MICHAIL STAMATAKIS, PhD

Associate Professor in Chemical Engineering

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EDUCATION

2004 – 2009 **Chemical & Biomolecular Engineering Department, Rice University, Houston, TX, USA**

Doctor of Philosophy

(Overall GPA: 3.96/4.00)

1999 – 2004 **School of Chemical Engineering, National Technical University of Athens (NTUA), Greece**

Diploma in Chemical Engineering

Graduated 1st among class of 2004 (overall GPA: 9.70/10.00)

ACADEMIC APPOINTMENTS

2019 – 2020 **Visiting Professor, National Institute of Technology (KOSEN), Akashi College, Akashi, Japan**

2015 – Present **Honorary Research Fellow, Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, UK**

2018 – Present **Associate Professor in Chemical Engineering, University College London, UK**

2017 – 2018 **Senior Lecturer in Chemical Engineering, University College London, UK**

2012 – 2017 **Lecturer in Chemical Engineering, University College London, UK**

Research Interests:

- Development of multiscale stochastic modelling approaches for the simulation of realistic catalyst structures. *Zacros*, a software implementation of these approaches is distributed via http://zacros.org/
- Development of coarse-graining and meta-modelling techniques for accurate simulation of catalytic kinetics at the mesoscopic and macroscopic scales.
- Fundamental and feasibility computational studies on transition metals, highly dilute alloys (*single atom alloys*) and other materials (e.g. chalcogenides) as catalysts for various reactions. Applications encompass mature industrial processes (e.g. emissions control chemistries, water-gas

shift, hydrogenation reactions), but also niche applications (e.g. novel routes for chemicals manufacturing, methane and biomass valorisation).

RESEARCH EXPERIENCE

2009 – 2012 **Post-Doctoral: Research group of Prof. Dionisios G. Vlachos; Department of Chemical Engineering, University of Delaware, Newark, DE, USA**

- Multiscale modelling of catalytic processes pertinent to energy production and the environment.
- Multiscale modelling of intermolecular phenomena in cell membranes.

2008 – 2009 **Collaborative research with Prof. Gábor Balázsi; The University of Texas M. D. Anderson Cancer Center, Houston, TX, USA**

- Effects of competitive utilization of regulatory molecules on the determination of extrinsic and intrinsic noise.

2004 – 2009 **Doctoral: Research group of Prof. Kyriacos Zygourakis, co-advised by Dr Nikos V. Mantzaris; Rice University, Houston, TX, USA**

Thesis title: "Stochasticity and Cell Population Heterogeneity in an Artificial *lac* Operon Genetic Network".

Other projects:

- Computational analysis of the effects of noise on oscillatory behaviour, in presence or absence of frequency encoding and excitability.
- Theoretical and computational studies of wave propagation phenomena in astrocytic cellular networks.

2003 – 2004 **Undergraduate: Diploma thesis research, mentored by Prof. Andreas Boudouvis, National Technical University of Athens, Greece, and Dr Nikos V. Mantzaris, Rice University, Houston, TX, USA**

Thesis Title: "Mathematical and Computational Analysis of Signal Transduction Mechanisms in Cellular Networks".

INVITED JOURNAL ARTICLES

Darby, M. T., **Stamatakis, M.**, Michaelides, A. and E. Charles. H. Sykes (2018). "Lonely Atoms with Special Gifts: Breaking Linear Scaling Relationships in Heterogeneous Catalysis with Single-Atom Alloys". The Journal of Physical Chemistry Letters 9: 5636-5646. *[Invited perspective article].* ***[Featured on the front cover of the issue]*****.**

Darby, M. T., Sykes, E. C. H., Michaelides, A. and **M. Stamatakis** (2018). "Carbon Monoxide Poisoning Resistance and Structural Stability of Single Atom Alloys". Topics in Catalysis 61(5-6): 428-438. *[Invited paper for a special issue on "Catalyst Design across Reaction Conditions" in honour of Prof. Cynthia Friend]*.

Piccinin, S. and **M. Stamatakis** (2017). "Steady-State CO Oxidation on Pd(111): First-Principles Kinetic Monte Carlo Simulations and Microkinetic Analysis". Topics in Catalysis 60(1): 141-151. *[Invited article for a special issue of Topics in Catalysis "Catalysis and environmental protection"].*

M. Stamatakis. (2015). "Kinetic Modelling of Heterogeneous Catalytic Systems". Journal of Physics: Condensed Matter 27: 013001. *[Invited review article].*

Stamatakis, M. and D. G. Vlachos (2012). "Unraveling the Complexity of Catalytic Reactions via Kinetic Monte Carlo Simulation: Current Status and Frontiers". ACS Catalysis 2(12): 2648-2663. *[Invited review article].*

Stamatakis, M., Adams, R. and G. Balázsi (2011). "A Common Repressor Pool Results in Indeterminacy of Extrinsic Noise". Chaos 21: 047523. *[Invited paper for a focus issue on "Nonlinear and Stochastic Physics in Biology" dedicated to the memory of Prof. Frank Moss]*.

JOURNAL ARTICLES

Réocreux, R., Fampiou, I. and **Stamatakis, M.** (2020). "The role of oxygenated species in the catalytic self-coupling of MeOH on O pre-covered Au(111)". Faraday Discussions In press.

Papanikolaou, K. G., Darby, M. T. and **Stamatakis, M.** (2020). "Engineering the surface architecture of highly dilute alloys: an *ab initio* Monte-Carlo approach". ACS Catalysis 10(2): 1224-1236. ***[Featured on the front cover of the issue].***

Chutia, A., Thetford, A., **Stamatakis, M.** and Catlow, C. R. A. (2020). "A DFT and KMC Based Study on the Mechanism of Water Gas Shift Reaction on Pd(100) Surface". Physical Chemistry Chemical Physics 22: 3620-3632.

