Mechanism development for complexity and emergent behavior. *Chem. Eng. Sci.* **66**, 4319–4355 (2011). **As of 2015, it runs 7<sup>th</sup> in citations of the journal for that year and is one of the most cited Chem. Eng. Sci. papers since 2010.**
12. N. Kaisare and D. G. Vlachos, Micropower technology: A review and a research roadmap for portable and distributed power generation, *Prog. Energy Comb. Sci.* **38**, 321-359 (2012).
13. N. Guo, S. Caratzoulas, D. J. Doren, S. I. Sandler, and D. G. Vlachos, A Perspective on the Modeling of Biomass Processing, *Energy Environ. Sci.* **5(5)**, 6703-6716 (2012). **Perspective and cover art.**
14. D. G. Vlachos, Multiscale modeling for emergent behavior, complexity, and combinatorial explosion, *AIChE* **58(5)**, 1314–1325 (2012). **Perspective and cover art.**
15. S. Caratzoulas, M. E. Davis, R. J. Gorte, R. Gounder, R. F. Lobo, V. Nikolakis, S. I. Sandler, M. A. Snyder, M. Tsapatsis, D. G. Vlachos, Challenges of and insights into acid-catalyzed transformations of sugars, *J. Phys. Chem. C* **118(40)**, 22815-22833 (2014). **Feature Article and cover art.**
16. J. E. Sutton and D. G. Vlachos, Building large microkinetic models with first-principles' accuracy at reduced computational cost, *Chem. Eng. Sci.* **121**, 190-199 (2015). **Invited.**
17. K. Xiong, W. Yu, D. G. Vlachos and J. G. Chen, Reaction Pathways of Biomass-Derived Oxygenates over Metals and Carbides: From Model Surfaces to Supported Catalysts, *ChemCatChem* **7(9)**, 1402-1421 (2015). **Invited Review.**

### Refereed Publications

Summary and Highlights (Numbers refer to papers below):

*High Impact Factor Journal Publications*

- *Nature Chemistry*: [191]
- *Science* and featured also in C&E News and in Materials Today: [77]
- *Phys. Rev. Lett.*: [49, 55, 84, 180]
- *J. Am. Chem. Soc.*: [57, 133, 140, 186, 216]

- *Appl. Phys. Lett.*: [42, 79]
- *Bioinformatics journals*: [108, 153, 195]
- *Proc. Nat. Acad. Sci.*: [72]
- *Nano Letters*: [193, 196]
- *ACS Nano*: [218]
- *Energy Environ. Sci.*: [232, 236, 246] and one of them was highlighted in *Nature Chemistry*
- *Prog. Energy Comb. Sci.*: [234]

#### Highly Cited Papers

- [170] in *J. Catal.* was in the Top 25 Hottest Articles, October-December, 2008
- [179] was among the 10 most-cited articles in the *AIChE J.* in 2009
- [188]: most downloaded paper in 2010 in *Chem. Eng. Sci.*; Dec 7, 2010
- [147]: Most cited paper in *J. Comp. Aided Mat. Design* in 2007 (ISI Date 12/11/10)
- [150]: 4<sup>th</sup> Most cited paper in *Comb. Flame* in 2007
- [130]: ranked 2<sup>nd</sup> in number of times being accessed within 30 days from its publication (downloaded 834 times); 2996 times accessed from Nov. 2005 to Dec. 2007
- [72]: ranked 6<sup>th</sup> most frequently cited mathematics paper in *Proc. Nat. Acad. Sci.*
- [137]: was in the top 25 most accessed papers in *Biophys. Chem.*<sup>1</sup>
- [70]: received the *Chem. Eng. Sci.* Most Cited 2003-2006 Paper Award

#### Refereed Publications

1. D. G. Vlachos, L. D. Schmidt, and R. Aris, "The effects of phase transitions, surface diffusion, and defects on surface catalyzed reactions: Oscillations and fluctuations," *J. Chem. Phys.* **93**, 8306-8313 (1990).
2. D. G. Vlachos, L. D. Schmidt, and R. Aris, "The effect of phase transitions, surface diffusion, and defects on heterogeneous reactions: Multiplicities and fluctuations," *Surf. Science* **249**, 248-264 (1991).
3. D. G. Vlachos, F. Schuth, R. Aris, and L. D. Schmidt, "Spatial and temporal patterns in catalytic oscillations," *Physica A* **188**, 302-321 (1992).
4. D. G. Vlachos and K. F. Jensen, "The roles of supersaturation, terrace width, and impurities on the formation of macrosteps on crystal surfaces using the terrace-ledge-kink model," *Surf. Science* **262**, 359-370 (1992).
5. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Structure of small catalyst particles," *Chem. Engng Sci.* **47**, 2769-2774 (1992).
6. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Structures of small metal clusters: I Low temperature behavior," *J. Chem. Phys.* **96**, 6880-6890 (1992).
7. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Structures of small metal clusters: II Phase transitions and isomerization," *J. Chem. Phys.* **96**, 6891-6901 (1992).
8. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Ignition and extinction of flames near surfaces: Combustion of H<sub>2</sub> in air," *Combust. Flame* **95**, 313-335 (1993).
9. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Kinetics of faceting of crystals in growth, etching, and equilibrium," *Phys. Rev. B* **47**, 4896-4909 (1993).
10. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Comparison of small metal clusters: Ni, Pd, Pt, Cu, Ag, Au," *Z. Phys. D-Atoms, Molecules and Clusters* **26**, S156-S158 (1993).
11. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Ignition and extinction of flames near surfaces: Combustion of CH<sub>4</sub> in air," *AIChE J.* **40(6)**, 1005-1017 (1994).
12. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Products in methane combustion near surfaces," *AIChE J.* **40(6)**, 1018-1025 (1994).
13. D. G. Vlachos, "The interplay of transport, kinetics, and thermal interactions in the stability of premixed hydrogen/air flames near surfaces," *Combust. Flame* **103(1-2)**, 59-75 (1995).
14. D. G. Vlachos, "Growth of elongated nanostructures," *Mater. Sci. Eng. A* **204(1-2)**, 90-95 (1995).

---

<sup>1</sup> Apr-Jun 06 (19th): [http://top25.sciencedirect.com/index.php?cat\\_id=8&subject\\_area\\_id=3&journal\\_id=03014622](http://top25.sciencedirect.com/index.php?cat_id=8&subject_area_id=3&journal_id=03014622);  
Jul-Sept 06 (12th): [http://top25.sciencedirect.com/index.php?cat\\_id=9&subject\\_area\\_id=3&journal\\_id=03014622](http://top25.sciencedirect.com/index.php?cat_id=9&subject_area_id=3&journal_id=03014622)

15. S. Kalamatianos and D. G. Vlachos, "Bifurcation behavior of premixed hydrogen/air mixtures in a continuous stirred tank reactor," *Combust. Sci. Technol.* **109(1-6)**, 347-371 (1995).
16. D. G. Vlachos, "Instabilities in homogeneous nonisothermal reactors: Comparison of deterministic with Monte Carlo simulations," *J. Chem. Phys.* **102(4)**, 1781-1790 (1995).
17. P. A. Bui, D. G. Vlachos, and P. R. Westmoreland, "Homogeneous ignition of hydrogen/air mixtures over platinum," in *Twenty Sixth Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, 1996, p. 1763-1770.
18. D. G. Vlachos, "Homogeneous-heterogeneous oxidation reactions over platinum and inert surfaces," *Chem. Engng Sci.* **51(10)**, 2429-2438 (1996).
19. D. G. Vlachos, "Reduction of detailed kinetic mechanisms for ignition and extinction of premixed hydrogen/air flames," *Chem. Engng Sci.* **51(16)**, 3979-3993 (1996).
20. D. G. Vlachos and P. A. Bui, "Catalytic ignition and extinction of hydrogen: Comparison of simulations and experiments," *Surf. Science* **364(3)**, L625-L630 (1996).
21. D. G. Vlachos, "Growth of nanophase clusters and potential energy minima: Hysteresis, oscillations, and phase transitions," *J. Global Optimization* **11(1)**, 69-82 (1997).
22. M. Ziauddin, A. Balakrishna, D. G. Vlachos, and L. D. Schmidt, "Ignition of methane flames in oxygen near inert surfaces: Effects of composition, pressure, preheat, and residence time," *Combust. Flame* **110(3)**, 377-391 (1997).
23. P.-A. Bui, D. G. Vlachos, and P. R. Westmoreland, "Modeling ignition of catalytic reactors with detailed surface kinetics and transport: Combustion of H<sub>2</sub>/air mixtures over platinum surfaces," *Ind. Eng. Chem. Res.* **36(7)**, 2558-2567 (1997).
24. P.-A. Bui, E. A. Wilder, D. G. Vlachos, and P. R. Westmoreland, "Hierarchical reduced models for catalytic combustion: H<sub>2</sub>/air mixtures near platinum surfaces," *Combust. Sci. Technol.* **129**, 243-275 (1997).
25. D. G. Vlachos, "Multiscale integration hybrid algorithms for homogeneous-heterogeneous reactors," *AIChE J.*, **43(11)**, 3031-3041 (1997).
26. Y. K. Park and D. G. Vlachos, "Kinetically driven instabilities and selectivities in methane oxidation," *AIChE J.* **43**, 2083-2095 (1997).
27. P.-A. Bui, D. G. Vlachos, and P. R. Westmoreland, "Catalytic ignition of methane/oxygen mixtures over platinum surfaces: Comparison of detailed simulations and experiments," *Surf. Science* **385(2-3)**, L1029-L1034 (1997).
28. D. G. Vlachos, "Stochastic modeling of chemical microreactors with detailed kinetics: Induction times and ignitions of H<sub>2</sub> in air," *Chem. Eng. Sci.* **53**, 157-168 (1998).
29. S. Kalamatianos, Y. K. Park, and D. G. Vlachos, "Two-parameter continuation algorithms for computing ignitions and extinctions: Sensitivity analysis, parametric dependence, mechanism reduction, and stability criteria," *Combust. Flame*, **112(1-2)**, 45-61 (1998).
30. Y. K. Park and D. G. Vlachos, "Isothermal chain-branching, reaction exothermicity, and transport interactions in the stability of methane/air mixtures," *Combust. Flame*, **114 (1-2)**, 214-230 (1998).
31. Y. K. Park and D. G. Vlachos, "Chemistry reduction and thermokinetic criteria for ignition of hydrogen/air mixtures at high pressures," *J. Chem. Soc. Faraday Trans.*, **94(6)**, 735-743 (1998).
32. V. Nikolakis, D. G. Vlachos, and M. Tsapatsis, "Modeling of zeolite crystallization: The role of gel microstructure," *Microporous and Mesoporous Materials* **21(4)**, 337-346 (1998).
33. P. Aghalayam and D. G. Vlachos, "NO<sub>x</sub> and fuel emissions in combustion of hydrogen/air mixtures near inert surfaces," in *Twenty Seven Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, 1435-1442 (1998).
34. P.-A. Bui, D. G. Vlachos, and P. R. Westmoreland, "On the local stability of multiple solutions and oscillatory dynamics of spatially distributed flames," *Combust. Flame*, **117(1-2)**, 307-322 (1999).
35. Y. K. Park, P. A. Bui, and D. G. Vlachos, "Operation regimes in catalytic combustion: H<sub>2</sub>/air mixtures near Pt," *AIChE J.* **44(9)**, 2035-2043 (1998).
36. P. Aghalayam and D. G. Vlachos, "The roles of thermal and chemical quenching in NO<sub>x</sub> and fuel emissions: Combustion of surface-stabilized hydrogen/air mixtures," *AIChE J.* **44(9)**, 2025-2034 (1998).  
**Highlighted in Chem. Eng. Progress (paper of the month), p. 10, 12, Sept. issue, 1998.**
37. P. Aghalayam, P. -A. Bui, and D. G. Vlachos, "The role of radical wall quenching in flame stability and wall heat flux: Hydrogen-air mixtures," *Combust. Theory Modeling* **2**, 515-530 (1998).
38. Y. K. Park, N. Fernandes, and D. G. Vlachos, "Effect of dilution on catalytic oxidation: Model validation through experiments and prediction of operation regimes," *Chem. Engng Sci.*, **54**, 3635-3642 (1999).



39. N. Fernandes, Y. K. Park, and D. G. Vlachos, "The autothermal behavior of platinum catalyzed hydrogen oxidation: Experiments and modeling," *Combust. Flame* **118(1-2)**, 164-178 (1999).
  40. S. Raimondeau, M. Gummalla, Y. K. Park, and D. G. Vlachos, "Reaction network reduction for distributed systems by model training in lumped reactors: Application to bifurcations in combustion," *Chaos: an Interdisciplinary Journal of Nonlinear Science* **9(1)**, 95-107 (1999).
  41. M. Gummalla, P. A. Bui, and D. G. Vlachos, "Nonlinear dynamics of surface stabilized premixed and diffusion flames: Current trends and future directions," *Chem. Engng Sci.* **55**, 311-319 (2000).
  42. D. G. Vlachos, "The role of macroscopic transport phenomena in film microstructure during the epitaxial growth," *Appl. Phys. Lett.* **74(19)**, 2797-2799 (1999).
  43. V. Nikolakis, D. G. Vlachos, and M. Tsapatsis, "Modeling zeolite L crystallization using continuum time Monte Carlo simulations," *J. Chem. Phys.* **111(5)**, 2143-2150 (1999).
  44. R. J. Olsen and D. G. Vlachos, "A complete pressure-temperature diagram for air oxidation of hydrogen in a continuous-flow stirred tank reactor," *J. Phys. Chem A* **103(40)**, 7990-7999 (1999).
  45. M. Gummalla, D. G. Vlachos, and M. A. Delichatsios, "Bifurcations and structure of surface stabilized methane-air diffusion flames," *Combust. Flame* **120(3)**, 333-345 (2000).
  46. Y. K. Park, P. Aghalayam, and D. G. Vlachos, "A generalized approach for predicting coverage-dependent reaction parameters of complex surface reactions: Application to H<sub>2</sub> oxidation over platinum," *J. Phys. Chem. A* **103(40)**, 8101-8107 (1999).
  47. M. Gummalla and D. G. Vlachos, "Complex dynamics of combustion flows by direct numerical simulations," *Phys. Fluids* **12(2)**, 252-255 (2000).
  48. V. Nikolakis, E. Kokkoli, M. Tirrell, M. Tsapatsis, and D. G. Vlachos, "Zeolite growth by addition of subcolloidal particles: Modeling and experimental validation," *Chem. Mater.* **12**, 845-853 (2000).
  49. M. A. Katsoulakis and D. G. Vlachos, "From microscopic interactions to macroscopic laws of cluster evolution," *Phys. Rev. Letters* **84(7)**, 1511-1514 (2000).
  50. S. Raimondeau and D. G. Vlachos, "Low-dimensional approximations of multiscale epitaxial growth models for microstructure control of materials," *J. Comp. Phys.* **160**, 564-576 (2000).
  51. P. Aghalayam, Y. K. Park, and D. G. Vlachos, "Partial oxidation of light alkanes in short contact time microreactors," *Catalysis* **15**, Spivey, J. J., ed., pp. 98-137 (2000) invited.
  52. P. Aghalayam, Y. K. Park, and D. G. Vlachos, "A detailed surface reaction mechanism for CO oxidation on Pt," *Symposium (International) on Combustion* **28**, 1331-1339 (2000).
  53. P. Aghalayam, Y. K. Park, and D. G. Vlachos, "Construction and optimization of complex surface reaction mechanisms," *AIChE J.* **46(10)**, 2017-2029 (2000).
- Highlighted in Chem. Eng. Progress (paper of the month), Oct. issue, 2000.**
54. G. Bonilla, M. Tsapatsis, D. G. Vlachos, and G. Xomeritakis, "Fluorescence confocal optical microscopy of the grain boundary structure of zeolite MFI membranes made by secondary (seeded) growth," *J. Membrane Sci.* **182(1-2)**, 103-109 (2001).
  55. \* D. G. Vlachos and M. A. Katsoulakis, "Derivation and validation of mesoscopic theories for diffusion of interacting molecules," *Phys. Rev. Letters* **85(18)**, 3898-3901 (2000).
  56. G. Bonilla, D. G. Vlachos, and M. Tsapatsis, "Simulations and experiments on the growth and microstructure of zeolite MFI films and membranes by secondary growth", *Micropor. Mesopor. Mat.* **42(2-3)**, 191-203 (2001).
  57. \* M. Tsapatsis, D. G. Vlachos, S. Kim, H. Ramanan, and G. R. Gavalas, "Spontaneous formation of periodically patterned deposits by chemical vapor deposition", *J. Am. Chem. Soc.* **122(51)**, 12864-12865 (2000).
  58. V. Nikolakis, G. Xomeritakis, A. Abibi, M. Dickson, M. Tsapatsis, and D. G. Vlachos, "Growth of faujasite-type zeolite membrane and its application in the separation of saturated/unsaturated hydrocarbon mixtures," *J. Membrane Sci.* **184(2)**, 209-219 (2001).
  59. N. E. Fernandes, S. M. Fisher, J. C. Poshusta, D. G. Vlachos, M. Tsapatsis, and J. J. Watkins, "Reactive deposition of metal thin films within porous supports from supercritical fluids," *Chem. Materials* **13**, 2023-2031 (2001).
  60. R. Lam and D. G. Vlachos, "A multiscale model for epitaxial growth of films: Growth mode transition," *Phys. Rev. B* **6403(3)**, 35401 (2001).
  61. J. Reese, S. Raimondeau, and D. G. Vlachos, "Monte Carlo algorithms for complex surface reaction mechanisms: Efficiency and accuracy," *J. Comp. Phys.* **173(1)**, 302-321 (2001).
  62. D. J. Hornthrop, M. A. Katsoulakis, and D. G. Vlachos, "Spectral methods for mesoscopic models of pattern formation," *J. Comp. Phys.* **173(1)**, 364-390 (2001).
  63. R. Lam, T. Basak, D. G. Vlachos, and M. A. Katsoulakis, "Validation of mesoscopic theories and their application to computing effective diffusivities," *J. Chem. Phys.* **115(24)**, 11278-11288 (2001).

64. R. Lam, D. G. Vlachos, and M. A. Katsoulakis, "Homogenization of mesoscopic theories: Effective properties of model membranes," *AIChE J.* **48(5)**, 1083-1092 (2002).
  65. S. Raimondeau and D. G. Vlachos, "Recent developments on multiscale, hierarchical modeling of chemical reactors," *Chem. Eng. J.* **90(1-2)**, 3-23 (2002).
  66. S. Raimondeau and D. G. Vlachos, "The role of adsorbate-layer nonuniformities in catalytic reactor design: Multiscale simulations for CO oxidation on Pt," *Comput. Chem. Eng.* **26(7-8)**, 965-980 (2002).
  67. A. B. Mhadeshwar, P. Aghalayam, V. Papavassiliou, and D. G. Vlachos, "Surface reaction mechanism development platinum catalyzed oxidation of methane," *Proc. Combust. Inst.* **29**, 997-1004 (2003).
  68. S. Raimondeau, D. A. Norton, D. G. Vlachos, and R. I. Masel, "Modeling of high temperature microburners," *Proc. Combust. Inst.* **29**, 901-907 (2003).
  69. P. Aghalayam, Y. K. Park, N. E. Fernandes, V. Papavassiliou, A. B. Mhadeshwar, and D. G. Vlachos, "A C1 mechanism for methane oxidation on platinum", *J. Catal.* **213**, 23-38 (2003).
  70. M. A. Snyder, D. G. Vlachos, and M. A. Katsoulakis, "Mesoscopic modeling of transport and reaction in microporous crystalline membranes", *Chem. Eng. Sci.* **58**, 895-901 (2003).
  71. S. Raimondeau and D. G. Vlachos, "Front propagation at low temperatures and multiscale modeling for the catalytic combustion of H<sub>2</sub> on Pt", *Chem. Eng. Sci.* **58**, 657-663 (2003).
  72. \* M. A. Katsoulakis, A. J. Majda, and D. G. Vlachos, "Coarse-grained stochastic processes for microscopic lattice systems", *Proc. Natl. Acad. Sci.* **100(3)**, 782-787 (2003).
- Ranked 6<sup>th</sup> among 'The 20 Most-Frequently-Read Applied Mathematics Papers' in PNAS during March 2003, updated monthly and recorded since ~1996 (see <http://www.pnas.org/reports/mfrAPP2.dtl>).**
73. M. A. Katsoulakis, A. J. Majda, and D. G. Vlachos, "Coarse-grained stochastic processes and Monte Carlo simulations in lattice systems", *J. Comp. Phys.* **186**, 250-278 (2003).
  74. S. Raimondeau, P. Aghalayam, A. B. Mhadeshwar, and D. G. Vlachos, "Parameter optimization in molecular models: Application to surface kinetics", *Ind. Eng. Chem. Res.* **42**, 1174-1183 (2003).
  75. D. G. Norton and D. G. Vlachos, "Combustion characteristics and flame stability at the microscale: A CFD study of premixed methane/air mixtures", *Chem. Eng. Sci.* **58**, 4871-4882 (2003).
- Ranked 3<sup>rd</sup> in citations on 4/12/13 among all papers published that year in the journal**
76. M. Gummalla, M. Tsapatsis, J. J. Watkins, and D. G. Vlachos, "The role of transients and nucleation in film deposition within a support", *Ind. Eng. Chem. Res.* **42**, 1321-1328 (2003).
  77. \* Z. Lai, G. Bonilla, G. Nery, I. Diaz-Carretero, K. Sujaoti, M. A. Amat, E. Kokkoli, O. Terasaki, R. W. Thompson, M. Tsapatsis, D. G. Vlachos, "Microstructural optimization of a zeolite membrane for organic vapor separation", *Science* **300**, 456-460, (2003). **Cover art.**
- See also in C&E News, Science Concentrates, March 10, 2003 and in Materials Today, May 2003, pg. 9.**
78. V. Nikolakis, M. Tsapatsis, and D. G. Vlachos, "Physicochemical characterization of silicalite-1 surface and its implications for crystal growth", *Langmuir* **19(11)**, 4619-4626 (2003).
  79. M. Bhattacharya, D. G. Vlachos and M. Tsapatsis, "Periodic patterning in materials deposition by self-regulating diffusion-reaction processes", *Appl. Phys. Letters* **82(19)**, 3357-3359 (2003).
- Selected in the May 19, 2003 issue of the Virtual Journal of Nanoscale Science & Technology (<http://www.vjnano.org>)**
80. D. D. Kragten, J. M. Fedeyko, K. R. Sawant, J. D. Rimer, D. G. Vlachos, R. F. Lobo, and M. Tsapatsis, "The structure of the silica phase extracted from silica/TPAOH solutions containing nanoparticles", *J. Phys. Chem. B* **107**, 10006-10016 (2003).
  81. A. B. Mhadeshwar, H. Wang, and D. G. Vlachos, "Thermodynamic consistency in microkinetic development of surface reaction mechanisms", *J. Phys. Chem. B* **107**, 12721-12733 (2003).
  82. S. G. Davis, A. B. Mhadeshwar, D. G. Vlachos, H. Wang, "A new approach to response surface development for detailed gas-phase and surface reaction kinetic model development and optimization", *Int. J. Chem. Kin.* **36**, 94-106 (2004).
  83. M. A. Katsoulakis and D. G. Vlachos, "Coarse-grained stochastic processes and kinetic Monte Carlo simulators for the diffusion of interacting particles", *J. Chem. Phys.* **119(18)**, 9412-9428 (2003).
  84. \* M. I. Lebedeva, D. G. Vlachos, and M. Tsapatsis, "Bifurcation analysis of Liesegang ring pattern formation", *Phys. Rev. Letters* **92(8)**, 088301-1-4 (2004).
  85. M. Gummalla, M. Tsapatsis, J. J. Watkins, D. G. Vlachos, "Multiscale hybrid modeling of film deposition within porous substrates", *AIChE J.* **50(3)**, 684-695 (2004).
  86. S. R. Deshmukh, A. B. Mhadeshwar, and D. G. Vlachos, "Microreactor modeling for hydrogen production from ammonia decomposition on ruthenium", *Ind. Eng. Chem. Res.* **43**, 2986-2999 (2004).
- Cited by the DOE report 'Potential Roles of Ammonia in a Hydrogen Economy', March 2006.**

87. S. R. Deshmukh, A. B. Mhadeshwar, M. I. Lebedeva, and D. G. Vlachos, "From density functional theory to microchemical device homogenization: Model prediction of hydrogen production for portable fuel cells", *Int. J. Multiscale Comp. Eng.* **2(2)**, 221-238 (2004).
88. M. A. Snyder and D. G. Vlachos, "Rational, hierarchical parameterization of complex zeolite-guest molecular models", *Mol. Sim.* **30(9)**, 561-577 (2004).
89. M. A. Snyder and D. G. Vlachos, "Development of thermodynamically consistent, experiment-based molecular models of diffusion through thin microporous membranes", *Stud. Surf. Sci. Catal.* **154**(Part A-C), 2062-2069 (2004).
90. D. G. Norton and D. G. Vlachos, "A CFD study for propane/air microflame stability", *Combust. Flame* **138**, 97-107 (2004).

**Ranked 5<sup>th</sup> in citations on 4/12/13 among all papers published in 2004 in the journal**

91. M. I. Lebedeva, D. G. Vlachos, and M. Tsapatsis, "Pattern Formation in porous media via the Liesegang ring mechanism", *Ind. Eng. Chem. Res.* **43**, 3073-3084 (2004).
92. A. B. Mhadeshwar, J. R. Kitchin, M. A. Barteau, and D. G. Vlachos, "The role of adsorbate-adsorbate interactions in the rate controlling step and most abundant reaction intermediate of NH<sub>3</sub> decomposition on Ru," *Cat. Letters*, **96(1-2)**, 13-22 (2004).
93. D. G. Norton, E. R. Wetzel, and D. G. Vlachos, "Fabrication of single-channel catalytic microburners: Effect of confinement on the oxidation of hydrogen/air mixtures", *Ind. Eng. Chem. Res.* **43**, 4833-4840 (2004).
94. J. M. Fedeyko, J. D. Rimer, R. F. Lobo, and D. G. Vlachos, "Spontaneous formation of silica nanoparticles in basic solutions of small tetraalkylammonium cations", *J. Phys. Chem. B* **108**, 12271-12275 (2004).
95. A. Chatterjee, D. G. Vlachos, and M. Katsoulakis "Numerical assessment of theoretical error estimates in coarse-grained kinetic Monte Carlo simulations: Application to surface diffusion", *Int. J. Multiscale Comp. Eng.* **3**, 59 (2005).
96. A. Chatterjee, D. G. Vlachos, and M. A. Katsoulakis, "Spatially adaptive lattice coarse-grained Monte Carlo simulations for diffusion of interacting molecules", *J. Chem. Phys.* **121(22)**, 11420-11431 (2004).

**Also selected in December 13, 2004 issue of Virtual Journal of Nanoscale Science & Technology.**

97. A. Chatterjee, M. A. Snyder, and D. G. Vlachos, "Mesoscopic modeling of chemical reactivity", *Chem. Engng Sci.* **59**, 5559-5567 (2004), invited.
98. A. B. Mhadeshwar and D. G. Vlachos, "Microkinetic modeling for water-promoted CO oxidation, water-gas shift, and preferential oxidation of CO on Pt", *J. Phys. Chem. B* **108**, 15246-15258 (2004).
99. M. A. Snyder, Z. Lai, M. Tsapatsis, and D. G. Vlachos, "Combining simultaneous reflectance and fluorescence imaging with SEM for conclusive identification of polycrystalline features of MFI membranes", *Micro. Meso. Mat.* **76(1-3)**, 29-33 (2004).
100. J. Ludwig and D. G. Vlachos, "First principles modeling of dissociative adsorption at crystal surfaces: Hydrogen on Pt(111)", *Mol. Sim.* **30(11-12)**, 765-771 (2004).
101. I. Diaz, G. Bonilla, Z. Lai, O. Terasaki, D. G. Vlachos, and M. Tsapatsis, "Silicalite-1 crystals with modified morphology: HRTEM imaging and synthesis of B-oriented films", *Stud. Surf. Sci. Catal.* **154**, 1160-1167 (2004).
102. J. M. Fedeyko, K. Sawant, D. Kragten, D. G. Vlachos, and R. F. Lobo, The Structure of Subcolloidal Zeolite Nanoparticle Precursors, *Stud. Surf. Sci. Catal.* **154**, 1267-1273 (2004).
103. G. Bonilla, G., I. Diaz, M. Tsapatsis, H.-K. Jeong, Y. Lee, and D. G. Vlachos, "Zeolite (MFI) crystal morphology control using organic structure-directing agents," *Chem. Mater.* **16**, 5697-5705, (2004).
104. M. A. Snyder, A. Chatterjee, and D. G. Vlachos, "Net-event kinetic Monte Carlo for overcoming stiffness in spatially homogeneous and distributed systems", *Comput. Chem. Eng.* **29(4)**, 701-712 (2005).
105. D. G. Norton and D. G. Vlachos, "Hydrogen assisted self-ignition of propane/air mixtures in catalytic microburners", *Proc. Combust. Inst.* **30**, 2473-2480 (2005).
106. A. Chatterjee, D. G. Vlachos, and M. A. Katsoulakis, "Binomial distribution based  $\tau$ -leap accelerated stochastic simulation", *J. Chem. Phys.* **122**, 024112-1-6 (2005).
107. A. Chatterjee, M. A. Katsoulakis, and D. G. Vlachos, "Spatially adaptive grand canonical ensemble Monte Carlo simulations", *Phys. Rev. E* **71**, 026702-1-6 (2005).
108. A. Chatterjee, K. Mayawala, J. S. Edwards, and D. G. Vlachos, "Time accelerated Monte Carlo simulations of biological networks using the binomial  $\tau$ -leap method", *Bioinformatics* **21(9)**, 2136-2137 (2005).
109. K. Mayawala, D. G. Vlachos, and B. J. Edwards, "Heterogeneities in EGF receptor density at the cell surface can lead to concave up Scatchard plot of EGF binding", *FEBS (The Federation of European Biochemical Societies) Letters* **579**, 3043-3047 (2005).

110. A. B. Mhadeshwar and D. G. Vlachos, "Is the water-gas shift reaction on Pt simple? Computer-aided microkinetic model reduction, lumped rate expression, and rate-determining step", *Cat. Today* **105**(1), 162-172 (2005).
111. J. M. Fedeyko, D. G. Vlachos, and R. F. Lobo, "Formation and Structure of Self-Assembled Silica Nanoparticles in Basic Solutions of Organic and Inorganic Cations", *Langmuir* **21**, 5197-5206 (2005).
112. M. A. Snyder and D. G. Vlachos, "Molecular sieve valves driven by adsorbate-adsorbate interactions: Hysteresis in permeation of microporous membranes", *J. Chem. Phys.* **122**, 204706-01-10 (2005).
113. M. A. Snyder and D. G. Vlachos, "Molecular valves actuated by intermolecular forces", *Phys. Rev. E Rapid Communications* **71**, 060201-1-4 (2005).  
*Selected also for the July 4, 2005 issue of Virtual Journal of Nanoscale Science & Technology, <http://www.vjnano.org>.*
114. J. D. Rimer, D. G. Vlachos, and R. F. Lobo, "Evolution of Self-Assembled Silica-Tetrapropylammonium Nanoparticles at Elevated Temperatures", *J. Phys. Chem. B* **109**(26), 12762-12771(2005).
115. S. R. Deshmukh and D. G. Vlachos, "CFD simulations of coupled, counter-current combustor/reformer microdevices for hydrogen production", *Ind. Eng. Chem. Res.* **44**(14), 4982-4992 (2005).
116. S. Caratzoulas, D. G. Vlachos, and M. Tsapatsis, "Molecular dynamics studies on the role of tetramethylammonium cations in the stability of the silica octamers  $\text{Si}_8\text{O}_{20}^{-8}$  in solution", *J. Phys. Chem. B* **109**(20), 10429-10434 (2005).
117. S. R. Deshmukh and D. G. Vlachos, "Effect of flow configuration on the operation of coupled combustor/reformer microdevices for hydrogen production", *Chem. Eng. Sci.* **60**(21), 5718-5728 (2005).
118. A. B. Mhadeshwar and D. G. Vlachos, "A thermodynamically consistent surface reaction mechanism for the CO oxidation on Pt", *Combust. Flame* **142**, 289-298 (2005).
119. A. B. Mhadeshwar and D. G. Vlachos, "Hierarchical, multiscale surface reaction mechanism development: CO and  $\text{H}_2$  oxidation, water-gas shift, and preferential oxidation of CO on Rh", *J. Catal.* **234**(1), 48-63 (2005).
120. J. D. Rimer, R. F. Lobo, and D. G. Vlachos, "Physical Basis for the Formation and Stability of Silica Nanoparticles in Basic Solutions of Monovalent Cations", *Langmuir* **21**, 8960-8971 (2005).
121. A. B. Mhadeshwar and D. G. Vlachos, "Hierarchical multiscale mechanism development for methane partial oxidation and reforming, and for thermal decomposition of oxygenates on Rh", *J. Phys. Chem. B* **109**, 16819-16835 (2005).
122. J. D. Rimer, J. M. Fedeyko, D. G. Vlachos, and R. F. Lobo, "Silica Self-Assembly and the Synthesis of Microporous and Mesoporous Silicates", *Chem. Eur. J.* **12**, 2926-2934 (2006).
123. J. M. Fedeyko, D. G. Vlachos, and R. F. Lobo, "Understanding the Differences between Microporous and Mesoporous Synthesis through the Phase Behavior of Silica", *Micro. Meso. Mat.* **90** (1-3), 102-111 (2006).
124. A. Samant and D. G. Vlachos, "Overcoming stiffness in stochastic simulation stemming from partial equilibrium: A multiscale Monte Carlo algorithm", *J. Chem. Phys.* **123**, 144114-1-8 (2005).
125. M. A. Snyder and D. G. Vlachos, "The role of molecular interactions and interfaces in diffusion: Transport diffusivity and evaluation of the Darken approximation", *J. Chem. Phys.* **123**, 184707-1-11 (2005).
126. M. A. Snyder and D. G. Vlachos, "The role of molecular interactions and interfaces in diffusion: Permeation through single-crystal and polycrystalline microporous membranes", *J. Chem. Phys.* **123**, 184708-1-11 (2005).  
*Also in Nov. 21, 2005 issue of Virtual Journal of Nanoscale Science & Technology.*
127. S. R. Deshmukh and D. G. Vlachos, "Novel micromixers driven by flow instabilities: Application to post-reactors", *AIChE J.* **51**(12), 3193-3204 (2005).
128. P. Liu, Y. Huang, Y. Zhang, M. J. Bonder, G. C. Hadjipanayis, D. Vlachos, and S. R. Deshmukh, Magnetic and transport properties of Co nanoparticles embedded in a carbon matrix, *J. Appl. Phys.* **97**(10) No. 10J303, 1-3 (2005).
129. D. G. Vlachos, "A review of multiscale analysis: Examples from systems biology, materials engineering, and other fluid-surface interacting systems", *Adv. Chem. Eng.* **30**, 1-61, invited (2005).
130. K. Mayawala, D. G. Vlachos, J. S. Edwards, 'Computational modeling reveals molecular details of epidermal growth factor binding', *BMC Cell Biology* 6: Art. No. 41 Nov. 30 (2005).
131. J. Ludwig, D. G. Vlachos, A. C. T. v. Duin, and W. A. G. III, "Dynamics of the Dissociation of Hydrogen on Stepped Platinum Surfaces Using ReaxFF", *J. Phys. Chem. B* **110**, 4274-4282 (2006).
132. A. Chatterjee and D. G. Vlachos, "Temporal acceleration of spatially distributed kinetic Monte Carlo simulations", *J. Comp. Phys.* **211**, 596-615 (2006).
133. \* S. Caratzoulas, D. G. Vlachos, and M. Tsapatsis, "On the role of tetramethylammonium cation and effects of solvent dynamics on the stability of the cage-like silicates  $\text{Si}_6\text{O}_{15}^{-6}$  and  $\text{Si}_8\text{O}_{20}^{-8}$  in aqueous solution. A molecular dynamics study", *J. Am. Chem. Soc.* **128**, 596-606 (2006).

