

## CURRICULUM VITAE

### Dionisios (Dion) G. Vlachos

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**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 Tech. Univ. of Athens, Athens, Greece, 1987

### Current Academic Appointments

Unidel Dan Rich Chair in Energy Professor of Chemical and Biomolecular Engineering, Univ. of Delaware, 2021-  
Professor (Joint) of Physics and Astronomy, University of Delaware, 9/1/15-8/31/21

ExxonMobil Visiting Chair Professor, National University of Singapore, Singapore, 2018-2021

Director, Delaware Energy Institute (DEI), 2016-

Director, Catalysis Center for Energy Innovation (CCEI), an Energy Frontier Research Center (EFRC) funded by DOE with \$42.7 M, 2009-2022

RAPID Manufacturing Institute UD Lead ~\$15 M (2018-2022)

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

Focus Area Leader of Intensified Process Fundamentals of RAPID Manufacturing Institute, 2017-2020

Allan and Myra Ferguson Prof. of Chemical and Biomolecular Engineering, Univ. of Delaware, 2016-2020

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

- Circular economy and waste derivatization, distributed (bio)chemical manufacturing, process intensification and novel catalytic reactors, renewable fuels and chemicals, catalyst informatics and in silico materials prediction, and kinetic modeling of biomass, shale gas, nitrogen cycle, and CO<sub>2</sub> cycle.
- Multiscale modeling, simulation, and dynamics: data science applied to multiscale modeling and experimental systems; hybrid, hierarchical, and coarse-grained branches of multiscale modeling; mesoscopic theory; model reduction; computational fluid dynamics; stochastic processes and kinetic Monte Carlo; molecular dynamics; density functional theory; nonlinear dynamics and bifurcation theory.

### Select Honors and Awards

Irving Wender Award for Excellence in Catalysis from the Pittsburgh-Cleveland Catalysis Society, 2020

ExxonMobil Visiting Chair Professorship, National University of Singapore, Singapore, 2018-2021  
Emerging Feedstocks and Opportunities, Distinguished Lecture in Energy, EPFL ChemE seminar series, EPFL, November 30<sup>th</sup>, 2018  
Lead of the Crosscut Panel for the Basic Energy Sciences (BES) Roundtable on Chemical Upcycling of Polymers, April 30 – May 1, Bethesda, MD  
Invited panelist and report writer, Basic Research Needs: Catalysis Science to Transform Energy Technologies workshop, 2017  
Doumas Lecture, Department of Chemical Engineering, Virginia Tech, 2016  
Philadelphia Catalysis Club Award, 2016  
Allan and Myra Ferguson Professorship of Chemical and Biomolecular Engineering, Univ. of Delaware, 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 (7/13/15-7/12/22); 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.*

*International Scientific Committee/Board Member: [IUPAC International Conference on Green Chemistry](#), Athens, Greece, October 18-22, 2020, [XXIV International Conference on Chemical Reactors CHEMREACTOR-24](#), Aug. 30-Sept. 4, 2020, Milan, Italy; [2<sup>nd</sup> International Process Intensification Conference](#) (Leuven, Belgium, 27-29 May 2019); Process Systems Engineering International Programming Committee, San Diego, CA, July 1-5, 2018; International Conference on Structured Catalysts and Reactors, ICOSCAR 6, Bad Herrenalb/Karlsruhe, Germany, on September 11-14, 2019; TU Delft Process Technology Institute (2013-2019); 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](#), 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**

A participant, presenter, and writer of DOE CSGB Reactions/Separations Workshop, January 11-14, 2021.  
A participant and presenter, DOE-Basic Energy Sciences-UK Catalysis Hub, October 8, 2020, joint virtual meeting.  
Co-organizer, Modeling – software – model library: The RAPID proposition, Modeling and Software Workshop, June 2019, Houston, TX  
Leader of the Crosscut Panel for the Basic Energy Sciences (BES) Roundtable on Chemical Upcycling of Polymers, April 30 – May 1, 2019, Bethesda, MD  
RAPID Leadership: Advised and co-developed with RAPID the research roadmap on modular manufacturing, 2018. Oversee the portfolio of RAPID projects in the Intensified Process Fundamentals Focus area, which consists of 6 large projects, of the order of 6 million per year or a total of >\$20 million for the duration of RAPID.  
ISCRE Vice President (2017-2018), President (2019-20), and Past President (2021-22)  
AIChE Awards Committee Member, 2012-2017  
Council of Fellows, Delaware Environmental Institute (DENIN), 2017-  
Modular Manufacturing Workshop Organizer, Arlington at Ballston, VA January 17/18, 2017, and [Roadmap](#) leader  
Director of ORCS, 2016  
The representative of Philadelphia Catalysis Club (CCP) in the North American Catalysis Society (NACS), 2015-