Réocreux, R., Uhlman, M., Thuening, T., Kress, P., Hannagan, R., **Stamatakis, M.** and Sykes, C. (2019). "Efficient and Selective Carbon-Carbon Coupling on Coke-Resistant PdAu Single-Atom Alloys". Chemical Communications 55: 15085-15088.

Apostolopoulou, M., Santos, M. S., Hamza, M., Bui, T., Economou, I. G., **Stamatakis, M.** and Striolo, A. (2019). "Quantifying Pore Width Effects on Diffusivity *via* a Novel 3D Stochastic Approach with Input from Atomistic Molecular Dynamics Simulations". Journal of Chemical Theory and Computation 15(12): 6907-6922.

Chen, B. W. J., **Stamatakis, M.** and M. Mavrikakis (2019). "Kinetic Isolation between Turnovers on Au_{18} Nanoclusters: Formic Acid Decomposition One Molecule at a Time". ACS Catalysis 9(10): 9446-9457.

Darby, M. T., Lucci, F. R., Marcinkowski, M. D., Therrien, A., Michaelides, A., **Stamatakis, M.** and E. C. H. Sykes (2019). "Carbon Monoxide Mediated Hydrogen Release from PtCu Single-Atom Alloys: The Punctured Molecular Cork Effect". The Journal of Physical Chemistry C 123(16): 10419-10428.

Papanikolaou, K. G., Darby, M. T. and **M. Stamatakis** (2019). "CO-Induced Aggregation and Segregation of Highly Dilute Alloys: A Density Functional Theory Study". The Journal of Physical Chemistry C 123(14): 9128-9138. ***[Featured on a supplementary cover of the issue. In the top 25% of all research outputs scored by Altmetric]*.**

Apostolopoulou, M., Dusterhoft, R., Day, R., **Stamatakis, M.**, Coppens, M.-O. and A. Striolo (2019). "Estimating Permeability in Heterogeneous Porous Media: Deterministic vs. Stochastic Investigations". International Journal of Coal Geology 205: 140-154.

Papanikolaou, K. G., Darby, M. T. and **M. Stamatakis** (2018). "Adlayer structure and lattice size effects on catalytic rates predicted from KMC simulations: NO oxidation on Pt(111)". The Journal of Chemical Physics 149(18): 184701.

Pineda, M. and **M. Stamatakis** (2018). “Non-Equilibrium Thermodynamics and Stochastic Dynamics of a Bistable Catalytic Surface Reaction”. Entropy 20(11): 811.

Pineda, M. and **M. Stamatakis** (2018). “On the stochastic modelling of surface reactions through reflected chemical Langevin equations”. Computers & Chemical Engineering 117: 145-158.

Darby, M. T., Réocreux, R., Sykes, E. C. H., Michaelides, A. and **M. Stamatakis** (2018). “Elucidating the Stability and Reactivity of Surface Intermediates on Single Atom Alloy Catalysts”. ACS Catalysis 8(6): 5038-5050. ***[In the top 5% of all research outputs scored by Altmetric].***

Marcinkowski, M. D., Darby, M. T., Liu, J., Wimble, J. M., Lucci, F. R., Lee, S., Michaelides, A., Flytzani-Stephanopoulos, M., **Stamatakis, M.** and E. C. H. Sykes (2018). “Pt/Cu single-atom alloys as coke-resistant catalysts for efficient C-H activation”. Nature Chemistry 10: 325-332. ***[Featured in 19 news stories from 17 outlets. In the top 5% of all research outputs scored by Altmetric].***

Apostolopoulou, M., Day, R., Hull, R., **Stamatakis, M.** and A. Striolo (2017). “A kinetic Monte Carlo approach to study fluid transport in pore networks”. The Journal of Chemical Physics 147(13): 134703.

Vignola, E., Steinmann, S. N., Vandegehuchte, B. D., Curulla, D., **Stamatakis, M.** and P. Sauté (2017). “A machine learning approach to graph-theoretical cluster expansions of the energy of adsorbate layers”. The Journal of Chemical Physics 147(5): 054106.

Liu, G., Robertson, A. W., Li, M. M.-J., Kuo, W. C. H., Darby, M. T., Muhieddine, M. H., Lin, Y.-C., Suenaga, K., **Stamatakis, M.**, Warner, J. H. and S. C. E. Tsang (2017). “MoS_2 monolayer catalyst doped with isolated Co atoms for the hydrodeoxygenation reaction”. Nature Chemistry 9(8): 810-816. ***[In the top 25% of all research outputs scored by Altmetric].***

Pineda, M. and **M. Stamatakis** (2017). “Beyond mean-field approximations for accurate and computationally efficient models of on-lattice chemical kinetics”. The Journal of Chemical Physics 147(2): 024105.

Teixeira, I. F., Lo, B. T. W., Kostetskyy, P., **Stamatakis, M.**, Ye, L., Tang, C. C., Mpourmpakis, G., and S. C. E. Tsang (2016). “A New Facilitated Process of Biomass-Derived Furans to p-Xylene with Ethanol over Zeolite”. Angewandte Chemie International Edition 55(42): 13061-13066. ***[Featured on the inside back cover of the issue]*.**

Campbell, C., Bowker, M., **Stamatakis, M.**, Hutchings, G., Davies, P., Earley, J., Howard, M., Garrett, B., Oloye, F., Gross, E., et al. (2016). “Bridging model and real catalysts: general discussion”. Faraday Discussions 188: 565-589.