134. D. G. Norton, E. D. Wetzel, and D. G. Vlachos, "Thermal management in catalytic microreactors", *Ind. Eng. Chem. Res.* **45**, 76-84 (2006).
135. D. G. Vlachos, A. B. Mhadeshwar, and N. Kaisare, "Hierarchical multiscale model-based design of experiments, catalysts, and reactors for fuel processing", *Comp. Chem. Eng.* **30**, 1712-1724 (2006).
136. A. Chatterjee and D. G. Vlachos, 'Multiscale spatial Monte Carlo simulations: Multigridding, computational singular perturbation, and hierarchical stochastic closures', *J. Chem. Phys.* **124**, 0641101-06411016 (2006).
137. K. Mayawala, D. G. Vlachos, and J. S. Edwards, "Spatial modeling of dimerization reaction dynamics in the plasma membrane: Monte Carlo vs. continuum differential equations", *Biophys. Chem.* **121**, 194-208 (2006).
138. J. L. Provis and D. G. Vlachos, 'Silica Nanoparticle Formation in the TPAOH-TEOS-H<sub>2</sub>O System: A Population Balance Model', *J. Phys. Chem. B* **110(7)**, 3098-3108 (2006).
139. J. A. Federici, D. G. Norton, T. Brüggemann, K. W. Voit, E. D. Wetzel, and D. G. Vlachos, "Catalytic microcombustors with integrated thermoelectric elements for portable power production", *J. Power Sources* **161**, 1469-1478 (2006).
140. \* S. Caratzoulas, D. G. Vlachos, and M. Tsapatsis, "Potential of mean force for tetramethylammonium binding to cage-like oligosilicates in aqueous solution", *J. Am. Chem. Soc.* **128(50)**, 16138-16147 (2006).
141. N. S. Kaisare and D. G. Vlachos, "Extending the region of stable homogeneous micro-combustion through forced unsteady operation", *Proc. Combust. Inst.* **31(2)**, 3293-3300 (2007).
142. N. S. Kaisare and D. G. Vlachos, "Optimal Reactor Dimensions for Homogeneous Combustion in Small Channels", *Catal. Today* **120**, 96-106 (2007).
143. M. A. Snyder, D. G. Vlachos, and V. Nikolakis, "Quantitative analysis of membrane morphology, microstructure, and polycrystallinity via laser scanning confocal microscopy: Application to NaX zeolite membranes", *J. Membrane Sci.* **290(1-2)**, 1-18 (2007).
144. J. D. Rimer, D. D. Roth, D. G. Vlachos, and R. F. Lobo, "Self-assembly and phase behavior of germanium oxide nanoparticles in basic aqueous solutions", *Langmuir* **23(5)**, 2784-2791 (2007).
145. J. M. Fedeyko, H. Egolf-Fox, D. W. Fickel, D. G. Vlachos, and R. F. Lobo, "Initial Stages of Self-Organization of Silica-Alumina Gels in Zeolite Synthesis", *Langmuir* **23**, 4532-4540 (2007).
146. A. Chatterjee and D. G. Vlachos, "Systems tasks in nanotechnology via hierarchical multiscale modeling: Nanopattern formation in heteroepitaxy", *Chem. Eng. Sci.* **62(18-20)**, 4852-4863 (2007).
147. A. Chatterjee and D. G. Vlachos, "An overview of spatial microscopic and accelerated kinetic Monte Carlo methods", *J. Comput.-Aided Mater. Des.* **14(2)**, 253-308 (2007) invited.
148. M. A. Snyder and D. G. Vlachos, "Nano-patterned standards for improving the quantitative capability of laser scanning confocal microscopy for materials characterization", *Micro. Meso. Mat.* **102**, 101-110 (2007).
149. K. Mayawala, D. G. Vlachos, and J. S. Edwards, "The role of reaction engineering in cancer biology: Bio-imaging informatics reveals implications of the plasma membrane heterogeneities", *Chem. Eng. Sci.* **62(18-20)**, 5222-5231 (2007).
150. S. Deshmukh and D. G. Vlachos, "A reduced mechanism for methane and one-step rate expressions for fuel-lean catalytic combustion of small alkanes on noble metals", *Combust. Flame* **149**, 366-383 (2007).
151. A. B. Mhadeshwar and D. G. Vlachos, "A catalytic reaction mechanism for methane partial oxidation at short contact times, reforming, and combustion, and for oxygenate decomposition and oxidation on Pt", *Ind. Eng. Chem. Res.* **46**, 5310-5324 (2007).
152. A.-M. S. Niehaus, D. G. Vlachos, J. S. Edwards, P. Plechac, and R. Tribe, "Microscopic Simulation of Epidermal Growth Factor Receptor Diffusion on Corralled Membrane Surfaces", *Biophys. J.* **94(5)**, 1551-1564 (2008).
153. A. Samant, B. A. Ogunnaike, and D. G. Vlachos, "A Hybrid Multiscale Monte Carlo Algorithm (HyMSMC) to Cope with Disparity in Time Scales and Species Populations in Well-Mixed Reaction Networks", *BMC Bioinformatics* **8:175**, 23 pages (24 May 2007); <http://www.biomedcentral.com/1471-2105/8/175>.
154. A. Chatterjee and D. G. Vlachos, "A continuum mesoscopic framework for multiple interacting species and processes on multiple site types and/or crystallographic planes", *J. Chem. Phys.* **127(3)**, 034705-1-16 (2007).  
*Also in Virtual Journal of Nanoscale Science & Technology, July 30, 2007.*
155. J. Ludwig and D. G. Vlachos, "Self-consistent ab-initio molecular dynamics of hydrogen dissociation on metal surfaces using neural networks and novelty sampling", *J. Chem. Phys.* **127**, 154716-1-16 (2007).
156. J. D. Rimer, O. Trofymuk, A. Navrotsky, R. F. Lobo, and D. G. Vlachos, 'Kinetic and Thermodynamic Studies of Silica Nanoparticle Dissolution', *Chem. Mat.* **19(17)**, 4189-4197 (2007).
157. N. Kaisare, S. R. Deshmukh, and D. G. Vlachos, Stability and performance of catalytic microreactors: Simulations of propane catalytic combustion on Pt, *Chem. Engng Sci.* **63**, 1098-1116 (2008).
158. S. Caratzoulas and D. G. Vlachos, "Molecular dynamics study on the stabilization of the silica hexamer Si<sub>6</sub>O<sub>6</sub><sup>-15</sup> in aqueous and methanolic solutions", *J. Phys. Chem. B Letters* **112**, 7-10 (2008).

159. M. Maestri, T. Faravelli, G. Groppi, E. Tronconi, and D. G. Vlachos, "Two-dimensional detailed modeling of fuel-rich H<sub>2</sub> combustion over Rh/Al<sub>2</sub>O<sub>3</sub> catalyst ", *Chem. Engng Sci.* **63**(10), 2657-2669 (2008).
160. J. Federici and D. G. Vlachos, "A computational fluid dynamics study of propane/air microflame stability in a heat recirculation reactor", *Combust. Flame* **153**, 258–269 (2008).
161. J. Ludwig and D. G. Vlachos, "Molecular dynamics of hydrogen dissociation on an oxygen covered Pt(111) surface", *J. Chem. Phys.* **128**, 154708 (2008).
162. A. Karim, J. Federici, and D. G. Vlachos, "Portable power production from methanol in an integrated thermoelectric/microreactor system", *J. Power Sources* **179**, 113–120 (2008).
163. G. Mpourmpakis and D. G. Vlachos, Insights into the early stages of metal nanoparticle formation via first-principle calculations: The roles of citrate and water. *Langmuir* **24**(14), 7465-7473 (2008).
164. G. D. Stefanidis and D. G. Vlachos, Millisecond Methane Steam Reforming via Process and Catalyst Intensification. *Chem. Eng. Tech.* **31**(8), 1201-1209, (2008).
165. G. D. Stefanidis, N. Kaisare, and D. G. Vlachos, Modeling ignition in catalytic microreactors. *Chem. Eng. Tech.* **31**(8), 1170-1175 (2008).
166. M. -Y. Hsieh, S. Yang, M. A. Raymond-Stinz, S. Steinberg, D. G. Vlachos, W. Shu, B. Wilson, and J.S. Edwards, Stochastic simulations of ErbB homo and heterodimerisation: potential impacts of receptor conformational state and spatial segregation. *IET Systems Biology* **2**(5), 256-272 (2008).
167. V. Prasad and D. G. Vlachos, Multiscale model and informatics-based optimal design of experiments: Application to the catalytic decomposition of ammonia on ruthenium. *Ind. Eng. Chem. Res.* **47**, 6555-6567 (2008).
168. L. J. Provis, J. D. Gehman, C. E. White, and D. G. Vlachos, Modeling silica nanoparticle dissolution in TPAOH-TEOS-H<sub>2</sub>O solutions. *J. Phys. Chem. C* **112**, 14769–14775 (2008).
169. J. D. Rimer, O. Trofymuk, R. F. Lobo, A. Navrotsky, and D. G. Vlachos, Thermodynamics of Silica Nanoparticle Self-Assembly in Basic Solutions of Monovalent Cations. *J. Phys. Chem. C* **112**, 14754–14761 (2008).
170. M. Maestri, D. G. Vlachos, A. Beretta, G. Groppi, and E. Tronconi, Steam and dry reforming of methane on Rh: Microkinetic analysis and hierarchy of kinetic models. *J. Catal.* **259**, 211–222 (2008).
- Top 25 Hottest Articles, October-December, 2008.**
171. D. G. Vlachos, Temporal coarse-graining of microscopic-lattice kinetic Monte Carlo simulations via  $\tau$ -leaping. *Phys. Rev. E* **78**(4), 046713-1-7 (2008).
- Selected in the November 1, 2008 issue of Virtual Journal of Biological Physics Research, published by the American Physical Society and the American Institute of Physics; <http://www.vjbio.org>.*
172. S. Collins, A. Chatterjee, and D. G. Vlachos, Coarse-grained kinetic Monte Carlo models: Complex lattices, multicomponent systems, and homogenization at the stochastic level. *J. Chem. Phys.* **129**, No. 184101, pg. 1-15 (2008).
173. G. D. Stefanidis, D. G. Vlachos, N. S. Kaisare, and M. Maestri, Methane steam reforming at microscales: Operation strategies for variable power output at millisecond contact times. *AIChE J.* **55**(1), 180-191 (2009).
174. N. Kaisare, G. D. Stefanidis, and D. G. Vlachos, "Comparison of ignition strategies for catalytic microburners", *Proc. Comb. Inst.* **32**(2), 3027–3034 (2009).
175. G. D. Stefanidis and D. G. Vlachos, Controlling Homogeneous Chemistry in Homogeneous-Heterogeneous Reactors: Application to Propane Combustion. *Ind. Eng. Chem. Res.* **48**(13), 5962–5968 (2009).
176. J. Federici, E. D. Wetzel, B. R. Geil, and D. G. Vlachos, "Single channel and heat recirculation catalytic microburners: an experimental and computational fluid dynamics study", *Proc. Comb. Inst.* **32**, 3011–3018 (2009).
177. A. Scarpa, R. Pirone, G. Russo, and D. G. Vlachos, Effect of heat recirculation on the self-sustained catalytic combustion of propane/air mixtures in a quartz reactor. *Combust. Flame* **156**, 947–953 (2009).
178. V. Prasad, A. Karim, A. Arya, and D. G. Vlachos, Assessment of Overall Rate Expressions and Multiscale, Microkinetic Model Uniqueness via Experimental Data Injection: Ammonia Decomposition on Ru/g-Al<sub>2</sub>O<sub>3</sub> for Hydrogen Production. *Ind. Eng. Chem. Res.* **48**, 5255-5265 (2009).
179. M. Maestri, D. G. Vlachos, A. Beretta, G. Groppi, and E. Tronconi, A C1 microkinetic model for methane conversion to syngas on Rh/Al<sub>2</sub>O<sub>3</sub>. *AIChE J.* **55**(4), 993-1008 (2009).
180. \* G. Mpourmpakis and D. G. Vlachos, Growth Mechanisms of Metal Nanoparticles via First Principles. *Phys. Rev. Letters* **102**, No. 155505, pg. 1-4 (2009).
- Selected in April 27, 2009 issue of Virtual Journal of Nanoscale Science & Technology.**

181. N. Kaisare, G. D. Stefanidis, and D. G. Vlachos, Millisecond Production of Hydrogen from Alternative, High Hydrogen Density Fuels in a Cocurrent Multifunctional Microreactor. *Ind. Eng. Chem. Res.* **48**, 1749–1760 (2009).
182. G. Mpourmpakis and D. G. Vlachos, The Effects of the MgO Support and Alkali Doping on the CO Interaction with Au. *J. Phys. Chem. C* **113**, 7329–7335 (2009).
183. M. N. Costa, K. Radhakrishnan, B. S. Wilson, D. G. Vlachos, J. S. Edwards, Coupled Stochastic Spatial and Non-Spatial Simulations of ErbB1 Signaling Pathways Demonstrate the Importance of Spatial Organization in Signal Transduction, *PLoS One* **4(7)** e6316, pg. 1-9 (2009).
184. G. D. Stefanidis and D. G. Vlachos, High vs. low temperature reforming for hydrogen production via microtechnology, *Chem. Eng. Sci.* **64**, 4856-4865 (2009).
185. W. Hauptmann, M. Votsmeier, J. Gieshoff, D. G. Vlachos, A. Drochner, and H. Vogel, A Fast Approach to Predictive Models: NO-Oxidation in Exhaust Gas Aftertreatment Systems, *Topics Catal.* **52(13-20)**, 1925-1928 (2009).
186. \* A. M. Karim, V. Prasad, G. Mpourmpakis, W. W. Lonergan, A. I. Frenkel, J. G. Chen, and D. G. Vlachos, Correlating Particle Size and Shape of Supported Ru/g-Al<sub>2</sub>O<sub>3</sub> with NH<sub>3</sub> Decomposition Activity, *J. Am. Chem. Soc.* **131**, 12230–12239 (2009).
187. M. Maestri, D. G. Vlachos, A. Beretta, P. Forzatti, G. Groppi, and E. Tronconi, Dominant Reaction Pathways in the Catalytic Partial Oxidation of CH<sub>4</sub> on Rh, *Topics Catal.* **52**, 1983–1988 (2009).
188. D. G. Vlachos and S. Caratzoulas, The roles of catalysis and reaction engineering in overcoming the energy and the environment crisis, *Chem. Eng. Sci.* **65**, 18–29 (2010), Invited as part of the plenary lecture.
189. G. D. Stefanidis and D. G. Vlachos, Intensification of steam reforming of natural gas: Choosing combustible fuel and reforming catalyst, *Chem. Eng. Sci.* **65**, 398-404 (2010).
190. V. Prasad, A. M. Karim, Z. Ulissi, M. Zagrobelny, and D. G. Vlachos, High throughput multiscale modeling for design of experiments, catalysts, and reactors: Application to hydrogen production from ammonia, *Chem. Eng. Sci.* **65**, 240-246 (2010).
191. V. Papavassiliou, P. Pacouloute, K. T. Wu, R. Drnevich, D. Vlachos, J. Hemmings, and L. Bonnel, Catalytic Partial Oxidation Pilot Plant Study, *Ind. Eng. Chem. Res.* **49(1)**, 94–103 (2010).
192. \* D. A. Hansgen, D. G. Vlachos, and J. G. Chen, Using first principles to predict bimetallic catalysts for the ammonia decomposition reaction, *Nature Chemistry* **2**, 484-489 (2010).
193. W. W. Lonergan, D. G. Vlachos, and J. G. Chen, Correlating extent of Pt–Ni bond formation with low-temperature hydrogenation of benzene and 1,3-butadiene over supported Pt/Ni bimetallic catalysts, *J. Catal.* **271(2)**, 239-250 (2010).
194. \* G. Mpourmpakis, A. N. Andriotis, and D. G. Vlachos, Identification of Descriptors for the CO Interaction with Metal Nanoparticles, *Nano Letters* **10**, 1041-1045 (2010).
195. Y. Chen and D. G. Vlachos, Hydrogenation of Ethylene and Dehydrogenation and Hydrogenolysis of Ethane on Pt(111) and Pt(211): A Density Functional Theory Study, *J. Phys. Chem. C* **114**, 4973–4982 (2010).
196. S. Collins, M. Stamatakis, and D. G. Vlachos, Adaptive coarse-grained Monte Carlo simulation of heterogeneous plasma membranes, *BMC Bioinformatics* **11**, 218 (2010).
197. \* G. Mpourmpakis, S. Caratzoulas, and D. G. Vlachos, What Controls Au Nanoparticle Dispersity during Growth?, *Nano Letters* **10(9)**, 3408–3413 (2010).
198. M. S. Mettler, G. D. Stefanidis, D. G. Vlachos, Scale out strategies for microchemical devices: Application to natural gas to syngas conversion, *Ind. Eng. Chem. Res.* **49**, 10942–10955 (2010).
199. D. G. Vlachos, J. G. Chen, R. J. Gorte, G. W. Huber, and M. Tsapatsis, Catalysis Center for Energy Innovation for Biomass Processing: Research Strategies and Goals, *Cat. Letters* **140**, 77–84 (2010).
200. A. Donazzi, M. Maestri, B. C. Michael, A. Beretta, P. Forzatti, G. Groppi, E. Tronconi, L. D. Schmidt and D. G. Vlachos, Microkinetic modeling of spatially resolved autothermal CH<sub>4</sub> catalytic partial oxidation experiments over Rh-coated foams, *J. Catal.* **275(2)**, 270-279 (2010).
201. K. A. Al-Majnouni, N. D. Hould, W. W. Lonergan, D. G. Vlachos, and R. F. Lobo, High Temperature Decomposition of Brønsted Acid Sites in Gallium-Substituted Zeolites, *J. Phys. Chem.* **114**, 19395–19405 (2010).
202. M. Saliccioli, Y. Chen, and D. G. Vlachos, DFT derived group additivity and linear scaling methods for prediction of oxygenate stability on metal catalysts: Adsorption of open-ring alcohol and polyol dehydrogenation intermediates on Pt based metals, *J. Phys. Chem. C* **114**, 20155–20166 (2010).
203. H. Y. Wang, M. Stamatakis, D. A. Hansgen, S. Caratzoulas, and D. G. Vlachos, Understanding mixing of Ni and Pt in the Ni/Pt(111) bimetallic catalyst via molecular simulation and experiments, *J. Chem. Phys.* **133**, No. 224503 pg. 1-11 (2010).

204. K. Radhakrishnan, A. Halasz, D. G. Vlachos, and J. S. Edwards, Quantitative understanding of cell signaling: The importance of membrane organization, *Curr. Opinion Biotech.* **21**(5), 677-682 (2010).
205. K. Bijjula and D. G. Vlachos, Catalytic ignition and autothermal combustion of JP-8 over a Pt/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalyst, *Proc. Comb. Inst.* **33**, 1801-1807 (2011).
206. M. Saliccioli, Y. Chen, and D. G. Vlachos, Microkinetic modeling and reduced rate expressions of ethylene hydrogenation and ethane hydrogenolysis on platinum, *Ind. Eng. Chem. Res.* **50**, 28-40 (2011).
207. M. S. Mettler, G. D. Stefanidis and D. G. Vlachos, Enhancing stability in parallel plate microreactor stacks for syngas production, *Chem. Eng. Sci.* **66**, 1051-1059 (2011).
208. J. A. Federici and D. G. Vlachos, Experimental studies on syngas catalytic combustion on Pt/Al<sub>2</sub>O<sub>3</sub> in a microreactor, *Combust. Flame* **158**, 2540-2543 (2011).
209. S. Caratzoulas and D. G. Vlachos, Converting fructose to 5-hydroxymethylfurfural: A quantum mechanics/molecular mechanics study of the mechanism and energetics, *Carb. Res.* **346**, 664-672 (2011).
210. W. Hauptmann, M. Votsmeier, H. Vogel, and D. G. Vlachos, Modeling the simultaneous oxidation of CO and H<sub>2</sub> on Pt - Promoting effect of H<sub>2</sub> on the CO-light-off, *Appl. Cat. A: General* **397**, 174-182 (2011).
211. G. Mpourmpakis and D. G. Vlachos, Computational-based catalyst design for thermochemical transformations, *MRS Bulletin* **36**, 211-215 (2011).
212. N. M. Abukhdeir, D. G. Vlachos, M. Katsoulakis, and M. Plexousakis, Long-time integration methods for mesoscopic models of pattern-forming systems, *J. Comp. Phys.* **230**, 5704-5715 (2011).
213. D. A. Hansgen, L. M. Thomanek, J. G. Chen, and D. G. Vlachos, Experimental and theoretical studies of ammonia decomposition activity on Fe-Pt, Co-Pt, and Cu-Pt bimetallic surfaces, *J. Chem. Phys.* **134** (No. 184701), pg. 1-7 (2011).
214. M. Stamatakis and D. G. Vlachos, A graph-theoretical kinetic Monte Carlo framework for on-lattice chemical kinetics, *J. Chem. Phys.* **134** (No. 214115), pg. 1-13 (2011).
215. M. Stamatakis, Y. Chen, and D. G. Vlachos, First-Principles-Based Kinetic Monte Carlo Simulation of the Structure Sensitivity of the Water-Gas Shift Reaction on Platinum Surfaces, *J. Phys. Chem. C* **115**(50), 24750-24762 (2011).
216. Z. Ulissi, V. Prasad, and D. G. Vlachos, Effect of multiscale model uncertainty on identification of optimal catalyst properties, *J. Catal.* **281**, 339-344 (2011).
217. \* M. Saliccioli, W. Yu, M. A. Barteau, J. G. Chen, and D. G. Vlachos, Differentiation of O-H and C-H bond scission mechanisms of ethylene glycol on Pt and Ni/Pt using theory and isotopic labeling experiments, *J. Am. Chem. Soc.* **133**(20), 7996-8004 (2011).
218. M. Saliccioli and D. G. Vlachos, Kinetic modeling of Pt catalyzed and computation-driven catalyst discovery for ethylene glycol decomposition, *ACS Catal.* **1**(10), 1246-1256 (2011). **Cover art.**
219. \* N. M. Abukhdeir and D. G. Vlachos, Nano-scale surface pattern evolution in heteroepitaxial bimetallic films, *ACS Nano* **5**(9), 7168-7175 (2011).
220. M. Saliccioli, M. Stamatakis, S. Caratzoulas, and D. G. Vlachos, A review of multiscale modeling of catalytic reactions: Mechanism development for complexity and emergent behavior. *Chem. Eng. Sci.* **66**, 4319-4355 (2011). **As of 2015, it runs 7<sup>th</sup> in citations among 614 papers published in the journal that year.**
221. T. C. Brüggemann, D. G. Vlachos, and F. J. Keil, Microkinetic Modeling of the Fast Selective Catalytic Reduction of Nitrogen Oxide with Ammonia on H-ZSM5 Based on First Principles, *J. Catal.* **283**, 178-191 (2011).
222. N. Nikbin, G. Mpourmpakis, and D. G. Vlachos, A Combined DFT and statistical mechanics study for the CO oxidation on the Au<sub>10</sub><sup>-1</sup> cluster, *J. Phys. Chem. C* **115**, 20192-20200 (2011).
223. D. Hansgen, D. G. Vlachos, and J. G. Chen, Ammonia decomposition activity on monolayer Ni supported on Ru, Pt and WC substrate, *Surf. Sci.* **605**, 2055-2060 (2011).
224. M. Stamatakis and D. G. Vlachos, Equivalence of on-Lattice Stochastic Chemical Kinetics with the Well-Mixed Chemical Master Equation in the Limit of Fast Diffusion, *Comput. Chem. Eng.* **35**(12), 2602-2610 (2011).
225. W. W. Lonergan, T. Wang, D. G. Vlachos, and J. G. Chen, Effect of Oxide Support Surface Area on Hydrogenation Activity: Pt/Ni Bimetallic Catalysts Supported on Low and High Surface Area Al<sub>2</sub>O<sub>3</sub> and ZrO<sub>2</sub>, *App. Cat. A: General* **408**, 87-95 (2011).
226. G. Mpourmpakis, M. Stamatakis, S. Herrmann, D. G. Vlachos, and A. N. Andriotis, Predicting the adsorption behavior in bulk from metal clusters, *Chem. Phys. Letters* **518**, 99-103 (2011).
227. Y. Chen, M. Saliccioli, and D. G. Vlachos, An efficient reaction pathway search method applied to the Decomposition of Glycerol on Platinum, *J. Phys. Chem. C* **115**(38), 18707-18720 (2011).
228. \*V. Choudhary, A. B. Pinar, S. I. Sandler, D. G. Vlachos, and R. F. Lobo, Xylose Isomerization to Xylulose and its Dehydration to Furfural in Aqueous Media, *ACS Catal.* **1**, 1724-1728 (2011).



**Ranked 8<sup>th</sup> in citations on 4/12/13 among all papers published in 2011 in ACS Catal. and 9<sup>th</sup> on 6/7/15.**

229. R. C. Xiong, S. I. Sandler, and D. G. Vlachos, Alcohol Adsorption onto Silicalite from Aqueous Solution, *J. Phys. Chem. C* **115**(38), 18659-18669 (2011).
230. S. Caratzoulas, T. Courtney, and D. G. Vlachos, Hybrid Quantum Mechanics/Molecular Mechanics-Based Molecular Dynamics Simulation of Acid-Catalyzed Dehydration of Polyols in Liquid Water, *J. Phys. Chem. A* **115**(32), 8816-8821 (2011).
231. L. Yang, S. I. Sandler, D. G. Vlachos, C. Peng, H. Liu, and Y. Hu, Adsorption and Diffusion of Methanol, Glycerol, and Their Mixtures in a Metal Organic Framework, *Ind. Eng. Chem. Res.* **50**, 14084-14089 (2011).
232. E. Kalligiannaki, M. Katsoulakis, P. Plechac, and D. G. Vlachos, Multilevel coarse graining and nano-pattern discovery in many particle stochastic systems, *J. Comp. Phys.* **231**(6), 2599-2620 (2012).
233. \* M. S. Mettler, S. H. Mushrif, A. D. Paulsen, A. D. Javadekar, D. G. Vlachos, and P. J. Dauenhauer, Revealing Pyrolysis Chemistry for Biofuels Production: Conversion of Cellulose to Furans and Small Oxygenates, *Energy Environ. Sci.* **5**, 5414-5424 (2012).

**Highlighted in Nature Chemistry 4, 68-69 (2012).**

234. C. Bramsiepe, S. Sievers, T. Seifert, G. D. Stefanidis, D. G. Vlachos, H. Schnitzer, B. Muster, C. Brunner, J. P. M. Sanders, M. E. Bruins, and G. Schembecker, Low-cost small scale processing technologies for production applications in various environments—Mass produced factories, *Chem. Eng. Processing: Process Intensification* **51**, 32– 52 (2012).
235. \* N. Kaisare and D. G. Vlachos, A review on microcombustion: Fundamentals, devices and applications, *Prog. Energy Comb. Sci.* **38**, 321-359 (2012).
236. V. Choudhary, R. Burnett, D. G. Vlachos and S. I. Sandler, Dehydration of Glucose to 5-(Hydroxymethyl)furfural and Anhydroglucose: Thermodynamic Insights, *J. Phys. Chem. C* **116**, 5116-5120 (2012).
237. \* N. Guo, S. Caratzoulas, D. J. Doren, S. I. Sandler and D. G. Vlachos, A Perspective on the Modeling of Biomass Processing, *Energy Environ. Sci.* **5**(5), 6703-6716 (2012). **Perspective and cover art.**
238. J. McGill, B. Ogunnaike and D. G. Vlachos, Efficient Gradient Estimation Using Finite Differencing and Likelihood Ratios for Kinetic Monte Carlo Simulations, *J. Comp. Phys.* **231**(21), 7170-7186 (2012).
239. S. H. Mushrif, S. Caratzoulas and D. G. Vlachos, Understanding solvent effects in the selective conversion of fructose to 5-hydroxymethyl-furfural: A molecular dynamics investigation, *Phys. Chem. Chem. Phys.* **14**, 2637–2644 (2012).
240. N. Nikbin, S. Caratzoulas and D. G. Vlachos, A first principles-based microkinetic model for the conversion of fructose to 5-hydroxymethylfurfural, *ChemCatChem* **4**, 504-511 (2012).
241. M. Saliccioli, S. M. Edie and D. G. Vlachos, Adsorption of Acid, Ester, and Ether Functional Groups on Pt: Fast Prediction of Thermochemical Properties of Adsorbed Oxygenates via DFT-Based Group Additivity Methods, *J. Phys. Chem. C* **116**, 1873–1886 (2012).
242. R. Xiong, S. I. Sandler and D. G. Vlachos, Molecular Screening of Alcohol and Polyol Adsorption onto MFI-type Zeolites, *Langmuir* **28**, 4491–4499 (2012).
243. D. G. Vlachos, Multiscale modeling for emergent behavior, complexity, and combinatorial explosion, *AIChE J.* **58**(5), 1314–1325 (2012). **Cover art.**
244. M. Saliccioli and D. G. Vlachos, Kinetic modeling of Pt-catalyzed glycolaldehyde decomposition to syngas, *J. Phys. Chem. A* **116**(18), 4621-4628 (2012).
245. Y. Huang, D. G. Vlachos and J. G. Chen, Synthesis of rigid and stable large-inner-diameter multiwalled carbon nanotubes, *RSC Advances* **2**, 2685–2687 (2012).
246. \* M. S. Mettler, A. D. Paulsen, D. G. Vlachos and P. J. Dauenhauer, Pyrolytic Conversion of Cellulose to Fuels: Levoglucosan Deoxygenation via Elimination and Cyclization within Molten Biomass, *Energy Environ. Sci.* **5**, 7864-7868 (2012). **Cover art.**
247. M. S. Mettler, A. D. Paulsen, D. G. Vlachos and P. J. Dauenhauer, The Chain Length Effect in Pyrolysis: Bridging the Gap Between Glucose and Cellulose, *Green Chem.* **14**, 1284-1288 (2012).
248. \* M. S. Mettler, D. G. Vlachos and P. J. Dauenhauer, Top Ten Fundamental Challenges of Biomass Pyrolysis for Biofuels, *Energy Environ. Sci.* **5**, 7797-7809 (2012).
249. \*C. L. Williams, C.-C. Chang, P. Do, N. Nikbin, S. Caratzoulas, D. G. Vlachos, R. F. Lobo, W. Fan and P. J. Dauenhauer, Cycloaddition of Biomass-derived Furans for Catalytic Production of p-Xylene, *ACS Catal.* **2**, 935-939 (2012).
250. M. A. Christiansen and D. G. Vlachos, Microkinetic modeling of Pt-catalyzed ethylene glycol steam reforming, *App. Cat. A: General* **431-432**, 18-24 (2012).

251. J. S. Kruger, V. Nikolakis and D. G. Vlachos, Carbohydrate dehydration using porous catalysts, *Current Opinion Chem. Eng.* **1**, 312-320 (2012).
252. Y. Huang, F. Deng, C. Ni, J. G. Chen and D. G. Vlachos, Synthesis of Mesoporous Silica Nanobamboo with Highly Dispersed Tungsten Carbide Nanoparticles, *Dalton Trans.* **41**, 6914-6918 (2012).
253. V. Nikolakis, S. H. Mushrif, B. Herbert, K. S. Booksh and D. G. Vlachos, Fructose-Water-Dimethylsulfoxide Interactions by Vibrational Spectroscopy and Molecular Dynamics Simulations, *J. Phys. Chem. B* **116**(36), 11274-11283 (2012).
254. M. Stamatakis, M. A. Christiansen, D. G. Vlachos and G. Mpourmpakis, Multiscale Modeling Reveals Poisoning Mechanisms of MgO-Supported Au Clusters in CO Oxidation, *Nano Lett.* **12**, 3621-3626 (2012).
255. S. Tupy, A. Karim, C. Bagia, W. Deng, Y. Huang, D. G. Vlachos and J. G. Chen, Correlating ethylene glycol reforming activity with in-situ EXAFS detection of Ni segregation in supported NiPt bimetallic catalysts, *ACS Catal.* **2**, 2290-2296 (2012).
256. R. C. Catapan, A. A. M. Oliveira, Y. Chen and D. G. Vlachos, DFT Study of the Water-Gas Shift Reaction and Coke Formation on Ni(111) and Ni(211) Surfaces, *J. Phys. Chem. C* **116**(38), 20281-20291 (2012).
257. \*V. Choudhary, S. I. Sandler and D. G. Vlachos, Conversion of Xylose to Furfural using Lewis and Brønsted Acid Catalysts in Aqueous Media, *ACS Catal.* **2**(9), 2022-2028 (2012).
258. J. R. McManus, W. Yu, M. Saliccioli, D. G. Vlachos, J. G. Chen and J. M. Vohs, Biomass-derived Oxygenate Reforming on Pt(111): A Demonstration of Surface Science Using D-glucose and its Model Surrogate Glycolaldehyde, *Surf. Sci.* **606**(23-24), L91-L94 (2012).
259. \*S. Roy, G. Mpourmpakis, D.-Y. Hong, D. G. Vlachos, A. Bhan and R. J. Gorte, Mechanistic Study of Alcohol Dehydration on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, *ACS Catal.* **2**(9), 1846-1853 (2012).
260. \*V. Vorotnikov, G. Mpourmpakis and D. G. Vlachos, A DFT Study of Furfural Conversion to Furan, Furfuryl Alcohol, and 2-Methylfuran on Pd(111), *ACS Catal.* **2**, 2496-2504 (2012).
261. T. D. Courtney, V. Nikolakis, G. Mpourmpakis, J. G. Chen and D. G. Vlachos, Liquid-phase Dehydration of Propylene Glycol using Solid-Acid Catalysts, *Appl. Catal. A: General* **449**, 59-68 (2012).
262. Y. Chen and D. G. Vlachos, Density Functional Theory Study of Methane Oxidation and Reforming on Pt(111) and Pt(211), *Ind. Eng. Chem. Res.* **51**(38), 12244-12252 (2012).
263. J. R. McManus, M. Saliccioli, W. Yu, D. G. Vlachos, J. G. Chen and J. M. Vohs, Correlating the Surface Chemistry of C<sub>2</sub> and C<sub>3</sub> Aldoses with a C<sub>6</sub> Sugar: Reaction of Glucose, Glyceraldehyde, and Glycolaldehyde on Pd(111), *J. Phys. Chem. C* **116**(35), 18891-18898 (2012).
264. N. R. Peela, I. C. Lee and D. G. Vlachos, Design and Fabrication of a High-Throughput Microreactor and Its Evaluation for Highly Exothermic Reactions, *Ind. Eng. Chem. Res.* **51**(50), 16270-16277 (2012).
265. \*M. Stamatakis and D. G. Vlachos, Unraveling the Complexity of Catalytic Reactions via Kinetic Monte Carlo Simulation: Current Status and Frontiers, *ACS Catal.* **2**(12), 2648-2663 (2012).
266. \*J. E. Sutton and D. G. Vlachos, A Theoretical and Computational Analysis of Linear Free Energy Relations for the Estimation of Activation Energies, *ACS Catal.* **2**(8), 1624-1634 (2012).
267. N. Nikbin, P. T. Do, S. Caratzoulas, R. F. Lobo, P. J. Dauenhauer and D. G. Vlachos, A DFT Study of the Acid-catalysed Conversion of 2,5-Dimethylfuran and Ethylene to p-Xylene, *J. Catal.* **297**, 35-43 (2013).
268. J. E. Sutton and D. G. Vlachos, Error Estimates in Semi-empirical Estimation Methods of Surface Reactions, *J. Catal.* **297**, 202-216 (2013).
269. J. E. Sutton, P. Panagiotopoulou, X. E. Verykios and D. G. Vlachos, Combined DFT, Microkinetic, and Experimental Study of Ethanol Steam Reforming on Pt, *J. Phys. Chem. C* **117**(9), 4691-4706 (2013).
270. V. Choudhary, S. Caratzoulas and D. G. Vlachos, Insights into the Isomerization of Xylose to Xylulose and Lyxose by a Lewis Acid Catalyst, *Carbohydr. Res.* **368**, 89-95 (2013).
271. \*V. Choudhary, S. H. Mushrif, C. Ho, A. Anderko, V. Nikolakis, N. S. Marinkovic, A. I. Frenkel, S. I. Sandler and D. G. Vlachos, Insights into the Interplay of Lewis and Brønsted Acid Catalysts in Glucose and Fructose Conversion to 5-(Hydroxymethyl)furfural and Levulinic Acid in Aqueous Media, *J. Am. Chem. Soc.* **135**(10), 3997-4006 (2013).
272. M. A. Delichatsios, M. Gummala and D. G. Vlachos, Extinction of Surface Stabilized Gaseous Diffusion Flames: Part I Simplified Numerical Model and Implications for Solid Fuels in Fires, *Fire Safety J.* **55**, 152-159 (2013).
273. M. A. Delichatsios, M. Gummala and D. G. Vlachos, Extinction in Solid Fuel Combustion: Part II Detailed Model, *Fire Safety J.* **56**, 1-8 (2013).
274. W. Guo and D. G. Vlachos, Effect of Local Metal Microstructure on Adsorption on Bimetallic Surfaces: Atomic Nitrogen on Ni/Pt (111), *J. Chem. Phys.* **138**(17), 174702 (2013).
275. J. S. Kruger, V. Choudhary, V. Nikolakis and D. G. Vlachos, Elucidating the Roles of Zeolite H-BEA in Aqueous-Phase Fructose Dehydration and HMF Rehydration, *ACS Catal.* **3**(6), 1279-1291 (2013).