International Program Committee Member of the TU Delft Process Technology Institute, 2012-2019  
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 the workshop ‘Harnessing DOE’s High-Performance Computing Expertise to Strengthen the US Chemical Enterprise,’ 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, Gore

### Overview of Research and Educational Impact

- **>430 refereed publications; >19,600 total citations, >2,000 citations per year** in 2018-2020, and an **h-index of 75 (by ISI)**; **>26,600 total citations, >3,000 citations per year** in 2020, and an **h-index of 90 (by google scholar)**
- **High Impact Journal Papers:** Science (1), Sciences Advances (2), Nature Family Journals (10), ACS Catalysis (35), ACS Central Science (2), Energy & Environmental Science (5), Green Chemistry (8), J. Amer. Chem. Soc. (8), Nano Letters (3), Chemical Sciences (1)
- Research funding from recent grants (as the lead principal investigator) over **\$74,000,000**
- 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)
- Co-inventor in **10 disclosures, patent applications, or patents**
- 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 many institutions with funding of **\$42.7 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, the first introduction of Lewis acid catalysts for the hydrodeoxygenation of furans, and the production of detergents, dienes, lubricants, and adhesives. One of the four centers, and the only one in catalysis, that has been renewed twice from the original 46 awarded centers
- 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, by collaborators and the broader community, transforming the rather empirical field of biomass chemistry 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. Teaching frequently multiscale kinetics tutorials at workshops. Created an exchange program of undergraduate, graduate, and postdoctoral fellows among CCEI institutions and 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 five high school students, including students with special needs and from underrepresented groups over the past nine years. Created four new courses on applied mathematics (2), kinetics (1), and energy principles (1) at the graduate and advanced undergraduate level. Headed software implementation and tutorial development across the undergraduate and graduate curriculum of chemical engineering of UD.

- **Journal Covers by Group Publications**



**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.

## PATENTS, PATENT APPLICATIONS, AND DISCLOSURES

1. D. Norton, E. Wetzel, D. G. Vlachos, 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).
4. L. Wang, S. Advani, A. Prasad, D. G. Vlachos, W. Zheng, Nanosizing Early Transition Metal Carbides Within Composite Membranes for Fuel Cell Applications. PCT/US2017/029306 (filed 4/25/17)
5. R. F. Lobo, D. G. Vlachos, E. Saraci, Precursor to Terephthalic Acid, U.S. Provisional Patent Application 62/375,915 (filed on 8/17/16)
6. D. G. Vlachos, B. Saha, S. Sadula, An Integrated Process for Direct Saccharification and Dehydration of Intact Biomass to Furfurals, PCT/US2017/46874 (filed on 8/15/17)
7. D. G. Vlachos, B. Saha, S. Dutta, A Process for Production of C-C Coupled Long Carbon Fuel Precursors Using Improved Graphene Oxide. U.S. Provisional Patent Application 62/375,995 (filed 8/17/16)
8. D. G. Vlachos, B. Saha, S. Dutta, Hydrophobic Graphene Oxide Sponge (GOS) for Efficient Oil Separation and C-C Coupling Reaction. U.S. Provisional Patent Application 62/465,864 (filed on 3/2/17)
9. B. Saha, S. Liu, D. G. Vlachos, Production of Furan-based Renewable Lubricants. U.S. Provisional Patent Application 62/546,603 (filed on 8/17/17)
10. T. Epps, S. Wang, B. Saha, L. Shuai, D. G. Vlachos, Lignin-Based Pressure Sensitive Adhesives, U.S. Provisional Patent Application 62/615,040 (filed on 1/9/18)
11. B. Saha, S. Liu, D. G. Vlachos, A. Norton, Bio-based base oils from fatty acids and biomass, PTC/US20 19/063325 (filed 11/29/28)
12. E. Ebikade and D. G. Vlachos, Production of Antioxidants, Furfurals, and Biochar From Food Waste (filed on 6/5/19)
13. E. Gottlieb, R. O'Dea, E. Ebikade, T. H. Epps, III, D. G. Vlachos, Low-pressure depolymerization of lignocellulosic biomass, PCT/US2020/046384 (filed on 6/27/19)
14. S. Liu and D. G. Vlachos, A new process for the production of fuels and lubricants from recycled plastics (filed 1/28/20)
15. S. Sadula, B. Saha, and D. G. Vlachos, A cost-efficient process for the production of monosaccharides and lignin from biomass (filed on 3/29/20)
16. W. Chen, A. Malhotra, and D. G. Vlachos, Reactor Configuration using a Microwave Absorbing Scaffold for Endothermic Reactions (filed on 8/28/20)