Campbell, C., van Santen, R., **Stamatakis, M.**, Collis, N., Freund, H.-J., Plaisance, C., Sauer, J., Garrett, B., Gross, E., et al. (2016). “Catalyst design from theory to practice: general discussion”. Faraday Discussions 188: 279-307.

Wang, Z.-T., Darby, M. T., Therrien, A. J., El-Soda, M., Michaelides, A., **Stamatakis, M.**, and E. C. H. Sykes (2016). “Preparation, Structure, and Surface Chemistry of Ni-Au Single Atom Alloys”. The Journal of Physical Chemistry C 120: 13574-13580.

Stamatakis, M. and S. Piccinin (2016). “Rationalising the relation between adlayer structure and observed kinetics in catalysis”. ACS Catalysis 6: 2105-2111.

Lucci, F., Darby, M., Mattera, M., Ivimey, C., Therrien, A., Michaelides, A., **Stamatakis, M.** and E. C. Sykes (2016). "Controlling Hydrogen Activation, Spillover, and Desorption with Pd-Au Single Atom Alloys". The Journal of Physical Chemistry Letters 7: 480-485.

Nikbin, N., Austin, N., Vlachos, D. G., **Stamatakis, M.** and G. Mpourmpakis (2015). "Catalysis at the Sub-Nanoscale: Complex CO Oxidation Chemistry on a Few Au Atoms". Catalysis Science & Technology 5(1): 134-141. ***[Featured on the front cover of the issue. In the top 5% of all research outputs scored by Altmetric]*.**

Piccinin, S. and **M. Stamatakis** (2014). "CO Oxidation on Pd(111): A First-Principles Based Kinetic Monte Carlo Study". ACS Catalysis 4: 2143-2152.

Herrmann, S., **Stamatakis, M.**, Andriotis, A. N. and G. Mpourmpakis (2014). "Adsorption Behavior of Noble Metal Clusters and Their Alloys". Journal of Computational and Theoretical Nanoscience 11(2): 511-520.

Nielsen, J., d'Avezac, M., Hetherington, J. and **M. Stamatakis** (2013). "Parallel Kinetic Monte Carlo Simulation Framework Incorporating Accurate Models of Adsorbate Lateral Interactions". The Journal of Chemical Physics 139(22): 224706.

Guo, W., **Stamatakis, M.** and D. G. Vlachos (2013). "Design Principles of Heteroepitaxial Bimetallic Catalysts". ACS Catalysis 3: 2248-2255.

Marcinkowski, M. D., Jewell, A. D., **Stamatakis, M.**, Boucher, M. B., Lewis, E. A., Murphy, C. J., Kyriakou, G. and E. C. H. Sykes (2013). "Controlling a Spillover Pathway with the Molecular Cork Effect". Nature Materials 12(6): 523-528.

M. Stamatakis. (2013). "Cell Population Balance and Hybrid Modeling of Population Dynamics for a Single Gene with Feedback". Computers and Chemical Engineering 53: 25-34.

Stamatakis, M., Christiansen, M., Vlachos, D. G. and G. Mpourmpakis (2012). "Multiscale Modeling Reveals Poisoning Mechanisms on MgO-supported Au Catalysts in CO Oxidation". Nano Letters 12(7): 3621-3626.

Stamatakis, M., Chen, Y. and D. G. Vlachos (2011). "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.

Mpourmpakis, G., **Stamatakis, M.**, Herrmann, S., Vlachos, D. G. and A. N. Andriotis (2011). "Predicting the Adsorption Behavior in Bulk from Metal Clusters". Chemical Physics Letters 518: 99-103.

Stamatakis, M. and D. G. Vlachos (2011). "Equivalence of on-Lattice Stochastic Chemical Kinetics with the Well-Mixed Chemical Master Equation in the Limit of Fast Diffusion". Computers and Chemical Engineering 35(12): 2602-2610.

Salciccioli, M., **Stamatakis, M.**, Caratzoulas, S. and D. G. Vlachos (2011). "A Review of Multiscale Modeling of Metal-Catalyzed Reactions: Mechanism Development for Complexity and Emergent Behavior". Chemical Engineering Science 66(19): 4319-4355.

Stamatakis, M. and K. Zygourakis (2011). "Deterministic and Stochastic Population-Level Simulations of an Artificial *lac* Operon Genetic Network". BMC Bioinformatics 12: 301.

Stamatakis, M. and D. G. Vlachos (2011). "A Graph-Theoretical Kinetic Monte Carlo Framework for on-Lattice Chemical Kinetics". The Journal of Chemical Physics 134(21): 214115.

Wang, H., **Stamatakis, M.**, Hansgen, D., Caratzoulas, S. and D. Vlachos (2010). "Understanding Mixing of Ni and Pt in the Ni/Pt(111) Bimetallic Catalyst via Molecular Simulation and Experiments". The Journal of Chemical Physics 133(22): 224503.

Stamatakis, M. and N. V. Mantzaris (2010). "Intrinsic Noise and Division Cycle Effects on an Abstract Biological Oscillator". Chaos 20: 033118. ***[Among the top 20 Chaos articles with the most full-text downloads during October 2010. Selected for the October 1, 2010 issue of the Virtual Journal of Biological Physics Research].***

Stamatakis, M. and K. Zygourakis (2010). "A Mathematical and Computational Approach for Integrating the Major Sources of Cell Population Heterogeneity". Journal of Theoretical Biology 266(1): 41-61.

Collins, S., **Stamatakis, M.** and D. G. Vlachos (2010). "Adaptive Coarse-Grained Monte Carlo Simulation of Reaction and Diffusion Dynamics in Heterogeneous Plasma Membranes". BMC Bioinformatics 11: 218.