276. M. León, T. D. Swift, V. Nikolakis and D. G. Vlachos, Adsorption of the Compounds Encountered in Monosaccharide Dehydration in Zeolite Beta, *Langmuir* **29**(22), 6597-6605 (2013).
277. H. Ren, W. Yu, M. Saliccioli, Y. Chen, Y. Huang, K. Xiong, D. G. Vlachos and J. G. Chen, Selective Hydrodeoxygenation of Biomass-Derived Oxygenates to Unsaturated Hydrocarbons using Molybdenum Carbide Catalysts, *ChemSusChem* **6**(5), 798-801 (2013).
278. J. Jae, W. Zheng, R. F. Lobo and D. G. Vlachos, Production of Dimethylfuran from Hydroxymethylfurfural through Catalytic Transfer Hydrogenation with Ruthenium Supported on Carbon, *ChemSusChem* **6**(7), 1158-1162 (2013).
279. T. D. Swift, C. Bagia, P. Dornath, V. Nikolakis, W. Fan and D. G. Vlachos, Reactive Adsorption for the Selective Dehydration of Sugars to Furans: Modeling and Experiments, *AIChE J.* **59**(9), 3378-3390 (2013).
280. T. Wang, G. Mpourmpakis, W. W. Lonergan, D. G. Vlachos and J. G. Chen, Effect of Oxide Supports in Stabilizing Desirable Pt–Ni Bimetallic Structures for Hydrogenation and Reforming Reactions, *Phys. Chem. Chem. Phys.* **15**(29), 12156-12164 (2013).
281. S. A. Tupy, J. G. Chen and D. G. Vlachos, Comparison of Ethylene Glycol Steam Reforming over Pt and NiPt Catalysts on Various Supports, *Top. Catal.* **56**, 1644-1650 (2013).
282. V. Choudhary, A. B. Pinar, R. F. Lobo, D. G. Vlachos and S. I. Sandler, Comparison of Homogeneous and Heterogeneous Catalysts for Glucose-to-Fructose Isomerization in Aqueous Media, *ChemSusChem* **6**(12), 2369-2376 (2013).
283. M. A. Christiansen, G. Mpourmpakis and D. G. Vlachos, Density Functional Theory-Computed Mechanisms of Ethylene and Diethyl Ether Formation from Ethanol on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>(100), *ACS Catal.* **3**(9), 1965-1975 (2013).
284. \*W. Guo, M. Stamatakis and D. G. Vlachos, Design Principles of Heteroepitaxial Bimetallic Catalysts, *ACS Catal.* **3**(10), 2248-2255 (2013).
285. N. Nikbin, S. Caratzoulas and D. G. Vlachos, On the Brønsted Acid-Catalyzed Homogeneous Hydrolysis of Furans, *ChemSusChem* **6**(11), 2066-2068 (2013).
286. Y. Pantazis, M. A. Katsoulakis and D. G. Vlachos, Parametric sensitivity analysis for biochemical reaction networks based on pathwise information theory, *BMC Bioinformatics* **14**, Article 311 (2013).
287. N. R. Peela, W. Zheng, I. C. Lee, A. M. Karim and D. G. Vlachos, Core–Shell Nanocatalyst Design by Combining High-Throughput Experiments and First-Principles Simulations, *ChemCatChem* **5**(12), 3712-3718 (2013).
- Cover art:** <http://onlinelibrary.wiley.com/doi/10.1002/cctc.201300553/abstract>
288. \*N. Rai, S. Caratzoulas and D. G. Vlachos, Role of Silanol Group in Sn-Beta Zeolite for Glucose Isomerization and Epimerization Reactions, *ACS Catal.* **3**, 2294-2298 (2013).
289. J. Jae, E. Mahmoud, R. F. Lobo and D. G. Vlachos, Cascade of Liquid-Phase Catalytic Transfer Hydrogenation and Etherification of Hydroxymethylfurfural to Potential Bio-diesel Components over Lewis Acid Zeolites, *ChemCatChem* **6**(2), 508-513 (2014).
- Cover art:** <http://onlinelibrary.wiley.com/doi/10.1002/cctc.201490013/abstract>
290. J. Jae, W. Zheng, A. M. Karim, W. Guo, R. F. Lobo and D. G. Vlachos, The Role of Ru and RuO<sub>2</sub> in the Catalytic Transfer Hydrogenation of 5-Hydroxymethylfurfural for the Production of 2,5-Dimethylfuran, *ChemCatChem* **6**(3), 848-856 (2014).
291. W. Guo and D. G. Vlachos, On Factors Controlling Activity of Submonolayer Bimetallic Catalysts: Nitrogen Desorption, *J. Chem. Phys.* **140**(1), Article Number: 014703 (2014).
- 2014 Editors' Choice**
292. J. S. Kruger, V. Nikolakis and D. G. Vlachos, Aqueous-Phase Fructose Dehydration Using Brønsted Acid Zeolites: Catalytic Activity of Dissolved Aluminosilicate Species, *Appl. Catal. A: General* **469**, 116-123 (2014).
293. J. McGill, B. Ogunnaike and D. G. Vlachos, A robust and efficient triangulation-based optimization algorithm for stochastic black-box systems, *Comput. Chem. Eng.* **60**, 143-153 (2014).
294. H. Ren, Y. Chen, Y. Huang, W. Deng, D. G. Vlachos and J. G. Chen, Tungsten carbides as selective deoxygenation catalysts: experimental and computational studies of converting C3 oxygenates to propene, *Green Chem.* **16**, 761-769 (2014).
295. \*T. D. Swift, C. Bagia, V. Choudhary, G. Peklaris, V. Nikolakis and D. G. Vlachos, Kinetics of Homogeneous Brønsted Acid Catalyzed Fructose Dehydration and 5-Hydroxymethyl Furfural Rehydration: A Combined Experimental and Computational Study, *ACS Catal.* **4**, 259-267 (2014).
296. \*S. Wang, V. Vorotnikov, J. E. Sutton and D. G. Vlachos, Brønsted-Evans-Polanyi and Transition State Scaling Relations of Furan Derivatives on Pd(111) and Their Relation to Those of Small Molecules, *ACS Catal.* **4**, 604-612 (2014).
297. S. Wang, V. Vorotnikov and D. G. Vlachos, A DFT study of furan hydrogenation and ring opening on Pd(111),

- Green Chem.* **16**, 736-747 (2014).
298. R. Xiong, M. León, V. Nikolakis, S. I. Sandler and D. G. Vlachos, Adsorption of HMF from Water/DMSO Solutions onto Hydrophobic Zeolites: Experiment and Simulation, *ChemSusChem* **7**(1), 236-244 (2014).
  299. \*W. Yu, M. Saliccioli, K. Xiong, M. A. Barteau, D. G. Vlachos and J. G. Chen, Theoretical and Experimental Studies of C-C versus C-O Bond Scission of Ethylene Glycol Reaction Pathways via Metal-Modified Molybdenum Carbides, *ACS Catal.* **4**(5), 1409-1418 (2014).
  300. P. Panagiotopoulou and D. G. Vlachos, Liquid Phase Catalytic Transfer Hydrogenation of Furfural Over Ru/C Catalyst, *Appl. Catal. A: General* **480**, 17-24 (2014).
  301. G. R. Jenness, M. A. Christiansen, S. Caratzoulas, D. G. Vlachos and R. J. Gorte, Site-Dependent Lewis Acidity of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> and Its Impact on Ethanol Dehydration and Etherification, *J. Phys. Chem. C* **118**(24), 12899-12907 (2014).
  302. N. R. Peela, J. E. Sutton, I. C. Lee and D. G. Vlachos, Microkinetic Modeling of Ethane Total Oxidation on Pt, *Ind. Eng. Chem. Res.* **53**(24), 10051-10058 (2014).
  303. W. S. Lee, Z. S. Wang, W. Q. Zheng, D. G. Vlachos and A. Bhan, Vapor phase hydrodeoxygenation of furfural to 2-methylfuran on molybdenum carbide catalysts, *Catal. Sci. Technol.* **4**(8), 2340-2352 (2014).
  304. J. Luo, J. Y. Yu, R. J. Gorte, E. Mahmoud, D. G. Vlachos and M. A. Smith, The effect of oxide acidity on HMF etherification, *Catal. Sci. Technol.* **4**(9), 3074-3081 (2014).
  305. P. Panagiotopoulou, N. Martin and D. G. Vlachos, Effect of hydrogen donor on liquid phase catalytic transfer hydrogenation of furfural over a Ru/RuO<sub>2</sub>/C catalyst, *J. Mol. Catal. A: Chem.* **392**, 223-228 (2014).
  306. V. Vorotnikov, S. G. Wang and D. G. Vlachos, Group Additivity for Estimating Thermochemical Properties of Furanic Compounds on Pd(111), *Ind. Eng. Chem. Res.* **53**(30), 11929-11938 (2014).
  307. S. H. Mushrif, J. J. Varghese and D. G. Vlachos, Insights into the Cr(III) catalyzed isomerization mechanism of glucose to fructose in the presence of water using *ab initio* molecular dynamics, *Phys. Chem. Chem. Phys.* **16**(36), 19564-19572 (2014).
  308. R. C. Xiong, S. I. Sandler, D. G. Vlachos and P. J. Dauenhauer, Solvent-tuned hydrophobicity for faujasite-catalyzed cycloaddition of biomass-derived dimethylfuran for renewable *p*-xylene, *Green Chem.* **16**(9), 4086-4091 (2014).
  309. S. Caratzoulas, M. E. Davis, R. J. Gorte, R. Gounder, R. F. Lobo, V. Nikolakis, S. I. Sandler, M. A. Snyder, M. Tsapatsis and D. G. Vlachos, Challenges of and Insights into Acid-Catalyzed Transformations of Sugars, *J. Phys. Chem. C* **118**(40), 22815-22833 (2014). **Feature article and cover art.**
  310. M. S. Mettler, A. D. Paulsen, D. G. Vlachos and P. J. Dauenhauer, Tuning cellulose pyrolysis chemistry: selective decarbonylation via catalyst-impregnated pyrolysis, *Catal. Sci. Technol.* **4**(11), 3822-3825 (2014). **Cover art.**
  311. N. Nikbin, S. Caratzoulas and D. G. Vlachos, On the oligomerization mechanism of Brønsted acid-catalyzed conversion of furans to diesel-range fuels, *Appl. Catal. A-Gen.* **485**, 118-122 (2014).
  312. N. Nikbin, S. T. Feng, S. Caratzoulas and D. G. Vlachos, *p*-Xylene Formation by Dehydrative Aromatization of a Diels-Alder Product in Lewis and Bronsted Acidic Zeolites, *J. Phys. Chem. C* **118**(42), 24415-24424 (2014).
  313. T. R. Josephson, G. Tsilomelekis, C. Bagia, V. Nikolakis, D. G. Vlachos and S. Caratzoulas, Solvent-Induced Frequency Shifts of 5-Hydroxymethylfurfural Deduced via Infrared Spectroscopy and *ab Initio* Calculations, *J. Phys. Chem. A* **118**(51), 12149-12160 (2014).
  314. J. E. Sutton and D. G. Vlachos, Building large microkinetic models with first-principles' accuracy at reduced computational cost, *Chem. Eng. Sci.* **121**, 190-199 (2015). **Invited.**
  315. \*R. E. Patet, N. Nikbin, C. L. Williams, S. K. Green, C.-C. Chang, W. Fan, S. Caratzoulas, P. J. Dauenhauer, and D. G. Vlachos, Kinetic Regime Change in the Tandem Dehydrative Aromatization of Furan Diels-Alder Products, *ACS Catalysis* **5**(4), 2367-2375 (2015). **ACS Editors' Choice; Date: March 21, 2015.**
  316. A. V. Mironenko, M. J. Gilkey, P. Panagiotopoulou, G. Facas, D. G. Vlachos, and B. Xu, Ring Activation of Furanic Compounds on Ruthenium-Based Catalysts, *J. Phys. Chem. C* **119**(11), 6075-6085 (2015).
  317. G. R. Jenness, and D. G. Vlachos, DFT Study of the Conversion of Furfuryl Alcohol to 2-Methylfuran on RuO<sub>2</sub> (110), *J. Phys. Chem. C* **119**(11), 5938-5945 (2015).
  318. M. A. Christiansen, G. Mpourmpakis, and D. G. Vlachos, DFT-driven multi-site microkinetic modeling of ethanol conversion to ethylene and diethyl ether on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>(111), *J. Catal.* **323**, 121-131 (2015).
- Selected as a Featured Article in the March 2015 issue.**
319. J. Luo, L. Arroyo-Ramirez, R. J. Gorte, D. Tzoulaki and D. G. Vlachos, Hydrodeoxygenation of HMF Over Pt/C in a Continuous Flow Reactor, *AIChE J.* **61**(2), 590-597 (2015).
  320. \*S. G. Wang, V. Vorotnikov and D. G. Vlachos, Coverage-Induced Conformational Effects on Activity and

- Selectivity: Hydrogenation and Decarbonylation of Furfural on Pd(111), *ACS Catal.* **5(1)**, 104-112 (2015).
321. K. Xiong, W. Yu, D. G. Vlachos and J. G. Chen, Reaction Pathways of Biomass-Derived Oxygenates over Metals and Carbides: From Model Surfaces to Supported Catalysts, *ChemCatChem* **7(9)**, 1402-1421 (2015).

**Invited Review.**

322. L. Yang, G. Tsilomelekis, S. Caratzoulas and D. G. Vlachos, Mechanism of Brønsted Acid-Catalyzed Glucose Dehydration, *ChemSusChem* **8(8)**, 1334-1341 (2015).

**Cover art.**

323. T. D. Swift, H. Nguyen, A. Anderki, V. Nikolakis, D. G. Vlachos, Tandem Lewis/Bronsted homogeneous acid catalysis: conversion of glucose to 5hydroxymethylfurfural in an aqueous chromium(III) chloride and hydrochloric acid solution, *Green Chem.* **17(10)**, 4725-4735 (2015).
324. K. Lee, G. H. Gu, C. A. Mullen, A. A. Boateng and D. G. Vlachos, Guaiacol Hydrodeoxygenation Mechanism on Pt(111): Insights from Density Functional Theory and Linear Free Energy Relations, *ChemSusChem* **8(2)**, 315-322 (2015).
325. N. Nikbin, N. Austin, D. G. Vlachos, M. Stamatakis and G. Mpourmpakis, Catalysis at the Sub-nanoscale: Complex CO Oxidation Chemistry on a Few Au Atoms, *Catal. Sci. Technol.* **5(1)**, 134-141 (2015).

**Cover art.**

326. M. Nunez and D. G. Vlachos, Steady State Likelihood Ratio Sensitivity Analysis for Stiff Kinetic Monte Carlo Simulations, *J. Chem. Phys.* **142(4)**, No. 0441087, 7 pages (2015).
327. V. Vorotnikov and D. G. Vlachos, Group Additivity and Modified Linear Scaling Relations for Estimating Surface Thermochemistry on Transition Metal Surfaces: Application to Furanics, *J. Phys. Chem. C* **119(19)**, 10417-10426 (2015).
328. P. Panagiotopoulou, N. Martin and D. G. Vlachos, Liquid-Phase Catalytic Transfer Hydrogenation of Furfural over Homogeneous Lewis Acid-Ru/C Catalysts, *ChemSusChem* **8(12)**, 2046-2054 (2015).

**Cover art.**

329. J.E. Sutton and D.G. Vlachos, Ethanol Activation on Closed-Packed Surfaces, *Ind. Eng. Chem. Res.* **54(16)**, 4213-4225 (2015).
330. \*M.J. Gilkey, P. Panagiotopoulou, A.V. Mironenko, G.R. Jenness, D.G. Vlachos and B. Xu, Mechanistic Insights into Metal Lewis Acid-Mediated Catalytic Transfer Hydrogenation of Furfural to 2-Methylfuran, *ACS Catal.* **5(7)**, 3988-3994 (2015).
331. \*J. Rosen, G.S. Hutchings, Q. Lu, S. Rivera, Y. Zhou, D.G. Vlachos and F. Jiao, Mechanistic Insights into the Electrochemical Reduction of CO<sub>2</sub> to CO on Nanostructured Ag Surfaces, *ACS Catal.* **5(7)**, 4293-4299 (2015).
332. \*J.R. Christianson, S. Caratzoulas and D.G. Vlachos, Computational Insight into the Effect of Sn-Beta Na Exchange and Solvent on Glucose Isomerization and Epimerization, *ACS Catal.* **5(9)**, 5256-5263 (2015).
333. \*W. Guo and D.G. Vlachos, Patched bimetallic surfaces are active catalysts for ammonia decomposition, *Nature Communications* **6**, No. 8619 (2015).

**Highlighted in Chemistry Views (chemistry.views.org), Bimetallic Catalysts with Important Defects, October 10, 2015.**

334. \*S.K. Green, R.E. Patet, N. Nikbin, C.L. Williams, C.C. Chang, J.Y. Yu, R.J. Gorte, S. Caratzoulas, W. Fan, D.G. Vlachos, P.J. Dauenhauer, Diels-Alder cycloaddition of 2 methylfuran and ethylene for renewable toluene, *Appl. Catal. B-Env.* **180**, 487-496 (2016).
335. C.L. Williams, K.P. Vinter, C.C. Chang, R.C. Xiong, S.K. Green, S.I. Sandler, D.G. Vlachos, W. Fan, P. J. Dauenhauer, Kinetic regimes in the tandem reactions of HBEA catalyzed formation of p-xylene from dimethylfuran, *Catal. Sci. Technol.* **6(1)**, 178-187 (2016).
336. \*Z. Zhuang, S.A. Giles, J. Zheng, G.R. Jenness, S. Caratzoulas, D.G. Vlachos, Y. Yan, Nickel supported on nitrogen-doped carbon nanotubes as hydrogen oxidation reaction catalyst in alkaline electrolyte, *Nature Communications* **7**, No. 10141 (2016).

**Highlighted in Energy Storage - today, Green Car Congress, the Trendy Things, and 'A New Milestone for Fuel Cell Cost' in New Energy and Fuel, January 15, 2016.**

337. \*S.S.M. Konda, S. Caratzoulas, and D.G. Vlachos, Computational Insights into the Role of Metal and Acid Sites in Bifunctional Metal/Zeolite Catalysts: A Case Study of Acetone Hydrogenation to 2-Propanol and Subsequent Dehydration to Propene. *ACS Catal.* **6(1)**, 123-133 (2016).

338. \*J.E. Sutton, W. Guo, M.A. Katsoulakis and D.G. Vlachos, Effects of correlated parameters and uncertainty in electronic-structure-based chemical kinetic modelling, *Nature Chemistry* **8**, 331–337 (2016); doi:10.1038/nchem.2454 [in the 96% of the 252,381 tracked articles of a similar age in all journals and 77% in *Nature Chemistry* as of 10/5/16].
339. T.D. Swift, H. Nguyen, Z. Erdman, J.S. Kruger, V. Nikolakis, and D.G. Vlachos, Tandem Lewis acid/Bronsted acid-catalyzed conversion of carbohydrates to 5-hydroxymethylfurfural using zeolite beta. *J. Catal.* **333**, 149-161, (2016).
340. C.P. O'Brien, G.R. Jenness, H. Dong, D.G. Vlachos, I.C. Lee, Deactivation of Pt/Al<sub>2</sub>O<sub>3</sub> during propane oxidation at low temperatures: Kinetic regimes and platinum oxide formation. *J. Catal.* **337**, 122-132 (2016).
341. J.E. Sutton, J.E. and D.G. Vlachos, Effect of errors in linear scaling relations and Bronsted-Evans-Polanyi relations on activity and selectivity maps. *J. Catal.* **338**, 273-283 (2016).
342. G. Tsilomelekis, M.J. Orella, Z.X. Lin, Zheng, W.Q., Nikolakis, V., Vlachos, D.G., Molecular structure, morphology and growth mechanisms and rates of 5-hydroxymethyl furfural (HMF) derived humins. *Green Chem.* **18**, 1983-1993 (2016).
343. C.L. Williams, K.P. Vinter, C.C. Chang, R.C. Xiong, S.K. Green, S.I. Sandler, D.G. Vlachos, W. Fan, and P.J. Dauenhauer, Kinetic regimes in the tandem reactions of H-BEA catalyzed formation of p-xylene from dimethylfuran. *Catal. Sci. Technol.* **6**, 178-187 (2016).
344. R.E. Patet, S. Caratzoulas, and D.G. Vlachos, Adsorption in zeolites using mechanically embedded ONIOM clusters. *Phys. Chem. Chem. Phys.* **18**, 26094-26106 (2016).
345. \*D.S. Park, K.E. Joseph, M. Koehle, C. Krumm, L.M. Ren, J.N. Damen, M.H. Shete, H.S. Lee, X.B. Zuo, B. Lee, W. Fan, and D.G. Vlachos, R.F. Lobo, M. Tsapatsis, and P.J. Dauenhauer, Tunable Oleo-Furan Surfactants by Acylation of Renewable Furans. *ACS Central Sci.* **2**, 820-824 (2016).
346. \*H. Nguyen, V. Nikolakis, and D.G. Vlachos, Mechanistic Insights into Lewis Acid Metal Salt-Catalyzed Glucose Chemistry in Aqueous Solution. *ACS Catal.* **6**, 1497-1504 (2016).
347. \*A.V. Mironenko and D.G. Vlachos, Conjugation-Driven "Reverse Mars-van Krevelen"-Type Radical Mechanism for Low-Temperature C-O Bond Activation. *J. Am. Chem. Soc.* **138**, 8104-8113 (2016).
348. \*J. Luo, H. Yun, A.V. Mironenko, K. Goulas, J.D. Lee, M. Monai, C. Wang, V. Vorotnikov, C.B. Murray, D.G. Vlachos, P. Fornasiero, and R.J. Gorte, Mechanisms for High Selectivity in the Hydrodeoxygenation of 5-Hydroxymethylfurfural over PtCo Nanocrystals. *ACS Catal.* **6**, 4095-4104 (2016).
349. \*J. Lee, B. Saha, and D.G. Vlachos, Pt catalysts for efficient aerobic oxidation of glucose to glucaric acid in water. *Green Chem.* **18**, 3815-3822 (2016).
350. \*G.R. Jenness, W.M. Wan, J.G.G. Chen, and D.G. Vlachos, Reaction Pathways and Intermediates in Selective Ring Opening of Biomass-Derived Heterocyclic Compounds by Iridium. *ACS Catal.* **6**, 7002-7009 (2016).
351. A. Hashemi, M. Nunez, P. Plechac, and D.G. Vlachos, Stochastic averaging and sensitivity analysis for two scale reaction networks. *J. Chem. Phys.* **144**, 074104 (2016).
352. G.H. Gu and D.G. Vlachos, Group Additivity for Thermochemical Property Estimation of Lignin Monomers on Pt(111). *J. Phys. Chem. C* **120**, 19234-19241 (2016).
353. \*G.H. Gu, C.A. Mullen, A.A. Boateng, and D.G. Vlachos, Mechanism of Dehydration of Phenols on Noble Metals via First-Principles Microkinetic Modeling. *ACS Catal.* **6**, 3047-3055 (2016).
354. \*S.K. Green, R.E. Patet, N. Nikbin, C.L. Williams, C.C. Chang, J.Y. Yu, R.J. Gorte, S. Caratzoulas, W. Fan, D.G. Vlachos, and P.J. Dauenhauer, Diels-Alder cycloaddition of 2-methylfuran and ethylene for renewable toluene. *Appl. Catal. B-Environ.* **180**, 487-496 (2016).
355. S.K. Brand, T.R. Josephson, J.A. Labinger, S. Caratzoulas, D.G. Vlachos, and M.E. Davis, Methyl-ligated tin silsesquioxane catalyzed reactions of glucose. *J. Catal.* **341**, 62-71 (2016).
356. \*T.R. Josephson, S.K. Brand, S. Caratzoulas, and D.G. Vlachos, 1,2-H- versus 1,2-C-Shift on Sn-Silsesquioxanes. *ACS Catal.* **7**(1), 25-33 (2017).

**\* High impact journal article (IF>8)**

**Book Chapters**

1. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Bifurcation and global stability in surface catalyzed reactions using the Monte Carlo method," in *Patterns and Dynamics in Reactive Media*, edited by H. Swinney, R. Aris, and D. Aronson, Springer-Verlag, 1992, p. 187-206.
2. M. M. Zacharias and D. G. Vlachos, "Simulated annealing calculations for optimization of nanoclusters: The roles of quenching, nucleation, and isomerization in cluster morphology," in *Global minimization of nonconvex*

- energy functions: Molecular conformation and protein folding, edited by P. M. Pardalos, D. Shalloway, and G. Xue, Vol. 23, American Mathematical Society, 1996, p. 251-271.
3. D. G. Vlachos, P. -A. Bui, Y. K. Park, and P. Aghalayam, "Numerical bifurcation theory applied to real chemistry premixed flames: Flame stability and pollution abatement," in *Advanced Computation & Analysis of Combustion*, edited by G. D. Roy, S. M. Frolov, and P. Givi, ENAS Publishers, Moscow, 1997, p. 100-113.
  4. P. Aghalayam, P. -A. Bui, and D. G. Vlachos, "The role of flame-surface interactions in flame stability and pollutant emissions," in *Advances in Chemical Propulsion-Science to Technology*, CRC Press, edited by G. Roy, 2001.
  5. M. A. Katsoulakis and D. G. Vlachos, "Mesoscopic modeling of surface processes," in *Dispersive Transport Equations and Multiscale Models*, Edited by: N. B. Abdallah, A. Arnold, P. Degond, I. Gamba, R. Glassey, C. D. Levermore, and C. Ringhofer (Springer-Verlag, IMA, Vol. 136, 2003), p. 179-198.
  6. Díaz, I., G. Bonilla, Z. Lai, O. Terasaki, D. G. Vlachos, and M. Tsapatsis, *Silicalite-1 crystals with modified morphology: HRTEM imaging and synthesis of b-oriented films*. ed. E.V. Steen, L.H. Callanan, and M. Claeys. *Studies in Surface Science and Catalysis*. Vol. 154, 1160-1167 (2004).
  7. Norton, D. G., S. R. Deshmukh, E. D. Wetzel, and D. G. Vlachos, "Downsizing chemical processes for portable hydrogen production", in *Microreactor Technology and Process Intensification*, Y. Wang and J. D. Holladay, Editors. ACS Symposium Series 914, Washington, DC, p. 179-193 (2005).
  8. D. G. Vlachos, *Microreaction Engineering: Processes, Detailed design and Modeling*, in *Microfabricated Power Generation Devices*, ed. P. I. Barton and A. Mitsos, Wiley-VCH, Berlin (2009), p. 179-198.
  9. C. Catapan, M. A. Christiansen, A. A. M. Oliveira, and D. G. Vlachos, eds. *Catalytic Kinetics and Dynamics. Heterogeneous Catalysis at the Nanoscale for Energy Applications*, ed. F. Tao, W. Schneider, and P.V. Kamat. 2015, Wiley, pg. 161-189.

#### Chapters in Encyclopedias and Handbooks

1. M. A. Katsoulakis and D. G. Vlachos, "Mathematical strategies for the coarse-graining of microscopic models", in *Handbook of Materials Modeling*, Ed. by S. Yip, Springer, Dordrecht, Netherlands, pg. 1477-1490 (2005).
2. D. G. Vlachos, "Molecular modeling for non-equilibrium chemical processes", in *Encyclopedia of Chemical Processing*, Ed. Lee, S., Decker Encyclopedia of Chemical Processing, Taylor & Francis, New York, pg. 1717-1726 (2006).
3. N. Kaisare, G. D. Stefanidis, and D. G. Vlachos, *Transport Phenomena in Microscale Reacting Flows*, in *Handbook of Micro Reactors: Fundamentals, Operations and Catalysts*, V. Hessel et al., Editors. Wiley-VCH, Berlin (2009), p. 283-302.

#### Proceedings Publications and Reports

1. D. G. Vlachos and K. F. Jensen, "Crystal growth at high supersaturation based on the step propagation mechanism," *UMSI Report 90/95* (1990).
2. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Kinetics of facet formation during growth and etching of crystals," in *Interface Dynamics and Growth*, edited by K. S. Liang, M. P. Anderson, R. F. Bruinsma, and G. Scoles, Vol. 237, (Mat. Res. Soc. Symp. Proc., 1992), p. 145-150.
3. A. Balakrishna, D. G. Vlachos, L. D. Schmidt, and R. Aris, "Effect of pressure on ignition and extinction of methane near inert surfaces," in *Central States Section, Combustion Fundamentals & Applications*, The Combustion Institute, Madison, WI, 1994, p. 463-467.
4. P. A. Bui, D. G. Vlachos, and P. R. Westmoreland, "Inhibition of homogeneous ignition by a catalytic surface," in *Eastern States Section, Chemical and Physical Processes in Combustion*, The Combustion Institute, Worcester, MA, 1995, p. 147-150.
5. S. Kalamatianos and D. G. Vlachos, "Dynamics near ignitions and extinctions of premixed H<sub>2</sub>/air mixtures," in *Eastern States Section, Chemical and Physical Processes in Combustion*, The Combustion Institute, Worcester, MA, 1995, p. 131-134.
6. M. A. Delichatsios and D. G. Vlachos, "Critical conditions for extinction and transient pyrolysis decay in solid material fires," in *Eastern States Section, Chemical and Physical Processes in Combustion*, Hilton Head, SC, 1996, p. 285-288.
7. M. Tsapatsis and D. G. Vlachos, "Continuum and stochastic modeling on the role of gel microstructure in zeolite crystallization," in *Microporous and macroporous materials*, edited by J. S. Beck, L. E. Iton, D. R. Corbin, R. F. Lobo, and M. E. Davis, Vol. 431, (Mat. Res. Soc. Symp. Proc., San Francisco, CA, 1996), p. 197-202.
8. D. G. Vlachos and S. -J. He, "Particle formation in chemical reactors," in *Fifth World Congress of Chemical Engineering*, Vol. 5, San Diego, CA, 1996, p. 79-84.

9. P. -A. Bui, D. G. Vlachos, and P. R. Westmoreland, "Self-sustained oscillations in distributed flames modeled with detailed chemistry," in *Eastern States Section, Chemical and Physical Processes in Combustion, October 27-29*, The Combustion Institute, 1997, p. 337-340.
10. R. J. Olsen and D. G. Vlachos, "A multiparameter investigation of oscillatory ignition in the air oxidation of hydrogen in a continuous-flow stirred tank reactor," in *Eastern States Section, Chemical and Physical Processes in Combustion, October 27-29*, The Combustion Institute, 1997, p. 233-236.
11. Y. K. Park and D. G. Vlachos, "Methane/air instabilities driven by chain-branching and thermal feedback: The premixed nature of ignition," in *Eastern States Section, Chemical and Physical Processes in Combustion, October 27-29*, The Combustion Institute, 1997, p. 229-232.
12. D. G. Vlachos, "Two-dimensional detailed chemistry simulations in catalytic monoliths for methane combustion," in *Eastern States Section, Chemical and Physical Processes in Combustion, October 27-29*, The Combustion Institute, 1997, p. 305-308.
13. D. G. Vlachos, P. Aghalayam, and M. H. Zullo, "NO<sub>x</sub> formation and destruction near inert and catalytic surfaces," in *Eastern States Section, Chemical and Physical Processes in Combustion, October 27-29*, The Combustion Institute, 1997, p. 395-398.
14. P. R. Westmoreland, P. -A. Bui, I. B. Graff, and D. G. Vlachos, "Experimental gas-phase kinetics for parallel-plate PECVD," Fundamental gas-phase and surface chemistry of vapor-phase materials synthesis, (M.D. Allendorf, M.R. Zachariah, T.J. Mountziaris, A.H. McDaniel, eds.), The Electrochemical Society, Pennington NJ: Proceedings Volume 98-23, pp. 167-178 (1999).
15. P. Aghalayam, Y. K. Young, and D. G. Vlachos, "Detailed surface reaction mechanisms for methane oxidation on platinum," in Joint Combustion Meeting of the U.S. Sections of the Combustion Institute, March 14-17, The Combustion Institute, Washington, DC, 1999, p. 745-748.
16. M. Gummalla, H. Bermudez, D. G. Vlachos, and M. A. Delichatsios, "Flammability of diffusion flames near surfaces," in Joint Combustion Meeting of the U.S. Sections of the Combustion Institute, March 14-17, The Combustion Institute, Washington, DC, 1999, p. 741-744.
17. M. Gummalla, H. Bermudez, D. G. Vlachos, and M. A. Delichatsios, "Flammability, multiplicity and oscillation in surface stabilized diffusion flames: Application to fire extinction," in Mediterranean Combustion Symposium, Antalya, Turkey, June 20-25, 1999.
18. S. Raimondeau and D. G. Vlachos, "Two-dimensional detailed chemistry simulation of methane in short contact time catalytic monoliths," in Mediterranean Combustion Symposium, Antalya, Turkey, June 20-25, 1999.
19. M. Gummalla, D. G. Vlachos, and M. A. Delichatsios, "Effect of dilution on extinction limits of surface interacting diffusion flames with detailed chemistry and transport," in *Eastern States Section, Chemical and Physical Processes in Combustion*, The Combustion Institute, Raleigh, NC, Oct. 10-13, 1999, p. 188-191.
20. P. Aghalayam and D. G. Vlachos, "Development of an analytical criterion for the ignition of premixed alkane/air mixtures near platinum surfaces," in *Eastern States Section, Chemical and Physical Processes in Combustion*, The Combustion Institute, Raleigh, NC, Oct. 10-13, 1999, p. 217-220.
21. M. Gummalla and D. G. Vlachos, "Oscillatory instabilities and chaotic dynamics in premixed hydrogen-air flames", Proceedings of FEDSM: 2000 ASME Fluids Engineering Division, June 11-15, Boston, MA.
22. S. Raimondeau, P. Aghalayam, M. A. Katsoulakis, and D. G. Vlachos, "Bridging the gap of multiple scales: From microscopic, to mesoscopic, to macroscopic models," P. T. Cummings and P. R. Westmoreland (eds.), Foundations of Molecular Modeling and Simulations, AIChE Symposium Series No. 325, **97**, 155-158 (2001).
23. D. E. Zak, F. J. Doyle, D. G. Vlachos, and J. S. Schwaber, "Stochastic Kinetic Analysis of Transcriptional Feedback Models for Circadian Rhythms", Proc. 40th IEEE Conf. Decision & Control 2001, pg. 849-854.
24. S. Raimondeau, D. G. Vlachos, and R. I. Masel, "Two-dimensional modeling of homogeneous and catalytic microburners", Proceedings of the 40th Power Sources Conference, June 10-13, 2002, Cherry Hill, NJ, p. 415-418.
25. M. A. Snyder and D. G. Vlachos, "Mesoscopic modeling of binary diffusion through microporous zeolite membranes", MRS proceedings, 752, 161-166, (2002), Boston, MA 2002.
26. D. G. Norton, K. W. Voit, T. Brüggemann, D. G. Vlachos, and E. D. Wetzel, "Portable power generation via integrated catalytic microcombustion-thermoelectric devices", 24<sup>th</sup> Army Science Conference (2004).D. G. Norton, E. D. Wetzel, and D. G. Vlachos, "Design and Development of Catalytic Microburners", in Proceedings of the Joint Comb. Mtg. of the Comb. Inst., Philadelphia, PA, March 20-23, 2005 (paper #B41, session B-8).S. R. Deshmukh and D. G. Vlachos, "The power of microreactors", Fluent News, Summer 2005, p. 15.
29. D. G. Vlachos, A. B. Mhadeshwar, and N. Kaisare, "Hierarchical multiscale model-based design of experiments, catalysts, and reactors for fuel processing", *Proc. Chem. Proc. Control* 7, Paper No. 45, (2006). Lake Louise, Alberta, Canada, January 8-13, 2006.



30. M. Maestri, D. G. Vlachos, A. Beretta, P. Forzatti, G. Groppi, E. Tronconi, Microkinetic modeling of heterogeneous catalysis: from the rate equation to the rate constant, Italian Ass. Chem. Eng., 2008.

## INVITED TALKS

1. "Combustion near surfaces: Flame structure and numerical bifurcation", SANDIA National Laboratories, Livermore, CA, February 1, 1993.
2. "Combustion near surfaces: Flame structure and numerical bifurcation", Dept. Mech. Eng., Univ. of California at Berkeley, Berkeley, CA, February 2, 1993.
3. "Ignitions and extinctions near surfaces", Dept. Chem. Eng., University of Massachusetts, Amherst, MA, October 14, 1993.
4. "Structures and dynamics of nanophase systems: Surface reactions and materials processing", Dept. Chem. Eng., University of Nebraska, Lincoln, NE, March 14, 1994.
5. "Simulated annealing calculations for structure optimization of nanoclusters", workshop on *Global minimization of nonconvex energy functions: Molecular conformation and protein folding* (P. M. Pardalos, D. Shalloway, and G. Xue, eds.), AMS, Center for Discrete Mathematics and Theoretical Computer Science, Rutgers University, March 20-21, 1995.
6. "Transport phenomena, kinetics, and safety in oxidation reactors for chemical and materials synthesis", Minnesota Supercomputer Institute, University of Minnesota, Minneapolis, MN, May 24, 1995.
7. "Homogeneous-heterogeneous oxidation reactors: Reactor safety, chemical synthesis, and pollution abatement," Tufts University, Medford, MA, September 11, 1995.
8. "Oxidation reactors: Flames, chemical synthesis, and pollution abatement," State Univ. of NY at Buffalo, NY, April 22, 1996.
9. "A multiscale approach to homogeneous-heterogeneous oxidation reactors: Reactor safety, chemical synthesis, and pollution abatement", Dept. Chem. Eng., University of Massachusetts, Amherst, MA, September 18, 1997.
10. "A multiscale approach to homogeneous-heterogeneous oxidation reactors: Reactor safety, chemical synthesis, and pollution abatement", Dept. of Chem. Eng., Penn State Univ., PA, October 14, 1997.
11. "Modeling of homogeneous-heterogeneous oxidation reactors: Recent progress and future directions", Praxair Inc., NY, January 15, 1998.
12. "A multiscale approach to homogeneous-heterogeneous oxidation reactors", Dept. of Chem. Eng., Northwestern University, Evanston, IL, January 22, 1998.
13. "A multiscale approach to homogeneous-heterogeneous oxidation reactors", Dept. of Chem. Eng., University of Delaware, Newark, DE, January 22, 1998.
14. "Experimental Gas-Phase Kinetics for Parallel Plate PECVD," in *Fundamental Gas-Phase and Surface Chemistry of Vapor-Phase Materials Synthesis*, 194th Meeting of Electrochemical Society, Boston, MA, Nov. 1-6, 1998 (with P. R. Westmoreland, B. Graff, and P. -A. Bui).
15. "New reactor designs for minimization of waste byproducts and performance optimization," in *Second Annual Green Chemistry and Engineering Conference*, Washington, DC, June 30-July 2, 1998 (with Z. -T. Liu, and M. Tsapatsis).
16. "A multiscale approach to chemical reactors: From partial oxidation to complete combustion", in Dept. of Chem. Eng., University of Pennsylvania, Philadelphia, PA, November 30, 1998.
17. "A multiscale approach to chemical reactors: From partial oxidation to complete combustion," in Dept. of Chem. Eng., Kansas University, Manhattan, December 7, 1998.
18. "Ignitions, extinctions, and emissions of flames interacting with inert and catalytic surfaces", Univ. of Tokyo, January 21, 1999.
19. "Recent advances in oxidation microreactors and microstructure control in materials synthesis", in Dept. of Chem. and Biochemical Eng., Rutgers Univ., April 18, 1999.
20. "Recent advances in oxidation microreactors", Exxon Research and Engineering Company, Annandale, May 19, 1999.
21. "Recent advances in oxidation microreactors and microstructure control in materials synthesis", in Dept. of Chem. Eng., Drexel Univ., January 24, 2000.
22. "Multiscale models for complex systems: Chemistry, microstructure, and pattern formation", in Dept. of Chem. Eng., The City College of the City University of New York, NY, March 17, 2000.
23. "Multiscale models for complex systems: Chemistry, microstructure, and pattern formation", in Dept. of Chem. Eng., Univ. of California at Santa Barbara, CA, April 18, 2000.
24. "Multiscale models for complex systems: Chemistry, microstructure, and pattern formation", Fritz Haber Institute der Max Blank, Berlin, May 12, 2000.
25. "Recent advances in catalytic combustion", Paul Scherrer Institute, Zurich, Switzerland, May 16, 2000 (ERCOFTAC visitor).
26. "Nonlinear dynamics in laminar flames", ETH, Zurich, Switzerland, May 15, 2000.