## 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. Eng. 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).
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).
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\* Impact journal article (IF>8)

## RESEARCH TEXTBOOKS, SOFTWARE, EDITORIALS, PROCEEDINGS, AND OTHER REPORTS

### Textbooks

- An introduction to multiscale analysis for well-mixed, chemical and biological reacting systems (in preparation).
- Graduate kinetics and reactor textbook; anticipated publication date in June 2019.

### Software

- **pMuTT**: Python Multiscale Thermochemistry Tool; J. Lym, G. Wittreich and D. G. Vlachos
- **OpenMKM**: Microkinetic Modeling for Complex Reaction Networks; B. Medasani and D. G. Vlachos
- **ReNView**: Reaction Network Viewer; An open-source framework for reaction path visualization of chemical reaction systems; U. Gupta and D. G. Vlachos

### Perspectives (Not Peer Reviewed)

B. Saha and D. G. Vlachos, Bio-based lubricant base-oils: Tuning synthesis to meet market desirability. *The catalyst reviews, Inc.* **32**(5), pgs. 1 & 6 (2019).

### 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.
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### Invited Papers

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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). **In 2015, it run 7<sup>th</sup> in citations of the journal for that year and remains as 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.**
18. Invitations by ACS Catal. and Nature Catal.

#### Book Chapters and Chapters in Encyclopedias and Handbooks

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. 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).

9. 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).
10. 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.
11. 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.
12. 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.
13. G. R. Wittreich, K. Alexopoulos, and D. G. Vlachos, *Microkinetic Modeling of Surface Catalysis*, Springer International Publishing AG, Part of Springer Nature 2018, W. Andreoni, S. Yip (eds.), *Handbook of Materials Modeling*, [https://doi.org/10.1007/978-3-319-50257-1\\_5-1](https://doi.org/10.1007/978-3-319-50257-1_5-1).

### 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 AND PLENARY 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, 13th 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.
236. Process Intensification for Reactions and Reactors, Process Intensification Topical Conference at the AIChE Spring Meeting in San Antonio, TX, March 27-29, 2017.
237. Mechanisms of lignin and furan derivative upgrade on metal surfaces, 253<sup>rd</sup> ACS National Meeting in San Francisco, CA, April 2-6, 2017.
238. Recent advances in biomass conversion for bioproducts and fuels, 253<sup>rd</sup> ACS National Meeting in San Francisco, CA, April 2-6, 2017.
239. Renewable chemicals and fuels from biomass, Technical University of Eindhoven, Eindhoven, Netherlands, May 17, 2017.
240. Renewable chemicals and fuels from biomass, 254<sup>th</sup> ACS National Meeting, Washington, DC, August 20-24, 2017.
241. In silico prediction of materials for energy applications, 254<sup>th</sup> ACS National Meeting, Washington, DC, August 20-24, 2017.
242. Process Intensification and Modularization for Sustainability, 2017 AIChE Annual Meeting, Minneapolis, MN, October 29-November 3, 2017.

