

**MULTISCALE MATHEMATICS FOR BIOMASS CONVERSION TO RENEWABLE
HYDROGEN
DE-FG02-05ER25702**

FINAL PROGRESS REPORT (AUGUST 15, 2012 – AUGUST 14, 2013)

Co-PIs: Petr Plechac^{1,4}, Markos Katsoulakis², and Dionisios Vlachos³ (Project leader)*

¹Department of Mathematics, University of Tennessee

²Department of Mathematics and Statistics, University of Massachusetts

³Department of Chemical and Biomolecular Engineering, University of Delaware

⁴ As of Sept. 1, 2010: Department of Mathematical Sciences, University of Delaware

* Contact information: vlachos@udel.edu; Tel. (302)-831-2830; Fax (302)-831-1048

OVERVIEW AND OBJECTIVES

The overall objective of this project is to develop multiscale models for understanding and eventually designing complex processes for renewables. To the best of our knowledge, our work is the first attempt at modeling complex reacting systems, whose performance relies on underlying multiscale mathematics. Our specific application lies at the heart of biofuels initiatives of DOE and entails modeling of catalytic systems, to enable economic, environmentally benign, and efficient conversion of biomass into either hydrogen or valuable chemicals. Specific goals include:

- (i) Development of rigorous *spatio-temporal coarse-grained kinetic Monte Carlo (KMC)* mathematics and simulation for microscopic processes encountered in biomass transformation.
- (ii) Development of *hybrid multiscale simulation* that links *stochastic* simulation to a *deterministic partial differential equation (PDE) model* for an entire reactor.
- (iii) Development of *hybrid multiscale simulation* that links *KMC simulation* with *quantum density functional theory (DFT) calculations*.
- (iv) Development of *parallelization* of models of (i)-(iii) to take advantage of Petaflop computing and enable real world applications of complex, multiscale models.

In this NCE period, we continued addressing these objectives and completed the proposed work. Main initiatives, key results, and activities are outlined below.

1. RESEARCH ACCOMPLISHMENTS FOR THE UD-SUPPORTED WORK

Below we describe our major accomplishments.

1.1 Multiscale Simulation of Structure Sensitivity of Catalytic Systems for Energy Applications

Steam methane reforming (SMR) is an important process for the industrial production of syngas. The structure sensitivity of SMR on metal clusters remains unresolved, as computational studies have been unable to reproduce experimental structural trends. A hierarchical multiscale modeling framework is employed to develop a model for SMR which takes into account nanoparticle structure and closes the gap between model predictions and experimental data.

Our prior DFT data have been used in mean-field microkinetic modeling to simulate the SMR chemistry on the Pt(111) and Pt(211) surfaces (preliminary kinetic Monte Carlo

simulations have also been performed). Parameters have been adjusted within the error of DFT to obtain better agreement with experiments. Very good agreement has been obtained as shown in Figure 1 and Table 1. The Pt(211) model gives though very low activation energy (E_a) compared to experiments indicating that steps are potentially blocked under reaction conditions and terraces (Pt(111)) play a major role in the structure sensitivity of this reaction.

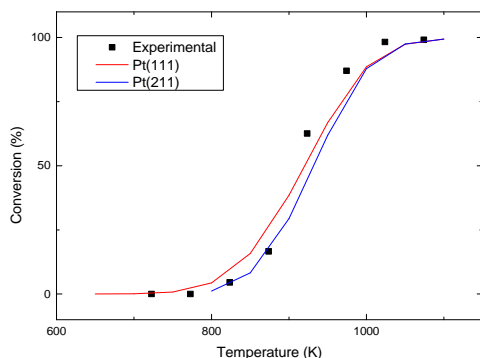


Table 1: Reaction orders and activation energy.

Surface	CH ₄	H ₂ O	E _a
Expts ²	1	0	20.4
Pt(111) model	0.95	0.04	20.6
Pt(211) model	0.83	0.05	12.4

Figure 1. Conversion on Pt(111) and Pt(211) surfaces compared to data from Hegarty et al. (*Catal. Today* 1998, 42, 225-232). The feed consisted of 13 kPa CH₄, 34 kPa H₂O, 46.8 kPa H₂, and 6 kPa Ar. A catalyst surface area to reactor volume ratio of 10000cm⁻¹ was assumed.