27. "Recent advances in catalytic combustion", ABB Co., Zurich, Switzerland, May 18, 2000.
28. "Multiscale models for chemical reactors", in "Multiscale Models for Surface Evolution and Reacting Flows, Institute of Mathematics and its Applications (IMA) Workshop", Minneapolis, MN, June 5-9, 2000 (with S. Raimondeau, P. Aghalayam, V. Nikolakis, G. Bonilla, and M. Tsapatsis).
29. "Nonlinear dynamics in homogeneous and catalytic combustion", in Oscillations and dynamics, Gordon Research Conference, Bristol, RI, Aug. 20-25, 2000 (with M. Gummalla, P. K. Young, P. Aghalayam, and R. J. Olsen).
30. "Methods for continuation/bifurcation", 2<sup>nd</sup> Int. Workshop on Chemkin in Combustion, Edinburgh, Scotland, July 30, 2000.
31. "Multiscale modeling for chemical reactors: From atoms to reactor design", Technical university of Delft, Netherlands, July 5, 2001.
32. "Multiscale modeling for chemical reactors and membranes", Knowledge Foundation Workshop on Multiscale Modeling, Boston, MA, Aug 13-14, 2001.
33. Keynote Lecture of Chemical kinetics and Reactor Design: "Multiscale modeling for chemical reactors: From atoms to reactor design", EuropaCat V, Limerick, Ireland, Sept. 6, 2001.
34. "Multiscale modeling for chemical reactors", in AIChE meeting, Catalysis and Reaction Engineering and Topical T1 - Applying Molecular Simulations and Computational Chemistry, Session: "Multi-scale approaches to reaction engineering", Reno, 2001.
35. Modeling of high temperature microchemical systems, ExxonMobil, Annandale, 2001.
36. "Short contact time microreactors", Rohm Haas, Springhouse, PA, January 9, 2002.
37. "Short contact time microreactors: Chemistry and design", DuPont, Wilmington, DE, February 6, 2002.
38. "Recent advances in multiscale modeling of oxidation microreactors", Department of Mechanical and Aerospace Engineering, Univ. of Southern California, Los Angeles, CA, Feb. 13, 2002.
39. "Multiscale modeling for linking growth, microstructure, and transport-chemistry properties of inorganic microporous films", NASA workshop, Hampton, VA, March 5-6, 2002.
40. "Multiscale modeling: Application to materials nanotechnology and microreactors", Department of Mechanical and Industrial Engineering, Univ. of Illinois at Urbana-Champaign, IL, April 21, 2002.
41. "Bridging length and time scales in materials modeling", DOE workshop on Nanosciences, San Francisco, CA, May 10-11, 2002.
42. "Bridging length and time scales in materials modeling", in Methods for Advancing Length and Time Scales in Modeling Nanostructured Materials Session, AIChE meeting, Indianapolis, IN, Nov. 3-8, 2002.
43. "Bridging length and time scales in materials modeling", Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, March 25, 2003.
44. Microchemical Systems for Lightweight Multifunctional Structures, ARL, Aberdeen, MD, April 17, 2003.
45. "Bridging length and time scales in materials modeling", SIAM, Snowbird, UT, May 29, 2003.
46. "Short contact time microreactors: Chemistry and design", BOC, NJ, June 25, 2003.
47. Multiscale simulations for zeolite membrane growth and permeation, Department of Chemical and Biomolecular Engineering, Georgia Tech., Atlanta, Sept. 24, 2003.
48. Multiscale simulation for zeolite nanoparticle and membrane growth, CECAM-SIMU Workshop: "Molecular simulation of zeolites, towards *in silico* design?" Lyon, France, October 2-4, 2003.
49. From chemistry to design concepts of portable fuel processing devices, Catalysis Center, Northwestern University, Oct. 29, 2003.
50. From chemistry to design concepts of portable fuel processing devices, Department of Chemical Engineering, Lehigh University, Nov. 12, 2003.
51. Multiscale simulations of zeolite nanoparticle and membrane growth, 7<sup>th</sup> NECZA meeting, Philadelphia, PA, December 12, 2003.
52. Multiscale modeling and simulation in materials growth, Department of Mathematics, Univ. of Delaware, April 24, 2004.
53. Surface reactivity as a many body multiscale problem, in "molecular modeling and reaction chemistry" Symposium, ACS meeting, March 31<sup>st</sup>, Anaheim, CA, 2004.
54. Multiscale simulation of zeolite nanoparticle and membrane growth, in honor of the Ipatief Award recipient, ACS meeting, March 31<sup>st</sup>, Anaheim, CA, 2004.
55. Energy integration for microchemical systems, in "Thermal management for micro power sources", ARO/DARPA meeting, Chicago, IL, May 17<sup>th</sup>, 2004.
56. Multiscale simulations of nucleation and growth of ceramic and metal-composite nanoparticles and membranes, in Simulation of nano-world, Sicily, Italy, May 30-June 4, 2004.

57. Challenges and opportunities from hierarchical multiscale simulation for catalyst design and reactor optimization and control, ISCRE 18<sup>th</sup> meeting, Chicago, IL, June 6-9, 2004.
58. Coarse-Graining of Stochastic Processes and Associated Lattice Monte Carlo Simulations, *in* session "Simulation and control of multiscale processes", American Control Conference, Boston, MA, June 30<sup>th</sup>, 2004.
59. Portable Microchemical Devices for Hydrogen Production, Department of Chemical Engineering, University of Houston, Houston, TX, Oct. 15, 2004.
60. The emerging field of multiscale simulation in the chemical sciences, Department of Chemical Engineering, Drexel University, Philadelphia, PA, Oct. 29, 2004.
61. Multiscale Simulations of Nucleation and Growth in Porous Media, In memory of Stratis Sotirchos, AIChE meeting, Austin, TX, Nov. 8, 2004.
62. 14th International Zeolite Conference, Cape Town, South Africa, April 25-30, 2004.
63. J. M. Fedeyko, J. D. Rimer, D. G. Vlachos, and R. F. Lobo, "The First Stage of Microporous Silicate growth: Characterization of Zeolite Nanoparticle Precursors and Role of Nanoparticles in the Growth Mechanism of Silicalite-1", invited talk at National Institute of Standards and Technology, Center for Neutron Research, Gaithersburg, MD (2004).
64. Quantitative characterization of grain boundaries and defects within microporous zeolite membranes and their effect upon transport properties, keynote presentation, 8<sup>th</sup> International Conference in Inorganic Membranes, Cincinnati, Ohio, July 18-22, 2004 (with M. A. Snyder, D. G. Vlachos, Z. Lai, and M. Tsapatsis).
65. The emerging field of multiscale simulation in the chemical sciences, Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute, Troy, NY, Jan. 26, 2005.
66. The emerging field of multiscale simulation in the chemical and biological sciences, Department of Chemical Engineering, UCLA, Feb. 25, 2005.
67. Chemical kinetics and design concepts of portable fuel processing devices, Philadelphia Catalysis Club, April 27, 2005.
68. Design concepts of portable power generators: Hierarchical multiscale simulations and experiments, Aerospace Engineering, Univ. of Maryland, College Park, MD, May 13, 2005.
69. Design concepts of portable power generators: Hierarchical multiscale simulations and experiments, GE, Albany, NY, June 3, 2005.
70. The emerging field of multiscale simulation in the chemical and biological sciences, in Institute of Chemical Engineering and High Temperature Chemical Processes (ICE-HT), Patras, Greece, June 17, 2005.
71. Multiscale CFD simulations of Portable Microchemical Devices for Hydrogen Production, in "Single and multiphase chemically reacting flows: CFD with detailed chemistry, population balances, fine-particle formation, and other mixing-sensitive processes" as part of the Conference on "Computational Fluid Dynamics in Chemical Reaction Engineering IV", Il Ciocco, Barga, Italy, June 26 – July 1, 2005.
72. Combustion and partial oxidation at the microscale: Hierarchical multiscale simulations and experiments, Praxair, Buffalo, NY, Aug. 2, 2005.
73. On the understanding of zeolite nanoparticle and membrane growth mechanisms, in International Symposium entitled "Catalytic processes on advanced micro- and mesoporous materials", Nessebar, Bulgaria, September 2-5, 2005.
74. Design concepts for portable power generators: Hierarchical multiscale simulations and experiments, *China/USA/Japan Joint Chemical Engineering Conference*, Beijing, China, October 11-13, 2005. Keynote Lecture
75. Multiscale Methods for Stochastic Simulation, in Workshop II: Multiscale Modeling in Condensed Matter and Materials Sciences, including Mini-Workshop: Time Acceleration Methods in Atomistic Simulations, IPAM, Los Angeles, CA, October 17-22, 2005.
76. The emerging field of multiscale simulation, Fluent Inc., Nov. 16, 2005.
77. Hierarchical multiscale model-based design of experiments, catalysts, and reactors for portable power generators, in Emerging Applications: Microchemical and Fuel Cell Systems of the Chemical Process Control 7<sup>th</sup> (CPC7) Meeting, Lake Louise, Canada, January 8-13, 2006.
78. Insights into stochasticity of Liesegang ring formation from nonlinear analysis and multiscale Monte Carlo simulation, in the workshop "Stochastic Effects in Liesegang Patterns Formation", Sils-Maria, Switzerland, January 15-19, 2006.
79. The emerging field of multiscale simulation in the chemical and biological sciences, UD Computational Science Day, Feb. 14, 2006.
80. The role of catalysis in the hydrogen cycle, NSF Workshop on Research Frontiers for Combustion in the Hydrogen Economy, Arlington, VA, March 9-10, 2006.

81. Multiscale model-based process and product engineering, Imperial College, London, UK, March 17, 2006.
82. Trends in energy research, Department of Chemical Engineering, Univ. of Patras, March 20, 2006.
83. Multiscale simulations and experiments of zeolite-nanoparticle self-assembly and growth, Department of Chemical Engineering, Univ. of Patras, March 24, 2006.
84. Catalytic Microcombustors for Compact Power Generation, Army Research Lab, Delphi, MD, April 4, 2006.
85. The emerging field of multiscale simulation: Relation to cyber-infrastructure and educational needs, NSF Workshop on Cyber-based Combustion Science, Arlington, VA, April 19-20, 2006.
86. The emerging field of multiscale simulation in the biological sciences, Department of Molecular Genetics and Microbiology, University of New Mexico Cancer Research and Treatment Center, Albuquerque, NM, May 3<sup>rd</sup>, 2006.
87. The emerging field of multiscale simulation in the biological sciences, Los Alamos National Laboratories, Los Alamos, NM, May 4, 2006.
88. Microkinetic modeling: Development, model-based design of experiments, catalysts, and reactors for fuel processing, ExxonMobil Research and Engineering Company, Annandale, NJ, June 5, 2006.
89. On the understanding of zeolite precursor nanoparticles: Implications for control of zeolite particle and membrane morphology, ExxonMobil Research and Engineering Company, Annandale, NJ, June 5, 2006.
90. Multiscale modeling of catalytic processes and catalyst synthesis, ExxonMobil Research and Engineering Company, Annandale, NJ, June 23, 2006.
91. Hierarchical multiscale model-based design of experiments, catalysts and reactors, in 16<sup>th</sup> European Symposium on Computer Aided Process Engineering (ESCAPE) and 9<sup>th</sup> International Symposium on Process Systems Engineering (PSE), Garminsch-Partkenkirchen, Germany, July 9-13, 2006.
92. Insights into the nucleation and growth of zeolite nanoparticles from multiscale modeling, CECAM workshop on 'Computational aspects of building blocks, nucleation, and synthesis of porous materials', Lyon, France, Aug. 29-31, 2006.
93. Microkinetic modeling: Development and use, General Motors, Warren, MI, Sept. 14, 2006.
94. Hierarchical multiscale model-based design of experiments, catalysts, and reactors for portable power generation, UPenn, Philadelphia, PA, Oct. 4, 2006.
95. The emerging field of multiscale simulation in the chemical, materials, and biological sciences, School of Chemical, Biological, and Materials Engineering, The University of Oklahoma, Norman, OK, Oct. 26, 2006.
96. The emerging field of multiscale simulation in the chemical, materials, and biological sciences, UW-Madison Chemical & Biological Engineering Dept., October 31, 2006.
97. Multiscale model-based process engineering: Application to portable and decentralized power generation, NASCRE II meeting, Houston, Feb. 4-7, 2007.
98. The emerging field of multiscale simulation in the chemical, materials, and biological sciences, Stevens, March 28, 2007.
99. The emerging field of multiscale simulation: Application to scale-up of nanotechnological processes and control of cellular engineering, Univ. of Florida, April 23, 2007.
100. The emerging field of multiscale simulation: Application to scale-up of nanotechnological processes and control of cellular engineering, Department of Chemical and Biological Engineering, Tufts University, Boston, MA, April 30, 2007.
101. The emerging field of multiscale simulation: Application to scale-up of nanotechnological processes and control of cellular engineering, EPFL (Ecole Polytechnique Federale de Lausanne), Lausanne, Switzerland, June 7, 2007.
102. Temporal acceleration of stochastic simulation, Workshop on 'Mathematical and Computational Methods for Accelerated Molecular and Stochastic Simulations', Institute for Computational and Applied Mathematics (IACM), Foundation for Research and Technology-Hellas (FORTH), Heraklion, Crete, Greece, June 25-27, 2007.
103. Methods for spatial acceleration of stochastic simulation, Workshop on 'Mathematical and Computational Methods for Accelerated Molecular and Stochastic Simulations', Institute for Computational and Applied Mathematics (IACM), Foundation for Research and Technology-Hellas (FORTH), Heraklion, Crete, Greece, June 25-27, 2007.
104. The multiple branches of the emerging field of multiscale simulation in the chemical, materials, and biological sciences, Workshop on 'Mathematical and Computational Methods for Accelerated Molecular and Stochastic Simulations', Institute for Computational and Applied Mathematics (IACM), Foundation for Research and Technology-Hellas (FORTH), Heraklion, Crete, Greece, June 25-27, 2007.

105. Multiscale model-based product engineering, Plenary at the Association of Crystallization Technology Meeting on the topic "Molecular Modeling in Crystallization", Madison, WI, October 7-10, 2007.
106. Multiscale Simulation for Cellular Engineering and Scale-up of Nanotechnological Processes, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, October 18, 2007.
107. The role of microreaction engineering in portable and distributed energy, Eastern Mediterranean Meeting of Chemical Engineering, Italy, May 20-24, 2008.
108. Uncertainty in multiscale modeling of materials, SIAM meeting, May, 2008.
109. Hierarchical Multiscale Modeling of Nanopattern Formation in Heteroepitaxy, IUTAM Symposium on Modeling Nanomaterials and Nanosystems, Aalborg, May 19-22, 2008.
110. The role of microreaction engineering in portable and distributed energy Production, Cetrato, Italy, 5<sup>th</sup> Chemical Engineering Conference for Collaborative Research in the Eastern Mediterranean Countries, May 25-29, 2008.
111. Molecular insights into nucleation and growth of zeolitic materials, Nanoporous Materials Gordon Conference, Maine, June 16, 2008.
112. Molecular Simulations: MD, KMC & TST, Lecture for the EC-funded Marie Curie Training Course, 'EF2: Nanostructured material and membrane modeling and simulation', Patras, Greece, June 19, 2008.
113. Multiscale modeling for development of surface reaction mechanisms and design of catalysts and reactors for decentralized hydrogen production, Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, June 25, 2008.
114. Multiscale Simulation for Bioimaging Informatics of Cells, in mini-symposium 'Multiscale Methods in Biological Modeling: Hybrid Systems and Coarsening Methods', SIAM Conference on Life Sciences, Montreal, Quebec, Canada, August 4-7, 2008.
115. Coping with the challenges of energy and the environment: Emerging opportunities for reaction engineering, Plenary Lecture in ISCRE 20<sup>th</sup> meeting, Kyoto, Japan, September 7-10, 2008.
116. The role of microreaction engineering in portable and distributed energy production, 7th International Workshop on Catalytic Combustion and Future Concepts in Energy Related Catalysis, Pfäffikon SZ, Switzerland, September 29-October 1, 2008.
117. Catalysis for decentralized hydrogen production, Panhellenic Symposium of Catalysis, Metsovo, Greece, Oct. 3-4, 2008.
118. Multiscale Monte Carlo simulations for biological, materials, and chemical engineering applications, in workshop "Stochastic Differential Equations: Models and Numerics", Stockholm, Sweden, Oct. 20-22, 2008.
119. The role of catalysis and reaction engineering in coping with the energy crisis, Univ. of South Carolina, Dec. 4, 2008.
120. The role of catalysis and reaction engineering in coping with the energy crisis, UCLA, Jan. 30, 2009.
121. The role of catalysis and reaction engineering in coping with the energy crisis, Penn State, March 17, 2009.
122. Catalysis for decentralized hydrogen production, Spring Symposium of the Catalysis Society of Metropolitan New York, Princeton University, March 18, 2009.
123. Hierarchical Multiscale Modeling and Control of Nanomaterials, Foundations of Molecular Modeling and Simulation (FOMMS), Plenary lecture, Washington, July 12-17, 2009.
124. Microkinetic modeling development and use in exhaust gas after-treatment technologies, 12<sup>th</sup> U.S. Department of Energy's Cross-Cut Lean Exhaust Emissions Reduction Simulation (CLEERS) workshop, Michigan, April 28-30, 2009.
125. Overcoming Complexity and Emergent Behavior via Multiscale Modeling, in Future Directions in Reaction Engineering, CRE Division, AIChE meeting, Nashville, Tennessee, Nov. 8-13, 2009.
126. The role of catalysis and reaction engineering in the energy arena, Department of Chemical and Biomolecular Engineering, University of Notre Dame, November 17, 2009.
127. Kinetic Monte Carlo Simulations of Receptor Clustering in Heterogeneous Cell Membranes, The New Mexico Center for the Spatiotemporal Modeling of Cell Signaling, Univ. of New Mexico, Dec. 4, 2009.
128. Living in a multiscale world, Inaugural lecture, Univ. of Delaware, Newark, DE, Dec. 8, 2009.
129. Kinetic Monte Carlo Simulations of EGFR Clustering in Heterogeneous Cell Membranes, Tokyo Medical and Dental University, Biomedical Science International PhD School, Systems Biology, December 7 - 11, 2009.
130. Scale-out strategies for portable and distributed processing, Int. Conf. on Microreactor Technology (IMRTE) 11, Kyoto, Japan, March 8-11, 2010; keynote lecture.
131. The role of catalysis and reaction engineering in the energy arena, General Electric, Albany, NY, February 24, 2010.
132. Complexity and emergent behavior in catalytic reactions: CO oxidation on gold and ammonia decomposition on single metals and bimetallics, Tokyo Univ., Tokyo, Japan, March 10, 2010.

133. Modern catalytic technologies for converting biomass to fuels, Biomass 2010 Conference, Crystal City, VA, March 30<sup>th</sup> - 31, 2010, Panel talk.
134. Emerging frontiers in multiscale modeling: Combinatorial complexity, uncertainty, and emergent behavior, DOE Applied Mathematics Meeting, Berkeley, CA, May 3, 2010, Plenary talk.
135. The role of catalysis and reaction engineering in the energy arena, Chemical & Biomolecular Engineering Department, Ohio State University, May 6, 2010.
136. Emerging frontiers in multiscaling: Combinatorial complexity, uncertainty, and emergent behavior, Department of Applied Mathematics, University of Crete, Crete, Greece, July 26<sup>th</sup>, 2010.
137. Highlights of the Catalysis Center for Energy Innovation, BESAC meeting, Rockville, MD, August 5-6, 2010.
138. An introduction to the Catalysis Center for Energy Innovation, UD Energy & Sustainability 2010 conference, Newark, DE, 09/23/10-09/25/10; <http://www.energy-sustainability-2010.com>.
139. Complexity and emergent behavior in catalytic reactions: CO oxidation on gold, biomass processing, and ammonia decomposition, Frontiers in Catalysis Science and Engineering talk, Pacific Northwest National Labs, Richland, WA, September 14, 2010.
140. Complexity and emergent behavior in catalytic reactions: Biomass processing and ammonia decomposition, Department of Chemical and Petroleum Engineering, Kansas University, Lawrence, KS, November 16<sup>th</sup>, 2010.
141. Complexity and emergent behavior in catalytic reactions, Department of Chemical Engineering, Michigan University, Ann Arbor, MI, December 7, 2010.
142. Modern catalytic technologies for converting biomass to renewable fuels and chemicals, NECZA, PA, December 10<sup>th</sup>, 2010.
143. Mechanism and energetics of fructose dehydration in solution and on nanomaterials for green chemicals, Pacificchem meeting, Honolulu, Hawaii, December 15-20, 2010.
144. Enablers for renewable chemicals and fuels, Department of Chemical Engineering, University of Delaware, Newark, DE, February 3, 2011.
145. Sustainable chemistry via catalysis: UD Capabilities and Prospects, Delaware Sustainable Chemistry Alliance (DESCA), Delaware Technology Park - Biotechnology Institute, Univ. of Delaware, Newark, DE, February 11, 2011.
146. Multiscale modeling in the catalysis center for energy innovation for biomass conversion to fuels and chemicals, Invited talk at Energy Frontier Symposium, ACS Spring meeting, Anaheim, CA, March 27-31, 2011.
147. Combinatorial complexity, uncertainty, and emergent behavior in the design of catalytic materials, Invited talk in Honor of Arvind Varma, ACS Spring meeting, Anaheim, CA, March 27-31, 2011.
148. Modern catalytic technologies for converting biomass to renewable fuels and chemicals, Invited talk at Special Symposium on Acid, Base and Zeolite Catalysis, ACS Spring meeting, Anaheim, CA, March 27-31, 2011.
149. Design of Emergent-Behaving Catalytic Materials, Chicago Catalysis Club, Chicago, IL, April 11, 2011.
150. Plenary talk: The role of microcombustion in portable and distributed energy, 13<sup>th</sup> International Conference on Numerical Combustion, April 27-29, 2011, Corfu, Greece.
151. Development of detailed reaction mechanisms for catalytic combustion, Invited Talk at Microcombustion Minisymposium, 13<sup>th</sup> International Conference on Numerical Combustion, April 27-29, 2011, Corfu, Greece.
152. Advanced Catalytic Reactor Technologies for Energy Applications, Keynote talk at the North American Catalysis Meeting, Detroit, MI, June 5-10, 2011.
153. Combinatorial complexity, uncertainty, and emergent behavior in the design of catalytic materials, Invited talk, Applied Math Center, Heraklion, Crete, Greece, June 27-July 1, 2011.
154. Design of Emergent-Behaving Catalytic Materials, EuropaCat X, Glasgow, Scotland, August 28-September 2, 2011.
155. Modern Catalytic Technologies for Converting Biomass to Renewable Fuels and Chemicals, BES/DOE Contractors meeting, Annapolis, MD, October 2-5, 2011.
156. Advanced Catalytic Reactor Technologies for Energy Applications, CCST Symposium, Newark, DE, October 6, 2011.
157. The role of catalysis and reaction engineering in the energy arena, Pennergy Institute, University of Pennsylvania, Philadelphia, October 24, 2011.
158. Modern catalytic technologies for converting biomass to renewable fuels and chemicals: An overview of the Catalysis Center for Energy Innovation, the Catalysis Society of Metropolitan New York, ExxonMobil, Clinton, NJ, March 14, 2012.
159. Hierarchical multiscale microkinetic modeling for chemical processing, ExxonMobil, Clinton, NJ, March 19, 2012.

160. Modern catalytic technologies for converting biomass to renewable fuels and chemicals: An overview of the Catalysis Center for Energy Innovation, Division of Physical Chemistry, Frontiers in Heterogeneous Catalysis, 243rd ACS National Meeting, San Diego, CA, March 25-29 2012.
161. High-throughput Multiscale Modeling: Informatics Strategies for Experimental Assessment, Catalyst Screening, Model Reduction, and Uncertainty Analysis, 243rd ACS National Meeting, San Diego, CA, March 25-29, 2012.
162. Recent Advances in Multiscale Modeling for Biomass Conversion, 243rd ACS National Meeting, San Diego, CA, March 25-29, 2012.
163. The role of catalysis and reaction engineering in the energy arena, Department of Chemical & Biochemical Engineering, Rutgers University, April 18, 2012.
164. Recent advances in multiscale modeling: Application to biomass conversion, Plenary talk at Int. Conf. on Theoretical Aspects of catalysis-14 (ICTAC-14), Vlissingen, the Netherlands, June 26-30, 2012.
165. An overview of multiscale simulation: Application to reactions and reactors, ExxonMobil, Clinton, NJ, July 26, 2012.
166. Modern Catalytic Technologies for Converting Biomass Derived Sugars to Chemicals: An Overview of the Catalysis Center for Energy Innovation, 244th ACS National Meeting & Exposition, Philadelphia, PA, August 19-23, 2012.
167. First-Principles-Based Multiscale Modeling of the Water-Gas Shift Reaction on Platinum and Nickel Surfaces, 244th ACS National Meeting & Exposition, Philadelphia, PA, August 19-23, 2012.
168. Challenges in multiscale model-based process systems engineering, in Future Innovation in Process System Engineering (FIPSE 1), Aldemar-Olympian Village, Greece, August 29-31, 2012.
169. Recent advances in catalysis: Application to renewable chemicals. 3M Company, St. Paul, MN, October 1, 2012.
170. Combinatorial complexity, uncertainty, and emergent behavior in the design of catalytic materials and processes, Chemical & Biomolecular Engineering, Cornell University, Ithaca, NY, November 12, 2012.
171. Modern catalytic technologies for converting biomass to renewable fuels and chemicals, Delft University, Netherlands, November 26, 2012.
172. Combinatorial complexity, uncertainty, and emergent behavior in the design of catalytic materials and processes, Department of Chemical Engineering, University of Washington, Seattle, WA, December 3, 2012.
173. The role of catalysis and reaction engineering in the energy arena, Department of Chemical & Environmental Engineering, Yale University, New Haven, CT, February 27, 2013.
174. Process and catalyst intensification for biomass processing, Keynote lecture, 3rd North American Symposium on Chemical Reaction Engineering (NASCRE-3), Chemical Reaction Engineering for a Sustainable Future: Addressing New Challenges and Revisiting Persistent Problems in Energy, Environmental, and Chemicals Research, Houston, TX, March 17-20, 2013.
175. Modern Catalytic Technologies for Converting Biomass to Renewable Fuels and Chemicals, The Michigan Catalysis Society, Detroit, MI, April 17, 2013.
176. Process and Catalyst Intensification for Biomass Processing, Archer Daniels Midland Company (ADM), Decatur, IL, May 15, 2013.
177. W. Guo and D. G. Vlachos, Multiscale KMC-DFT Simulation on Bimetallic Catalysts, Society for Industrial and Applied Mathematics (SIAM) 2013, Philadelphia, PA, June 8-12, 2013.
178. Multiscale Simulation of Chemical Reactions and Reactors: Combinatorial Complexity, Uncertainty, and Emergent Behavior, Symposium on 'Frontiers in Chemical Reaction Engineering', Gent, Belgium, June 25, 2013.
179. Renewable Chemicals and Fuels from Biomass, ExxonMobil, Clinton, NJ, August 22, 2013.
180. Combinatorial complexity, uncertainty, and emergent behavior in the design of catalytic materials, Symposium on New Theoretical Concepts and Directions in Catalysis, Santa Barbara, CA, August 27-30, 2013.
181. Design principles of bimetallic core-shell catalysts, CCST symposium, Newark, DE, October 10, 2013.
182. Multiscale Simulation of Chemical Reactions and Reactors: Combinatorial Complexity, Uncertainty, and Emergent Behavior, AIChE Symposium on Multiscale Modeling, San Francisco, CA, November 4, 2013.
183. Heteroepitaxial materials: self-assembly, control, and emergent properties, Waterloo Institute for Nanotechnology, Waterloo, Canada, March 13, 2014.
184. Renewable fuels and chemicals, Princeton Plasma Physics Laboratory Colloquium (PPPL), Princeton, NJ, March 19, 2014.
185. Multiscale ab initio modeling of catalysts, Workshop on Catalysis from first principles (Cat1P): Heterogeneous catalysis meets electrocatalysis, Castle Reissensburg, Germany, May 25-28, 2014.
186. Renewable Chemicals and Fuels from Biomass, Gordon Research Conference, Catalysis: From Art to Science, New London, NH, June 22-27, 2014.



187. Renewable fuels and chemicals, DuPont Co., Wilmington, DE, July 1, 2014.
188. Process and Catalyst Intensification for Distributed Energy and Chemicals, NSF Workshop on Process Intensification, Washington DC, Sept. 30 – October 1, 2014.
189. Renewable fuels and chemicals, J. D. Lindsay Lecture Series, Department of Chemical Engineering, Texas A&M University, October 8, 2014.
190. Modern catalytic technologies for converting biomass to renewable fuels and chemicals, Plenary lecture for the conference, *Advanced Materials, Energy and Sustainability*, 64th Canadian Chemical Engineering Conference (CSChE 2014), Niagara Falls, Ontario, October 19-22, 2014.
191. Heteroepitaxial materials in the energy arena: Self-assembly, control, and emergent properties, 2014-2015 ICI Distinguished DB Robinson Lectureship Series at the University of Alberta, Department of Chemical and Materials Engineering, Univ. of Alberta, October 23, 2014.
192. Multiscale Simulation of Chemical Reactions and Reactors: Combinatorial Complexity, Uncertainty, and Emergent Behavior, 2014-2015 ICI Distinguished Lecture, DB Robinson Lectureship Series at the University of Alberta, Department of Chemical and Materials Engineering, Univ. of Alberta, October 24, 2014.
193. Modeling reaction pathways, in *Theory and Computation for Interface Science and Catalysis: Fundamentals, Research and Hands-on Engagement using VASP*, A Joint Workshop of the Center for Functional Nanomaterials at Brookhaven National Laboratory and the Institute for Advanced Computational Science at Stony Brook University, November 2-7, 2014.
194. Tools for kinetic modeling, in *Theory and Computation for Interface Science and Catalysis: Fundamentals, Research and Hands-on Engagement using VASP*, A Joint Workshop of the Center for Functional Nanomaterials at Brookhaven National Laboratory and the Institute for Advanced Computational Science at Stony Brook University, November 2-7, 2014.
195. Multiscale ab initio modeling of catalysts, Inorganic Materials Plenary: Honorary Session I for Prof. Michael Tsapatsis, AIChE Meeting, Atlanta, GA, 2014.
196. Design principles of bimetallic core-shell catalysts, in honor of Arvind Varma, AIChE Meeting, Atlanta, GA, 2014.
197. Catalyst and process intensification, Dow Chemicals, Midland, MI, January 14, 2015.
198. Renewable Chemicals and Fuels from Biomass, Air Liquide, Newark, DE, January 19, 2015.
199. Multiscale simulations: Application to biological systems, UT Southwestern Medical Center, Dallas, TX 75390-8816, January 26, 2015.
200. Catalyst and process intensification, Department of Chemical & Biomolecular Engineering, Univ. of Connecticut, Storrs, CT, February 5, 2015.
201. Design principles of bimetallic core-shell catalysts, in George Olah Award Symposium, 249th ACS Meeting, Denver, Colorado, March 22-26, 2015.
202. Mechanisms and catalyst design principles in the conversion of sugars and furans to renewable monomers and fuels, 249th ACS Meeting, Denver, Colorado, March 22-26, 2015.
203. Insights into the hydrodeoxygenation mechanisms for lignin upgrade, 249th ACS Meeting, Denver, Colorado, March 22-26, 2015.
204. In Silico Prediction of Emergent Catalysts, in session on 'Design of materials and chemical processes: the genomic approach', 249th ACS Meeting, Denver, Colorado, March 22-26, 2015.
205. Correlated Uncertainty Quantification: Application to Complex Chemical Kinetics Mechanisms, Fifteenth International Conference on Numerical Combustion Program, Avignon, France, April 21, 2015.
206. Renewable Chemicals and Fuels from Biomass, CCP, Wilmington, DE, May 7, 2015.
207. In Silico Prediction of Core-Shell Bimetallic Catalysts, Thalys Program, Ioannina, Greece, June 29, 2015.
208. Renewable Chemicals and Fuels from Biomass, Thalys Program, Ioannina, Greece, June 29, 2015.
209. Comparing simulation and experiments: Successes and gaps, Catalysis Research PI Meeting, Benchmarking Catalysis Science, DOE BES meeting, July 19-22, 2015, Keynote lecture.
210. Renewable Chemicals and Fuels from Biomass, Discovery Days, Purdue University, West Lafayette, IN, October 2, 2015.
211. Renewable Chemicals and Fuels from Biomass, EFRC, Purdue University, West Lafayette, IN, October 2, 2015.
212. Multiscale Modeling for Energy Applications, Department of Chemical Engineering, MIT, Boston, MA, October 16, 2015.
213. Design Principles of Bifunctional Catalysts: Hydrogenation, dehydration, and hydrogenolysis, in honor of the 2015 CRE Practice Award winner Dan Hickman, AIChE meeting, Salt Lake city, Utah, Nov. 2015.
214. Design Principles of Bimetallic Core-Shell Catalysts, in Honor of Curt Conner, AIChE meeting, Salt Lake city, Utah, Nov. 2015.

215. Modern Catalytic Technologies for Converting Biomass to Renewable Fuels and Chemicals, in honor of Stan Sandler, AIChE meeting, Salt Lake city, Utah, Nov. 2015.
216. Multiscale simulation of chemical reactions and catalyst discovery, in Advanced Ab Initio Methods I, MRS Symposium YY, Boston, MA, November 29-December 4, 2015.
217. How predictive are multiscale materials simulations? Keynote lecture in Predictive Multiscale Materials Modelling, Isaac Newton Institute, Cambridge, England, December 1-4, 2015.
218. In Silico Prediction of Materials for Energy Applications, Department of Chemistry, University of Pennsylvania, Philadelphia, PA, March 9, 2016.
219. Modern catalytic technologies for converting biomass to renewable aromatics, 251<sup>st</sup> ACS Meeting, San Diego, CA, March 13-17, 2016.
220. Multifunctional catalysts for low temperature upgrade of biomass, 251<sup>st</sup> ACS Meeting, San Diego, CA, March 13-17, 2016.
221. Tuning Catalytic Performance via Active Site Design, 251<sup>st</sup> ACS Meeting, San Diego, CA, March 13-17, 2016.
222. Renewable fuels and chemicals from biomass, Plenary Lecture, Academia Mexicana de Investigacion y Docencia en Ingenieria Quimica (AMIDIQ), Puerto Vallarta, Mexico, May 3-6, 2016.
223. First principles prediction of optimal catalyst active site, SIAM meeting, Philadelphia, May 8-12, 2016.
224. Kinetics short-course, ISCRE meeting, Minneapolis, MN, June 2016.
225. Hydrogenolysis Mechanism of Furanics on Metal/Metal Oxide Catalysts, ACS Meeting, Philadelphia, PA, August 21-25, 2016.
226. In Silico Prediction of Materials for Energy Applications, Department of Chemical Engineering, UCL, London, September 13, 2016.
227. In Silico Prediction of Materials for Energy Applications, Catalysis Club of Philadelphia Award Lecture, Wilmington, DE, September 15, 2016.
228. Mechanisms and Kinetics in Complex Systems: Application to Biomass Processing, Plenary Lecture, X International Conference on Mechanisms of Catalytic Reactions, Svetlogorsk, Kaliningrad, Russia, October 3-7, 2016.
229. In Silico Prediction of Materials for Energy Applications, Katholieke Universiteit Leuven, Leuven, Belgium, October 12, 2016.
230. Design Principles for New Catalytic Materials for Energy Applications, Gent University, Gent, Belgium, October 14, 2016.
231. Maria Burka and the Reaction Engineering Community, In honor of Maria Burka, AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
232. In Silico Prediction of Materials for Energy Applications, Dumas Lecture, Department of Chemical Engineering, Virginia Tech, VA, December 2, 2016.
233. Robust Self-Sustainment in Austere Environments – Enablers for Comprehensive Power and Energy Efficiencies, Army Science Planning and Strategy Meeting, Materials for Sustainable and Mission Flexible Intelligent Systems, Aberdeen, MD, December 8-9, 2016.
234. In Silico Prediction of Materials for Energy Applications, Department of Chemical and Biomolecular Engineering, Clemson Univ., Clemson, SC, February 2, 2017.
235. Renewable chemicals and fuels from biomass, Department of Energy, Polytechnic Di Milano, Milan, Italy, February 21, 2017.