243. Predictive Multiscale Modeling of Complex Systems for Sustainability, 8<sup>th</sup> Asian-Pacific Chemical Reaction Engineering Symposium (APCRE 2017), Shanghai, China, November 12-15, 2017. Plenary talk.
244. Renewable chemicals and fuels from biomass, State Key Laboratory of Physical Chemistry of Solid Surfaces, Xiamen University, Xiamen, China, November 15<sup>th</sup>, 2017.
245. Small molecules, big challenges, National University of Singapore, Singapore, November 17, 2017.
246. Emerging Feedstocks and Opportunities, Lehigh University, Bethlehem, PA, January 24, 2018.
247. Renewable Chemicals and Fuels: From First Principles to Chemical Manufacturing, New York University: Tandon School of Engineering, January 26, 2018.
248. Predictive Multiscale Modeling of Complex Systems for Sustainability, Georgia Institute of Technology, Atlanta, GA, April 4, 2018.
249. Renewable chemicals and fuels from biomass, Invited Talk, Washington University, St. Louis, MO, April 13, 2018.
250. Machine Learning for Reducing Parametric and Model Form Uncertainty of Predictive, Complex Chemical-Reaction Models. Keynote, ISCRE 25<sup>th</sup>, Florence, Italy, May 20-23, 2018.
251. Predictive Modeling of Complex Chemical Reactions: Correlated Data, Uncertainty Quantification, And Machine Learning, Invited, First Conference on Machine Learning in Science and Engineering, Pittsburgh, PA, CMU, June 7<sup>th</sup>, 2018.
252. In Silico Prediction of Materials for Energy Applications, Pittsburgh-Cleveland Catalysis Society (PCCS) Annual Symposium, Pittsburgh, PA, June 8<sup>th</sup>, 2018.
253. In Silico Prediction of Materials for Energy Applications, FIPSE (Future Innovation in Process Systems), Chalkidiki, Greece, June 25-27, 2018.
254. Modular Manufacturing for Emerging Energy Industries: Shale Gas and Biomass Upgrade, Plenary (with Stratos Pistikopoulos), Process Systems Engineering (PSE 2018), San Diego, CA, July 1-5, 2018.
255. Renewable Chemicals and Fuels: From First Principles to Chemical Manufacturing, National Technical University of Athens, Athens, Greece, October 17, 2018.
256. From First Principles to Chemical Manufacturing of Renewable Chemicals, AIChE Invited talk in honor of CRE Young Investigators, AIChE Annual Meeting, Pittsburgh, PA, October 29-November 2, 2018.
257. Multi-level Bridge between Reaction Engineering and Computational Catalysis, Plenary lecture, XXIII International conference on Chemical Reactors, CHEMREACTOR-23, Ghent, Belgium, November 5-9, 2018.
258. Emerging Feedstocks and Opportunities, Distinguished Lecture in Energy, EPFL ChemE seminar series, EPFL, November 30<sup>th</sup>, 2018.
259. Data Science for Chemistry and Chemical Engineering, National University of Singapore, Singapore, January 7-11, 2019.
260. From First Principles to Chemical Manufacturing of Renewable Chemicals, National University of Singapore, Singapore, January 7-11, 2019.
261. Non-oxidative Conversion of Methane to Value-added Chemicals, Spring ACS National Meeting, Orlando, FL, March 31 – April 4, 2019
262. Computational Operando Spectroscopy and Kinetics for Single Atom Catalysis, Spring ACS National Meeting, Orlando, FL, March 31 – April 4, 2019
263. Artificial Intelligence for Chemical Sciences, Spring ACS National Meeting, Orlando, FL, March 31 – April 4, 2019
264. Renewable Chemicals and Fuels: From First Principles to Chemical Manufacturing, Chemical Engineering Department Seminar, University of California at Santa Barbara, May 9, 2019.
265. Modular Manufacturing for Emerging Energy Industries: Green Ammonia, Shale Gas, and Biomass Upgrade, Plenary at Second International Process Intensification Conference (IPIC2), Leuven, Belgium, May 27-29, 2019.
266. Modular Manufacturing for Emerging Energy Industries: Green Ammonia, Shale Gas, and Biomass Upgrade, Plenary at 12<sup>th</sup> Panhellenic Symposium of Chemical Engineering, Athens, May 29-31, 2019.
267. Catalyst and Process Intensification for Modular and Improved Manufacturing of Emerging Energy Industries, LyondellBasell Company, Houston, TX, June 11<sup>th</sup>, 2019.
268. Chemical Manufacturing of Renewable Bioproducts from Diverse Feedstocks, Plenary at CatBior V, Turku / Åbo, Finland, September 23-27, 2019.
269. Chemical Manufacturing of Renewable Bioproducts from Diverse Feedstocks, Oklahoma State University, October 8<sup>th</sup>, 2019.
270. Business Case for Process Intensification and Modularization, Panel Presentation and Discussion at SOCMA (Synthetic Organic Chemical Manufacturers) Meeting, Philadelphia, PA, October 10, 2019.