M. Stamatakis. (2010). "Cell Population Balance, Ensemble and Continuum Modeling Frameworks: Conditional Equivalence and Hybrid Approaches". Chemical Engineering Science 65(2): 1008-1015.

Stamatakis, M. and N. V. Mantzaris (2009). "Comparison of Deterministic and Stochastic Models of the *lac* Operon Genetic Network". Biophysical Journal 96(3): 887-906.

Stamatakis, M. and N. V. Mantzaris (2007). "Astrocyte Signaling in the Presence of Spatial Inhomogeneities". Chaos 17: 033123.

Stamatakis, M. and N. V. Mantzaris (2006). "Modeling of ATP-Mediated Signal Transduction and Wave Propagation in Astrocytic Cellular Networks". Journal of Theoretical Biology 241(3): 649-668.

BOOK CHAPTERS

Darby, M. T., Piccinin, P. and **M. Stamatakis** (2006). "Chapter 4: First Principles-based Kinetic Monte Carlo Simulation in Catalysis". Institute of Physics e-book on *"Physics of Surface, Interface and Cluster Catalysis"*, edited by Kasai, H. and M. C. S. Escaño.

CONFERENCE PROCEEDINGS

Inyang, U., Cortez-Montalvo, J., Dusterhoft, R., Apostolopoulou, M., Striolo, A. and **M. Stamatakis** (2019). "A Kinetic Monte Carlo Study to Investigate the Effective Permeability and Conductivity of Microfractures within Unconventional Reservoirs". SPE Oklahoma City Oil and Gas Symposium, 9-10 April, Oklahoma City, Oklahoma, USA. Doc. ID: SPE-195220-MS (doi: 10.2118/195220-MS)

INVITED TALKS/ SEMINARS

M. Stamatakis. "Kinetic Monte Carlo simulation for high-fidelity modelling of heterogeneously catalysed reactions". 1st International Symposium on Computational and Experimental Solid Catalysis – Dynamics & Kinetics, National Institute of Technology, Akashi College, Hyogo, Japan, Mar 5, 2020.

M. Stamatakis. "Unraveling the oxidative coupling of methanol on Au(111) using first-principles-based kinetic modelling". American Chemical Society Fall 2019 National Meeting

& Exposition, Session: Advances in Multiscale Computational Modeling of Biomass Conversion Processes, San Diego, USA, Aug 25, 2019.

M. Stamatakis. "Activation of small molecules using single atom alloy catalysts". American Chemical Society Fall 2019 National Meeting & Exposition, 2019 ACS Catalysis Lectureship for the Advancement of Catalytic Science: Symposium in Honor of Maria Flytzani-Stephanopoulos & Charles Sykes, San Diego, USA, Aug 26, 2019.

M. Stamatakis. "Towards Understanding and Engineering Surface Ensembles on Highly Dilute Alloys for Catalysis Applications". The International Materials Simulation Workshop, University of York, York, UK. Jul 20, 2019.

M. Stamatakis. "„Lonely Atoms with Special Gifts": Accelerating Chemical Reactions on Single-Atom Alloys". TYC Soiree, UCL, London, UK. Jun 6, 2019.

M. Stamatakis. "Modelling the Kinetics of Heterogeneously Catalysed Reactions: Predictive Power at Low Computational Cost". CECAM Workshop *Computational mathematics for model reduction and predictive modelling in molecular and complex systems*. École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland. May 28, 2019.

M. Stamatakis. "Catalytic Systems Modelling across Scales: towards First-Principles-based Reactor and Process Design". TYC – BP Molecular Computational Masterclass Series, BP Sunbury (London), UK. May 16, 2019.

M. Stamatakis. "Multiscale Modelling and Synergy with Experiments towards a Fundamental Understanding of Heterogeneous Catalysts". Chalmers University of Technology, Gothenburg, Sweden. Mar 28, 2019.

M. Stamatakis. "From Molecules to Reactors: Methods, Applications and Opportunities for Catalytic Process Design". Dial-a-Molecule *Predictive Scalability of Processes in Fine Chemical and Pharmaceutical Manufacturing* Meeting, GSK Stevenage. Nov 29, 2018.

Stamatakis, M. and S. van Gisbergen, "Products on Marketplaces – SWO: Software for modelling catalytic materials and chemical processes at the molecular and mesoscopic scales: current status and broader vision". EMMC IntOP2018, Freiburg, Germany. Nov 6, 2018.

M. Stamatakis. "Bridging the Scales from the Molecule to the Reactor: Tackling the Accuracy-Efficiency Dillema". The 18th IEEE International Conference on Nanotechnology (IEEENano), Cork, Ireland. Jul 23-26, 2018.

M. Stamatakis. "Understanding and Harnessing the 'Odd One Out': Designing Single Atom Alloy Materials for Catalysis". International Conference on Theoretical Aspects of Catalysis (ICTAC), UCLA, Los Angeles, CA, USA. Jun 24-28, 2018.

M. Stamatakis. "From Atomistic Events to Catalytic Performance: Bridging the Mesoscale in Chemical Reaction Engineering". King's College London, London, UK. Jan 22, 2018.

M. Stamatakis. "Lonely Atoms with Special Gifts: Understanding the Chemical Properties of Single Atom Alloys for the Design of Superior Catalysts". Tufts University, Boston, MA, USA. Nov, 6, 2017.

M. Stamatakis. "Escaping Linear Scaling Relations With Single Atom Alloys for the Design of Superior Catalysts". Joint UK-Japan Symposium on Nanomaterials, Catalysis & Hydrogen Research, University of Kent, Canterbury, Kent, UK. Jul 5, 2017.