A sensitivity analysis of the model before adjustments to parameters (Figure 2) suggests that the dissociative adsorption of methane as well as the C-O bond formation reactions are kinetically important and therefore warrant further investigation through additional DFT calculations on various configurations of platinum atoms. Accurate parameterization of these important reactions along with a graph-theoretical KMC framework capable of explicitly including catalyst structure will be able to elucidate the role of different sites in the SMR chemistry, and this work is near completion.

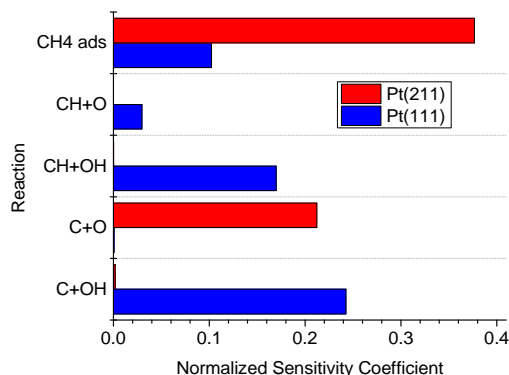


Figure 2. Sensitivity analysis of kinetic model on two structures.

1.2 Coupling of Quantum Mechanical, Density Functional Theory (DFT) and Kinetic Monte Carlo (KMC) Simulation

The ability to understand and eventually tailor the materials' properties over multiple length scales has always been a primary research goal. Toward this goal, we have completed the first-principles simulations of CO oxidation on Au nanoclusters to rationalize the magic size behavior of this exciting system.

Our detailed quantum mechanical (DFT) investigation of the CO oxidation activity on Au_6^- has been expanded to subnanometer Au clusters of different size, namely Au_8^- and Au_{10}^- . Specifically for Au_8^- cluster, which has been experimentally observed to be highly active towards CO oxidation, we identified a low-barrier reaction mechanism through the formation of a 4-center intermediate ($\text{CO}^* + \text{O}_2^*$). Interestingly, similarly to the Au_6^- case, a catalyst breathing mechanism has been observed, leading to reversible and irreversible deformations of the cluster. The slowest surface reactions are the formation of CO_2 either from the 4-center intermediate or from carbonate (species that poison the catalyst on Au_6). All carbonate structures are monodentate on Au_8^- and bidentate on Au_{10}^- and Au_6^- . We observe higher rate constants on Au_8^- than on Au_{10}^- . A low-energy pathway contributing to the CO oxidation activity on Au_8^- is the one presented in Figure 3a.

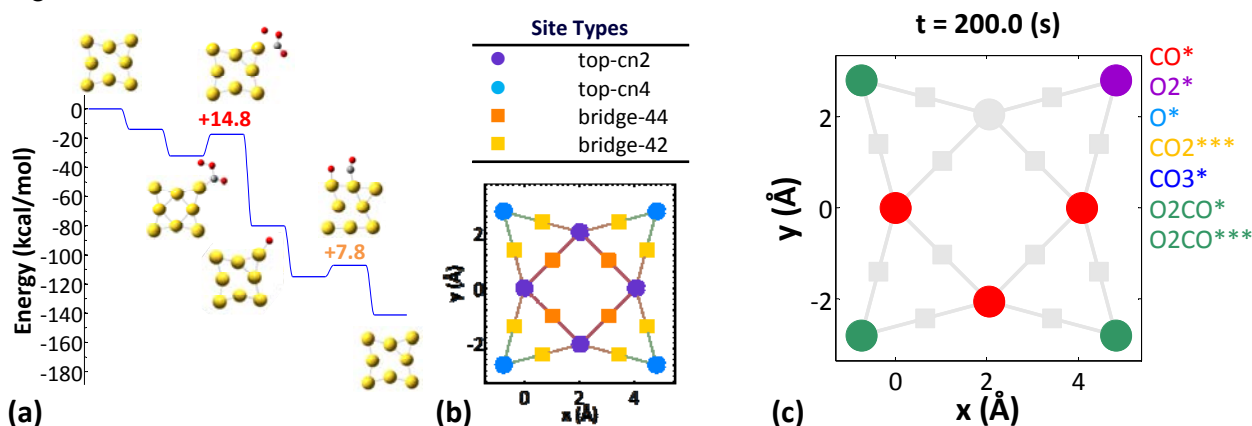


Figure 3. (a) Low-energy reaction pathway on Au_8^- contributing to CO oxidation activity of this cluster size. (b) The site types and lattice structure incorporated into the KMC simulation. (c) Snapshot from a KMC simulation showing the various adsorbates on the Au_8^- nanocluster.