271. Computation-driven catalyst discovery, Plenary at International Conference on Unconventional Catalysis, Reactors and Applications, Zaragoza, Spain, October 16-18, 2019.
272. Renewable Chemicals and Fuels: From First Principles to Chemical Manufacturing, Iowa State University, Ames, IA, January 23<sup>rd</sup>, 2020.
273. Biorefinery separations, Gordon Conference on Chemical Separations, Galveston, TX, January 26-31, 2020.
274. Data Science for Chemistry and Chemical Engineering, Johns Hopkins University, Baltimore, MD, February 6, 2020.
275. Data Science and Multiscale Modeling in Sciences and Engineering, DARWIN HPC symposium, Newark, DE, February 12, 2020.
276. Renewable Chemicals and Fuels: From First Principles to Chemical Manufacturing, Lectures at the Leading Edge, Chemical Engineering and Applied Chemistry, Univ. of Toronto, March 18<sup>th</sup>, 2020. Rescheduled as a Webinar for October 14, 2020.
277. Graph Theoretical Approaches for Thermochemistry, Uncertainty Quantification, and Atomically Resolved Kinetic Monte Carlo Simulations, Spring National ACS Meeting, Philadelphia, PA, March 22 – 26, 2020. Postponed.
278. Data Science and Fundamentals for Closing the Materials Gap, Spring National ACS Meeting, Philadelphia, PA, March 22 – 26, 2020. Postponed.
279. Non-oxidative Conversion of Methane to Value-added Chemicals, Spring National ACS Meeting, Philadelphia, PA, March 22 – 26, 2020. Postponed.
280. Operando Spectroscopy, Kinetics, and Stability of Single-Atom Catalysts for CO Oxidation, Spring National ACS Meeting, Philadelphia, PA, March 22 – 26, 2020. Postponed.
281. Emergent Behavior of Catalysts Exposes Fundamental Limitations of Sabatier's Principle, Spring National ACS Meeting, Philadelphia, PA, March 22 – 26, 2020. Postponed.
282. Closing the gap between experiments and calculations: How far are we? Keynote Lecture at [GRC Catalysis](#), New London, New Hampshire, June 28-July 2, 2020, 2020. Postponed.
283. Computational Catalysis: A Process Intensification Tool; RAPID Webinar Series, July 30, 2020.
284. The roles of catalysis and reaction engineering in a circular economy, Plenary at ISCRE 26 & APCRE 9, New Delhi, India, December 6-9, 2020. Postponed.
285. Data science for catalyst discovery and process intensification, Webinar to the Department of Chemical Engineering at Texas Tech University, October 2, 2020.
286. Data science for catalyst discovery and process intensification, Webinar to Physical Science and Engineering Division, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia, October 12, 2020.
287. Data science and multiscale modeling for chemical sciences, Distinguished Seminar Series in Computational Science and Engineering, MIT, Webinar, November 19, 2020.
288. International Symposium on Green Chemistry ([ISGC](#)), La Rochelle, France, May 3-7, 2021.