M. Stamatakis. "Capturing Chemical Kinetics on Catalytic Surfaces: Striving for Efficiency without Compromising on Accuracy". Centre Blaise Pascal, École Normale Supérieure de Lyon, France. May 29, 2017.

M. Stamatakis. *"Beyond-Mean-Field Approaches for Modelling Catalytic Kinetics"*. Southeast Asia Catalysis Conference (SACC) 2017, Nanyang Technological University, Singapore, May 23, 2017.

M. Stamatakis. " 'Decoding' the Rich Behaviour of Single Atom Alloys and Identifying Opportunities for Catalyst Design". 253rd American Chemical Society National Meeting & Exposition, Symposium: Designed Catalysis: Materials Genome Approach to Heterogeneous Processes, San Francisco, USA, Apr 4, 2017.

M. Stamatakis. "From the Molecular to the Reactor Scale with Accurate and Efficient Computational Frameworks for Reaction Kinetics". Oxford Centre for Industrial and Applied Mathematics, University of Oxford, Oxford, UK. Oct 20, 2016.

M. Stamatakis. "Accurate and Efficient Computational Frameworks for Reaction Kinetics: Towards First-Principles Based Reactor Design". XXII International conference on Chemical Reactors (CHEMREACTOR-22), University College London, London, UK. Sep 19, 2016.

M. Stamatakis. "Elucidating Surface Phenomena and Reaction Mechanisms for Emissions Control Catalysis". Energy Frontier Research Center "Integrated Mesoscale Architectures for Sustainable Catalysis", Harvard University, Boston, USA. Sep 16, 2016.

Darby, M. T., **Stamatakis, M.**, Michaelides, A. and E. C. H. Sykes "Catalysis on Single Atom Alloys: Theoretical Investigations and Opportunities". Tufts University, Boston, USA. Sep 14, 2016.

M. Stamatakis. "Elucidating Complexity in Transition Metal Catalysis via First Principles Kinetic Modelling". ChemEngDay UK 2016, University of Bath, UK, Mar 31, 2016.

M. Stamatakis. "Unravelling the complexity of catalytic kinetics: computational method development, applications and perspective". 251st American Chemical Society National Meeting & Exposition, Symposium: Computational Chemistry Across Catalysis, San Diego, USA, Mar 13, 2016.

M. Stamatakis. "Unravelling the Complexity of Catalytic Kinetics: Computational Method Development and Applications to CO Oxidation on Noble Metals". Faculty of Physical Sciences and Science Institute, University of Iceland, Iceland, Feb 26, 2016.

Stamatakis, M., Michaelides, A. and E. C. H. Sykes "Catalysis on Single Atom Alloys: Theoretical Investigations and Opportunities". Energy Frontier Research Center *"Integrated Mesoscale Architectures for Sustainable Catalysis"*, Harvard University, Boston, USA, Oct 16, 2015. *[Invited seminar via teleconference]*

M. Stamatakis. "Unravelling the Complexity of Catalytic Kinetics: Computational Method Development, Applications and Perspective". Institute of Energy and Process Systems Engineering, Technische Universität Braunschweig, Germany, Mar 9, 2015.

M. Stamatakis. "Elucidating the Catalytic Activity of Transition Metal Surfaces via First-Principles Kinetic Modelling: Method Development and Applications". International Max Planck Research School *Functional Interfaces in Physics and Chemistry*, Workshop "Micro to Macro", Schloss Ringberg, Kreuth, Germany, Feb 12, 2015.

M. Stamatakis. "Pushing the Frontiers of *Ab Initio* Kinetic Simulations in Heterogeneous Catalysis". Centre Blaise Pascal, École Normale Supérieure de Lyon, France. Oct 24, 2014.

M. Stamatakis. "Unravelling the complexity of catalytic kinetics: computational method development, applications and perspective". Chemical Engineering Department, University of Newcastle, UK. Oct 21, 2014.

M. Stamatakis. "Pushing the Frontiers of *Ab Initio* Kinetic Simulations in Heterogeneous Catalysis". Workshop: From the Chemical Bond to the Chemical Plant: Computational and Materials Challenges in Gas Conversion Technologies, International Centre for Materials Science, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore, India. Aug 25, 2014.

M. Stamatakis. "From Fundamental Understanding to Catalyst Design: Pushing the Frontiers of First-Principles Kinetic Simulation in Catalysis". Workshop on International Research and Education on Computational Materials Design in Asia, Department of Applied Physics, Osaka University, Osaka, Japan. Jun 3, 2014.

M. Stamatakis. "Structure Sensitive or Not? The Effect of Catalytic Surface Morphology on H_2 Production via the Water-Gas Shift Reaction". JSPS Core-to-Core Program: A. Advanced Research Networks - International Workshop of Computational Nano-Materials Design on Green Energy, Toyonaka Campus, Osaka University, Osaka, Japan. Jun 2, 2014.

M. Stamatakis. "From Virtual Catalysis to Practical Applications: Understanding and Designing Catalysts *in Silico*". Department of Chemistry, UCL, London, UK, Feb 27, 2013.

M. Stamatakis. "From Virtual Catalysis to Practical Applications: Understanding and Designing Catalysts *in Silico*". TYC Lunchtime Get-Together, London, UK, Feb 15, 2013.

M. Stamatakis. "Multiscale Stochastic Simulations of Transition Metal Catalysts for Energy Applications". Accelrys, Inc., Cambridge, UK. Nov 15, 2012.