To assess the complete CO oxidation activity of the Au nanoclusters, we performed kinetic Monte Carlo (KMC) simulations using as input detailed reaction information from the quantum mechanical results. Our KMC models of this reaction on Au_8^- and Au_{10}^- explicitly take into account the different binding configurations of the adsorbates participating in the chemistry, the oxidation mechanisms via the 4-center intermediates, as well as the direct oxidation steps. Carbonate formation on these two structures occurs only in the presence of CO_2 and was also included in the KMC model (Figure 3b). Using our previously developed Graph-Theoretical KMC method, we simulated the CO oxidation on Au_8 and Au_{10} revealing the most important reaction pathways contributing to the oxidation activity as well as the rate limiting steps.

On Au_8 the dominant pathway was found to be the one presented in Figure 3c, which entails the formation of the 4-center intermediate ($\text{CO}^* + \text{O}_2^*$), the decomposition thereof that leaves an O adatom on a corner site, and the subsequent CO oxidation that involves this leftover O. A similar mechanism involving a 4-center intermediate was found to be prominent on Au_{10}^- . For this structure our simulations suggest that the rate limiting step is the tilting of O_2 from bidentate (inactive) to monodentate (reactive) configurations. For Au_8^- , the 4-center intermediate decomposition was found to be rate limiting. No deactivation was observed for either Au_8^- or Au_{10}^- , in contrast to what was previously observed for Au_6^- (poisoning by carbonate). Moreover,

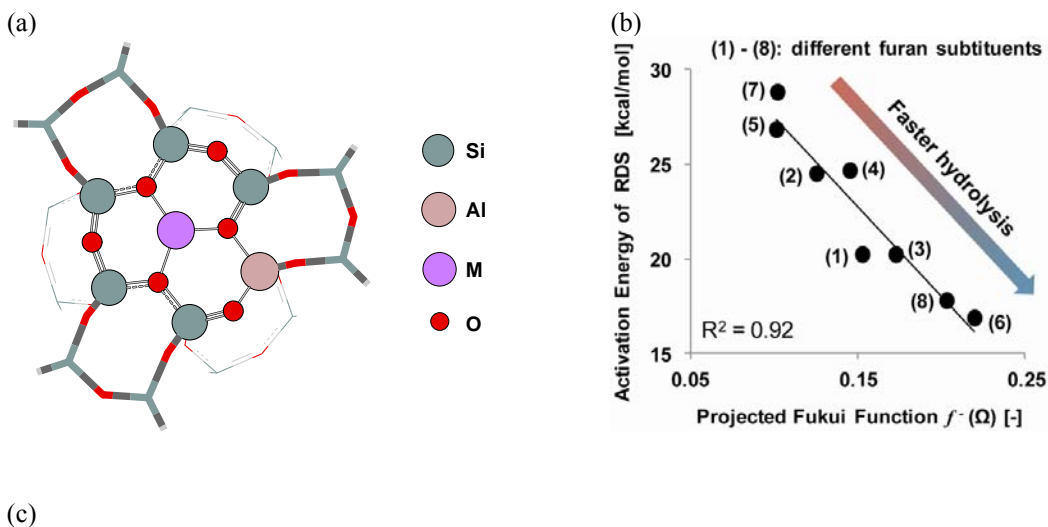
the turnover frequencies calculated for Au_8^- and Au_{10}^- match experimental observations, with Au_8^- being at least two times more active than Au_{10}^- . A publication on this work is in preparation.