## CONTRIBUTED PRESENTATIONS AT (INTER)NATIONAL 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", 229th 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. Guliants, 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
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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.
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- 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  $\text{CrCl}_3$  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  $\gamma\text{-Al}_2\text{O}_3$ , 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, Jingguang 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.
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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.
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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.
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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.
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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.
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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 Sylvan 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.
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392. Hannah Nguyen, Nick Xiao, Anatoly Frenkel, Stavros Caratzoulas, Dionisios G. Vlachos, On the Mechanism of Metal Chloride Catalysts in Reductive Etherification of Furan Derivatives, North American Catalysis Society Meeting, Denver, CO, June 5, 2017.
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423. Yifan Wang, Ya-qiong Su, Jin-Xun Liu, Ivo Filot, Konstantinos Alexopoulos, Dionisios G. Vlachos, Emiel J.M. Hensen, First-Principles Modeling of Single Atom Catalysis: CO Oxidation over Atomically Dispersed Pt on CeO<sub>2</sub>, AIChE Annual Meeting, Pittsburgh, PA, October 29-November 2, 2018.
424. Pierre Desir, Basudeb Saha, Dionisios G. Vlachos, Two-Phase Microreactor Design for the Reactive Extraction of Biomass Derivatives, AIChE Annual Meeting, Pittsburgh, PA, October 29-November 2, 2018.
425. Elvis Ebikade, Jonathan Lym, Basudeb Saha, Dionisios G. Vlachos, Kinetic Studies of Acid Hydrolysis of Linear Polysaccharides from Food Waste, AIChE Annual Meeting, Pittsburgh, PA, October 29-November 2, 2018.
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429. Natalia Rodriguez Quiroz, Dionisios G. Vlachos, A Fundamental Study of Cellulose Hydrolysis in Super Acidic Molten Salt Hydrate Media, 2018, AIChE Annual Meeting, Pittsburgh, PA, October 29-November 2, 2018.
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435. Joshua Lansford, Dionisios G. Vlachos, Catalyst Characterization from Complex Infrared Spectroscopy: A Machine Learning Approach, 2018, AIChE Annual Meeting, Pittsburgh, PA, October 29-November 2, 2018.
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437. Geun Ho Gu, Petr Plechac, Jonathan Lym, Dionisios G. Vlachos, Thermochemistry of Gas-Phase and Surface Species Via Lasso-Assisted Subgraph Selection, AIChE Annual Meeting, Pittsburgh, PA, October 29-November 2, 2018.
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440. Angela M. Norton, Sibao Liu, Basudeb Saha, Dionisios G. Vlachos, Renewable Lubricant Alkanes from Biomass-Derived Platform Chemicals, AIChE Annual Meeting, Pittsburgh, PA, October 29-November 2, 2018.
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442. Natalia Rodriguez-Quiroz, Dionisios G. Vlachos, Understanding Acidity of Molten Salt Hydrate Media for Cellulose Hydrolysis by Coupling Kinetic Studies, Electrolyte Solution Modeling, and 13C-NMR Experiments, 2019 North American Catalysis Society Meeting, Chicago, IL, June 23-28, 2019.
443. Geun Ho Gu, Yousung Jung, Dionisios G. Vlachos, Predicting Multi-Dentate Adsorbate Conformation on Metal Surfaces, 2019 North American Catalysis Society Meeting, Chicago, IL, June 23-28, 2019.
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445. Yifan Wang, Yaqiong Su, Emiel J. M. Hensen, Dionisios G. Vlachos, Statistical-Learning, First-Principles Modeling of the Stability and Dynamics of Single Atom Catalysts, 2019 North American Catalysis Society Meeting, Chicago, IL, June 23-28, 2019.