#### **Contributed Presentations to National and International Meetings**

1. D. G. Vlachos and K. F. Jensen, "Step Dynamics on Crystal Surfaces", American Institute of Chem. Eng., November 5-10, 1989, San Francisco, CA.
2. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Monte Carlo Studies of Rate Multiplicities and Self-Sustained Oscillations in Surface Reactions", American Institute of Chem. Eng., November 11-16, 1990, Chicago, IL.
3. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Structure of Small Catalyst Particles", American Institute of Chem. Eng., November 17-22, 1991, Los Angeles, CA.
4. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Kinetics of Facet Formation during Growth or Etching of Crystals", Materials Research Society, December 2-6, 1991, Boston, MA.
5. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Structure of Small Catalyst Particles", 12th International Symposium on Chemical Reaction Eng., 6/29/92-7/2/92, Torino, Italy.
6. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Comparison of Small Metal Clusters: Ni, Pd, Pt, Cu, Ag, Au", 6th International Symposium on Small Particles and Inorganic Clusters, September 16-22, 1992, Chicago, IL.

7. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Structure and Dynamics of Small Particles", American Institute of Chem. Eng., November 1-6, 1992, Miami, FL.
8. D. G. Vlachos, R. Olsen, L. D. Schmidt, and R. Aris, "Homogeneous-Heterogeneous Combustion Near Surfaces", American Institute of Chem. Eng., November 1-6, 1992, Miami, FL.
9. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Ignition and Extinction of Flames near Surfaces", American Institute of Chem. Eng., 1993, St. Lewis.
10. Balakrishna, D. G. Vlachos, L. D. Schmidt, and R. Aris, "Combustion of Natural Gas near Surfaces", American Institute of Chem. Eng., 1993, St. Lewis.
11. D. G. Vlachos, L. D. Schmidt, and R. Aris, "Methane Flames Near Surfaces", Twenty Fifth Symposium (International) on Combustion, July 31-August 5, 1994, Irvine, CA.
12. D. G. Vlachos, "Instabilities in homogeneous non-isothermal reactors: Comparison of deterministic and Monte Carlo Simulations", Gordon Conference on Oscillations and Dynamical Instabilities, August 7-12, 1994, Newport, RI.
13. S. Kalamatianos and D. G. Vlachos, "The interplay of transport and kinetics on flame stability", American Institute of Chem. Eng., November 13-18, 1994, San Francisco, CA.
14. S. -J. He and D. G. Vlachos, "Sintering of Supported Metal Catalysts: A Molecular Approach", American Institute of Chem. Eng., November 13-18, 1994, San Francisco, CA.
15. D. G. Vlachos, "Stochastic simulations of nanophase materials", American Institute of Chem. Eng., November 13-18, 1994, San Francisco, CA.
16. M. M. Zacharias and D. G. Vlachos, "Simulated annealing calculations of nanoclusters", Materials Research Society, November 27-December 2, 1994, Boston, MA.
17. D. G. Vlachos, "Growth of elongated nanostructures", Materials Research Society, November 27-December 2, 1994, Boston, MA.
18. S. Kalamatianos and D. G. Vlachos, "Mechanism reduction of complex reaction networks," American Institute of Chem. Eng., November 12-17, 1995, Miami, FL.
19. D. G. Vlachos, "The role of catalysis in homogeneous ignition and extinction of hydrogen," American Institute of Chem. Eng., November 12-17, 1995, Miami, FL.
20. S. -J. He and D. G. Vlachos, "The interplay of thermodynamics and kinetics in the formation of nanoparticles," American Institute of Chem. Eng., November 12-17, 1995, Miami, FL.
21. S. -J. He and D. G. Vlachos, "Hysteresis, oscillations, and phase transitions in growth of particles," American Institute of Chem. Eng., November 12-17, 1995, Miami, FL.
22. D. G. Vlachos, "Stochastic modeling of chemical reactors," American Institute of Chem. Eng., November 12-17, 1995, Miami, FL.
23. P. Bui, I. Graff, D. G. Vlachos, and P. R. Westmoreland, "Measurement of consumption and generation rates in a plasma-enhanced chemical vapor deposition reactor," American Institute of Chem. Eng., November 12-17, 1995, Miami, FL.
24. D. G. Vlachos and P. -A. Bui, "Homogeneous-heterogeneous ignitions and extinctions of hydrogen/air mixtures," in Sixth International Conference on Numerical Combustion, New Orleans, LA, March 4-6, 1996.
25. D. G. Vlachos and P. -A. Bui, "Homogeneous-heterogeneous oxidation reactors: Reactor safety, chemical synthesis, and pollution abatement," in AIChE Spring meeting, New Orleans, LA, Feb. 25-29, 1996.
26. D. G. Vlachos, "Homogeneous-heterogeneous oxidation reactions over platinum and inert surfaces," in 14th International Symposium on Chemical Reaction Engineering, Brugge, Belgium, May 5-8, 1996.
27. M. Tsapatsis and D. G. Vlachos, "Continuum and Stochastic Modeling on the Role of Gel Microstructure in Zeolite Crystallization," in Materials Research Society meeting, CA, April 8-12, 1996.
28. P. -A. Bui, D. G. Vlachos, and P. R. Westmoreland, "Homogeneous ignition of hydrogen/air mixtures over platinum," in Twenty Sixth Symposium (International) on Combustion, The Combustion Institute, Napoli, Italy, July 28-August 2, 1996.
29. P. -A. Bui, D. G. Vlachos, and P. R. Westmoreland, "On the self-inhibition of surface fuel ignition in catalytic oxidation reactors," in Twenty Sixth Symposium (International) on Combustion, The Combustion Institute, Napoli, Italy, July 28-August 2, 1996.
30. Y. K. Park and D. G. Vlachos, "Ignitions, extinctions, and oscillations in natural gas combustion," in American Institute of Chem. Eng., Chicago, IL, November 10-15, 1996.
31. M. Ziauddin, A. Balakrishna, L. D. Schmidt, R. Aris, and D. G. Vlachos, "Methane flames near inert surfaces: Effect of composition, pressure, preheat, and residence time," in American Institute of Chem. Eng., Chicago, IL, November 10-15, 1996.

32. D. G. Vlachos and M. Tsapatsis, "Mathematical modeling and experiments in zeolites: Nucleation and growth," in American Institute of Chem. Eng., Chicago, IL, November 10-15, 1996.
33. P. -A. Bui, D. G. Vlachos, and P. R. Westmoreland, "On the self-inhibition of surface fuel ignition in catalytic oxidation reactors," in American Institute of Chem. Eng., Chicago, IL, November 10-15, 1996.
34. D. G. Vlachos, "Stochastic modeling of chemical reactors with detailed kinetics: Induction times and explosions," in American Institute of Chem. Eng., Chicago, IL, November 10-15, 1996.
35. D. G. Vlachos and P. A. Monson, "Free energy of solid-phase clusters," in American Institute of Chem. Eng., Chicago, IL, November 10-15, 1996.
36. D. G. Vlachos, P.-A. Bui, Y. K. Park, and P. Aghalayam, "Numerical bifurcation theory applied to real chemistry premixed flames: Flame stability and pollution abatement," in International colloquium on advanced computation & analysis of combustion, Moscow, Russia, May 12-14, 1997.
37. M. Tsapatsis and D. G. Vlachos, "Continuum and stochastic models of zeolite crystallization," in International Symposium on Zeolites and Microporous Crystals, Tokyo, Japan, August 24-27, 1997.
38. Y. K. Park and D. G. Vlachos, "Ignitions and oscillations in methane/air mixtures," in *Gordon Conference on Oscillations and Dynamical Instabilities*, July 13-18, 1997, Newport, RI, 1997.
39. Y. K. Park, P.-A. Bui, and D. G. Vlachos, "Simulations of flammability and ignitability of catalytic oxidation reactors with detailed reaction mechanisms," American Institute of Chem. Eng., Los Angeles, CA, November 16-21, 1997.
40. V. Nikolakis, M. Tsapatsis, and D. G. Vlachos, "Mathematical modeling of zeolite nucleation and growth," American Institute of Chem. Eng., Los Angeles, CA, November 16-21, 1997.
41. P. Aghalayam and D. G. Vlachos, "Simulations of NO<sub>x</sub> production and destruction paths in H<sub>2</sub>/air premixed flames near surfaces," American Institute of Chem. Eng., Los Angeles, CA, November 16-21, 1997.
42. D. G. Vlachos, "Multiscale integration hybrid algorithms for homogeneous-heterogeneous process modeling," American Institute of Chem. Eng., Los Angeles, CA, November 16-21, 1997.
43. Y. K. Park and D. G. Vlachos, "Ignitions, extinctions, oscillations, and chemical synthesis in methane oxidation," American Institute of Chem. Eng., Los Angeles, CA, November 16-21, 1997.
44. R. Olsen, Y. K. Park, and D. G. Vlachos, "Reaction set reduction at oscillatory ignition points," ACS National Meeting, Dallas, TX, March 29-April 2, 1998.
45. P. Aghalayam and D. G. Vlachos, "NO<sub>x</sub> and fuel emissions in the combustion of hydrogen/air mixtures," in Twenty Seven Symposium (International) on Combustion, The Combustion Institute, Boulder, CO August 2-7, 1998.
46. P. Aghalayam and D. G. Vlachos, "An integrated microreactor/heat exchanger for natural gas Combustion: Efficiency and pollutant emissions," American Institute of Chem. Eng., Miami, FL, November 15-20, 1998.
47. P.-A. Bui and D. G. Vlachos, "Oscillations in complex reacting flows: H<sub>2</sub>/air flames near surfaces," American Institute of Chem. Eng., Miami, FL, November 15-20, 1998.
48. M. Gummalla, D. G. Vlachos, and M. A. Delichatsios, "Bifurcations and structure of surface stabilized methane-air diffusion flames," in Twenty Seven Symposium (International) on Combustion, The Combustion Institute, Boulder, CO August 2-7, 1998.
49. Y. K. Park, P. -A. Bui, N. E. Fernandes, and D. G. Vlachos, "Catalytic Combustion of H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> mixtures near Pt: Model validation through experiments and prediction of operation regimes," in Twenty Seven Symposium (International) on Combustion, The Combustion Institute, Boulder, CO August 2-7, 1998.
50. Y. K. Park, N. Fernandes, and D. G. Vlachos, "Pt catalyzed combustion of diluted H<sub>2</sub>/O<sub>2</sub> mixtures: Experimental validation of detailed modeling," American Institute of Chem. Eng., Miami, FL, November 15-20, 1998.
51. V. Nikolakis, M. Tsapatsis, and D. G. Vlachos, "Study of zeolite L growth using lattice Monte Carlo simulations", American Institute of Chem. Eng., Miami, FL, November 15-20, 1998.
52. D. G. Vlachos and J. Reese, "Linking molecular and macroscopic simulations in epitaxial film growth", American Institute of Chem. Eng., Miami, FL, November 15-20, 1998.
53. D. G. Vlachos, M. Gummalla, P. -A. Bui, P. R. Westmoreland, and R. J. Olsen, "Recent advances and future directions in nonlinear dynamics of complex reactions in combustion," in 13th Int. Congress of Chemical and Process Eng., Prague, Czech Republic, August 23-28, 1998.
54. D. G. Vlachos, "Two-dimensional simulations with detailed chemistry in fast flow partial oxidation monolith reactors," in ISCRE 15th, Newport Beach, CA, Sept. 13-16, 1998.
55. Y. K. Park, N. E. Fernandes, and D. G. Vlachos, "Effect of dilution on catalytic oxidation: Model validation through experiments and prediction of operation regimes," in ISCRE 15th, Newport Beach, CA, Sept. 13-16, 1998.

56. S. Raimondeau and D. G. Vlachos, "Two-dimensional detailed chemistry simulation of methane in short contact time catalytic monoliths," in Mediterranean Combustion Symposium, Antalya, Turkey, June 20-25, 1999.
57. M. Gummalla, H. Bermudez, D. G. Vlachos, and M. A. Delichatsios, "Flammability, multiplicity and oscillation in surface stabilized diffusion flames: Application to fire extinction," in Mediterranean Combustion Symposium, Antalya, Turkey, June 20-25, 1999.
58. S. Fisher, N. Fernandes, D. G. Vlachos, M. Tsapatsis, and J. J. Watkins, "Fabrication of supported thin film metal membranes for hydrogen separation by reactive deposition from supercritical fluids," AICHE meeting, Dallas, TX, Oct. 31-Nov. 5, 1999.
59. M. Gummalla, D. G. Vlachos, and M. A. Delichatsios, "Counterflow diffusion flames: Flame extinction, flammability, and fire suppression," in American Institute of Chem. Eng., Dallas, TX, Oct. 31-Nov. 5, 1999.
60. M. Gummalla, D. G. Vlachos, and M. A. Delichatsios, "Chaotic dynamics and isola of periodic orbits at high pressures in a distributed flow and reaction system," in AICHE meeting, Dallas, TX, Oct. 31-Nov. 5, 1999.
61. V. Nikolakis, D. G. Vlachos, and M. Tsapatsis, "Theoretical and experimental studies of the seeded growth of TPA-silicalite-1," AICHE meeting, Dallas, TX, Oct. 31-Nov. 5, 1999.
62. D. G. Vlachos, J. S. Reese, R. Lam, S. Raimondeau, and M. Katsoulakis, "Bridging the gap of multiple scales: From microscopic, to mesoscopic, to macroscopic models for catalytic and deposition reactors," AICHE meeting, Dallas, TX, Oct. 31-Nov. 5, 1999.
63. M. Katsoulakis and D. G. Vlachos, "A multiscale approach to cluster growth problems", in "Multiscale Models for Surface Evolution and Reacting Flows, Institute of Mathematics and its Applications (IMA) Workshop", Minneapolis, MN, June 5-9, 2000.
64. V. Nikolakis, G. Bonilla, D. G. Vlachos, and M. Tsapatsis, "Theoretical and experimental studies of the seeded growth of TPA-silicalite-1 nanoparticles and membranes", Int. Symp. Zeolites and Microporous Materials, Sendai, Japan, Aug. 6-9, 2000.
65. P. Aghalayam, Y. K. Park and D. G. Vlachos, "A detailed surface reaction mechanism for CO oxidation on Pt", Twenty Eight Symposium (International) on Combustion, The Combustion Institute, Edinburgh, Scotland, July 30-August 4, 2000.

***Bernard Lewis Award from the Combustion Institute***

66. M. Gummalla, M. A. Delichatsios, and D. G. Vlachos, "A criterion for critical solid fuel extinction", Twenty Eight Symposium (International) on Combustion, The Combustion Institute, Edinburgh, Scotland, July 30-August 4, 2000.
67. M. Gummalla and D. G. Vlachos, "Oscillatory instabilities and chaotic dynamics in premixed H<sub>2</sub>-air flames", Twenty Eight Symposium (International) on Combustion, The Combustion Institute, Edinburgh, Scotland, July 30-August 4, 2000.
68. D. G. Vlachos, V. Nikolakis, G. Bonilla, and M. Tsapatsis, "Modeling Growth of Zeolites: From nanoclusters to membranes," in PDEs with Chemical Engineering Applications, First SIAM Conference on Computational Science and Engineering, Washington, DC, Sept. 21-23, 2000.
69. J. C. Poshusta, S. M. Fisher, N. E. Fernandes, T. Basak, D. G. Vlachos, M. Tsapatsis, and J. Watkins, "Fabrication of palladium membranes in porous supports by reactive deposition from supercritical fluids", Annual AICHE meeting, Los Angeles, CA, Nov. 12-17, 2000.
70. G. Bonilla, D. G. Vlachos, and M. Tsapatsis, "Simulation of the polycrystalline film growth of zeolite membranes," Annual AICHE meeting, Los Angeles, CA, Nov. 12-17, 2000.
71. G. Bonilla, D. G. Vlachos, and M. Tsapatsis, "Characterization of the microstructure of zeolite membranes using fluorescence confocal microscopy," Annual AICHE meeting, Los Angeles, CA, Nov. 12-17, 2000.
72. S. Raimondeau, P. Aghalayam, Y. K. Park, and D. G. Vlachos, "Multiscale models of chemical reactors", Annual AICHE meeting, Los Angeles, CA, Nov. 12-17, 2000.
73. V. Nikolakis, G. Xomeritakis, M. Tsapatsis, and D. G. Vlachos, "Development of a new aluminosilicate-type zeolite membrane and its application to hydrocarbon isomers separation," Annual AICHE meeting, Los Angeles, CA, Nov. 12-17, 2000.
74. G. Bonilla, V. Nikolakis, M. Tsapatsis, D. G. Vlachos, "Growth Studies of Silicalite-1 Crystals and Thin Films", Gordon Research Conference on: Membranes Materials and Processes, New London, CT (July 29 - August 3, 2000).
75. P. Aghalayam, D. G. Vlachos, and V. Papavassiliou, "Construction and optimization of elementary surface reaction mechanisms for catalytic oxidation", 5<sup>th</sup> International Conference on Chemical Kinetics, NIST, Gaithersburg, MD, July 16-20, 2001.

76. D. G. Vlachos, R. Lam, M. Snyder, M. A. Katsoulakis, "A Novel approach to molecular modeling of transport through inorganic nanoporous membranes", International Workshop on Zeolitic and Microporous Membranes, IWZMM2001, Purmerend, Netherlands, July 1-4, 2001.
  77. S. Raimondeau and D. G. Vlachos, "Modeling of high temperature microreactors," AIChE meeting, Reno, Nov. 4-9, 2001.
- Catalysis and Reaction Engineering Student Award***
78. M. A. Snyder, R. Lam, D. G. Vlachos, and M. A. Katsoulakis, "A novel approach to molecular modeling of transport through nanoporous membranes," AIChE meeting, Reno, Nov. 4-9, 2001.
  79. D. G. Vlachos, R. Lam, M. A. Snyder, and M. A. Katsoulakis, and Z. Chen, "Mesoscopic models and simulations of transport in nanoporous films," AIChE meeting, Reno, Nov. 4-9, 2001.
  80. M. Gummalla, M. Tsapatsis, and J. J. Watkins, and D. G. Vlachos, "Multiscale Modeling for Deposition of Thin Films in Porous Media," AIChE meeting, Reno, Nov. 4-9, 2001.
  81. R. Harikrishnan, M. I. Lebedeva, D. G. Vlachos and M. Tsapatsis, "Periodic patterning in materials deposition by self-regulating diffusion-reaction processes," AIChE meeting, Reno, Nov. 4-9, 2001.
  82. P. Aghalayam, D. G. Vlachos, and V. Papavassiliou, "Construction and optimization of elementary surface reaction mechanisms for catalytic oxidation", AIChE meeting, Reno, Nov. 4-9, 2001.
  83. M. A. Snyder, D. G. Vlachos, and M. A. Katsoulakis, "Novel approach to molecular modeling of transport through inorganic nanoporous membranes", ACS meeting, Orlando, FL, April 7-11, 2002.
  84. A. B. Mhadeshwar, P. Aghalayam, V. Papavassiliou, and D. G. Vlachos, "Surface reaction mechanism development for partial oxidation of methane to synthesis gas", ACS meeting, Orlando, FL, April 7-11, 2002.
  85. D. G. Vlachos, M. A. Snyder, R. Lam, V. Nikolakis, G. Bonilla, M. Tsapatsis, and M. A. Katsoulakis, "Multiscale modeling for linking growth, microstructure, and transport-chemistry properties of inorganic microporous films", Mathematics in Chemical Kinetics and Engineering, Int. Workshop, Ghent, Belgium, May 5-8, 2002.
  86. D. G. Vlachos, M. Lebedeva, H. Ramanan, and M. Tsapatsis, "Mechanisms of Pattern Formation in Materials", AIChE meeting, Indianapolis, IN, Nov. 3-8, 2002.
  87. M.A. Snyder, D. G. Vlachos, and M. A. Katsoulakis, "Mesoscopic Modeling of Transport through Anisotropic Microporous Membranes", AIChE meeting, Indianapolis, IN, Nov. 3-8, 2002.
  88. D. G. Norton, S. Raimondeau, and D. G. Vlachos, "Design Rules for Exothermic Microchemical Systems", AIChE meeting, Indianapolis, IN, Nov. 3-8, 2002.
  89. D. Kragten, J. Fedeyko, J. Rimer, K. R. Sawant, R. Lobo, D. G. Vlachos, and M. Tsapatsis, "Nanoscale Zeolite Crystal Growth", AIChE meeting, Indianapolis, IN, Nov. 3-8, 2002.
  90. G. Bonilla, Z. Lai, J. G. Nery, M. Tsapatsis, and D. G. Vlachos, "Use of Organic SDAs to Control Morphology of Zeolite Crystals and Its Implications on Membrane Microstructure", AIChE meeting, Indianapolis, IN, Nov. 3-8, 2002.
  91. D. G. Norton and D. G. Vlachos, "Oscillations in microburners: Premixed methane/air mixtures", in *Third Joint Meeting of the U.S. Sections of The Combustion Institute*, March 16-19, 2003. Chicago, IL.
  92. A. B. Mhadeshwar, D. D. Kragten, and D. G. Vlachos, "Application of quantum mechanical density functional theory as a fundamental basis for microkinetic modeling of catalytic combustion", in *Third Joint Meeting of the U.S. Sections of The Combustion Institute*, March 16-19, 2003. Chicago, IL.
  93. R. F. Lobo, et al., "Nanoscale Zeolite Crystal Growth", Nanostructured Catalysts Session, AIChE meeting, Indianapolis, IN, Nov. 3-8, 2002 (invited).
  94. J. D. Rimer, D. Kragten, R. Lobo, and D. Vlachos, "The growth of zeolite crystals from the deposition of subcolloidal silica-template nanoparticles", 77<sup>th</sup> ACS Colloid & Surface Science Symposium, Atlanta, GA, June 15-18, 2003.
  95. J. Fedeyko, D. Kragten, K. Sawant, D. Vlachos, and R. Lobo "The structure of subcolloidal zeolite nanoparticles", 77<sup>th</sup> ACS Colloid & Surface Science Symposium, Atlanta, GA, June 15-18, 2003.
  96. D. G. Vlachos, A. Chatterjee, and M. A. Katsoulakis, "Hierarchical, multiscale simulations for pattern formation", 77<sup>th</sup> ACS Colloid & Surface Science Symposium, Atlanta, GA, June 15-18, 2003.
  97. A. B. Mhadeshwar, S. Raimondeau, J. Ludwig, and D. G. Vlachos, "Multiscale simulations for catalytic reactions: Application to hydrogen production", 77<sup>th</sup> ACS Colloid & Surface Science Symposium, Atlanta, GA, June 15-18, 2003.
  98. D. G. Vlachos, A. Chatterjee, and M. A. Katsoulakis, "Coarse-Graining of Stochastic Processes and Associated Lattice Monte Carlo", 3rd International Workshop on Nonequilibrium Thermodynamics and Complex Fluids, Princeton, NJ, August 14-17 2003.
  99. A. B. Mhadeshwar, H. Wang, and D. G. Vlachos, "Thermodynamic Consistency in Microkinetic Development of Surface Reaction Mechanisms", 226 ACS Fall Meeting, New York, NY Sept. 7-11, 2003.

100. D. G. Norton and D. G. Vlachos, "The Role of Fuel in the Stability of Exothermic Microchemical Systems", 226 ACS Fall Meeting, New York, NY Sept. 7-11, 2003.
101. S. R. Deshmukh, A. B. Mhadeshwar and D. G. Vlachos, "Microkinetic Modeling of Ammonia Synthesis & Decomposition on Ruthenium and Microreactor Design for Hydrogen Production", 226 ACS Fall Meeting, New York, NY Sept. 7-11, 2003.
102. D. G. Norton, S. R. Deshmukh, A. B. Mhadeshwar, E. Wetzel, and D. G. Vlachos, "Fuel processing at the microscale for portable fuel cells", 226 ACS Fall Meeting, New York, NY Sept. 7-11, 2003.
103. J. D. Rimer, J. M. Fedeyko, D. Kragten, K. R. Sawant, R. F. Lobo, D. G. Vlachos, "Growth of zeolite nanocrystals via the self-assembly of subcolloidal silica-template nanoparticles", AIChE meeting, San Francisco, CA, Nov. 2003. D. G. Norton, S. R. Deshmukh, A. Mhadeshwar, E. Wetzel, D. G. Vlachos, "Fuel Processing at the Microscale for Portable Fuel Cells", AIChE meeting, San Francisco, CA, Nov. 2003.
105. D. G. Norton and D. G. Vlachos, "The Role of Fuel in the Stability of Exothermic Microchemical Systems", AIChE meeting, San Francisco, CA, Nov. 2003.
106. A.B. Mhadeshwar, H. Wang, and D. G. Vlachos, "Thermodynamic Consistency in Microkinetic Development of Surface Reaction Mechanisms", AIChE meeting, San Francisco, CA, Nov. 2003.
107. S. R. Deshmukh, M. B. Mhadeshwar, and D. G. Vlachos, "Microreactor Design for Hydrogen Production from Ammonia: Microkinetic Modeling and CFD simulations", AIChE meeting, San Francisco, CA, Nov. 2003. A. Chatterjee, D. G. Vlachos and M. A. Katsoulakis, "Beyond microscopic simulation for materials growth: spatially adaptive coarse-grained stochastic theory and Monte Carlo simulation", AIChE meeting, San Francisco, CA, Nov. 2003.
109. M. A. Snyder and D. G. Vlachos, "Multiscale modeling of transport in microporous membranes", AIChE meeting, San Francisco, CA, Nov. 2003.
110. M. A. Snyder, D. G. Vlachos, Z. Lai, and M. Tsapatsis, "Toward quantitatively assessing the size and distribution of grain boundaries and defects in polycrystalline microporous membranes", AIChE meeting, San Francisco, CA, Nov. 2003.
111. D. G. Vlachos and M. A. Katsoulakis, "Novel coarse grained kinetic Monte Carlo simulations: Application to patterning of materials", AIChE meeting, San Francisco, CA, Nov. 2003.
112. G. Bonilla, I. Diaz, O. Terasaki, M. Tsapatsis, and D. G. Vlachos, "Silicalite-1 Crystal Morphology Modification", AIChE meeting, San Francisco, CA, Nov. 2003.
113. J. D. Rimer, R. F. Lobo, and D. G. Vlachos, "The role of self-assembled silica-tetrapropylammonium nanoparticles in the growth of silicalite-1 crystals", 78<sup>th</sup> ACS Colloid and Surf. Sci. Symp., Yale, CT, June 20-23, 2004.
114. J. Fedeyko, R. F. Lobo, and D. G. Vlachos, 'A new class of self-assembled organic-silica nanoparticles', 78<sup>th</sup> ACS Colloid and Surf. Sci. Symp., Yale, CT, June 20-23, 2004.
115. A. B. Mhadeshwar and D. G. Vlachos, "Microkinetic Analysis of Water-Promoted CO oxidation, Water-Gas Shift, and Preferential Oxidation of CO on Pt for Hydrogen Generation", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
116. M. A. Snyder, D. G. Vlachos, Z. Lai, and M. Tsapatsis, "Fluorescence confocal optical microscopy for quantitatively characterizing polycrystalline features of microporous zeolite membranes and their effect upon membrane performance", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
117. M. A. Snyder and D. G. Vlachos, "Mesoscopic modeling for bridging disparate scales of molecular transport through microporous crystalline membranes", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
118. Energy Integration in Microchemical Devices for Hydrogen Production", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
119. J. Ludwig and D. G. Vlachos, "Prediction of sticking coefficients for use in microkinetic models using density functional theory and molecular dynamics: H<sub>2</sub>/Pt(111)", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
120. S. R. Deshmukh and D. G. Vlachos, "Microreactor dynamics", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
121. K. Mayawala, D. G. Vlachos, and J. S. Edwards, "Surface Dynamics of Epidermal Growth Factor Receptors: Study of Ligand Binding and Oligomerization Events", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
122. V. Nikolakis, D. G. Vlachos, S. Caratzoulas, and M. Tsapatsis, 'Complexation of tetrapropylammonium cation on silicalite-1 surface. Model development, experimental validation and crystal growth related predictions", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
123. D. G. Norton and D. G. Vlachos, "The Design and Development of Hydrocarbon Fueled Catalytic Microburners", AIChE meeting, Austin, TX, Nov. 7-12, 2004.

124. A. Chatterjee, M. A. Katsoulakis, and D. G. Vlachos, "Adaptive Coarse-Grained Monte Carlo Methods: A Novel Multiscale Stochastic Simulation for Large Length and Time Scales", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
125. J. M. Fedeyko, D. G. Vlachos, and R. F. Lobo, "A New Class of Self-Assembled Organic-Silica Nanoparticles", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
126. J. D. Rimer, D. G. Vlachos, and R. F. Lobo, "The Role of Self-Assembled Silica-Tetrapropylammonium Nanoparticles in the Growth of Silicalite-1 Crystals", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
127. A. Chatterjee, M. A. Katsoulakis, and D. G. Vlachos, "Time Acceleration of Spatially Homogeneous and Distributed Kinetic Monte Carlo Simulations", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
128. A. Chatterjee, M. A. Katsoulakis, and D. G. Vlachos, "Hierarchical Continuum/Stochastic Simulations for Pattern Formation of Nanomaterials", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
129. K. Mayawala, D. G. Vlachos, and J. S. Edwards, "Superagonistic Activation of Epidermal Growth Factor Receptor (EGFR) by EGF-related Growth Factors: An In-silico Study", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
130. A. Chatterjee, M. A. Katsoulakis, and D. G. Vlachos, "Optimally designed spatially adaptive kinetic Monte Carlo simulations: Nonlinear behavior on catalytic surfaces", AIChE meeting, Austin, TX, Nov. 7-12, 2004.
131. J. M. Fedeyko, D. G. Vlachos, and R. F. Lobo, "A New Class of Self-Assembled Organic-Silica Nanoparticles", 78<sup>TH</sup> ACS Colloid and Surface Science Symposium, New Haven, CT (2004).
132. J. D. Rimer, D. G. Vlachos, and R. F. Lobo, "The Role of Self-Assembled Silica-Tetrapropylammonium Nanoparticles in the Growth of Silicalite-1 Crystals", 78<sup>TH</sup> ACS Colloid and Surface Science Symposium, New Haven, CT (2004).
133. A. B. Mhadeshwar and D. G. Vlachos, "Molecular modeling of water-gas shift and preferential oxidation of CO reactions", ISCRE 18<sup>th</sup> meeting, Chicago, IL, June 6-9, 2004.
134. D. G. Norton and D. G. Vlachos, "Hydrogen assisted self-ignition of propane/air mixtures in catalytic microburners", *Proc. Combust. Inst.*, Chicago, IL, July 25-30, 2004.
135. ACS meeting talks of Rimer and Fedeyko
136. "Structural evolution of silica-tetrapropylammonium nanoparticles in the synthesis of silicalite-1", 229<sup>th</sup> ACS National Meeting, San Diego, CA, March 13-17, 2005.
137. D. G. Norton, E. D. Wetzel, and D. G. Vlachos, "Catalytic Microcombustion For Portable Power Generation", Army Science Conference, FL, 2004.
138. J. D. Rimer, R. F. Lobo, and D. G. Vlachos, "Growth Mechanisms of High-Silica Zeolites", 14<sup>th</sup> International Zeolite Conference, Cape Town, South Africa (2004).
139. Cape Town, South Africa meeting papers (2)
140. M. A. Snyder and D. G. Vlachos, "Mesoscopic modeling of transport through polycrystalline microporous membranes," 8<sup>th</sup> International Conference in Inorganic Membranes, Cincinnati, Ohio, July 18-22, 2004.
141. M. A. Snyder and D. G. Vlachos, "Mesoscopic modeling of transport through polycrystalline microporous membranes", 3<sup>rd</sup> Intl. Zeolite Membrane Meeting (IZZ), Breckenridge, CO, July 25-28, 2004.
142. M. A. Snyder, Z. Lai, M. Tsapatsis, and D. G. Vlachos, "Quantitative characterization of grain boundaries and defects within microporous zeolite membranes and their effect upon transport properties", 3<sup>rd</sup> Intl. Zeolite Membrane Meeting (IZZ), Breckenridge, CO, July 25-28, 2004.
143. J. M. Fedeyko, D. G. Vlachos, and R. F. Lobo, "Structure Determination of Subcolloidal Zeolite Nanoparticle Precursors", American Conference on Neutron Scattering, College Park, MD (2004).
144. J. D. Rimer, R. F. Lobo, and D. G. Vlachos, "Silica Nanoparticle Formation and Evolution in the Synthesis of All-Silica Zeolites", 19<sup>th</sup> North American Catalysis Society Meeting, Philadelphia, PA, May 22-27 (2005).
145. R. F. Lobo, J. M. Fedeyko, J. D. Rimer, and D. G. Vlachos, "Self-assembly of Silica Nanoparticles in Basic Solutions of Tetraalkylammonium Cations", 229<sup>th</sup> American Chemical Society Annual Meeting, San Diego, CA, (2005).
146. J. D. Rimer, J. M. Fedeyko, R. F. Lobo and D. G. Vlachos, "Structural Evolution of Silica-Tetrapropylammonium Nanoparticles in the Synthesis of Silicalite-1", 229<sup>th</sup> American Chemical Society Annual Meeting, San Diego, CA, (2005).
147. S. Deshmukh and D. G. Vlachos, "Design Principles of Multifunctional Microdevices", Microreaction Technology (IMRET8), Spring AIChE meeting, Atlanta, GA, April 10-24, 2005.
148. S. Deshmukh and D. G. Vlachos, "Mixing in Structured Microchemical Devices", Microreaction Technology (IMRET8), Spring AIChE meeting, Atlanta, GA, April 10-24, 2005.



149. S. Deshmukh, A. Mhadeshwar, and D. G. Vlachos, "Hydrogen Production from Ammonia Decomposition: Hierarchical, Multiscale Microkinetic Modeling and Microreactor Simulation", Microreaction Technology (IMRET8), Spring AIChE meeting, Atlanta, GA, April 10-24, 2005.
150. A. Benderly, A. Gaffney, N. Chadda, J. Lampert, W. Ruettinger, D. G. Vlachos, "Millisecond Oxidation of Alkanes", Spring AIChE meeting, Atlanta, GA, April 10-24, 2005.
151. "Silica Nanoparticle Formation and Evolution in the Synthesis of All-Silica Zeolites", in the "Nanotechnology as applied to catalysis" session, 19th North American Catalysis Society Meeting, Philadelphia, PA (2005).
152. D. G. Norton, S. R. Deshmukh, E. Wetzel, and D. G. Vlachos, 'Design concepts of portable fuel processing devices', EuropaCat-VII, Sofia, Bulgaria, Aug. 28 – Sept. 1, 2005.
153. B. J. Feist, J. Lauterbach, and D. G. Vlachos, 'High-throughput experimentation and microkinetic modeling of ammonia decomposition on Ru supported catalysts', EuropaCat-VII, Sofia, Bulgaria, Aug. 28 – Sept. 1, 2005.
154. J. Ludwig and D. G. Vlachos, 'Prediction of sticking coefficients for use in microkinetic models using density functional theory and classical molecular dynamics: H<sub>2</sub>/Pt(111)', EuropaCat-VII, Sofia, Bulgaria, Aug. 28 – Sept. 1, 2005.
155. A. B. Mhadeshwar and D. G. Vlachos, 'Hierarchical multiscale modeling of chemical kinetics: Water-gas shift and preferential oxidation of CO on noble metals', EuropaCat-VII, Sofia, Bulgaria, Aug. 28 – Sept. 1, 2005.
156. D. G. Vlachos, 'An Introduction to Multiscale Analysis', in Tutorial of Multiscale Topical Conference, AIChE meeting, Cincinnati, OH, Oct. 30-Nov. 4, 2005.
157. D. G. Vlachos, 'Multiscale Methods for Stochastic Simulation', in Tutorial of Multiscale Topical Conference, AIChE meeting, Cincinnati, OH, Oct. 30-Nov. 4, 2005.
158. M. A. Snyder and D. G. Vlachos, 'Multiscale Modeling for Bridging Disparate Scales of Diffusion in Polycrystalline Microporous Membranes', AIChE meeting, Cincinnati, OH, Oct. 30-Nov. 4, 2005.
159. N. Kaisare, S. Deshmukh, and D. G. Vlachos, 'On the Stability of Micro-Scale Heat Sources', AIChE meeting, Cincinnati, OH, Oct. 30-Nov. 4, 2005.
160. A. Chatterjee, D. G. Vlachos, 'Hierarchical Multiscale Stochastic Simulations', AIChE meeting, Cincinnati, OH, Oct. 30-Nov. 4, 2005.
161. M. A. Snyder, D. G. Vlachos, Z. Lai, M. Tsapatsis, V. Nikolakis, 'Non-Destructive, Quantitative Characterization of Microporous Thin Film Polycrystallinity for Elucidating Structure-Properties Relations', AIChE meeting, Cincinnati, OH, Oct. 30-Nov. 4, 2005.
162. A. B. Mhadeshwar and D. G. Vlachos, 'Methane Oxidation on Noble Metals for Hydrogen Production: a Hierarchical, Multiscale Microkinetic Modeling Approach', AIChE meeting, Cincinnati, OH, Oct. 30-Nov. 4, 2005.
163. Z. Zheng, V. Gulians, Y.S. Lin, M. A. Snyder, and D. G. Vlachos, 'Synthesis and Gas Permeation Properties of Sodalite Membranes', AIChE meeting, Cincinnati, OH, Oct. 30-Nov. 4, 2005.
164. S. Deshmukh, A. Chatterjee, and D. G. Vlachos, 'Multiscale Modeling of Catalytic Activity: from Single Crystals to Defected and Polycrystalline Materials', AIChE meeting, Cincinnati, OH, Oct. 30-Nov. 4, 2005.
165. S. Deshmukh, N. Kaisare, and D. G. Vlachos, 'Hierarchical Modeling of Integrated Microdevices for Hydrogen Production', AIChE meeting, Cincinnati, OH, Oct. 30-Nov. 4, 2005.
166. K. Mayawala, D. G. Vlachos, and J. S. Edwards, 'Implications of Spatial Organization of Epidermal Growth Factor Receptors', AIChE meeting, Cincinnati, OH, Oct. 30-Nov. 4, 2005.
167. J. D. Rimer, R. F. Lobo, and D. G. Vlachos, 'Physical Basis for the Formation and Stability of Silica Nanoparticles in Basic Solutions of Monovalent Cations', AIChE meeting, Cincinnati, OH, Oct. 30-Nov. 4, 2005.
168. S. Caratzoulas, D. G. Vlachos, and M. Tsapatsis, 'Molecular Dynamics Studies on the Stability of Cage-like Polysilicate Ions in TMA Aqueous Solution', AIChE meeting, Cincinnati, OH, Oct. 30-Nov. 4, 2005.
169. A. Samant, A. Chatterjee, and D. G. Vlachos, 'Multiscale Stochastic Simulations of the Mitogen Activated Protein (MAP) Kinase Cascade', AIChE meeting, Cincinnati, OH, Oct. 30-Nov. 4, 2005.
170. J. M. Fedeyko, R. F. Lobo, and D. G. Vlachos, 'Self-assembly of aluminosilicate solutions: The role of nanoparticles in zeolite synthesis', ACS meeting, Atlanta, GA, March 26-30, 2006.
171. J. Rimer, D. Roth, R. Lobo and D. G. Vlachos, Self-assembly and Role of Silica Nanoparticles in the Nucleation and Growth of Silicalite-1, CECAM workshop on 'Computational aspects of building blocks, nucleation, and synthesis of porous materials', Lyon, France, Aug. 29-31, 2006.
172. A. Chatterjee and D. G. Vlachos, 'Systems tasks in nanotechnology via hierarchical multiscale modeling: Nanopattern formation in heteroepitaxy' (final paper number 96), 232nd ACS National Meeting, San Francisco, CA, September 10-14, 2006.
173. N. S. Kaisare and D. G. Vlachos, Extending the Region of Stable Homogeneous Micro-Combustion through Forced Unsteady Operation, Symp. Int. Comb., Heidelberg, Germany, Aug. 2006.