1.3 Extending the Hierarchical Multiscale Approach to Complex Reaction Mechanisms for Renewable Chemicals

The hierarchical multiscale methodology developed as part of this program has been applied to prototype molecules. There is a need to extend it to more interesting energy relevant applications. In this last grant period, we combine semi-empirical (descriptor-based) methods and DFT calculations to provide an efficient search-method of key intermediates and reactions and point out the most likely reaction pathways for conversion of dimethylfuran (DMF) to para-xylene (p-xylene). This is the first modeling effort of making ‘green monomers’ used to produce plastics, such as bottles and diapers, and of very complex system using hierarchical multiscale modeling. Here we describe insights gained about the chemistry and touch upon descriptors that can be used to optimize such systems.

According to our electronic structure calculations, the cycloadduct is facily converted to p-xylene on HY, a Brønsted acidic zeolite (Figure 4a). We have thus predicted that, on HY, the rate-limiting step in the conversion of DMF and ethylene to p-xylene is in fact the uncatalyzed cycloaddition reaction (Figure 4c). This finding was able to explain why in the reported kinetics, the rate of p-xylene production was independent of the density of the acid sites whereas the turnover frequency depended strongly the zeolite’s Si/Al ratio, i.e., on the density of the active sites. Our calculations also predicted that the Diels-Alder cycloaddition can be accelerated by Lewis acids and in particular by alkali exchanged zeolites Y, among which NaY is the most effective. A corollary of our computational work is that a bifunctional, Brønsted-Lewis acidic zeolite, like NaHY, would enhance the rate of p-xylene production over that on pure HY.

Our calculations have also helped elucidate the most important side reactions: the Brønsted-catalyzed hydrolysis and oligomerization of furans. Oligomerization follows the much slower hydrolysis. We have found that site-specific Fukui descriptors (Figure 4b) as well as proton affinities correlate, quantitatively, with the activation energy associated with the proton attack on the β -C. Since this elementary step limits the overall hydrolysis rate, we assert that the aforementioned descriptors allow for a priori prediction of the protonation barrier and thus screening of furan derivatives according to their propensity to hydrolysis and oligomerization.



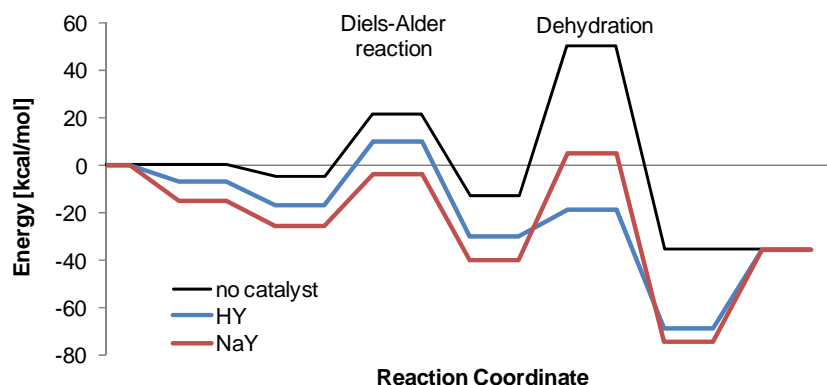


Figure 4. (a) Zeolite Y active site cluster model of Site II. Atoms of the six-ring window are shown as balls. Upward arms (tubes) are part of the supercage and wall of hexagonal prism between two sodalite cages, downward legs (wireframe) represent quadrilateral window between supercage and sodalite cage. (b) Activation energies of the rate-determining step (RDS), the proton transfer to the β -C of furan, plotted against projected Fukui indices for different proton acceptor positions on the ring of different furans; (c) Energy profiles for the conversion of DMF and ethylene to p-xylene: uncatalyzed, black line; HY, blue line; NaY, red line. The catalytic effect on the Diels-Alder reaction is minor. The presence of a Brønsted acidic proton lowers the dehydration barrier significantly.