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453. Konstantinos Goulas, Jennifer D. Lee, Christopher B. Murray, Dionisios G. Vlachos, Spectroscopic Insights into the Origins of Selectivity of Bimetallic Hydrodeoxygenation Catalyst, 2019 North American Catalysis Society Meeting, Chicago, IL, June 23-28, 2019. Poster.
454. Joshua Lansford, Dionisios G. Vlachos, Catalyst Site Characterization from Complex Infrared Spectroscopy, 2019 North American Catalysis Society Meeting, Chicago, IL, June 23-28, 2019.
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461. Yifan Wang, Ziwei Cheng, Dionisios G. Vlachos, Model-Driven Design of Experiments and Optimization, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019.
462. Angela M. Norton, Weiqing Zheng, Dionisios G. Vlachos, Michael Tsapatsis, Jorge A. Boscoboinik, Probing Hydroxyl Groups on Metal-Supported 2-D Silica Films, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019.
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465. M. Alexander Ardagh, Shizhong Liu, Gerhard R. Wittreich, Omar A. Abdelrahman, Qi Zhang, Dionisios G. Vlachos, Paul Dauenhauer, Transcending the Volcano Plot: Enhancing NH<sub>3</sub> Synthesis with Dynamic Catalysis, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019.
466. Jonathan Lym, Gerhard R. Wittreich, Udit Gupta, Bharat Medasani, Dionisios G. Vlachos, Reaction Software Ecosystem and Data Hub for Heterogeneous Catalysis, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019. Poster.
467. Natalia Rodriguez Quiroz, Joshua Lansford, George Tsilomelekis, Dionisios G. Vlachos, Combining Experimental Kinetics and Thermodynamic Modeling with IR Spectroscopy and Machine Learning for Fundamental Studies and Fast Product Quantification, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019. Poster.
468. Maximilian R. Cohen, Dionisios G. Vlachos, A Computational Investigation of Catalytic Upgrading of CO<sub>2</sub> to Methanol over Indium Oxide, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019. Poster.
469. Jon Wilson, Stavros Caratzoulas, Dionisios G. Vlachos, Yushan Yan, pH Effects in the Hydrogen Oxidation Reaction: A DFT/MD Approach to Understand Adsorbed Hydroxyl on Platinum, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019.
470. Sai Praneet Batchu, Stavros Caratzoulas, Dionisios G. Vlachos, Mechanistic Understanding of the Role of Ga in the Dehydrogenation of Ethane on Ga/Al<sub>2</sub>O<sub>3</sub> Catalyst, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019. Poster.
471. Hilal Ezgi Toraman, Gerhard R. Wittreich, Dionisios G. Vlachos, Mechanism of Oxidative Dehydrogenation of Ethane at High Temperatures, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019. Poster.
472. Konstantinos Alexopoulos, Dionisios G. Vlachos, Descriptor-Based Modeling of CO Oxidation over Alumina-Supported Single Metal Atoms, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019. Poster.
473. Jiayi Fu, Weiqing Zheng, Shizhong Liu, Cong Wang, Stavros Caratzoulas, Raymond J. Gorte, Dionisios G. Vlachos, Structure-Property Relations of PtWO<sub>x</sub>/C Inverse Catalysts, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019. Poster.
474. Natalia Rodriguez Quiroz, Joshua Lansford, George Tsilomelekis, Dionisios G. Vlachos, Coupling Experimental Kinetics and Thermodynamic Modeling with IR Spectroscopy and Machine Learning for Fundamental Studies and Fast Product Quantification, 2019AIChE Annual Meeting, Orlando, FL, November 10-15, 2019. Poster.
475. Elvis Ebikade, Dionisios G. Vlachos, Food Waste Repurposing to an Integrated Biorefinery, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019. Poster.
476. Shizhong Liu, Jiayi Fu, Weiqing Zheng, Stavros Caratzoulas, Dionisios G. Vlachos, Brønsted Acid Sites on Tungsten Oxide/Platinum Catalysts, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019.
477. Sebastian Prodingler, Basudeb Saha, Dionisios G. Vlachos, Raul F. Lobo, Challenges and Opportunities in the Production of Dimethylfuran from Sugars By Performing Tandem Catalysis, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019.
478. Sibao Liu, Basudeb Saha, Dionisios G. Vlachos, Catalytic Production of Renewable Lubricant Base Oils from Biomass, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019.
479. Athanasios Kritikos, Yung Wei Hsiao, Dionisios G. Vlachos, Marianthi Ierapetritou, George Tsilomelekis, Adsorption of Biomass-Derived Value-Added Chemicals in a Micro-Packed-Bed Reactor. a CFD Study AIChE Annual Meeting, Orlando, FL, November 10-15, 2019.