M. Stamatakis. "Multiscale Stochastic Simulations in Cell Population Biology and Transition Metal Catalysis". Princeton University, Princeton, NJ, USA. May 4, 2012.

M. Stamatakis. "Novel Approaches on Modeling Cell Population Heterogeneity". Laboratory of Computational Systems Biotechnology (LCSB), Institute of Chemical Sciences and Engineering, École Polytechnique Fédérale de Lausanne, Switzerland. Jul 5, 2010.

Stamatakis, M. and D. G. Vlachos. "Kinetic Monte Carlo Simulations of EGFR Clustering in Heterogeneous Cell Membranes". Advanced Computational Sciences Department, RIKEN Advanced Science Institute, Yokohama, Japan. Dec 8, 2009.

Stamatakis, M., Mantzaris, N. V. and K. Zygourakis. "Stochasticity and Cell Population Heterogeneity in an Artificial *lac* Operon Genetic Network". Department of Systems Biology, The University of Texas M. D. Anderson Cancer Center, Houston, TX, USA. Mar 10, 2009.

Stamatakis, M. and K. Zygourakis. "A Mathematical and Computational Approach for Integrating the Major Sources of Cell Population Heterogeneity". Department of Systems Biology, The University of Texas, M. D. Anderson Cancer Center, Houston, TX, USA. May 1, 2008.

TALKS/ SEMINARS

M. Stamatakis. "Computational Catalysis for Sustainable Process Design". Centre for Process

Systems Engineering – Annual Industrial Consortium Meeting, Imperial College London, London, UK, Dec 6, 2019.

M. Stamatakis. "Improving the Efficiency of Kinetic Monte Carlo Simulations for Catalysis with a Parallel Caching Algorithm". American Institute of Chemical Engineering Annual Meeting, Pittsburgh, PA, USA, Oct 29, 2018.

Pineda, M. and **M. Stamatakis**. "Overcoming the Compromise between Accuracy and Efficiency in Modelling Catalytic Kinetics". American Institute of Chemical Engineering Annual Meeting, Minneapolis, MN, USA, Oct 29, 2017.

Darby, M., Michaelides, A. and **M. Stamatakis**. "Escaping Linear Scaling Relations: Catalysis Beyond Constraints on Single Atom Alloys". American Institute of Chemical Engineers Annual Meeting 2017 Annual Meeting. *Keynote talk* in Session 52: Atomically Dispersed Supported Metal Catalysts I. Minneapolis, MN, USA. Oct. 30, 2017.

M. Stamatakis. "First-principles Kinetic Monte Carlo Simulations of C1 Chemistries on Pure Metals and Single Atom Alloys". EFRC-HUB-CMS PI Meeting, Washington DC, USA, Jul 25, 2017.

M. Stamatakis. "Catalytic Process Design across Scales: Method Development, Applications and Opportunities". Centre for Process Systems Engineering – Annual Industrial Consortium Meeting, Imperial College London, London, UK, Dec 2, 2016.

Nikbin, N., Austin, N., Christiansen, M., Vlachos, D. G., **Stamatakis, M.** and G. Mpourmpakis. "Unravelling the Complexity of CO Oxidation Catalysis on Au Nanoclusters". UK Catalysis Conference 2016, Loughborough, UK. Jan 7, 2016.

Piccinin, S. and **M. Stamatakis**. "Rationalising the Relation Between Adlayer Structure and Observed Kinetics in CO Oxidation on Pd(111)". American Institute of Chemical Engineers Annual Meeting, Salt Lake, UT, USA. Nov 10, 2015.

Nikbin, N., Austin, N., Christiansen, M., Vlachos, D. G., **Stamatakis, M.** and G. Mpourmpakis. "Unravelling the Complexity of CO Oxidation Catalysis on Au Nanoclusters". Short oral presentation within the *Discussion symposium 6 - "Oxidation Catalysis - Pollution control"*, XII European Congress on Catalysis (EuropaCatXII), Kazan, Russia. Sep 2, 2015.

Piccinin, S. and **M. Stamatakis**. "Coverage Effects for the CO Oxidation Reaction on O-Rich Pd(111)". Inaugural UK Catalysis Conference, Loughborough, UK. Jan 9, 2015.

Piccinin, S. and **M. Stamatakis**. "CO Oxidation on O-Rich Pd(111): How Does Adlayer Structure Affect Reactivity?". American Institute of Chemical Engineers Annual Meeting, Atlanta, GA, USA. Nov 17, 2014.

M. Stamatakis. "From Virtual Catalysis to Practical Applications: Understanding and Designing Catalysts *in Silico*". American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, USA. Nov 5, 2013.

Ruscillo, F., Darby, M., Sykes, C. and **M. Stamatakis**. "Investigation of Hydrogen Spillover Pathways on a Bimetallic Hydrogenation Catalyst". American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, USA. Nov 5, 2013.

M. Stamatakis. "Reduction Techniques and Hybrid Modelling Approaches for Cell Population Heterogeneity". American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, USA. Nov 4, 2013.

Stamatakis, M., Chen, Y. and D. G. Vlachos. "Active Sites and Structure Sensitivity Effects of the Water-Gas Shift Reaction on Platinum". Recent Appointees in Materials Science 2012 Conference, Glasgow, Scotland, UK. Sep 2, 2012.

Stamatakis, M., and D. G. Vlachos. "Investigation of Structure Sensitivity for the CO Oxidation Chemistry on Pt and Au". American Institute of Chemical Engineers Annual Meeting, Minneapolis, MN, USA. Oct 18, 2011.