174. N. S. Kaisare and D. G. Vlachos, 'Stability limits of homogeneous combustion in a reverse-flow microreactor,' IMRET meeting, Postdam, Germany, Sept. 6-8, 2006.
175. D. G. Vlachos, Temporal Coarse-Graining of Lattice Kinetic Monte Carlo Simulations, AIChE meeting, San Francisco, CA, Nov. 12-17, 2006.
176. Chatterjee and D. G. Vlachos, Generation of Kinetic "Phase Diagrams" for Self-Assembled Nanopattern Formation in Heteroepitaxy Via Hierarchical Multiscale Modeling, AIChE meeting, San Francisco, CA, Nov. 12-17, 2006.
177. N. Kaisare, S. Deshmukh, D. G. Vlachos, Effect of Combustion Mode on Performance and Startup of Microburners, AIChE meeting, San Francisco, CA, Nov. 12-17, 2006.
178. D. G. Vlachos, Multiscale Model-Based Design of Experiments and Catalysts, AIChE meeting, San Francisco, CA, Nov. 12-17, 2006.
179. K. Mayawala, D. G. Vlachos, and J. S. Edwards, Spatial Organization of EGF Receptors and Its Implications for Signaling, AIChE meeting, San Francisco, CA, Nov. 12-17, 2006.
180. A. Samant, D. G. Vlachos, and B. A. Ogunnaike, Hybrid, Multiscale Algorithm for Simulating Stochastic Systems, AIChE meeting, San Francisco, CA, Nov. 12-17, 2006.
181. V. Papavassiliou, P. Pacouloute, R. Drnevich, D. G. Vlachos, J. Hemmings, L. Bonnell, Catalytic Hot Oxygen Reactor, AIChE meeting, San Francisco, CA, Nov. 12-17, 2006.
182. J. A. Federici, N. Kaisare, D. G. Vlachos, Enhancing Microburner Stability for Portable Power through Heat Recuperation, AIChE meeting, San Francisco, CA, Nov. 12-17, 2006.
183. J. A. Federici, D. G. Norton, E. D. Wetzel, and D. G. Vlachos, Catalytic Microcombustors with Integrated Thermoelectric Elements for Portable Power Production, AIChE meeting, San Francisco, CA, Nov. 12-17, 2006.
184. J. J. Ludwig and D. G. Vlachos, Molecular Dynamics Simulations of the Dissociation of Hydrogen on Single Crystal Surfaces Using Neural Networks, AIChE meeting, San Francisco, CA, Nov. 12-17, 2006.
185. A.-M. S. Niehaus, D. G. Vlachos, and J. S. Edwards, Microscopic and Coarse Grained Stochastic Simulation of Epidermal Growth Factor Receptor Diffusion on Corralled Membrane Surfaces, AIChE meeting, San Francisco, CA, Nov. 12-17, 2006.
- R. F. Lobo, J. M. Fedeyko, D. G. Vlachos, J. D. Rimer, Mechanistic Links between Mesoporous and Microporous Silicate Synthesis, AIChE meeting, San Francisco, CA, Nov. 12-17, 2006.
187. K. Mayawala, A.-M. S. Niehaus, D. G. Vlachos, J. S. Edwards, Multiscale Stochastic Simulations for Systems Biology Modeling: Implications of Spatial Organization of EGF Receptor, MACKiE II meeting, Houston, Feb. 7 & 8, 2007.
188. A. Chatterjee and D. G. Vlachos, Systems Tasks in Nanotechnology via Hierarchical Multiscale Modeling: Nanopattern Formation in Heteroepitaxy, MACKiE II meeting, Houston, Feb. 7 & 8, 2007.
189. D. G. Vlachos, Multiscale simulations of nucleation and growth in porous media, meeting, MACKiE II meeting, Houston, Feb. 7 & 8, 2007.
190. D. G. Vlachos, A. Mhadeshwar, and N. Kaisare, Microkinetic modeling: Hierarchical multiscale model development and use, NASCRE II meeting, Houston, Feb. 4-7, 2007.
191. N. S. Kaisare and D. G. Vlachos, Optimization of Heat Recuperating Reactor Strategies for Autothermal Fuel Reforming to Hydrogen, North American Catalysis Meeting, Houston, June 17-22, 2007.
192. V. Prasad, A. Karim, N. S. Kaisare, D. Hansgen, and D. G. Vlachos, A Unified Modeling Framework for Design of Multi-Site Catalysts: Application to NH<sub>3</sub> Decomposition for H<sub>2</sub> Production, North American Catalysis Meeting, Houston, June 17-22, 2007.
193. E. D'Addio, R. Vijay, J. Binz, W. D. Pyrz, D. G. Vlachos, D. J. Buttrey, J. Lauterbach, K-Promoted Ru Catalysts for Ammonia Decomposition Discovered Using High-Throughput Experimentation, AIChE meeting, Salt Lake City, Utah, Nov. 4-9, 2007.
194. W. D. Pyrz, R. Vijay, J. Binz, D. G. Vlachos, J. Lauterbach, D. Buttrey, Characterization of K-Promoted Ru Catalysts for Hydrogen Production Via Ammonia Decomposition, AIChE meeting, Salt Lake City, Utah, Nov. 4-9, 2007.
195. V. Prasad and D. G. Vlachos, Hierarchical Multiscale Model-Based Design of Experiments: Application to Catalytic Systems for Portable and Distributed Energy Generation, AIChE meeting, Salt Lake City, Utah, Nov. 4-9, 2007.
196. M. Maestri, D. G. Vlachos, A. Beretta, G. Groppi and E. Tronconi, Insights into the CH<sub>4</sub> partial oxidation on Rh: a microkinetic perspective, 14<sup>th</sup> Int. Congress on Catalysis, Seoul, Korea, July 13-18, 2008
197. M. Maestri, D. G. Vlachos, A. Beretta, G. Groppi, E. Tronconi, Insights into the CH<sub>4</sub> partial oxidation on Rh: A microkinetic perspective, Rideal Conference, March 17-19, Cambridge, UK, 2008

198. M. Maestri, D. G. Vlachos, A. Beretta, G. Groppi, E. Tronconi, Insights into the CH<sub>4</sub> partial oxidation on Rh: A microkinetic perspective, 235<sup>th</sup> American Chemical Society National Meeting, April 6-10, New Orleans, LA, 2008
199. S. Caratzoulas and D. G. Vlachos, Molecular insights into nucleation and growth of zeolitic materials, 235<sup>th</sup> ACS National Meeting, New Orleans, LA, April 6-10, 2008
200. G. Mpourmpakis and D. G. Vlachos, Understanding the silver nanoparticle growth via first principle methods, 235<sup>th</sup> ACS National Meeting, New Orleans, LA, April 6-10, 2008
201. G. D. Stefanidis and D. G. Vlachos, Manipulating Homogeneous Chemistry in Catalytic Microreactors: Operation Strategies and Design Principles, IMRET 10<sup>th</sup> Meeting, New Orleans, LA, April 6-10, 2008
202. G. D. Stefanidis, N. Kaisare, and D. G. Vlachos, Ignition Strategies for Catalytic Microdevices, IMRET 10<sup>th</sup> Meeting, New Orleans, LA, April 6-10, 2008
203. G. D. Stefanidis, N. Kaisare, and D. G. Vlachos, Design Principles of Multifunctional Microdevices for Hydrogen Production Via Short Contact Time Steam Reforming, IMRET 10<sup>th</sup> Meeting, New Orleans, LA, April 6-10, 2008
204. Maestri et al., C1 microkinetic model for methane conversion to syngas on Rh", IWCC7 web site (<http://iwcc7.web.psi.ch/>), 2008
205. A. Chatterjee and D. G. Vlachos, Control of self-assembled nanoparticle array structures in heteroepitaxy, Cetrato, Italy, 5<sup>th</sup> Chemical Engineering Conference for Collaborative Research in the Eastern Mediterranean Countries, May 25-29, 2008
206. V. Prasad, A. M. Karim, Z. Ulissi, M. Zagrobelny, and D. G. Vlachos, HIGH throughput multiscale modeling for design of experiments, catalysts, and reactors: application to hydrogen production from ammonia, ISCRE 20<sup>th</sup> meeting, Kyoto, Japan, September 7-10, 2008
207. D. G. Vlachos, Multiscale Simulation for Scale-up of Nanotechnological Processes: Symbiosis of Traditional and Modern Tools, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
208. J. A. Federici and D. G. Vlachos, Design and Testing of Microreactors for Kinetic Experiments of Catalytic Oxidation of Small Alkanes Over Platinum, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
209. G. Mpourmpakis and D. G. Vlachos, Understanding the Silver Nanoparticle Growth Via First Principle Methods, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
210. Y. Chen and D. G. Vlachos, Insights into Partial Oxidation and Reforming of Ethane on Pt: Density Functional Theory, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008.
211. G. Mpourmpakis and D. G. Vlachos, First Principle Calculations of Supported Catalysts: CO Binding on MgO Supported Gold Clusters and Nanoparticles, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
212. J. Synowczynski, J. Andzelm, and D. G. Vlachos, DFT Study of the Dissociation of H<sub>2</sub>O and H<sub>2</sub> on Al<sub>2</sub>O<sub>3</sub> Supported Pt Clusters, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
213. D. A. Hansgen, J. G. Chen, D. G. Vlachos, Theoretical and Experimental Studies of Hydrogen Production from Ammonia Decomposition, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
214. G. D. Stefanidis, N. S. Kaisare, and D. G. Vlachos, Ignition Strategies for Catalytic Microdevices, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
215. S. D. Collins, A. Chatterjee, and D. G. Vlachos, Coarse-Grained Kinetic Monte Carlo Models: Applications to Membrane Receptor Dimerization, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
216. M. N. Costa, D. G. Vlachos, and J. S. Edwards, Stochastic Spatial and Non-Spatial Simulations of the Erbb Signaling Pathways Demonstrate the Importance of Spatial Organization In Signal Transduction, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
217. J. A. Federici, E. D. Wetzel, B. R. Geil, and D. G. Vlachos, Heat Recirculation Microreactors in Gas-Phase and Catalytic Reactions, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
218. J. D. Rimer, A. Navrotsky, D. G. Vlachos, and R. F. Lobo, Microporous Silicate Nucleation and Growth: Mechanistic Investigations toward Rational Design of Nanocrystalline Materials, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
219. K. Al-Majnouni, N. D. Hould, D. G. Vlachos, and R. F. Lobo, Crystallization of Mordenite from a Clear Solution, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
220. G. D. Stefanidis, N. S. Kaisare, M. Maestri, and D. G. Vlachos, Design Principles of Multifunctional Microdevices for Hydrogen Production Via Short Contact Time Steam Reforming, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
221. V. Prasad, Z. W. Ulissi, M. A. Zagrobelny, and D. G. Vlachos, Optimal Design of Catalysts Via Multiscale Modeling: Application to Hydrogen Production Reactions, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008

222. M. Maestri, E. Tronconi, G. Groppi, A. Beretta, and D. G. Vlachos, Steam and Dry Reforming and Partial Oxidation of Methane on Rh. A Comprehensive Kinetics Study, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
223. W. W. Lonergan, J. G. Chen, and D. G. Vlachos, Structure-Property Relationships of Supported Pt-Ni Bimetallic Catalysts, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
224. S. D. Collins, A. Chatterjee, and D. G. Vlachos, Multiscale Monte Carlo Study of Epidermal Growth Factor Receptor Diffusion and Dimerization, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
225. S. D. Collins, A. Chatterjee, and D. G. Vlachos, Coarse-Grained Kinetic Monte Carlo Models: Complex Lattices, Multicomponent Systems, and Homogenization at the Stochastic Level, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
226. N. O. Hanes, D. G. Vlachos, and J. A. Federici, Atomization, Ignition, and Sustained Catalytic Combustion of Liquid Fuels, AIChE meeting, Philadelphia, PA, Nov. 16-21, 2008
227. J. Synowczynski, J. Andzelm and D. G. Vlachos, Quantum Modeling of H<sub>2</sub> and H<sub>2</sub>O Chemistry on Pt/ $\alpha$ -Al<sub>2</sub>O<sub>3</sub>, Computational Catalysis III: Oxides and Oxide-Supported Transition Metals, AIChE meeting, Nashville, TN, Nov. 7-13, 2009
228. K. Al-majnouni and D. G. Vlachos, High Temperature Decomposition and Reactivity of Bronsted Acid Sites in Zeolites, Catalysis with Microporous and Mesoporous Materials I, AIChE meeting, Nashville, TN, Nov. 7-13, 2009
229. M. S. Mettler, G. D. Stefanidis and D. G. Vlachos, Scale-out of Microreactor Stacks for Syngas Production from Methane, Microreaction Engineering I, AIChE meeting, Nashville, TN, Nov. 7-13, 2009
230. G. D. Stefanidis and D. G. Vlachos, High vs. Low Temperature Reforming for Hydrogen Production via Microtechnology, Microreaction Engineering I, AIChE meeting, Nashville, TN, Nov. 7-13, 2009
231. Y. Chen, M. Saliccioli and D. G. Vlachos, Dehydrogenation, Hydrogenolysis and Oxidation of Ethane on Pt: Density Functional Theory Study and Microkinetic Analysis, Computational Catalysis II: Transition Metals, AIChE meeting, Nashville, TN, Nov. 7-13, 2009
232. M. Saliccioli and D. G. Vlachos, Microkinetic Modeling of Polyol Thermal Decomposition and Reforming on Platinum, Reaction Path Analysis I, AIChE meeting, Nashville, TN, Nov. 7-13, 2009
233. G. Mpourmpakis and D. G. Vlachos, Charging of Metal Oxide Supported Au Clusters and its Effect on the CO Oxidation Reaction, Computational Catalysis III: Oxides and Oxide-Supported Transition Metals, AIChE meeting, Nashville, TN, Nov. 7-13, 2009
234. D. A. Hansgen, J. G. Chen and D. G. Vlachos, Computational and Experimental Studies of a Ni/Pt Bimetallic Catalyst for H<sub>2</sub> Production, Rational Catalyst Design III, AIChE meeting, Nashville, TN, Nov. 7-13, 2009
- Catalysis and Reaction Engineering Student Award***
235. W. W. Lonergan, D. G. Vlachos and J. G. Chen, Structure-Property Relationships of Supported Pt/Ni Bimetallic Catalysts, Fundamentals of Supported Catalysis I, AIChE meeting, Nashville, TN, Nov. 7-13, 2009
236. W. W. Lonergan, D. G. Vlachos, J. G. Chen, Structure-Property Relationships of Supported Pt/3d Bimetallic Catalysts, Poster Session, New York Catalysis Society Spring Symposium, Bethlehem, PA, Mar. 17, 2010.
237. W. W. Lonergan, D. G. Vlachos, J. G. Chen, Structure-Property Relationships of Supported Pt/3d Bimetallic Catalysts, Poster Session, Catalysis Club of Philadelphia, Claymont, DE, Mar. 18, 2010.
238. W. W. Lonergan, D. G. Vlachos, J. G. Chen, Structure-Property Relationships of Supported Pt/3d Bimetallic Catalysts, Poster Session, Gordon Research Conference: Catalysis, New London, NH, Jun. 29, 2010.
239. W. W. Lonergan, D. G. Vlachos, J. G. Chen, Structure-Property Relationships of Supported Pt/3d Bimetallic Catalysts, New York Catalysis Society Meeting, Somerset, NJ, Sept. 15, 2010.
240. D. A. Hansgen, J. G. Chen and D. G. Vlachos, First Principles Based Bimetallic Catalyst Prediction for the Ammonia Decomposition Reaction, AIChE Meeting, Salt Lake City, UT, Nov. 7-12, 2010.
241. S. Caratzoulas and D. G. Vlachos, First Principles Based Bimetallic Catalyst Prediction for the Ammonia Decomposition Reaction, AIChE Meeting, Salt Lake City, UT, Nov. 7-12, 2010.
242. M. Saliccioli and D. G. Vlachos, Microkinetic Modeling of Ethylene Glycol Decomposition On Pt and Ni-Pt Bimetallic Catalysts, AIChE Meeting, Salt Lake City, UT, Nov. 7-12, 2010.
- Catalysis and Reaction Engineering Student Award***
243. M. S. Mettler, G. D. Stefanidis and D. G. Vlachos, Stability and Performance of Microreactor Stacks for Coupling of Exothermic and Endothermic Reactions, AIChE Meeting, Salt Lake City, UT, Nov. 7-12, 2010.
244. W. W. Lonergan, D. G. Vlachos and J. G. Chen, Structure Property Relationships of Supported Pt/Ni Bimetallic Catalysts: Correlating Pt-Ni Bimetallic Bond Formation to Catalytic Activity, AIChE Meeting, Salt Lake City, UT, Nov. 7-12, 2010.
245. N. M. Abukhdeir and D. G. Vlachos, Hierarchical Multi-Scale Modeling of Surface Pattern Formation Resulting from Complex Particle-Particle Interactions, AIChE Meeting, Salt Lake City, UT, Nov. 7-12, 2010.

246. N. M. Abukhdeir and D. G. Vlachos, Accelerated Simulation of Surface Pattern-Forming Systems Via Hierarchical Multi-Scale and Mesoscopic Modeling, AIChE Meeting, Salt Lake City, UT, Nov. 7-12, 2010.
247. M. Saliccioli and D. G. Vlachos, Microkinetic Modeling of Catalytic Reforming of Oxygenated Hydrocarbons, AIChE Meeting, Salt Lake City, UT, Nov. 7-12, 2010.
248. M. Stamatakis and D. G. Vlachos, Reduction of Stochastic on-Lattice Chemical Kinetics Models to Well-Mixed Descriptions via Singular Perturbation, AIChE Meeting, Salt Lake City, UT, Nov. 7-12, 2010.
249. M. Stamatakis and D. G. Vlachos, Structural Sensitivity of the Water Gas Shift Reaction on Platinum Surfaces, AIChE Meeting, Salt Lake City, UT, Nov. 7-12, 2010.
250. M. Saliccioli and D. G. Vlachos, Kinetic modeling of catalytic reforming of oxygenates on platinum based catalysts, Pacificchem meeting, Honolulu, Hawaii, December 15-20, 2010.
251. M. Stamatakis, Y. Chen and D. G. Vlachos, Structural Sensitivity of the Water-Gas Shift Reaction on Platinum Surfaces, 22nd North American Catalysis Society Meeting, Detroit, MI, June 5-10, 2011.
252. M. Saliccioli, D. G. Vlachos, Rational Catalyst Design for Reforming of Ethylene Glycol to Syngas, 22nd North American Catalysis Society Meeting, Detroit, MI, June 5-10, 2011.
253. Y. Chen, M. Saliccioli and D. G. Vlachos, Hierarchical Mechanism Development for Complex Reaction Networks of Biomass: Conversion of glycerol to synthesis gas over Platinum, 22nd North American Catalysis Society Meeting, Detroit, MI, June 5-10, 2011.
254. S. Caratzoulas and D. G. Vlachos, A theoretical study of two dehydration reactions in water: fructose to 5-hydroxymethylfurfural and glycerol to acrolein, 22nd North American Catalysis Society Meeting, Detroit, MI, June 5-10, 2011.
255. D. G. Vlachos, Mechanistic insights into the conversion of biomass derivatives to renewable fuels and chemicals, EuropaCat X, Glasgow, Scotland, August 28-September 2, 2011.
256. M. S. Mettler, D. G. Vlachos and P. J. Dauenhauer, A Novel Experimental Technique for Study of Isothermal Pyrolysis of Cellulose, AIChE Meeting, Minneapolis, MN, October 17-21, 2011.
257. S. A. Tupy, T. Vispute, G. W. Huber, J. G. Chen and D. G. Vlachos, Catalytic Studies of Reforming of Oxygenates, AIChE Meeting, Minneapolis, MN, October 17-21, 2011.
258. S. H. Mushrif, N. Nikbin, S. Caratzoulas, V. Choudhary, S. I. Sandler, V. Nikolakis and D. G. Vlachos, Molecular Investigation of Catalytic Isomerization of Glucose to Fructose, AIChE Meeting, Minneapolis, MN, October 17-21, 2011.
259. M. Stamatakis and D. G. Vlachos, Investigation of Structure Sensitivity for the CO Oxidation Chemistry On Pt and Au, AIChE Meeting, Minneapolis, MN, October 17-21, 2011.
260. V. Choudhary, D. G. Vlachos and S. I. Sandler, Reaction Free Energies in Solutions for Glucose Conversion into Biomass Intermediates, AIChE Meeting, Minneapolis, MN, October 17-21, 2011.
261. J. McGill, N. M. Abukhdeir, B. A. Ogunnaike and D. G. Vlachos, Optimization and Control of Heteroepitaxial Surface Morphologies, AIChE Meeting, Minneapolis, MN, October 17-21, 2011.
262. R. Xiong, D. G. Vlachos and S. I. Sandler, Molecular Screening of Alcohol Adsorption onto Zeolite from Aqueous Solution, AIChE Meeting, Minneapolis, MN, October 17-21, 2011.
263. V. Nikolakis, T. Courtney, S. Caratzoulas, R. F. Lobo, J. G. Chen and D. G. Vlachos, Investigation of Liquid Phase 1,2-Propanediol Dehydration Using Zeolite Catalysts, AIChE Meeting, Minneapolis, MN, October 17-21, 2011.
264. S. H. Mushrif, S. Caratzoulas and D. G. Vlachos, Understanding Solvent Effects In the Selective Conversion of Fructose to HMF: A Molecular Dynamics Investigation, AIChE Meeting, Minneapolis, MN, October 17-21, 2011.
265. T. Courtney, G. Mpourmpakis, J. G. Chen, D. G. Vlachos and S. Caratzoulas, Ab-Initio Study of Glycerol Dehydration Mechanisms with Explicit Solvent Treatment, AIChE Meeting, Minneapolis, MN, October 17-21, 2011.
266. M. S. Mettler, D. G. Vlachos and P. J. Dauenhauer, Condensed-Phase Cellulose Pyrolysis, Poster Session of CRE Division, AIChE Meeting, Minneapolis, MN, October 17-21, 2011.
267. M. Saliccioli and D. G. Vlachos, Rational Catalyst Design for Oxygenate Reforming, AIChE Meeting, Minneapolis, MN, October 17-21, 2011.
268. N. M. Abukhdeir and D. G. Vlachos. Nano-scale surface pattern evolution in heteroepitaxial bimetallic films. Materials Research Society Fall Meeting, Nov 2011, Boston, MA, USA, November 2011, (poster presentation).
269. A. M. Karim, S. Tupy, L. Zhang, D. L. King, D. G. Vlachos, G. Mpourmpakis, J. G. Chen, and Y. Wang, H<sub>2</sub> Production by Aqueous Phase Reforming of Bio-liquids: Correlating the Catalytic Activity and Selectivity to the Local Coordination and Electronic Structure of Pt and PtNi, Operando-IV Conference, Upton, NY, April 29-May 3, 2012.

270. V. Choudhary, A. B. Pinar, S. Caratzoulas, S. I. Sandler, D. G. Vlachos, and R. F. Lobo, Xylose Conversion to Furfural in a Cascade of Reactions Using Lewis and Brønsted Acid Catalysts in Aqueous Media, Gordon Research Conference on Catalysis, New London, NH, June 1, 2012.
271. V. Choudhary, S. Caratzoulas, A. B. Pinar, S. I. Sandler, D. G. Vlachos, and R. F. Lobo, Xylose Conversion to Furfural using Lewis and Brønsted Acid Catalysts in Aqueous Media, 244th ACS National Meeting, Philadelphia, PA, August 19-23, 2012.
272. M. A. Christiansen, D. G. Vlachos, Predictive Microkinetic Modeling of Pt-Catalyzed Ethylene Glycol Steam Reforming, 244th ACS National Meeting, Philadelphia, PA, August 19-23, 2012.
273. R. C. Catapan, A. A. M. Oliveira, M. Stamatakis, Y. Chen, M. A. Christiansen, D. G. Vlachos, First-principles-based Multiscale Modeling of the Water-gas Shift Reaction on Platinum and Nickel Surfaces, 244th ACS National Meeting, Philadelphia, PA, August 19-23, 2012.
274. J. S. Kruger, M. Leon-Garcia, V. Nikolakis, D. G. Vlachos, Aqueous-Phase Fructose Dehydration Using Zeolite Catalysts, 244th ACS National Meeting, Philadelphia, PA, August 19-23, 2012.
275. J. E. Sutton and D. G. Vlachos, Mechanistic Insights into Ethanol Steam Reforming on Pt(111) via Microkinetic Modeling, 244th ACS National Meeting, Philadelphia, PA, August 19-23, 2012.
276. J. E. Sutton and D. G. Vlachos, Error Distributions in Semi-Empirical Methods for Estimating Thermochemical and Kinetic Properties, 244th ACS National Meeting, Philadelphia, PA, August 19-23, 2012.
277. D. G. Vlachos, V. Choudhary, A. B. Pinar, V. Nikolakis, S. H. Mushrif, S. Caratzoulas, S. I. Sandler, and R. F. Lobo, Modern Catalytic Technologies for Converting Biomass Derived Sugars to Chemicals: An Overview of the Catalysis Center for Energy Innovation, 244th ACS National Meeting, Philadelphia, PA, August 19-23, 2012.
278. S. Caratzoulas, P. Daoutidis, P. J. Dauenhauer, M. E. Davis, W. Fan, M. Ierapetritou, R. F. Lobo, V. Nikolakis, M. Tsapatsis, D. G. Vlachos, Converting Biomass Feedstocks to Green Plastics, 3rd Annual Biobased Chemicals: Commercialization and Partnering Conference, San Francisco, CA, September 13-14, 2012.
279. M. A. Christiansen, D. G. Vlachos, Predictive Microkinetic Modeling of Pt-Catalyzed Ethylene Glycol Steam Reforming, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
280. J. S. Kruger, M. Leon-Garcia, V. Nikolakis, D. G. Vlachos, Aqueous-Phase Fructose Dehydration Using Zeolite Catalysts, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
281. M. Leon-Garcia, T. D. Swift, V. Nikolakis, D. G. Vlachos, Adsorption in Zeolites of Components Encountered in Hexose Dehydration, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
282. C. L. Williams, C. C. Chang, P. T. Do, N. Nikbin, S. Caratzoulas, D. G. Vlachos, R. F. Lobo, W. Fan, and P. J. Dauenhauer, Catalytic Cycloaddition of Ethylene to Dimethylfuran for the Production of p-Xylene, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
283. C. L. Williams, C. C. Chang, P. T. Do, N. Nikbin, S. Caratzoulas, D. G. Vlachos, R. F. Lobo, W. Fan, and P. J. Dauenhauer, Cycloaddition of Biomass Derived Furans for the Renewable Production of p-Xylene, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
284. G. Mpourmpakis, M. Stamatakis, N. Nikbin, M. A. Christiansen and D. G. Vlachos, Poisoning Mechanisms of MgO-Supported Au Clusters in CO Oxidation, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
285. G. Mpourmpakis, D. G. Vlachos and R. J. Gorte, Developing Relationships for the Lewis-Catalyzed Alcohol Dehydration on Alumina, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
286. N. Nikbin, S. Caratzoulas and D. G. Vlachos, Acid-Catalyzed Conversion of Dimethylfuran to p-Xylene in Catalytic Zeolite-Y. A Combined Computational and Experimental Study, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
287. V. Nikolakis, S. H. Mushrif, S. Caratzoulas, B. Herbert, K. S. Booksh and D. G. Vlachos, Understanding the Solvation of Fructose and 5-hydroxymethylfurfural in Water-dimethyl Sulfoxide Mixtures using Molecular Dynamics and Vibrational Spectroscopy, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
288. J. E. Sutton, P. Panagiotopoulou, X. E. Verykios and D. G. Vlachos, Combined DFT and Microkinetic Modeling Study of Ethanol Steam Reforming on Pt, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
289. J. E. Sutton and D. G. Vlachos, Analysis of Errors in Semi-Empirical Techniques for the Estimation of Microkinetic Model Parameters, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
290. S. H. Mushrif, S. Caratzoulas, V. Choudhary, S. I. Sandler, D. J. Doren and D. G. Vlachos, Modeling the Aldose-Ketose Isomerization by Lewis Acids in the Gas Phase and Aqueous Media. A Detailed Mechanistic Study, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
291. V. Vorotnikov and D. G. Vlachos, Reaction of Sugar Derivatives on Metal Surfaces, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.

292. V. Vorotnikov and D. G. Vlachos, Theoretical Insights into Reactions of Furans on Metal Surfaces, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
293. R. Xiong, S. I. Sandler and D. G. Vlachos, Molecular Screening of Alcohol and Polyol Adsorption onto MFI-Type Zeolites, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
294. P. J. Dauenhauer, R. F. Lobo and D. G. Vlachos, Renewable Catalytic Process for the Production of p-Xylene from Glucose, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
295. A. D. Paulsen, M. S. Mettler, D. G. Vlachos and P. J. Dauenhauer, Pyrolytic Conversion of Biomass to Fuels: Deoxygenation Via Elimination and Cyclization within Molten Cellulose, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
296. A. D. Paulsen, M. S. Mettler, D. G. Vlachos and P. J. Dauenhauer, Revealing Cellulose Pyrolysis Chemistry, AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
297. T. D. Swift, C. Bagia, P. Dornath, V. Nikolakis, W. Fan and D. G. Vlachos, Reactive Adsorption for the Selective Dehydration of Sugars to Furans: Modeling and Experiments, 3rd North American Symposium on Chemical Reaction Engineering (NASCRE-3), Houston, TX, March 17-20, 2013.
298. T. D. Courtney, V. Nikolakis, G. Mpourmpakis, J. G. Chen, and D. G. Vlachos, Effect of Solid-Acid Characteristics on Liquid-Phase Dehydration of Propylene Glycol, Catalysis Society of Metropolitan New York Spring Symposium, Princeton, NJ, March 20, 2013.
299. J. S. Kruger, M. Leon-Garcia, V. Nikolakis and D. G. Vlachos, Elucidating the Roles of Zeolite H-BEA in Aqueous-Phase Fructose Dehydration, Forest Products Laboratory, Madison, WI, April 17, 2013.
300. V. Choudhary, S. H. Mushrif, C. Ho, C. Mackintosh, M. Orella, A. Anderko, V. Nikolakis, N. Marinkovic, A. I. Frenkel, D. G. Vlachos and S. I. Sandler, Transformation of Aldose Sugars to Platform Furans Using CrCl<sub>3</sub> With HCl in Aqueous Media, 23<sup>rd</sup> North American Catalysis Society Meeting, Louisville, KY, June 2-7, 2013.
301. N. Nikbin, S. Caratzoulas and D. G. Vlachos, Theoretical Insights into the Conversion of 2,5-Dimethylfuran and Ethylene to p-Xylene, 23<sup>rd</sup> North American Catalysis Society Meeting, Louisville, KY, June 2-7, 2013.
302. J. E. Sutton and D. G. Vlachos, Error Analysis in Semi-Empirical Methods for Microkinetic Modeling, 23<sup>rd</sup> North American Catalysis Society Meeting, Louisville, KY, June 2-7, 2013.
303. M. A. Christiansen, G. Mpourmpakis and D. G. Vlachos, DFT-based Microkinetic Modeling of Ethanol Dehydration on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, 23<sup>rd</sup> North American Catalysis Society Meeting, Louisville, KY, June 2-7, 2013.
304. V. Vorotnikov and D. G. Vlachos, Theoretical Insights into Reactions of C5 Furans on Metal Surfaces, 23<sup>rd</sup> North American Catalysis Society Meeting, Louisville, KY, June 2-7, 2013.
305. W. Guo, M. Stamatakis and D. G. Vlachos, First-Principles TPD Simulation of Nitrogen Desorption on Ni/Pt(111) Bimetallic Catalyst, 23<sup>rd</sup> North American Catalysis Society Meeting, Louisville, KY, June 2-7, 2013. Poster.
306. A. M. Karim, S. Tupy, J. E. Sutton, M. Gray, H. M. Brown, D. G. Vlachos, J. G. Chen, D. L. King and Y. Wang, Correlating the Aqueous Phase Reforming Activity with the Structure of Pt-M Bimetallic Catalysts, 23<sup>rd</sup> North American Catalysis Society Meeting, Louisville, KY, June 2-7, 2013. Poster.
307. J. S. Kruger, M. Leon-Garcia, V. Nikolakis and D. G. Vlachos, Elucidating the Roles of an H-BEA Zeolite in Aqueous-Phase Fructose Dehydration, Energy Frontier Research Center (EFRC) PI Meeting, Washington, DC, July 18, 2013.
308. J. S. Kruger, M. Leon-Garcia, V. Nikolakis and D. G. Vlachos, Multiple Roles of Zeolites in Fructose Dehydration, Energy Frontier Research Center (EFRC) PI Meeting, Washington, DC, July 18, 2013.
309. W. Yu, M. Saliccioli, M. A. Barteau, D. G. Vlachos and J. G. Chen, First Principles Design of Metal-Modified Molybdenum Carbide Surfaces for Controlling the Activity and Selectivity of Ethylene Glycol Reactions, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
310. N. R. Peela, I. C. Lee, and D. G. Vlachos, Rational Design of Bimetallic Catalysts for Total Oxidation Reactions, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
311. J. S. Kruger, M. Leon-Garcia, V. Nikolakis and D. G. Vlachos, Elucidating the Roles of an H-BEA Zeolite in Aqueous-Phase Fructose Dehydration, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
312. N. R. Peela, I. C. Lee, J. E. Sutton and D. G. Vlachos, Density Functional Theory Based Microkinetic Modeling of Ethane Total Oxidation Over Pt(111), AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
313. N. Rai, S. Caratzoulas and D. G. Vlachos, Understanding the Role of Silanol Groups in Sn-Beta Zeolite for Glucose Isomerization and Epimerization Reactions, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
314. D. G. Vlachos, Multiscale Simulation of Chemical Reactions and Reactors: Combinatorial Complexity, Uncertainty, and Emergent Behavior, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.