2. HIGH IMPACT PUBLICATIONS ACKNOWLEDGING DOE FUNDING

- **Most highly cited paper of the journal for the year 2012 and 2013 and second most highly cited paper in other years since 2008:** An overview of spatial microscopic and accelerated kinetic Monte Carlo methods. *J. Comput-Aided Mater. Des.* 14(2), 253-308, (2007). This was published from a continuation grant.
- **High impact journal publications:** Phys. Rev. Letters, 2009. 102 (no. 155505); Nano Letters, 2010. 10: p. 1041–1045; Nano Letters, 2010. 10(9): p. 3408–3413.
- **Invited review:** M. Stamatakis and D. G. Vlachos, Unraveling the Complexity of Catalytic Reactions via Kinetic Monte Carlo Simulation: Current Status and Frontiers, *ACS Catal.* 2(12), 2648-2663 (2012).
- **Invited review; among top ten most highly cited papers of the journal for the year 2012:** M. Saliccioli, M. Stamatakis, S. Caratzoulas, and D. G. Vlachos, A review of multiscale modeling of metal-catalyzed reactions: Mechanism development for complexity and emergent behavior, *Chem. Eng. Sci.* 66, 4319–4355 (2011).
- **Invited perspective:** D. G. Vlachos, Multiscale Modeling for Emergent Behavior, Complexity, and Combinatorial Explosion, Perspective: AIChE 2011 R. H. Wilhelm Award in Chemical Reaction Engineering, *AIChE J.* 58(5), 1314-1325 (2012).

3. PUBLICATIONS ACKNOWLEDGING THIS AWARD (2009-2013)

- N. Nikbin, G. Mpourmpakis, and D. G. Vlachos, A Combined DFT and Statistical Mechanics Study for the CO Oxidation on the Au₁₀–1 Cluster, *The Journal of Physical Chemistry C* 115(41), 20192-20200 (2011).
- G. Mpourmpakis and D. G. Vlachos, Understanding metal nanoparticle growth by first principle methods, *Physical Review Letters* 102(No. 155505), 1-4 (2009).
- S. Collins, M. Stamatakis, and D. G. Vlachos, Adaptive coarse-grained Monte Carlo simulation of heterogeneous plasma membranes, *BMC Bioinformatics* 11, 218:211-213 (2010).

- G. Mpourmpakis, A. N. Andriotis, and D. G. Vlachos, Identification of Descriptors for the CO Interaction with Metal Nanoparticles, *Nano Letters* **10**, 1041–1045 (2010).
- G. Mpourmpakis, S. Caratzoulas, and D. G. Vlachos, What Controls Au Nanoparticle Dispersity during Growth?, *Nano Letters* **10**(9), 3408–3413 (2010).
- H. Y. Wang, M. Stamatakis, D. A. Hansgen, S. Caratzoulas, and D. G. Vlachos, Understanding mixing of Ni and Pt in the Ni/Pt(111) bimetallic catalyst via molecular simulation and experiments, *J. Chem. Phys.* **133**, 2245031-22450311 (2010).
- L. Xu, M. Taufer, S. Collins, and D. G. Vlachos. *Parallelization of Tau-Leap Coarse-Grained Monte Carlo Simulations on GPUs*. in *Proceedings of the IEEE/ACM International Parallel and Distributed Processing Symposium (IPDPS)*. 2010. Atlanta, Georgia, USA.
- T. C. Brüggemann, D. G. Vlachos, and F. J. Keil, Microkinetic Modeling of the Fast Selective Catalytic Reduction of Nitrogen Oxide with Ammonia on H-ZSM5 Based on First Principles, *Journal of Catalysis* **283**(2), 178–191 (2011).
- G. Mpourmpakis, M. Stamatakis, S. Herrmann, D. G. Vlachos, and A. N. Andriotis, Predicting the adsorption behavior in bulk from metal clusters, *Chem. Phys. Letters* **518**, 99-103 (2011).
- N. Nikbin, G. Mpourmpakis, and D. G. Vlachos, A Combined DFT and Statistical Mechanics Study for the CO Oxidation on the Au₁₀⁻¹ cluster, *J. Phys. Chem. C* **115**, 20192–20200 (2011).
- M. Saliccioli, M. Stamatakis, S. Caratzoulas, and D. G. Vlachos, A review of multiscale modeling of metal-catalyzed reactions: Mechanism development for complexity and emergent behavior, *Chem. Eng. Sci.* **66**, 4319–4355 (2011).
- M. Stamatakis, Y. Chen, and D. G. Vlachos, First-Principles-Based Kinetic Monte Carlo Simulation of the Structure Sensitivity of the Water-Gas Shift Reaction on Platinum Surfaces, *Journal of Physical Chemistry C* **115**(50), 24750-24762 (2011).
- M. Stamatakis and D. G. Vlachos, A Graph-Theoretical Kinetic Monte Carlo Framework for on-Lattice Chemical Kinetics, *Journal of Chemical Physics* **134**(No. 214115), 1-13 (2011).
- M. Stamatakis and D. G. Vlachos, Equivalence of on-Lattice Stochastic Chemical Kinetics with the Well-Mixed Chemical Master Equation in the Limit of Fast Diffusion, *Comput. Chem. Eng.* **35**(12), 2602-2610 (2011).
- M. Stamatakis and D. G. Vlachos, On the Structure Sensitivity of CO Oxidation on Pt and Au Catalysts, *Nano Letters*, In preparation (2011).
- Y. Chen and D. G. Vlachos, Density Functional Theory Study of Methane Oxidation and Reforming on Pt(111) and Pt(211), *Ind. Eng. Chem. Res.* **51**(38), 12244-12252 (2012). Article
- N. Nikbin, S. Caratzoulas, and D. G. Vlachos, A First Principles-Based Microkinetic Model for the Conversion of Fructose to 5-Hydroxymethylfurfural, *ChemCatChem* **4**(4), 504-511 (2012).
- M. Stamatakis, M. Christiansen, G. Mpourmpakis, and D. G. Vlachos, Multiscale Modeling Reveals Poisoning Mechanisms on MgO-supported Au Catalysts in CO Oxidation, *Nano Letters* **12**, 3621–3626 (2012).