M. Stamatakis. "Multiscale Modeling for the Fundamental Understanding of Heterogeneous Catalysis for Energy Applications". American Institute of Chemical Engineers Annual Meeting, Minneapolis, MN, USA. Oct 16, 2011.

Stamatakis, M., Chen, Y. and D. G. Vlachos. "Structural Sensitivity of the Water Gas Shift Reaction on Platinum Surfaces". North American Catalysis Society 22nd North American Meeting, Detroit, MI, USA. Jun 6, 2011.

Stamatakis, M., Chen, Y. and D. G. Vlachos. "Structural Sensitivity of the Water Gas Shift Reaction on Platinum Surfaces". American Institute of Chemical Engineers Annual Meeting, Salt-Lake, UT, USA. Nov 9, 2010.

Stamatakis, M. and D. G. Vlachos. "Reduction of Stochastic On-Lattice Chemical Kinetics Models to Well-Mixed Descriptions via Singular Perturbation". American Institute of Chemical Engineers Annual Meeting, Salt-Lake, UT, USA. Nov 8, 2010.

Stamatakis, M. and K. Zygourakis. "Deterministic and Stochastic Population Level Simulations of an Artificial *lac* Operon Genetic Network". American Institute of Chemical Engineers Annual Meeting, Nashville, TN, USA. Nov 9, 2009.

Stamatakis, M. and K. Zygourakis. "A Mathematical and Computational Approach for Integrating the Major Sources of Cell Population Heterogeneity". American Institute of Chemical Engineers Annual Meeting, Philadelphia, PA, USA. Nov 19, 2008.

Stamatakis, M. and N. V. Mantzaris. "Deterministic and Stochastic Modeling of a Caricature Biological Oscillator". American Institute of Chemical Engineers Annual Meeting, Salt Lake, UT, USA. Nov 8, 2007.

Stamatakis, M. and N. V. Mantzaris. "Deterministic and Stochastic Modeling of Genetic Networks with Positive Feedback Architecture". American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, USA. Nov 17, 2006.

Stamatakis, M., Contou-Carrere, P. and N. V. Mantzaris. "Wave Propagation Patterns in 2D Astrocytic Networks". American Institute of Chemical Engineers Annual Meeting, Cincinnati, OH, USA. Nov 3, 2005.

Stamatakis, M. and N. V. Mantzaris. "Astrocyte Signaling in the Presence of Spatial Inhomogeneities". American Institute of Chemical Engineers Annual Meeting, Cincinnati, OH, USA. Nov 1, 2005.

Stamatakis, M. and N. V. Mantzaris. "Modeling of Signal Transduction and Wave Propagation in Astrocytic Cellular Networks". The 22nd Annual Houston Conference on Biomedical Engineering Research, Houston, TX, USA. Feb 11, 2005.

Stamatakis, M. and N. V. Mantzaris. "Modeling of Signal Transduction and Wave Propagation in Astrocytic Cellular Networks". American Institute of Chemical Engineers Annual Meeting, Austin, TX, USA. Nov 12, 2004.

Mantzaris, N. V. and **M. Stamatakis.** "Theoretical and Computational Analysis of the Signal Transduction and Wave Propagation Mechanisms in Astrocytic Cellular Networks". The 21st Annual Houston Conference on Biomedical Engineering Research, Houston, TX, USA. Feb 12-13, 2004.

INVITED POSTER PRESENTATIONS

Stamatakis, M. and D. G. Vlachos. "Graph-Theoretical Kinetic Monte Carlo for on-Lattice Chemical Kinetics". Scientific Discovery through Advanced Computing Conference. Jul 13, 2011, Denver, CO, USA.

POSTER PRESENTATIONS

Nikbin, N., Austin, N., Christiansen, M., Vlachos, D. G., **Stamatakis, M.** and G. Mpourmpakis. "Unravelling the Complexity of CO Oxidation Catalysis on Au Nanoclusters". Designing New Heterogeneous Catalysts: Faraday Discussion, London, UK. Apr 4, 2016.

Nikbin, N., Austin, N., Christiansen, M., Vlachos, D. G., **Stamatakis, M.** and G. Mpourmpakis. "Unravelling the Complexity of CO Oxidation Catalysis on Au Nanoclusters". ChemEngDay UK 2016, University of Bath, UK. Mar 31, 2016.

Nikbin, N., Austin, N., Christiansen, M., Vlachos, D. G., **Stamatakis, M.** and G. Mpourmpakis. "Unravelling the Complexity of CO Oxidation Catalysis on Au Nanoclusters". XII European Congress on Catalysis (EuropaCatXII), Kazan, Russia. Sep 2, 2015.

M. Stamatakis. "Zacros Software Package: Pushing the Frontiers of Kinetic Simulation of Catalytic Materials". ChemEngDayUK 2015, Department of Chemical Engineering, The University of Sheffield, UK. Apr 8, 2015.

M. Stamatakis. "From Virtual Catalysis to Practical Applications: Understanding and Designing Catalysts *in Silico*". ChemEngDayUK 2014, Department of Chemical Engineering, University of Manchester, UK. Apr 7, 2014.

Stamatakis, M., Chen, Y. and D. G. Vlachos. "Structural Sensitivity of the Water Gas Shift Reaction in Platinum Catalysts". Gordon Research Conference on Catalysis, Colby-Sawyer College, New London, NH, USA. Jun 27, 2010.

Stamatakis, M., Mantzaris N. V. and K. Zygourakis. "Quantifying Stochastic Effects for an Artificial *lac* Operon Genetic Network". Computational Engineering & Science – High Performance Computing Workshop. Lehigh University, Bethlehem, PA, USA. Oct 5, 2009.