315. V. Choudhary, M. León, S. H. Mushrif, C. Ho, A. Anderko, V. Nikolakis, N. Marinkovic, A. I. Frenkel, S. I. Sandler and D. G. Vlachos, Mechanistic Insights in Catalytic Conversion of Sugars to Platform Furan Derivatives, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
316. W. Guo, M. Stamatakis and D. G. Vlachos, Multiscale KMC-DFT Simulation On Bimetallic Catalysts, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
317. M. León, R. Xiong, T. D. Swift, V. Nikolakis, S. I. Sandler and D. G. Vlachos, Adsorption of the Compounds Encountered in Monosaccharide Dehydration in Zeolites, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
318. G. Tsilomelekis, C. Bagia, T. R. Josephson, S. Caratzoulas, V. Nikolakis and D. G. Vlachos, Understanding Solvation Effects on Biomass Derived Platform Chemicals: A Combined Spectroscopic and Theoretical Approach, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
319. J. Jae, W. Zheng, R. F. Lobo and D. G. Vlachos, Production of Dimethylfuran from Hydroxymethylfurfural through Catalytic Transfer Hydrogenation with Ruthenium Supported on Carbon, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
320. T. D. Swift, C. Bagia, V. Nikolakis, D. G. Vlachos, P. Dornath and W. Fan, Reactive Adsorption for the Selective Production of Furans from Carbohydrates, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
321. N. Nikbin, S. Caratzoulas and D. G. Vlachos, Towards Catalyst Design for the Conversion of 2,5-Dimethylfuran to p-Xylene, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
322. R. Xiong, M. León, V. Nikolakis, S. I. Sandler and D. G. Vlachos, Adsorption of 5-Hydroxymethyl-Furfural (HMF) from Liquid Water/Dimethyl Sulfoxide (DMSO) Solutions onto Hydrophobic Zeolites: An Experimental and Simulation Study, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
323. T. D. Swift, C. Bagia, V. Choudhary, V. Nikolakis and D. G. Vlachos, On the Fructose Dehydration Kinetics in Aqueous HCl: An Integrated Experimental and Physics-Based Modeling Approach, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
324. T. D. Swift, C. Bagia, V. Choudhary, G. Peklaris, V. Nikolakis and D. G. Vlachos, An Experimental and Computational Study of Brønsted Acid-catalyzed Fructose Dehydration Kinetics, 247th ACS National Meeting, Dallas, TX, March 16-20, 2014.
325. Ryan Patet, Stavros Caratzoulas and Dionisios G. Vlachos, Modeling the Production of Aromatics from Biomass in Solid Acid Zeolites, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
326. Vinit Choudhary, Liu Yang, George Tsilomelekis, Stavros Caratzoulas, Vladimiro Nikolakis, Stanley I. Sandler and Dionisios G. Vlachos, Mechanistic Insights into Fructose Dehydration to 5-(hydroxymethyl)Furfural, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
327. George Tsilomelekis, Vladimiro Nikolakis and Dionisios G. Vlachos, Unraveling Solvation Effects on 5-Hydroxymethylfurfural Degradation: Insights from Catalytic and Spectroscopic Studies, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
328. Tyler R. Josephson, George Tsilomelekis, Christina Bagia, Stavros Caratzoulas, Vladimiro Nikolakis and Dionisios G. Vlachos, Solvent-Induced Frequency Shifts of 5-Hydroxymethylfurfural and Their Role in Its Stability, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
329. Paul Dauenhauer, Wei Fan, Dionisios Vlachos and Stavros Caratzoulas, Renewable Aromatic Chemicals By Diels-Alder Cycloaddition of Biomass-Derived Furans, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
330. Tim Courtney, Chun-Chih Chang, Wei Fan, Vladimiro Nikolakis, Jinguang G. Chen and Dionisios G. Vlachos, Understanding the Interaction of Water with the Sn Site of Sn-BEA Zeolites and Its Effect on Zeolite Activity, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
331. Vassili Vorotnikov and Dionisios G. Vlachos, Semi-Empirical Thermochemical Property Estimation for Biomass Derivatives on Transition Metal Surfaces, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
332. Dion G. Vlachos, Multiscale Ab Initio Modeling of Catalysts, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
333. Marcel Núñez and Dionisios G. Vlachos, Uncertainty Quantification in Stochastic Multiscale Models of Heterogeneous Catalysis, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
334. Bingjun Xu, Dion G. Vlachos, Paraskevi Panagiotopoulou and Matthew Gilkey, Mechanistic Studies on Hydrodeoxygenation of Furfural to 2-Methyl Furan Via Ring C-H Bond Activations, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
335. Glen Jenness, Matthew A. Christiansen, Stavros Caratzoulas, Dionisios G. Vlachos and Raymond J. Gorte, Site-Dependent Lewis Acidity of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> and Its Impact on Ethanol Dehydration and Etherification, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.



336. Vassili Vorotnikov and Dionisios G. Vlachos, Predictive Modeling for Understanding Biomass Upgrade over Metal Surfaces, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
337. Vinit Choudhary, Andre Bonill, Ana B. Pinar, Samir H. Mushrif, Vladimiro Nikolakis, Nebojsa Marinkovic, Anatoly I. Frenkel, Raul F. Lobo, Stanley I. Sandler and Dionisios G. Vlachos, Fundamental Insights and Similarities Between Homogeneous and Heterogeneous Catalysis in Biomass Conversion, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
338. Alex D. Paulsen, Matthew S. Mettler, Dionisios G. Vlachos and Paul Dauenhauer, Tuning Cellulose Pyrolysis Chemistry: Selective Decarbonylation via Catalyst-Impregnated Pyrolysis, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
339. Alexander V. Mironenko, Glen Jenness, Bingjun Xu and Dionisios G. Vlachos, Selective Hydrodeoxygenation on Ru Based Catalysts for the Conversion of Furfural to Methylfuran, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
340. Geun Ho Gu and Dionisios G. Vlachos, DFT and Microkinetic Modeling of p-Cresol Hydrodeoxygenation on Pt(111), AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
341. Tyler R. Josephson, George Tsilomelekis, Christina Bagia, Stavros Caratzoulas, Vladimiro Nikolakis and Dionisios G. Vlachos, Ab Initio Study of Solvent-Induced Frequency Shifts of 5-Hydroxymethylfurfural, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014. Poster.
342. Alex D. Paulsen, Matthew S. Mettler, Dionisios G. Vlachos and Paul Dauenhauer, Pyrolytic Conversion of Cellulose to Fuels: Tuning the Mechanisms of Cellulose Pyrolysis to Improve Bio-Oil Properties, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014. Poster.
343. Glen R. Jenness and Dionisios G. Vlachos, Understanding Reactivity of Metal Oxides: Case Studies of Alcohol Reduction on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> and Rutile RuO<sub>2</sub>, Catalysis Society of Metropolitan New York (CSMNY) Annual Symposium, March 18, 2015. Poster.
344. Dion Vlachos, Design Principles of Bimetallic Core-Shell Catalysts, in George Olah Award Symposium, 249th ACS Meeting, Denver, Colorado, March 22-26, 2015.
345. Dion Vlachos, In Silico Prediction of Emergent Catalysts, 249th ACS Meeting, Denver, Colorado, March 22-26, 2015.
346. Dion Vlachos, Insights Into the Hydrodeoxygenation Mechanisms for Lignin Upgrade, 249th ACS Meeting, Denver, Colorado, March 22-26, 2015.
347. Dion Vlachos, Mechanisms and Catalyst Design Principles in the Conversion of Sugars and Furans to Renewable Monomers and Fuels, 249th ACS Meeting, Denver, Colorado, March 22-26, 2015.
348. Christina Bagia, T. Dallas Swift, George Tsilomelekis, Ruichang Xiong, Liu Yang, Stavros Caratzoulas, Vladimiro Nikolakis and Dionisios G. Vlachos, Elucidating the Role of Organic Co-Solvents in Fructose Dehydration Kinetics, 24th North American Catalysis Society Meeting (NAM), Pittsburgh, PA, June 14-19, 2015.
349. Matthew J. Gilkey, Paraskevi Panagiotopolou, Alexander V. Mironenko, Glen R. Jenness, Dionisios G. Vlachos, Bingjun Xu, Mechanistic Investigation of the Hydrodeoxygenation of Furfural to 2-Methylfuran over Ru/C Using Isotopic Labeling Techniques, 24th North American Catalysis Society Meeting (NAM), Pittsburgh, PA, June 14-19, 2015.
350. Geun Ho Gu, Kyungtae Lee, Dionisios G. Vlachos, Computational Study of Hydrodeoxygenation of Lignin Compounds on Pt(111). 24th North American Catalysis Society Meeting (NAM), Pittsburgh, PA, June 14-19, 2015. Poster.
351. Glen R. Jenness, Stavros Caratzoulas, Dionisios G. Vlachos, Raymond J. Gorte, Understanding the Impact of Lewis Acidity of Oxide Surfaces on Adsorption and Dehydration, 24th North American Catalysis Society Meeting (NAM), Pittsburgh, PA, June 14-19, 2015.
352. Alexander V. Mironenko, Dionisios G. Vlachos, Hydrogenolysis Mechanism of Furfural on Ru/RuOx Catalyst, 24th North American Catalysis Society Meeting (NAM), Pittsburgh, PA, June 14-19, 2015. Poster.
353. T. Dallas Swift, Huong Nguyen, Vladimiro Nikolakis and Dionisios G. Vlachos, Optimization of the Brønsted-Lewis Catalyst for One-Pot Glucose Conversion to HMF, 24th North American Catalysis Society Meeting (NAM), Pittsburgh, PA, June 14-19, 2015.
354. Vassili Vorotnikov, Shengguang Wang and Dionisios G. Vlachos, Conformational Effects and Metal Catalyst Screening for Upgrade of Furanics, 24th North American Catalysis Society Meeting (NAM), Pittsburgh, PA, June 14-19, 2015.
355. Bingjun Xu, Matt Gilkey, Alexander Mironenko and Dionisios G. Vlachos, Aromatic Ring Activation of Furanic Compounds on Ru-Based Catalysts, 24th North American Catalysis Society Meeting (NAM), Pittsburgh, PA, June 14-19, 2015.

356. Alexander V. Mironenko, Dionisios G. Vlachos, Hydrogenolysis Mechanism of Furfuryl Alcohol on Ru/RuOx Catalyst, The 2015 Conference on Foundations of Molecular Modeling and Simulation (FOMMS 2015), Mt. Hood, OR, July 12-16, 2015. Poster.
357. Jeffrey R. Christianson, Stavros Caratzoulas and Dionisios G. Vlachos, Computational Insight into the Effect of Sn-Beta Na Exchange and Solvent on Glucose Isomerization and Epimerization, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
358. Paul J. Dauenhauer, Wei Fan, Stavros Caratzoulas and Dionisios G. Vlachos, Kinetic Regime Change in the Diels-Alder Cycloaddition of Biomass-Derived Furans with Solid Acids, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
359. Ioanna Fampiou, Stavros Caratzoulas and Dionisios G. Vlachos, Electronic Structure Effects on Adsorption on Bimetallic Surfaces, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
360. Geun Ho Gu and Dionisios G. Vlachos, Fast Estimation Methods of Catalytic Cycles of Lignin Molecules on Pt(111), AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
361. Glen Jenness, Ke Xiong, Geun Ho Gu, Dionisios G. Vlachos and Jingguang G. Chen, Understanding the Catalytic Ring Opening of Furfural on Iridium, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015. Poster.
362. Glen Jenness, Stavros Caratzoulas, Dionisios G. Vlachos and Raymond J. Gorte, Towards a Molecular Understanding of the Reactivity of Oxide Catalysts, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
363. Tyler R. Josephson, Kramer Brand, Jay Labinger, Mark E. Davis, Dionisios G. Vlachos and Stavros Caratzoulas, Investigation of Sugar Transformation Mechanisms on Homogeneous Sn-Silicate Catalysts, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015. Poster.
364. Tyler R. Josephson, Kramer Brand, Jay Labinger, Mark E. Davis, Dionisios G. Vlachos and Stavros Caratzoulas, Investigation of Sugar Isomerization Mechanism on Homogeneous Sn-Silicate Catalysts, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
365. Sai Konda, Stavros Caratzoulas and Dionisios G. Vlachos, Computational Investigation of Bifunctional Catalysts for Bio-Oil Upgrade, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
366. Alexander V. Mironenko and Dionisios G. Vlachos, C-O Bond Hydrogenolysis over Metal/Lewis Acid Catalysts, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
367. Alexander V. Mironenko and Dionisios G. Vlachos, Unraveling Metal/Lewis Acid Synergy in Hydrogenolysis of Furfuryl Alcohol, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015. Poster.
368. Marcel Núñez and Dionisios G. Vlachos, First Principles Prediction of Active Sites for Bimetallic Catalysts, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
369. Ryan Patet, Paraskevi Panagiotopoulou, Stavros Caratzoulas and Dionisios G. Vlachos, Dehydration Reactions in Lewis Acidic Zeolites, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015. Poster.
370. Ryan Patet, Stavros Caratzoulas and Dionisios G. Vlachos, The Effect of Brønsted Acidic Zeolites on the Synthesis of Aromatics from Furans, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
371. George Tsilomelekis, Vladimiro Nikolakis, Stavros Caratzoulas and Dionisios G. Vlachos, Solvent Effects on the Stability of 5-Hydroxymethylfurfural: Understanding the Undesirable Side Reactions, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
372. Dionisios G. Vlachos, Design Principles of Bifunctional Catalysts: Hydrogenation, Dehydrogenation, and Hydrogenolysis, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
373. Dionisios G. Vlachos, Design Principles of Bimetallic Core-Shell Catalysts, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
374. Dionisios G. Vlachos, Modern Catalytic Technologies for Converting Biomass to Renewable Fuels and Chemicals, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
375. Bingjun Xu, Matthew Gilkey and Dionisios G. Vlachos, Mechanistic Investigations of Furanics Upgrade Via Catalytic Transfer Hydrogenation, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
376. Weiqing Zheng, Liang Wang, Ajay K. Prasad, Suresh G. Advani and Dionisios G. Vlachos, Nano Tungsten Carbide Catalysts for Polymer Electrolyte Membrane Fuel Cells, AIChE Annual Meeting in Salt Lake City, Utah, November 8-13, 2015.
377. Alexander V. Mironenko, Dionisios G. Vlachos, Tools for Kinetic Modeling, ISCRE24 Conference Workshop, Minneapolis, MN, June 12, 2016.
378. Alexander V. Mironenko, Dionisios G. Vlachos, C-O Bond Activation via Low-Temperature Heterogeneous Catalysis, Spring Symposium, EFRC Catalysis Center for Energy Innovation, Newark, DE, April 11, 2016.

379. Marcel Nunez, Dionisios G. Vlachos, Identification of Active Sites On Transition Metal Catalysts, 24th International Symposium on Chemical Reaction Engineering, Minneapolis, MN, June 13, 2016. Poster.
380. Saikat Dutta, Ashish Bohre, Dionisios Vlachos, Basudeb Saha, Lattice Interrupted Graphene Oxide Catalyzed Selective and Solventless Hydroxyalkylation/alkylation of Sylan to Valorize to Fuel Reservoir, ACS 252nd National Meeting, Philadelphia, PA, August 21-25, 2016. Poster.
381. Marcel Nunez, Dionisios G. Vlachos, Optimization of Transition Metal Catalyst Structure for the Oxygen Reduction Reaction, 252nd American Chemical Society National Meeting & Exposition, Philadelphia, PA, Aug. 22, 2016.
382. Alexander V. Mironenko, Dionisios G. Vlachos, Hydrogenolysis Mechanism of Furanics on Metal/Metal Oxide Catalysts, 2016 ACS Meeting, Philadelphia, PA, August 23, 2016.
383. Alexander V. Mironenko, Glen R. Jenness, Dionisios G. Vlachos, Mechanism of Furfural Hydrodeoxygenation on Metal/Metal Oxide Catalysts, 2016 AIChE Annual Meeting, San Francisco, CA, November 14, 2016.
384. Konstantinos Goulas, Glen R. Jenness, Alexander V. Mironenko, Tobias Mazal, Dionisios G. Vlachos, Vacancy-Mediated Hydrodeoxygenation of Furfuryl Alcohol over Metal Oxide, 2016 AIChE Annual Meeting, San Francisco, CA, November 14, 2016.
385. Alexander V. Mironenko, Dionisios G. Vlachos, Radical Mechanism for Low Temperature C-O Bond Activation on Metal/Metal Oxide Catalysts, 2016 AIChE Annual Meeting, San Francisco, CA, November 14, 2016.
386. Stephen A. Giles, Stavros Caratzoulas, Dionisios G. Vlachos, Yushan Yan, Nanoparticle Catalysts Supported on Substitutionally Doped Graphene: Effects on Activity and Stability for Hydrogen Oxidation, 2016 AIChE Annual Meeting, San Francisco, CA, November 16, 2016.
387. Alexander V. Mironenko, Konstantinos Goulas, Christopher Murray, Ray Gorte, Dionisios G. Vlachos, Metal Core/Surface Oxide Shell Catalysts for C-O Bond Activation, 2016 AIChE Annual Meeting, San Francisco, CA, November 16, 2016.

### Regional Meetings

1. Balakrishna, D. G. Vlachos, L. D. Schmidt, and R. Aris, "Effect of pressure on ignition and extinction of methane near inert surfaces," Central States Section, The Combustion Institute, Combustion Fundamentals & Applications, June 5-7, 1994, Madison, WI.
2. S. -J. He and D. G. Vlachos, "Growth and sintering of small particles", The Catalysis Society of New England, Worcester, MA, December 10, 1994.
3. S. Kalamatianos and D. G. Vlachos, "Mechanism reduction at bifurcation points of lumped systems: Homogeneous combustion of H<sub>2</sub> in air," Thirteenth Meeting of the Capital District Regional Chemical Kinetics and Dynamics Group, Albany, NY, January 28, 1995.
4. P. -A. Bui, D. G. Vlachos, and P. R. Westmoreland, "Data Analysis of Gas-Phase Neutrals in a PECVD Reactor," Thirteenth Meeting of the Capital District Regional Chemical Kinetics and Dynamics Group, Albany, NY, January 28, 1995.
5. S. Kalamatianos and D. G. Vlachos, "Dynamics near ignitions and extinctions of premixed H<sub>2</sub>/air mixtures," Eastern States Section, Chemical and Physical Processes in Combustion, The Combustion Institute, Worcester, MA, October 16-18, 1995.
6. P. -A. Bui, D. G. Vlachos, and P. R. Westmoreland, "Inhibition of homogeneous ignition by a catalytic surface," Eastern States Section, Chemical and Physical Processes in Combustion, The Combustion Institute, Worcester, MA, October 16-18, 1995.
7. D. G. Vlachos and P.-A. Bui, "Simulations on catalytic ignition with detailed surface kinetics", in Western States Section, The Combustion Institute, Los Angeles, CA, October 28-29, 1996.
8. D. G. Vlachos, "Stochastic effects in ignition of hydrogen in air", in Western States Section, The Combustion Institute, Los Angeles, CA, October 28-29, 1996.
9. M. A. Delichatsios and D. G. Vlachos, "Critical conditions for extinction and transient pyrolysis decay in solid material fires", in Eastern States Section, Chemical and Physical Processes in Combustion, December 9-11, Hilton Head, SC, 1996.
10. D. G. Vlachos, "Oxidation reactions over inert and platinum surfaces", in Fifteen Meeting of the Capital District Regional Chemical Kinetics and Dynamics Group, RPI, Troy, NY, January 25, 1997.
11. Y. K. Park and D. G. Vlachos, "Kinetically driven instabilities and selectivities in methane oxidation," in Fifteenth Meeting of the Capital District Regional Chemical Kinetics and Dynamics Group, RPI, Troy, NY, January 25, 1997.
12. R. J. Olsen and D. G. Vlachos, "Oscillatory dynamics of the hydrogen/oxygen reaction," in Fifteenth Meeting of the Capital District Regional Chemical Kinetics and Dynamics Group, RPI, Troy, NY, January 25, 1997.

13. P. Aghalayam, Y. K. Park, and D. G. Vlachos, "Detailed surface reaction mechanisms for methane oxidation on platinum," in Joint Combustion Meeting, The Combustion Institute, Washington, DC, March, 1999.
  14. M. Gummalla, H. Bermudez, D. G. Vlachos, and M. Delichatsios, "Flammability of diffusion flames near surfaces," in Joint Combustion Meeting, The Combustion Institute, Washington, DC, March, 1999.
  15. M. Gummalla, D. G. Vlachos, and M. Delichatsios, "Effect of dilution on extinction limits of surface interacting diffusion flames with detailed chemistry and transport," in Eastern States Section of the U.S. Sections of the Combustion Institute, Raleigh, NC, October 11-13, 1999.
  16. P. Aghalayam, Y. K. Park and D. G. Vlachos, "Construction and optimization of detailed surface reaction mechanisms for catalytic oxidation," in 18th Annual Meeting of the Capital District Regional Chemical Kinetics and Dynamics Group, UMass, Amherst, MA, January 29, 2000.
  17. M. Gummalla and D. G. Vlachos, "Oscillatory instabilities and chaotic dynamics in premixed hydrogen-air flames," 2000 ASME Fluids Engineering Division Summer Meeting, Boston, June 11-15, 2000.
  18. G. Bonilla, V. Nikolakis, M. Tsapatsis and D. G. Vlachos, "Growth Studies of Zeolite Crystals and Thin Films", Annual Research Review, CCST, Newark, DE, Oct. 12, 2000.
  19. M. Gummalla and D. Vlachos, "Dynamics of chemical reactors", Annual Research Review, CCST, Newark, Oct. 12, 2000.
  20. P. Aghalayam, S. Raimondeau, and D. G. Vlachos, "Multiscale models for chemical reactors", Annual Research Review, CCST, Newark, Oct. 12, 2000.
  21. N. Fernandes, J. Poshusta, S. Fisher, M. Gummalla, J. Watkins, M. Tsapatsis, D. Vlachos, "Fabrication of palladium membranes in porous supports by reactive deposition from supercritical fluids", Annual student poster contest of the Philadelphia Catalysis Club, Wilmington, January 18, 2001.
- Alan Peters Memorial Award for the best poster presentation***
22. S. Raimondeau, R. Lam, and D. G. Vlachos, "Multiscale models for chemical reactors", Annual student poster contest of the Philadelphia Catalysis Club, Wilmington, January 18, 2001.
  23. P. Aghalayam, S. Raimondeau, and D. G. Vlachos, "Detailed surface reaction mechanisms for partial oxidation of methane", Annual student poster contest of the Philadelphia Catalysis Club, Wilmington, January 18, 2001.
  24. J. M. Fedeyko, D. G. Vlachos, and R. F. Lobo, "Structure Determination of Subcolloidal Zeolite Nanoparticle Precursors", North Eastern Corridor Zeolite Association Annual Meeting, Philadelphia, PA (2003).
  25. J. M. Fedeyko, D. G. Vlachos, and R. F. Lobo, "Structure Determination of Subcolloidal Zeolite Nanoparticle Precursors", International Fine Particle Research Institute Annual General Meeting, Newark, DE (2004).
  26. J. D. Rimer, D. D. Kragten, D. G., Vlachos, R. F. Lobo, "Growth of Zeolite Crystals From the Deposition of Subcolloidal Silica-template Nanoparticles", Philadelphia Catalysis Club, Wilmington, DE, January Meeting (2004).

## **FUNDING**

### **Current funding (single UD investigator unless otherwise indicated)**

AGENCY: DOE-RAPID

TITLE: Rapid Advancements in Process Intensification Deployment (RAPID)

TOTAL AMOUNT: \$140,000,000; UD's Center Anticipated Funding: \$20,000,000

DURATION: 4/1/2017-3/31/2022

UD PI and Focus Area Leader of Fundamentals of Intensified Processes; Grant Led by AIChE

AGENCY: DOE-EFRC DE-SC0001004

TITLE: Catalysis Center for Energy Innovation

TOTAL AMOUNT: \$29,900,000

DURATION: 8/1/09-7/31/2018

With several co-PIs

AGENCY: DARPA

TITLE: Information metrics for Reliable Uncertainty Quantification in Materials Design

TOTAL AMOUNT: \$826,522 (UD portion)

DURATION: 9/1/2015-8/31/2018

PI: P. Dupuis, Brown Univ. with other co-PIs

AGENCY: NSF/NSF Award No. 1415828

TITLE: International Collaboration in Chemistry: CDS&E: Multiscale Simulations of Bifunctional Catalysis

TOTAL AMOUNT: \$228,033

DURATION: 1/15/2015-12/31/2017

AGENCY: DOE DE-SC0010549

TITLE: DOE Collaborative Proposal: Mathematical Foundations for Uncertainty Quantification in Materials Design

TOTAL AMOUNT: \$450,000

DURATION: 9/1/2013-8/31/2017

PI: P. Plechac; UD Co-PI's: D. Vlachos

AGENCY: US Army Research Laboratory

TITLE: Combined Multiscale Modeling-High Throughput Experimentation for Design of Bimetallic Catalysts for Catalytic Combustion

TOTAL AMOUNT: \$ 240,000

DURATION: 4/15/14-4/14/17

AGENCY: NSF

TITLE: SusChEM: Collaborative Research: Process Optimization of Novel Routes for the Production of Bio-Based Para-Xylene

TOTAL AMOUNT: \$ 430,000

DURATION: 9/1/2014-8/31/2017

AGENCY: Univ. of Minnesota/ExxonMobil

TITLE: Chemistry of BisHydroxyMethyl Furan

TOTAL AMOUNT: \$ 250,000 (UD Portion)

DURATION: 1/1/2016-12/31/2018

PI: Paul Dauenhauer

### **Prior funding**

AGENCY: Pacific Northwest National Laboratory/DOE 205613

TITLE: Modeling of Aqueous Phase Upgrade of Bio-oil

TOTAL AMOUNT: \$625,000

DURATION: 3/1/2013-12/31/2015

AGENCY: USDA 59-1935-3-008

TITLE: Distributed On-Farm Bioenergy, Biofuels and Biochemicals (FarmBio3) Development and Production via Integrated Catalytic Thermolysis  
TOTAL AMOUNT: \$300,000  
DURATION: 10/1/2012-5/31/2015

AGENCY: Colorado School of Mines/Army Research Office  
Title: Heterogeneously-Catalyzed Endothermic Fuel Cracking  
TOTAL Amount: \$540,000  
Duration: 9/1/2012-10/31/2015  
UD Co-PI: R. Lobo

AGENCY: PET Technology Consortium  
TITLE: Renewable Terephthalic Acid by Catalytic Diels-Alder Cycloaddition of Ethylene and Furandicarboxylic Acid  
TOTAL AMOUNT: \$ 300,000  
DURATION: 9/2014 – 8/2015

AGENCY: Imperium Aviation Fuels, LLC/Department of Energy  
Title: Syngas to Fuels  
TOTAL Amount: \$180,000  
Duration: 3/1/2012-2/28/2015  
UD Co-PI: R. Lobo

AGENCY: NSF-EFRI A0000994102  
TITLE: EFRI:HyBi: One-pot Catalytic Conversion of Biomass to Fuels over Bifunctional Catalysts in Millisecond Contact Time Reactors  
TOTAL AMOUNT: \$400,000  
DURATION: 9/1/09-8/31/2014

AGENCY: US Army Research Laboratory  
TITLE: JP8 kinetics for design of thermoelectric devices  
TOTAL AMOUNT: \$ 277,957  
DURATION: 3/1/10-7/14/2014

AGENCY: America Air Liquide  
TITLE: Computational Studies for Feedstock  
TOTAL AMOUNT: \$400,000 (direct)  
DURATION: 3/1/2012-2/28/2014  
PI: M. Klein; UD Co-PI's: D. Vlachos, J. Chen

AGENCY: DOE DE-FG02-05ER25702  
TITLE: Multiscale mathematics for biomass conversion to renewable hydrogen  
TOTAL AMOUNT: \$544,545  
DURATION: 8/15/09-8/14/2013

AGENCY: DOE DE-FG02-03ER15468  
TITLE: From First Principles Design to Realization of Bimetallic Catalysts for Enhanced Selectivity  
TOTAL AMOUNT: \$2,996,651  
DURATION: 9/15/09-9/14/2013  
PI: R. Lobo; UD Co-PI's: M. Barteau, J. Chen, J. Lauterbach

AGENCY: NSF-CDI Type I 0940768  
TITLE: CDI-Type I: Complex Catalyst Design Enabled via Computational Thinking  
TOTAL AMOUNT: \$648,894  
DURATION: 12/1/09-11/30/2013

AGENCY: NSF/CHE-MRI 0922657  
TITLE: Acquisition of a Facility for Computational Approaches to Molecular-Scale Problems  
TOTAL AMOUNT: \$525,927  
DURATION: 09/15/09- 09/14/12  
PI: D. Doren and Co-PIs: S. Patel and M. Taufer

AGENCY: NSF/CDI-Type II 0835548  
TITLE: Hierarchical Stochastic Algorithms for Materials Engineering  
TOTAL AMOUNT (UD PART): \$889,451 out of a total of \$1,500,000  
DURATION: 9/1/08-8/31/13  
UD Co-PI: B. Ogunnaike; Other PIs: P. Plechac, M. Katsoulakis

AGENCY: UNM/NIH 3R96S  
TITLE: Center for Spatiotemporal Modeling of Cell Signaling (STMC)  
TOTAL AMOUNT: \$306,000  
DURATION: 7/1/09-6/30/11

AGENCY: NSF/CBET-0651043  
TITLE: Hierarchical multiscale model-based process engineering  
TOTAL AMOUNT: \$262,081  
DURATION: 3/15/07-2/28/11

AGENCY: NSF/CBET-0729714  
TITLE: Microchemical technology for future energy needs  
TOTAL AMOUNT: \$255,718  
DURATION: 9/1/07-8/31/11

AGENCY: NSF/CBET-0729701  
TITLE: Controlling Catalytic Microcombustors as Heat or Chemical Machines  
TOTAL AMOUNT: \$299,999  
DURATION: 9/1/07-8/31/11

AGENCY: COBRE/NIH-5P20RR015588  
TITLE: Spatial self-organization of plasma membrane proteins  
TOTAL AMOUNT: \$174,574  
DURATION: 6/1/08-5/31/11  
PI: A. Lenhoff

AGENCY: US Army Research Laboratory  
TITLE: Chemical Erosion of Silicon Nitride  
TOTAL AMOUNT: \$ 110,000  
DURATION: 1/1/09-31/12/10

AGENCY: DOE/DE-FG02-06ER15795  
TITLE: An Integrated Approach toward Rational Nanocatalyst Design for Hydrogen  
TOTAL AMOUNT: \$960,000  
DURATION: 7/1/06-12/31/10  
Co-PIs: D. J Buttrey, J. A. Lauterbach

AGENCY: DOE/DE-FG02-05ER25702  
TITLE: Multiscale modeling of spatially distributed biological systems  
TOTAL AMOUNT: \$ 1,120,747  
DURATION: 8/15/05-8/14/09  
Co-PIs: J. S. Edwards, M. Katsoulakis

AGENCY: DOE/ DE-FG02-03ER15468

Dion G. Vlachos-CV

TITLE: From first principles design to realization of bimetallic catalysts for enhanced selectivity  
TOTAL AMOUNT: \$ 2,506,000  
DURATION: 9/15/06-9/14/09  
PI: M. A. Barteau and 8 other co-PIs

AGENCY: US Army Research Laboratory  
TITLE: Microchemical devices for power production from JP-8  
TOTAL AMOUNT: \$ 95,000  
DURATION: 1/1/08-31/12/09

AGENCY: US Army Research Laboratory  
TITLE: Portable Power from Fuels Using High Temperature Thermoelectrics  
TOTAL AMOUNT: \$180,800  
DURATION: 6/1/06-12/31/08

AGENCY: NSF/CTS-0343757  
TITLE: Bridging length and time scales in catalytic reaction systems  
TOTAL AMOUNT: \$ 228,365  
DURATION: 3/1/04-8/31/07

AGENCY: Rohm & Haas/Engelhard/RANDH11232004  
TITLE: Microkinetic Models for Acrylic Acid Production  
TOTAL AMOUNT: \$ 479,338  
DURATION: 7/1/04-6/30/07

AGENCY: NSF/DMR  
TITLE: High Anisotropy Magnetic Nanoparticles and Nanocomposites  
TOTAL AMOUNT: \$ 600,000  
DURATION: 7/1/03-6/30/07  
PI: G. Hadjipanayis

AGENCY: US Army Research Laboratory  
TITLE: Microstructural Design of Lightweight Multifunctional Composite Armor  
TOTAL AMOUNT: \$ 320,000  
DURATION: 1/12/02-11/30/06

AGENCY: MURI, Department of Defense  
TITLE: Design Rules for High Temperature Microchemical Systems  
TOTAL AMOUNT: \$ 2,500,000  
UDeI TOTAL AMOUNT: \$ 437,927  
DURATION: 5/1/01-4/30/06  
Co-PIs: R. I. Masel (Leading PI), M. Shannon, P. Kenis, E. Seebauer

AGENCY: NSF/ITR (Information Technology), Division of Mathematics  
TITLE: Mesoscopic modeling and simulation: A novel approach to Monte Carlo methods  
TOTAL AMOUNT: \$ 420,000  
UDeI TOTAL AMOUNT: \$ 136,640  
DURATION: 9/1/02-8/31/05  
PI: M. A. Katsoulakis

AGENCY: DOE  
TITLE: From first principles design to realization of bimetallic catalysts for ultrahigh selectivity  
TOTAL AMOUNT: \$ 1,140,000  
DURATION: 9/1/03-8/31/06  
PI: M. Barteau



AGENCY: DOE

TITLE: Fuel Cell Research at the University of Delaware-Delaware Center for Clean Energy

TOTAL AMOUNT: \$ 996,000

DURATION: 6/1/04-10/31/05

Co-PIs: S. G. Advani (lead PI), J. G. Chen, A. Karlsson, J. A. Lauterbach, A. K. Prasad, M. H. Santare, N. J. Wagner, H. Wang, L.-P. Wang, B. G. Willis

AGENCY: PRF-ACS

TITLE: Multiscale Modeling for Chemical Kinetics of Ethane Oxidation

TOTAL AMOUNT: \$ 80,000

DURATION: 1/7/03-31/8/05

AGENCY: NSF/NIRT

TITLE: An Interdisciplinary Approach to Understanding the Growth of Nanoporous Materials

TOTAL AMOUNT: \$1,000,000

UDel TOTAL AMOUNT: \$ 344,025

DURATION: 7/1/01-6/30/05

Co-PIs: R.F. Lobo, P. A. Monson (leading PI), M. Tsapatsis

AGENCY: Conoco Co.

TITLE: Microkinetic analysis of catalytic pathways

TOTAL AMOUNT: ~\$ 85,000

DURATION: 1/1/04-31/12/04

AGENCY: NASA

TITLE: Thin film molecular sieve synthesis: Processing-microstructure relationships and the effect of microgravity on microstructure

TOTAL AMOUNT: \$ 340,000

DURATION: 6/1/00-12/31/03

PI: M. Tsapatsis

AGENCY: DOE/Praxair Inc.

TITLE: Partial oxidation of methane

TOTAL AMOUNT: \$ 150,000

DURATION: 1/1/01-12/31/03

AGENCY: NSF, Nanotechnology Initiative

TITLE: Preparation of nanostructured membranes by reactive depositions from supercritical fluids

TOTAL AMOUNT: \$ 510,000

DURATION: 9/1/98-8/31/03

PI: J. J. Watkins, co-PI: M. Tsapatsis

AGENCY: NSF, (Career Award)

TITLE: A multiscale hierarchical approach to reaction processes and its integration into the curriculum

TOTAL AMOUNT: \$ 200,000

DURATION: 5/1/97-4/30/02

AGENCY: NETI and Engelhard Co.

TITLE: Molecular sieve membranes: Processing-microstructure-separation properties

TOTAL AMOUNT: \$ 150,000

DURATION: 7/1/98-8/31/01

PI: M. Tsapatsis

AGENCY: NSF Plus Undergraduate Summer Support

TITLE: Linking fundamental investigations and engineering results for extinguishment of fires on solid materials

TOTAL AMOUNT: \$ 170,000

DURATION: 8/1/97-7/31/00

AGENCY: ONR, (Young Investigator Award)

TITLE: Dynamics of flames near surfaces: Flame stability and pollution abatement

TOTAL AMOUNT: \$ 300,000

DURATION: 6/1/96-12/31/99

AGENCY: National Environmental Technology Institute (NETI) and Praxair Inc.