- M. Stamatakis and D. G. Vlachos, Unraveling the Complexity of Catalytic Reactions via Kinetic Monte Carlo Simulation: Current Status and Frontiers, *ACS Catal.* **2**(12), 2648-2663 (2012). Review
- D. G. Vlachos, Multiscale Modeling for Emergent Behavior, Complexity, and Combinatorial Explosion, Perspective: AIChE 2011 R. H. Wilhelm Award in Chemical Reaction Engineering, *AIChE J.* **58**(5), 1314-1325 (2012).
- S. Herrmann, M. Stamatakis, A. N. Andriotis, and G. Mpourmpakis, Adsorption behavior of noble metal clusters and their alloys, *J. Comput. Theor. Nanos.*, Accepted (2013).
- N. Nikbin, P. T. Do, S. Caratzoulas, R. F. Lobo, P. J. Dauenhauer, and D. G. Vlachos, A DFT study of the acid-catalysed conversion of 2,5-dimethylfuran and ethylene to p-xylene, *J. Catal.* **297**, 35-43 (2013).
- N. Nikbin, S. Caratzoulas, and D. G. Vlachos, On the Brønsted Acid-Catalyzed Homogeneous Hydrolysis of Furans, *ChemSusChem*, In press (2013).
- N. Nikbin, S. Caratzoulas, and D. G. Vlachos, Toward catalyst design in the synthesis of p-xylene by Diels-Alder cycloaddition, *J. Am. Chem. Soc.*, Submitted (2013).

4. INVITED TALKS ACKNOWLEDGING THIS AWARD (2009-2013)

1. The role of catalysis and reaction engineering in coping with the energy crisis, UCLA, Jan. 30, 2009.
2. The role of catalysis and reaction engineering in coping with the energy crisis, Penn State, March 17, 2009.
3. Catalysis for decentralized hydrogen production, Spring Symposium of the Catalysis Society of Metropolitan New York, Princeton University, March 18, 2009.
4. Hierarchical Multiscale Modeling and Control of Nanomaterials, Foundations of Molecular Modeling and Simulation (FOMMS), Plenary lecture, Washington, July 12-17, 2009.
5. The role of catalysis and reaction engineering in the energy arena, Department of Chemical and Biomolecular Engineering, University of Notre Dame, November 17th, 2009.
6. 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. 4th, 2009.
7. Living in a multiscale world, Inaugural lecture, Univ. of Delaware, Newark, DE, Dec. 8th, 2009.
8. 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.
9. The role of catalysis and reaction engineering in the energy arena, General Electric, Albany, NY, February 24th, 2010.
10. Complexity and emergent behavior in catalytic reactions: CO oxidation on gold and ammonia decomposition on single metals and bimetallics, Tokyo Univ., Tokyo, Japan, March 10th, 2010.
11. Emerging frontiers in multiscale modeling: Combinatorial complexity, uncertainty, and emergent behavior, DOE Applied Mathematics Meeting, Berkeley, CA, May 3rd, 2010, Plenary talk.
12. The role of catalysis and reaction engineering in the energy arena, Chemical & Biomolecular Engineering Department, Ohio State University, May 6th, 2010.