480. Joshua Lansford, Dionisios G. Vlachos, Computational Modeling of Operando Infrared Spectroscopy for Site-Specific Catalyst Characterization, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019.
481. Zhaoxing Wang, Souryadeep Bhattacharyya, Dionisios G. Vlachos, Selective Extraction of Furfural and 5-Hydroxymethylfurfural from Mixed Lignocellulosic Biomass-Derived Feedstocks in Biphasic Solvent Systems, AIChE Annual Meeting, Virtual, November 16-20, 2020.
482. Abhinav Malhotra, Weiqi Chen, Ignacio Julian, José Manuel Catalá Civera, Jesús Santamaria, Dionisios G. Vlachos, Thermal Analysis of Structured Reactors for Microwave Reaction Engineering, AIChE Annual Meeting, Virtual, November 16-20, 2020.
483. Weiqi Chen, Kewei Yu, Abhinav Malhotra, Weiqing Zheng, Ignacio Julian, José Manuel Catalá Civera, Jesús Santamaria, Dionisios G. Vlachos, Ethane Oxidative Dehydrogenation in Microwave-Heated Fixed Bed and Structured Catalyst Reactors, AIChE Annual Meeting, Virtual, November 16-20, 2020.
484. Sai Praneet Batchu, Hsuan-Lan Wang, Weiqi Chen, Weiqing Zheng, Stavros Caratzoulas, Raul Lobo, Dionisios G. Vlachos, On the Reaction Mechanism and Kinetics of Ethane Dehydrogenation to Ethylene on Ga-Modified  $\text{Al}_2\text{O}_3$  Catalyst, AIChE Annual Meeting, Virtual, November 16-20, 2020.
485. Maximilian Cohen, Weiqi Chen, Dionisios G. Vlachos, A Data-Driven Investigation of Catalytic Upgrading of Ethane to Ethylene Over Ga/ $\text{Al}_2\text{O}_3$ , AIChE Annual Meeting, Virtual, November 16-20, 2020.
486. Yung Wei Hsiao, Dionisios G. Vlachos, Design and Characterization of a Microfixed-Bed for Reactive Separation of HMF, AIChE Annual Meeting, Virtual, November 16-20, 2020.
487. Seungyeon Lee, Ji Qi, Phillip Christopher, Stavros Caratzoulas, Dionisios G. Vlachos, Theoretical Insights into Heterogeneous Ethylene Hydroformylation on Atomically Dispersed Rh Supported By  $\text{ReO}_x$ -Modified  $\gamma\text{-Al}_2\text{O}_3$ , AIChE Annual Meeting, Virtual, November 16-20, 2020.
488. Yifan Wang, Ya-Qiong Su, Emiel J.M. Hensen and Dionisios G. Vlachos, Stability of Subnanometer Clusters in a CO Atmosphere via Machine Learning-Assisted Multiscale Modeling, AIChE Annual Meeting, Virtual, November 16-20, 2020.
489. Yunzhu Wang, Jiayi Fu, Weiqing Zheng, Dionisios G. Vlachos, Redispersions of Pt Nanoparticles to Single Atoms over Reducible Metal Oxides, AIChE Annual Meeting, Virtual, November 16-20, 2020.
490. Tai-Ying Chen, Montgomery Baker-Fales, Dionisios G. Vlachos, Data-Driven Optimization of Microwave-Assisted Continuous-Flow Microreactor for Biomass-Derived Carbohydrates' Conversion, AIChE Annual Meeting, Virtual, November 16-20, 2020.
491. Sophia Kurdziel, Joshua Lansford, Dionisios G. Vlachos, Vibrational Scaling Relationships for Transition States, AIChE Annual Meeting, Virtual, November 16-20, 2020.
492. Jiayi Fu, Shizhong Liu, Weiqing Zheng, Renjing Huang, Cong Wang, Raymond J. Gorte, Anatoly I. Frenkel, Stavros Caratzoulas, Dionisios G. Vlachos, Characterization and Activity of  $\text{WO}_x/\text{Pt}(111)$  Catalysts, CCEI Spring Symposium, Virtual, April 24, 2020.
493. Montgomery Baker-Fales, Tai-Ying Chen, Dionisios G. Vlachos, Electrification, Process Intensification, and Artificial Intelligence for Modular and Improved Chemical Manufacturing, AIChE Spring Meeting, Virtual, August 17-21, 2020.
494. Joshua Lansford and Dionisios G. Vlachos, Infrared Spectroscopy Data- and Physics-driven Machine Learning for Characterizing Complex Surface Structure, The Center for Dynamics and Control of Materials at UT Austin (Invited Talk) February 21, 2020.
495. James D. Sheehan, Elvis Ebikade, Dionisios G. Vlachos, Raul F. Lobo, Developing Lignin-based Polyelectrolytes for Applications as Eco-Friendly Flocculants, AIChE Annual Meeting, Virtual, November 16-20, 2020.