TITLE: A novel thin film microreactor for partial oxidation: Minimization of waste byproducts and optimization of reactor efficiency

TOTAL AMOUNT: \$ 100,000

DURATION: 7/1/97-6/30/99

AGENCY: NETI

TITLE: Environmentally benign products and processes based on homogeneous catalysis

TOTAL AMOUNT: \$ 300,000

DURATION: 7/1/98-6/30/01

PI: K. M. Ng

AGENCY: NSF, CTS

TITLE: Engineering research equipment: A high performance computer and graphics facility for research in molecular and materials modeling

TOTAL AMOUNT: \$ 96,688

DURATION: 5/1/99-6/30/00

(co-PI with P. A. Monson and P. R. Westmoreland)

AGENCY: AFOSR

TITLE: Acquisition of light scattering and electrophoresis equipment for studies on nanosol synthesis and processing for device fabrication

TOTAL AMOUNT: \$ 152,000

DURATION: 6/7/96-6/6/97

(co-PI with M. Tsapatsis and R. L. Rowell of Chemistry of UMass)

AGENCY: ACS-PRF & Summer Faculty Fellow Support

TITLE: A Microscopic approach to oxidation reactions and reactors

TOTAL AMOUNT: \$ 30,000

DURATION: 9/1/95-8/31/97

AGENCY: NSF, Research Equipment

TITLE: Engineering Research Equipment: A Computer Graphics Facility for Research in Applied Molecular and Materials Modeling

TOTAL AMOUNT: \$ 78,000

DURATION: \$ 9/1/94-8/31/95

(co-PI with P. A. Monson, P. R. Westmoreland, and M. R. Cook)

## **SERVICE**

### **Division/Area Programming Chair, National Committees**

Programming Chair of the Catalysis and Reaction Engineering Division of AIChE, 2008-2013  
Breakout leader of 'Harnessing DOE's High Performance Computing Expertise to Strengthen the US Chemical Enterprise', a workshop hosted by the Council for Chemical Research (CCR) and DOE, Washington, DC, March 10-11, 2011  
AIChE Executive Board of the National Planning Committee (*EBPC*), 2011-2014  
Chair, Philadelphia Catalysis Club, 2010-2011  
Chair-elect, Philadelphia Catalysis Club, 2009-2010  
President's Blue Ribbon Committee on Certification (BRCC), Member 2009-2010  
CAST programming chair of Area 10d - Applied Mathematics and Numerical Analysis, 2006-07

### **Major Meeting/Symposium Organizer**

Organizer, Spring Catalysis Club of Philadelphia Symposium, Villanova, PA, May 13<sup>th</sup>, 2010  
Co-organizer of the ISCRE 21 meeting, Philadelphia, PA, June 13-16, 2010  
Co-organizer of the 5th International Zeolite Membrane Meeting (IZMM), Loutraki, Greece, May 23-26, 2010  
Organizer of the reaction engineering topical area of the North American Catalysis Society meeting, San Francisco, CA, June 7-12, 2009  
Topical conference on Multiscale Simulation, AIChE meeting, 2005  
SIAM Minisymposium, "Multiscale modeling: Fundamentals and applications", First SIAM Conference on Computational Science and Engineering, Washington, DC, Sept. 21-23, 2000

### **Session Chair or Co-Chair**

Predictive Materials Modeling in the Energy Sector, Panel Discussion, Predictive Multiscale Materials Modelling Dec. 1-4, 2015, Isaac Newton Institute, Cambridge, England  
Advanced Ab Initio Methods I, MRS Symposium YY, Boston, MA, December 1, 2015 (with Enrique Martinez Saez)  
Fundamentals of Catalysis: Mechanisms and Elementary Steps III, 23<sup>rd</sup> NAM, Louisville, KY on June 2-7, 2013  
Reaction Engineering Fundamentals, NASCRE 3, Houston, TX, March 17-20, 2012  
Theory and Modeling, EuropaCat X, Glasgow, Scotland, August 28-September 2, 2011  
Flames V, 13th International Conference on Numerical Combustion, Corfu, Greece, April 27-29, 2011  
Reaction Engineering for Renewables, AIChE meeting, Nashville, Tennessee, Nov. 8-13, 2009  
Reaction Engineering, North American Catalysis Society meeting, San Francisco, CA, June 7-12, 2009  
Catalysts & catalytic reaction engineering, ISCRE 20<sup>th</sup> meeting, Kyoto, Japan, September 7-10, 2008  
Advanced modeling and reactor related experiments, Pfäffikon SZ, Switzerland, September 29-October 1, 2008  
Numerical Methods for Molecular and Mesoscopic Systems, CAST10D, AIChE meeting, 2008  
Sessions in honor of Gus Aris, AIChE meeting, 2008  
IMRET meeting and Spring AIChE, Modeling and characterization of microsystems, 2008  
Membrane reactors, International Zeolite Membrane Meeting, Zaragoza, Spain, July 22-25, 2007  
Numerical Methods and Simulation of Multiscale Systems, AIChE meeting, San Francisco, CA, 2006  
Preparation and Selection of Catalysts; Combinatorial Catalysis, EUROPACAT-7, Sofia, Bulgaria, Aug. 28 – Sept. 1, (2005)  
Kinetics of Catalytic Reactions and Reaction Engineering, EUROPACAT-7, Sofia, Bulgaria, Aug. 28 – Sept. 1, (2005)  
Nanomaterials, Acireale, Sicily, 2004  
Simulation and control of multiscale processes, American Control Conference, Boston, MA, June 30<sup>th</sup>-July 2<sup>nd</sup>, 2004 (with A. Armaou)  
Multiscale Modeling and Simulation I and II, AIChE meeting, 2004 (with M. Gallivan)  
Dynamics and Control of Multiscale Processes (with Christofides)-Area 10, 2003  
Multi-Scale Approaches to Reaction Engineering (with Neurock)-Area 20, 2003  
Microreactors: Fundamentals and Applications I (with Masel)-Area 20, 2003  
Ordering, Phase Transitions and Self-Assembly I (with R. Rajagopalan), ACS meeting, Atlanta, Georgia, June 16-18, 2003  
Computational methods in self-assembling systems (with J. de Joannis), ACS meeting, Atlanta, Georgia, June 16-18, 2003  
Microscale combustion, Joint Combustion Meeting, Chicago, March 16-19, 2003  
Detailed Reaction and Reactor Modeling I (with Androulakis)-Areas 20 and 10, 2002

Detailed Reaction and Reactor Modeling II (with Androulakis)-Areas 20 and 10, 2002  
Multiscale Modeling of Chemical and Materials Processing (with Maroudas)-Areas 20, 21, and T1, 2002  
ISCRE 17<sup>th</sup> session, Hong Kong, Aug. 2002  
Dynamics and control of multiscale processes, with P. Christofides, AIChE Joint 10b and 10d Session in Computing and Systems Technology Division, Indianapolis, Nov. 2002  
Session on Membranes, MRS meeting (with V. Bourganos), Boston, MA, December 2002  
AIChE Session in Group 20 - Detailed chemistry and reactor modeling, Indianapolis, Nov. 2002, with I. Androulakis  
Sessions in areas 21 - Computational Molecular Science and Engineering Forum; 20 - Catalysis and Reaction Engineering Division; T1 - Nanoscale Science and Engineering; 10 - Computing and Systems Technology Division, 2001  
AIChE session in Group 10 - Computing and Systems Technology: Multi-scale modeling in chemical and materials processing, Reno, 2001  
AIChE session in Group 20 - Catalysis and Reaction Engineering and Topical T1 - Applying Molecular Simulations and Computational Chemistry, "Multi-scale approaches to reaction engineering", Reno, 2001  
Detailed chemistry and reactor modeling sessions, AIChE, Los Angeles, CA Nov. 2000  
Reaction Engineering: Modeling and Simulation, NACS, Boston, June 1999  
Ignition and Detonation. Joint Combustion Meeting, Washington, DC, March 1999  
Detailed Kinetics Modeling, Eastern States Meeting, Raleigh, NC, Oct. 11-13, 1999  
Dynamics of Chemical Reactors, Dallas, TX, 1999  
Multiscale modeling of reactions and reactors, AIChE Annual Meeting, Miami, 1998  
Dynamics of Chemical Reactors, Los Angeles, CA, 1997  
Combustion Modeling, Eastern States Section of the Combust. Institute, Hartford, CT 1997  
Dynamics of Chemical Reactors, AIChE Annual Meeting, Chicago, IL, 1996  
Annual Fall Symposium, The Catalysis Society of New England, Worcester, MA, 1996  
Chemical Reactor Stability and Dynamics", AIChE Annual Meeting, San Francisco, CA, 1994 (with H. Viljoen)  
14th Regional Meeting on Kinetics and Dynamics, Amherst, 1996 (with P. R. Westmoreland)  
AIChE judge: National students paper competition, 1994

### **Reviewer for Meetings**

North American Catalysis Meeting, 2015  
ISCRE, 2015  
Third North American Symposium on Chemical Reaction Engineering (NASCRE3), North American Catalysis (NACS) meeting, 2012  
Int. Combustion Institute meeting, 2010  
Third Conference on Structured Catalysts and Reactors, ICOSCAR-3, 2009  
Organic Reactions Catalysis Society (ORCS) conference, 2010 (<http://www.orcs.org/>)  
Inst. Symposium Chemical Reaction Engineering, ISCRE 21<sup>st</sup>, 2009/2010 (many abstracts and papers)  
Int. Combustion Institute meeting, 2008 (7 papers)  
EuropaCat meeting, 2006  
Int. Combustion Institute meeting, 2006 (6 papers)  
EuropaCat VII abstracts for various symposia, 2005  
Thirtieth International Symposium on Combustion, 2004  
Twenty Ninth International Symposium on Combustion, 2001  
ISCRE 15th meeting abstracts, 1998

### **Referee for Journals (by Group) and Publishers**

Interdisciplinary: Science, Nature Chemistry, Nature Communications, Nature Materials, Nature Nanotechnology  
Engineering: Ind. Eng. Chem. Res., Chem. Eng. Sci., Comput. Chem. Eng., Chem. Eng. J., AIChE J., Chem. Eng. J., J. Membrane Sci.  
Physical chemistry, chemical physics, soft matter: Nature Chemistry, J. Am. Chem. Soc., J. Chem. Phys., J. Phys. Chem. B and C, Langmuir  
Catalysis: Appl. Cat. A, J. Catal., Cat. Letters, Cat. Today, ACS Catal., ChemCatChem, ChemSumChem

Physics: Phys. A: Mathematical and General, Surface Science, Phys. Rev. E, Phys. D, Phys. Rev. B, Phys. Rev. Lett.

Mathematical/computational: J. Comput. Physics

Energy: Energy Environ. Sci., Comb. Flame, Comb. Sci. Tech., Comb. Theory Modeling, J. Power Sources

Materials: Micropor. Mesopor. Mat., J. Crystal Growth, Chem. Mater., Nature Materials, Nature Nanotechnology

Biological: Biophys. J., Bioinformatics

Publishers: Cambridge Univ. Press, Elsevier, ACS

### **Referee for Funding Agencies**

PRF, NSF, DOE, European programs, Marie Curie, US-Eastern European Countries Contracts

### **Recommender**

Award recommendations

Promotion and tenure reviewer

### **University, College, and Department Service**

#### UD Service

Council of Community Engagement and Public Service Centers, 2017-

Manufacturing strategic plan developer, 2017

Data Science strategic plan developer, 2017

University Research Council Committee, 2016-

Sponsored Program Deputy Provost search committee, member 2016-2017

College of Engineering industrial director search committee and conception of the industrial development program, member, 2013-

University of Delaware Energy Institute (UDEI) Board Member, 2009-

Computational Science Faculty search committee member, 2009-2010

Senator, 2001-03

College Infrastructure Committee Member, 2001

#### UD Departmental Service

Chair of Faculty search committee, 2015-2016

Member of Faculty search committee, 2008-2011

$\Omega$ E advisor of undergraduates, 2000-2006, 2008-2011

Chemical engineering chairman search committee, 2005 (Member)

Chemical engineering faculty search committee, 2001-02, 2005-06 (Member)

Advisor of ~25 undergraduates, 2000-02, 2005-2007

Energy working group (Member), 2006-present

Graduate curriculum committee (Member), 2005-present

Graduate recruiting coordinator, 2001-2005

Safety committee, 2001-2005

Undergraduate curriculum committee, 2001-04

Departmental laboratory committee, 2000-2005

#### UMass College and University Service

Member: VIP Director search committee, summer 1998

Member: IT planning committee, 1995-96

Member: Students affairs committee, 1995-96

Member: Engineering Computing Services Committee, 1994, 1995-97

#### UMass Departmental Service

Graduate program director, 1997-99

Personnel committee member, 1998-99

AIChE Student Chapter Advisor, 1994-97; AIChE Student Chapter Co-advisor, 1993

Dion G. Vlachos-CV

Member: Faculty search committee, 1993-94

Member: Ph.D. Qualifying Exam Committee in Transport, 1993, 94; in Kinetics, 1994

Chair: Ph.D. Qualifying Exam Committee in Transport, 1995; in Kinetics 1996, 97-99

## TEACHING EXPERIENCE, ADVISING, AND MANAGING

### Graduate Students, Postdoctoral Scholars and International Scholars Advised

*Current graduate students (20):* Vassili Vorotnikov, Tyler Josephson, Alexander Mironenko, Marcel Nunez, Ryan Patet, Geun Ho Gu, Stephen Giles, Matthew Gilkey, Huong Thi Thanh (Hannah) Nguyen, Ziwei (Lily) Cheng, Zhiqiang (Jack) Zhang, Angela Norton, Joshua Lansford, Jiayi Fu, Jonathan Lym, Pierre Desir, Gerhard Wittreich, Elvis Ebikade, Natalia Rodriguez Quiroz, Yifan Wang.

*Ph.D Degrees Awarded (31):* T. Dallas Swift (June 2015; OSIssoft), Timothy Courtney (October 2014, Air Products), Matthew Christiansen (June 2014, Shell), Nima Nikbin (June 2014, Dow Chemicals), Jonathan Sutton (June 2014, Oak Ridge National Lab), Sarah Tupy (August 2013, 3M), Jacob McGill (October 2013, Apogee Research), Vinit Choudhary (May 2013, ExxonMobil), Matthew Mettler (June 2012, ExxonMobil), Michael Saliccioli (April 2012, Exxon Chemicals), Danielle Hansgen (June 2011, Intel), William Lonergan (May 2011, ExxonMobil); Khalid Ali Al-Majnouni (January 2011, Saudi Arabia); Mr. J. Federici (June 2009, ExxonMobil), Mr. A. Chatterjee (May 2007, Asst. Prof., IIT Kanpur), Mr. J. Ludwig (March 2007, Exxon Mobil), Mr. J. Rimer (Oct. 2006, Asst. Prof., Univ. of Houston), Mr. S. Deshmukh (June 2006, Velocys), Mr. M. Snyder (April 2006, Lehigh Univ.), Mr. J. Fedeyko (March 2006, Johnson Matthey), Mr. Kapil Mayawala (May 2006, Novartis), Mr. D. Norton (April 2005, GE), Mr. A. Mhadeshwar (June 2005, Univ. of Connecticut, Asst. Prof.), Ms. G. Bonilla (Jan. 2004, IBM), Mr. S. Fisher (Nov. 2003, GE Plastics), Ms. S. Raimondeau (Aug. 2002), Ms. M. Gummalla (Ph.D., Nov. 2001, UTRC), Mrs. P. Aghalayam (Dec. 2000, IIT Bombay), Mr. V. Nikolakis (Dec. 2000, UPatras), Mr. Y. K. Park (April 2000, Carrier), Mr. P. -A. Bui (May 1998, GE).

*MS (11):* Mr. Garam Lee (December 2016; Intel), Mr. Andrew Black (2014), Mr. Stephen Edie (May 2012), Mr. Jacob Weiner (December 2011), S. Collins (May 2009, OSIssoft), Mrs. A. -M. Schilthuis (April 2007, DuPont), Ms. A. Samant (June 2007, Mathworks), Mr. B. Feist (May 2006, Air Liquide), Mr. R. Lam (Feb. 2001), Mr. J. Reese (Dec. 99), Mr. S. Kalamatianos (Jan. 1995, Dimensions International, Inc.)

*International and Other Scholars Advising:* Adriano Sousa from Brazil (October 2014-September 2015), Stefano Tacchino from Torin, Italy (March 2011-February 2012); Till Brüggemann from Germany (3/1/10-5/30/10); Rafael de Camargo Catapan from Brazil (3/1/10-2/28/11); Wulf Hauptmann, Technische Universität Darmstadt, Germany (at UD in Summer and Fall 2006); Matteo Maestri, Polytechnique of Milan, Italy (at UD, July 2006-June 2007); Andrea Scarpa, Univ. of Naples, Italy (January 2008 – June 2008); Jennifer Synowczynski (2006-2009), ARL co-advised with Jan Andzelm; Anders Larsen (Fall 2007 and January 2008), Univ. of Minnesota in collaboration with Lanny Schmidt; Michelle Costa (2007-2008) in collaboration with Jeremy Edwards.

*Sabbatical host:* Blaž Likozar, Fulbright Fellow, from Slovenia (October 2014-April 2015)

*Current Postdoctoral Fellows (7):* Li Shuai (January 2017-), Weiqing Zheng (October 2012-), Glen Jenness (September 2013-), Konstantinos Goulas (September 2015-), Sha Li (2016-), Sibao Liu (2016-), Eugenio Souza (2016)

*Former Postdoctoral Scholars (37 total):* Ioanna Fampiou (September 2014-May 2016, Harvard Univ.), Evangelos Miliordos (June 2015-June 2016, Univ. of Alabama, Asst. Prof.), Davood Pourkargar (August 2015-July 2016), Jechan Lee (June 2015-February 2016), Sai Konda (June 2014-January 2016), Jeffrey Christianson (September 2014-October 2015, Cerner), Ruichang Xiong (July 2010-July 2015, AspenTech), George Tsilomelekis (October 2012-July 2015, Rutgers University), Liu Yang (April 2013-February 2015, Johnson Matthey), Wei Guo (October 2011-October 2014, Beijing Institute of Technology), Shengguang Wang (October 2012-October 2014, Univ. Houston), Despoina Tzoulaki (October 2013-September 2014, Haldor Topsoe A/S), Kyungtae Lee (July 2013-July 2014, Samsung Advanced Institute of Technology), Marta Leon Garcia (November 2011-May 2014, MeadWestvaco), Nageswara Rao Peela (April 2011-March 2014, Asst. Prof., IIT, Guwahati), Paraskevi (Vivi) Panagiotopoulou (October 2012-February 2014, Univ. of Crete), Yifang Zhao (January 2013-February 2014, Queen's University Belfast), JungHo Jae (May 2012-November 2013, KIST), Neeraj Rai (July 2012-August 2013, Asst. Prof., Mississippi Univ.), Santiago Builes Toro (August 2012-July 2013, Asst. Prof. EAFIT Univ., Columbia), Jacob Kruger (October 2011-July 2013, NREL), Prasad Vegendla (October 2011-December 2012, Argonne Nat. Lab), Yulin Huang (August 2012, DDH Advanced Materials & Systems, Inc.), Michail Stamatakis (May 2009-June 2012, Asst. Prof., UCL, London), Samir Mushrif (September 2010-July 2012, Asst. Prof., Nat'l Univ. of Singapore), Nasser Abukhdeir (Nov. 2009-April 2011, Asst. Prof., Univ. of Waterloo), Hangyao Wang (November 2009-March 2011, Dow Chemicals), K. Bijjula (Sept. 2008-March 2009, Intel), G. Stefanidis (Jan. 07-Jan. 09, Assoc. Prof., KU Leuven.), V. Prasad (Jan. 07-Dec.08, Asst.

Prof., Univ. of Alberta), Ayman Karim (Jan. 2007-June 2008, Assoc. Prof., Virginia Tech.), N. Kaisare (Jan. 2005-May 2007, Assoc. Prof., IIT-Madras), Altaf Karim (Sept. 2006-June 2007, BNL), N. Fernandes (Acumentrics Co.), T. Basak (Prof., IIT Madras), D. Kragten (Unimin), M. Lebedeva (Penn State)

Scientific Research Staff: Stavros Caratzoulas, Jeff Everhart, Basubed Saha

Previous Scientific Research Staff: Vladimiro Nikolakis (2011-2015; W.L. Gore), Weihua Deng (2012-2015; Lab Mgr., CBE, UD), Giannis Mpourmpakis (2011-2013; Asst. Prof., Univ. of Pittsburgh), Christina Bagia (2011-2013; Scientist, Duquesne University), Ying Chen (2009-2012, Self-employed)

Administrative (CCEI) Staff: Cindy King (2016-present; Admin. Asst.), Sheila Boulden (2009-2016; Admin. Asst. in CCST, 2008-2009), Gina Frushon (2011-2015), Michele Jennings (2012-2014), Kris Farmer (2011-2013), Jennifer Sykes (2011), John Pollock (2009-2011), Mark Stitz (2009-2010)

## **Courses**

### Graduate Courses

- Special Topics in Energy - CHEG 614, Spring 2015 (co-taught)
- Advanced Topics in Energy - CHEG 814, Spring 2015 (co-taught)
- Energy Engineering - CHEG 867-014/614-010, Spring 2013
- Applied Chemical Kinetics - CHEG 835, Fall 2000-2003, 2008, 2010
- Chemical Engineering Principles I - CHEG 867, (Applied Mathematics for first year graduate students), Fall 2001-2006 (co-taught with Prof. Beris in the Fall 2001)
- Chemical Engineering Principles II - CHEG 867, (Applied Mathematics for first year graduate students), Spring 2002-2006, 2008, 2009 (co-taught with Profs. Beris and Ogunnaike)
- Special Topics in Energy Engineering - CHEG867-014/614, co-taught with Profs. Chen and Beris, Spring 2006, 2008-2012, co-taught with Profs. Chen, Beris, Yan and Jiao, co-taught with Profs. Beris, Yan and Jiao
- Advanced Chemical Analysis I - ChE 661 (Applied Mathematics course), Fall 1993-1995
- Transport Processes - ChE 633, Spring 1994-1996
- Reactor Design Seminars - ChE 891, 1993-2000
- Advanced Kinetics and Reactor Design - ChE 625, Fall 1999

### Undergraduate Courses

- Introduction to Chemical Engineering - CHEG 112, Spring 2001-2005 (co-taught with Profs. Zydney, Wool, Chen, and Dr. Michaud)
- Honors Sections - CHEG 112, Spring 2001-2005
- Kinetics and Reactor Design - ChE 320, 1998-2000
- Applied Transport Phenomena (Transport based separations) - ChE 434, 1996-1999

### Video Instructional Program

- ChE 633 in VIP 1995-1999
- Applied Chemical Kinetics CHEG 835, Fall 2001
- Special Topics in Energy Engineering - CHEG867-014, Spring 2011-2012

### Multi-institutional teaching activities

- Taught two lectures at the Applied Mathematics Department, University of Crete, October 26<sup>th</sup>, 2009
- Taught part of the Multiscale Modeling course of the Institute of Multiscale Modeling of Biological Interactions (IMMBI) at John Hopkins University, Fall 2005

### Workshops/Tutorials

- Tutorials on multiscale modeling, UD, January 4-14, 2010
- A Marie Curie training program with nearly 100 students and postdocs from around the globe, Lectures on Molecular Simulations: MD, KMC & TST, for the EC-funded Marie Curie Training Course, 'EF2: Nanostructured material and membrane modeling and simulation', Patras, Greece, June 19, 2008



- Taught at the workshop on ‘Mathematical and Computational Methods for Accelerated Molecular and Stochastic Simulations’, Institute for Computational and Applied Mathematics (IACM), Foundation for Research and Technology-Hellas (FORTH), Heraklion, Crete, Greece, June 25-27, 2007
- Organized and taught part of a workshop on Multiscale Modeling of Biological Systems; Winter 2006 at UD
- Organized and offered tutorials (with Profs. Fichtorn and Maroudas) during the Topical Multiscale Conference at the 2005 AIChE meeting

### PhD Graduated Students and Thesis Title

#### Ph.D.

1. Mr. T. Dallas Swift (June 2015, OSISoft), Improving HMF Yield Using an Integrated Modelling Approach
2. Mr. Timothy Courtney (October 2014, Air Products), Experimental and Computational Analysis of Acid Catalysts for Biomass Conversion
3. Mr. Matthew Christiansen (June 2014, Shell), Kinetic Modeling and Mechanisms for Catalytic Upgrade of Biomass Derivatives
4. Mr. Nima Nikbin (June 2014, Dow Chemicals), First-Principles-Based Kinetic Modeling of the Zeolite-Catalyzed Conversion of Furans to Aromatics
5. Mr. Jonathan Sutton (June 2014, Oak Ridge National Lab), Error reduction, uncertainty quantification, and sensitivity analysis methods for microkinetic modeling: Application and insights into the catalytic conversion of ethanol on late transition metals
6. Mr. Jacob McGill (October 2013, Apogee Research), Control of pattern formation in self-assembly
7. Ms. Sarah Tupy (August 2013, 3M), Experimental studies on the reforming and hydrotreating of small oxygenates
8. Mr. Vinit Choudhary (May 2013, ExxonMobil), Mechanistic insights into Lewis and Brønsted acid catalyzed conversion of sugars to platform furan derivatives in aqueous media
9. Mr. Matthew Mettler (June 2012, ExxonMobil), Revealing cellulose pyrolysis chemistry for biofuels production
10. Mr. Michael Saliccioli (April 2012, ExxonChemicals), On the reforming mechanisms and rational catalyst design for chemical conversion of biomass-derived oxygenates
11. Ms. Danielle Hansgen (June 2011, Intel), Rational catalyst design for the ammonia decomposition reaction
12. Mr. William Lonergan, (May 2011, ExxonMobil), Structure-property relationship of supported Pt/3d bimetallic catalysts
13. Mr. Khalid Ali Al-Majnouni, (January 2011, Saudi Arabia), High temperature decomposition of Bronsted acid sites: Structures formed and their catalytic activity toward small alkanes activation
14. Mr. J. Federici, (June 2009, ExxonMobil), Catalytic kinetics and thermal management in microchemical systems for distributed energy and portable power generation
15. Mr. A. Chatterjee (May 2007, Los Alamos Nat. Lab), Nanoscale modeling and control of self-assembled nanoparticle arrays using a hierarchy of multiscale models
16. Mr. J. Ludwig (March 2007, Exxon Mobil), Molecular dynamics of the dissociation of hydrogen on catalytic surfaces
17. Mr. J. Rimer (Ph.D., Oct. 2006, NYU), Self-assembly of silica nanoparticles and their role in the mechanism of silicalite-1 crystallization
18. Mr. S. Deshmukh (Ph.D., June 2006, Velocys), Design principles for multifunctional microchemical systems: Application to portable hydrogen production
19. Mr. M. Snyder (April 2006, Univ. Minnesota), Multiscale approaches for elucidating structure-properties relations of molecular transport in polycrystalline microporous thin films
20. Mr. J. Fedeyko (March 2006, Johnson Matthey), Silica phase behavior and the formation of microporous and mesoporous materials
21. Mr. Kapil Mayawala (May 2006, Novartis), Spatiotemporal modeling of epidermal growth factor receptor signaling pathway
22. Mr. A. Mhadeshwar (June 2005, GE), A hierarchical multiscale approach for predictive microkinetic modeling of hydrogen production
23. Mr. D. Norton (April 2005, GE), Design and development of portable microchemical power generators
24. Ms. G. Bonilla (Jan. 2004, IBM), Modeling, analysis, and characterization of zeolite MFI crystal and membrane growth
25. Mr. S. Fisher (Nov. 2003, GE Plastics), The construction of palladium and palladium-alloy supported membranes for hydrogen separation using supercritical fluid deposition
26. Ms. S. Raimondeau (Aug. 2002, ExxonMobil), Multiscale and reduced models of chemical reactors

27. Ms. M. Gummalla (Ph.D., Nov. 2001, UTRC), Chemical synthesis and fire suppression in diffusion flames
28. Mrs. P. Aghalayam (Dec. 2000, IIT Bombay), Interactions of premixed flames with surfaces: Flame stability and pollutant abatement
29. Mr. V. Nikolakis (Dec. 2000, Univ. of Patras), Theoretical and experimental studies of zeolite nanocrystal growth
30. Mr. Y. K. Park (April 2000, Carrier), Homogeneous and catalytic oxidation of hydrogen and methane
31. Mr. P. -A. Bui (May 1998, GE), Modeling reacting flows near reactive surfaces: catalytic oxidation and PECVD

#### MS

32. Mr. Jacob Weiner (December 2011, UD), Ammonia decomposition on NiPt supported on  $\gamma$ -alumina: a study of stability of real catalysts
33. Mr. Matthew Mettler (July 2010, UD), Scale-out and stability of microreactor stacks for syngas production
34. Mr. Stuart D. Collins (May 2009), Multiscale Monte Carlo study of epidermal growth factor receptor diffusion and dimerization
35. Mrs. A.-M. Niehaus (April 2007, DuPont), Simulations of epidermal growth factor receptor dynamics on corralled membrane surfaces
36. Ms. A. Samant (June 2007, Mathworks), Multiscale Monte Carlo methods to cope with separation of scales in stochastic simulation of biological networks
37. Mr. B. Feist (May 2006, Air Liquide), High throughput experimentation and microkinetic modeling
38. Mr. R. Lam (Feb. 2001, EmKaltenbach-Thuring, France), Atomistic-continuum hybrid models for epitaxial growth of materials and homogenized mesoscopic theories for diffusion through nanoporous films
39. Mr. J. Reese (Dec. 99, Software developer), Coupled molecular and continuum scale models: Application to catalytic reactors
40. Mr. S. Kalamatianos (Jan. 1995, Dimensions International, Inc.), Bifurcation behavior and mechanism reduction in lumped systems: Combustion of hydrogen in air

#### **Undergraduate Student Research Advising**

- Joseph Hasse, Catalysis of Electrophilic Aromatic Substitution of Furans by Brønsted or Lewis Acidic Zeolites; Calculation of the Degree of Polymerization of Lithium Bromide Pretreated Cellulose (Summer 2014-Present)
- James Kennedy, Cellulose Hydrolysis in Acidified Molten Salt Hydrate (AMSH) Media; Kinetics of Cellulose Hydrolysis and the Determination of Lithium Bromide Concentration (Summer 2014-Present)
- Brian Dinkelacker, Partition Coefficient of 5-hydroxymethylfurfural in Its Extraction from Aqueous to Organic Solvents (Summer 2015)
- Ryan Dudek (Summer 2015)
- Rachel Muzzelo, On the Reversal of Electron Demand in Diels-Alder Cycloaddition of Non-Nucleophilic Furans using Nucleophilic Modifiers: A Theoretical Study (Summer 2015)
- Brittany Wiebe, Catalytic Transfer Hydrogenation of Hydroxymethylfurfural to 2,5-Dimethylfuran with Carbon-supported Ruthenium Catalysts: The Effect of Carbon Support (Summer 2015)
- Zhexi Lin, Elucidating the Structure, Reaction Pathway and Kinetics of the Carbohydrate Derived Humins; Designing Bimetallic Catalysts to Improve the Catalyst Selectivity and Stability (Summer 2013, Summer and Fall 2014, Spring 2015)
- Shuting Feng, Adsorption Calculations of Biomass Derivatives in Zeolites; Dehydration Chemistry-Proton Affinity Database (Summer 2012-Spring 2014)
- Nickolas Martin, Liquid Phase Catalytic Transfer Hydrogenation of Furfural over Ru/Lewis Acid Catalysts; Hydrodeoxygenation of Furans (Summer 2013-Present)
- Michael Orella, Humins Formation (Summer 2013-Spring 2014)
- Mohamed Eltahir, Hydrodeoxygenation of Furans (Summer 2013)
- Zach Erdman, Kinetics of Bronsted and Lewis Acid Sites in Zeolites (Summer 2013)
- Hannah Phillips, Ether Formation on RuO<sub>2</sub> and ReO<sub>3</sub> Oxide (Summer 2013)
- Zachary Mozer (high school student), Synthesis of Mono and Multimetallics and Multicondenser for High Throughput Experiments (Summer 2013)
- Juan Lucio-Vego, Mechanism of Terephthalic Acid via DFT (Summer 2012)
- George Peklaris, Understanding the Effect of Solvent - Solute Interaction, pH, & Temperature on Sugar Dehydration Chemistry (Summer 2012)

- Andrew Shah, Investigation of the adsorption of carbohydrates and furans in microporous catalysts (Summer 2012); Computations of composition in ionic liquids (Winter 2011, Summer 2011)
- Evan Sohodski, Reactive adsorption studies of fructose dehydration to maximize the HMF & levulinic acid yields (Summer 2012, Fall 2012)
- Catherine Halat, Measurements of solubilities (Winter 2011, Summer 2011)
- Colin Sweeney, Biomass reactions in ionic liquids (Summer 2010, Fall 2010); Biodiesel production (Winter and Spring 2011)
- Cory Mackintosh, Reactions in biphasic systems (Summer 2010, Fall 2010, Spring 2011)
- Deniz Dindi, Catalyst synthesis (Summer 2009)
- Shannon O'Brien, REU student from Manhattan College, Process intensification, (Summer 2009)
- Robert Jackson, REU student from MIT, Thermoelectric measurements (Summer 2009)
- Stanley Herrmann, DFT studies of bimetallic catalysts (Winter, Summer, and Fall 2009, Summer, Fall 2010, Winter and Spring of 2011)
- Megan Zagrobelny, Reactor optimization; Biomass reactor design (Winter 2008, Summer 2008, Winter 2009, Fall 2009, Spring 2010)
- Anshu Arya, Microreactor experiments (Summer 2007, Winter 2008, Summer 2008, Winter 2009, Spring 2009)
- Zack Ulissi, Multiscale modeling of chemical kinetics (Summer 2007; Winter 2007, Winter 2008, Summer 2008, Winter 2009, Spring 2009)
- Nick Hanes, JP8 kinetics (Summer 2008)
- Steven Zaritsky, Microchemical systems experiments (Summer 2006)
- Ryan Kenaley, Fabrication of portable fuel to electricity converters (Summer 2006; Winter 2007)
- Daniel D. Roth; Experimental studies of self-assembly of Germanium nanoparticles (Summer 2005; Winter 2006; Summer 2006)
- Eavan Murphy, modeling of self-assembly of EGFR receptors (Winter 2006, Summer 2006)
- Sumanth Swaminathan, multiscale modeling (summer and fall of 2004)
- Kevin Voit, fabrication of microreactors (winter break and summer of 2004)
- Dan Miller, Stochastic modeling of biological networks (summer of 2004)
- Justin Federici, Fabrication of microreactors (summer of 2004)
- Matthew Ginzberg, BS 05, Fabrication of and experiments in microreactors (2003)
- Laura Parrish, NSF-REU Undergraduate Research Student, 2003
- Pat Schilling, Mesoscopic modeling of catalytic processes (2002)
- Elizabeth Bell, Experiments and simulations for surface reaction mechanism development (2002)
- Harry Bermudez, Diffusion flames (1998-99)
- Petersen Hasjim, Polymer flammability (1998)
- Markus Zacharias, Simulated annealing optimization of nanoclusters (1995-96)
- Kevin Chasse, Free energy calculation of nanoclusters (1997)
- Elizabeth Wilder, Monte Carlo simulations of surface reactions and combustion studies (1994-95)
- Matthew Zullo, NO<sub>x</sub> reduction (1995)

### Student Awards

- Theodore A. Koch Award, Catalysis Club of Philadelphia, Alexander Mironenko, 2016
- ISCRE 24 Dow travel award, Marcel Nunez, 2016
- CCEI Achievement Award, Alexander Mironenko, 2016
- AIChE CRE Division Travel Award, Alexander Mironenko, 2016
- AIChE CRE Division Travel Award, Tyler Josephson, 2015
- FOMMS Fellowship, Alexander Mironenko, July 2015
- Kokes Award of 24th North American Catalysis Society (NACS) Meeting, Alexander Mironenko, June 2015
- Philip & Ruth Evans Chemical Engineering Fellowship, Tyler Josephson, April 2015
- AIChE CRE Division Travel Award, Vassili Vorotnikov, 2014
- Gordon Research Conference, first place poster award, Georgios Tsilomelekis, 2014
- Eastman Chemical Student Award of 2013 (CCST), Nima Nikbin, October 2013
- AIChE CRE Division Travel Award, T. Dallas Swift, 2013
- Kokes Award of 23<sup>rd</sup> North American Catalysis Society (NACS) Meeting, Nima Nikbin, June 2013

- Kokes Award of 23<sup>rd</sup> North American Catalysis Society (NACS) Meeting, Matthew Christiansen, 2013
- Catalysis Club of Philadelphia's poster competition award (1<sup>st</sup> runner-up) to Vinit Choudhary, 2012
- George W. Laird Merit Fellowship, Tyler Josephson, 2012
- NSF graduate research fellowship, Tyler Josephson, 2012
- Fraser and Shirley Russell Teaching Fellowship, Jacob McGill, 2012
- Bill Baron Fellowship Award, Michael Saliccioli, 2011
- Kokes Award of 22<sup>nd</sup> North American Catalysis Society (NACS) Meeting, Michael Saliccioli, 2011
- Catalysis Club of Philadelphia's poster competition award, Timothy Courtney, 2011
- AIChE CRE Division Travel Award, Matthew Mettler, 2011
- AIChE CRE Division Travel Award, Michael Saliccioli, 2010
- NSF graduate fellowship, Vassili Vorotnikov, 2010
- NSF graduate fellowship honorary mention, Jonathan Sutton, 2009
- NSF graduate fellowship, Zack Ulissi, 2009
- UD team takes top honors in math modeling contest (Zack Ulissi);  
<http://www.udel.edu/udaily/2009/apr/topmath041609.html>, 2009
- DOE Computational Fellowship, Zack Ulissi (4 years, \$250,000), 2009,  
[www.udel.edu/udaily/2009/mar/doefellowship033009.html](http://www.udel.edu/udaily/2009/mar/doefellowship033009.html),
- Humboldt Research Fellowship, Matteo Maestri, 2009
- American Institute of Chemical Engineers Sophomore Award, Stanley Herrmann, 2009
- Sylvia and Charles Joanedis Chemical Engineering Scholarship, Stanley Herrmann, 2009
- NSF EPSCoR Scholarship (Grant EPS-0447610) for the Summer Scholars Research at the University of Delaware, Stanley Herrmann, 2009
- Kokes Award, 21<sup>st</sup> North American Catalysis Society, Michael Saliccioli, 2009
- Kokes Award, 21<sup>st</sup> North American Catalysis Society, Danielle Hansgen, 2009
- AIChE CRE Division Travel Award, Danielle Hansgen, 2009
- Griselda Bonilla featured in GEM newsletter;  
[http://www.gemfellowship.org/gem\\_alumni\\_spotlight/bonilla.php?utm\\_medium=email&utm\\_source=Campaign+Monitor&utm\\_content=153553514&utm\\_campaign=June+eNewsletter](http://www.gemfellowship.org/gem_alumni_spotlight/bonilla.php?utm_medium=email&utm_source=Campaign+Monitor&utm_content=153553514&utm_campaign=June+eNewsletter)