13. Emerging frontiers in multiscale modeling: Combinatorial complexity, uncertainty, and emergent behavior, Department of Applied Mathematics, University of Crete, Crete, Greece, July 26th, 2010.
14. 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 14th, 2010.
15. Complexity and emergent behavior in catalytic reactions: Biomass processing and ammonia decomposition, Department of Chemical and Petroleum Engineering, Kansas University, Lawrence, KS, November 16th, 2010.
16. Complexity and emergent behavior in catalytic reactions, Department of Chemical Engineering, Michigan University, Ann Arbor, MI, December 7th, 2010.
17. Enablers for renewable chemicals and fuels, Department of Chemical Engineering, University of Delaware, Newark, DE, February 3, 2011.
18. 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.
19. 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.
20. 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.
21. Design of Emergent-Behaving Catalytic Materials, Chicago Catalysis Club, Chicago, IL, April 11, 2011.
22. Plenary talk: The role of microcombustion in portable and distributed energy, 13th International Conference on Numerical Combustion, April 27-29, 2011, Corfu, Greece.
23. Development of detailed reaction mechanisms for catalytic combustion, Invited Talk at Microcombustion Mini-symposium, 13th International Conference on Numerical Combustion, April 27-29, 2011, Corfu, Greece.
24. Development of detailed reaction mechanisms for catalytic combustion, Invited Talk at Microcombustion Mini-symposium, 13th International Conference on Numerical Combustion, April 27-29, 2011, Corfu, Greece.
25. 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.
26. Design of Emergent-Behaving Catalytic Materials, EuropaCat X, Glasgow, Scotland, August 28-September 2, 2011.
27. The role of catalysis and reaction engineering in the energy arena, Pennergy Institute, University of Pennsylvania, Philadelphia, October 24, 2011.
28. Hierarchical multiscale microkinetic modeling for chemical processing, ExxonMobil, Clinton, NJ, March 19, 2012.
29. 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.
30. Recent Advances in Multiscale Modeling for Biomass Conversion, 243rd ACS National Meeting, San Diego, CA, March 25-29, 2012.
31. The role of catalysis and reaction engineering in the energy arena, Department of Chemical & Biochemical Engineering, Rutgers University, April 18, 2012.
32. 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.

33. An overview of multiscale simulation: Application to reactions and reactors, ExxonMobil, Clinton, NJ, July 26, 2012.
34. 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.
35. 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.
36. Combinatorial complexity, uncertainty, and emergent behavior in the design of catalytic materials and processes, Chemical & Biomolecular Engineering, Cornell University, Ithaca, NY, November 12, 2012.
37. Modern catalytic technologies for converting biomass to renewable fuels and chemicals, Delft University, Netherlands, November 26, 2012.
38. 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.
39. The role of catalysis and reaction engineering in the energy arena, Department of Chemical & Environmental Engineering, Yale University, New Haven, CT, February 27, 2013.
40. 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.
41. Renewable Chemicals and Fuels from Biomass, ExxonMobil, Clinton, NJ, August 22nd, 2013.
42. Combinatorial complexity, uncertainty, and emergent behavior in the design of catalytic materials, in Symposium on New Theoretical Concepts and Directions in Catalysis, Santa Barbara, CA, August 27-30, 2013.

PERSONNEL FUNDED BY OR ASSOCIATED WITH THIS PROJECT AND BUDGET

Graduate students

Stuart Collins (supported from the previous award)

Nima Nikbin

Stephen Edie

Marcel Nunez

Lifan Xu (in collaboration with Prof. Michela Taufer in Computer Science)

Postdoctoral fellows

Michail Stamatakis

Ying Chen

Giannis Mpourmpakis (co-supervised part of Nima Nikbin's earlier work)

Undergraduates

Matt Christiansen

Stan Herrmann