Stamatakis, M., Adams, R. and G. Balázsi. "A Common Repressor Pool Results in Indeterminacy of Extrinsic Noise". The Third International Conference on Foundations of Systems Biology in Engineering. Denver, CO, USA. Aug 10, 2009.

Stamatakis, M. and K. Zygourakis. "A Mathematical and Computational Approach for Integrating the Major Sources of Cell Population Heterogeneity". The Third International Conference on Foundations of Systems Biology in Engineering. Denver, CO, USA. Aug 10, 2009.

Stamatakis, M. and K. Zygourakis. "A Mathematical and Computational Approach for Integrating the Major Sources of Cell Population Heterogeneity". Systems Biology Symposium. University of Pennsylvania. Philadelphia, PA, USA. Jun 24, 2009.

Stamatakis, M. and K. Zygourakis. "A Mathematical and Computational Approach for Integrating the Major Sources of Cell Population Heterogeneity". Biophysical Society 53rd Annual Meeting. Boston, MA, USA. Mar 2, 2009.

Stamatakis, M. and K. Zygourakis. "A Mathematical and Computational Approach for Integrating the Major Sources of Cell Population Heterogeneity". Computational & Theoretical Biology Symposium – Evolutionary Design Principles of Biological Networks. Houston, TX, USA. Dec 6, 2008.

Prakash, A., **Stamatakis, M.**, Jones, C. J., Mayo, J. T., Pasquali, M. and V. L. Colvin. "Optical Tracking of Monodisperse Magnetite Nanoparticles". American Institute of Chemical Engineers Annual Meeting, Philadelphia, PA, USA. Nov 17, 2008.

Stamatakis, M. and N. V. Mantzaris. "Stochastic Simulations of Cell Population Dynamics". American Institute of Chemical Engineers Annual Meeting, Cincinnati, OH, USA. Nov 2, 2005.

RESEARCH FUNDING

Primary Investigator

2018 "Computational Design of Poisoning-Resistant Catalysts for Methane-Steam Reforming". 42 months. £66,000.00. Impact Studentship sponsored by Johnson Matthey PLC.

2017 "From Molecules To Chemical Reactors By Boosting Kinetic Monte-Carlo". 42 months. £274,554. Project ID: RPG-2017-361. Sponsored by the Leverhulme Trust, UK.

2017 Subcontract with the Integrated Mesoscale Architectures For Sustainable Catalysis Energy Frontier Research Center (IMASC-EFRC) at Harvard University, sponsored by the Department of Energy, USA. 12 months. $100,000.

2017 "*Zacros* Software Package Development: Code Refactoring, Exact Spatial Parallelism and Algorithms for Emerging Hardware". 12 months. £102,170. Project ID: eCSE10-08. Sponsored by the Edinburgh Parallel Computing Centre through subcontracting from the Engineering and Physical Sciences Research Council and Natural Environment Research Council, UK.

2014 "*Zacros* Software Package Development: Pushing the Frontiers of Kinetic Monte Carlo Simulation in Catalysis". 12 months. £82,783. Project ID: eCSE01-001. Sponsored by the Edinburgh Parallel Computing Centre through subcontracting from the Engineering and Physical Sciences Research Council and Natural Environment Research Council, UK.

2014 "Accurate and Computationally Efficient Models for Virtual Catalyst Design". 24 months. £113,044. Project ID: RPG-2014-161. Sponsored by the Leverhulme Trust, UK.

Award Manager

Collaborative proposals led by institutions other than UCL; MS is the Award Manager at UCL.

2018 "Software Platform for Multiscale Modelling of Reactive Materials and Processes". 48 months. €501,695 (total value of grant: €4,114,411). Project ID: 814416. Sponsored by the European Commission (Horizon 2020).

2018 "Integrated Mesoscale Architectures For Sustainable Catalysis (IMASC)". 24 months. £183,167 (total value of grant: $15,660,740). Project ID: DE-SC0012573. Sponsored by the US Department of Energy.

Co-Investigator

2019 "CBET-EPSRC: Enhancing the CSMHyK fluid dynamics calculations via the inclusion of a stochastic model of hydrate nucleation, agglomeration and growth". 36 months. £479,771 (total value of grant: ~£774K). Project ID: EP/T004282/1. Sponsored by the Engineering and Physical Sciences Research Council and Natural Environment Research Council, UK, and the Chemical, Bioengineering, Environmental and Transport Systems (CBET) division of the National Science Foundation (NSF), USA.

2018 "New Paradigms In Catalyst Design: Efficient CH_4 Conversion By Single Atom Alloys". 42 months. £183,167 (collaboration between two UCL Departments: Chemical Engineering; Physics and Astronomy). Project ID: RPG-2018-209. Sponsored by the Leverhulme Trust, UK.

2018 "Cognitive Chemical Manufacturing". 48 months. £497,052 (total value of grant: £2,007,487). Project ID: EP/R032807/1. Sponsored by the Engineering and Physical Sciences Research Council and Natural Environment Research Council, UK.

HONORS, FELLOWSHIPS AND AWARDS

2015 Research project "Catalysis at the Sub-Nanoscale: Unravelling the Complexity of CO Oxidation on a Few Au Atoms" shortlisted for the IChemE Global Awards 2015 (Category "Research Project of the Year").

2013 Identified as one of the Top Reviewers for Computers & Chemical Engineering in 2012-2013.

2010 Registration support award by the committee chair of the Gordon Research Conference in Catalysis Prof. Abhaya K. Datye.

2009 Second prize in the Poster Competition of the Computational Engineering & Science – High Performance Computing Workshop held in Lehigh University, Bethlehem, PA, Oct 5-6.

2009 Second prize in the Poster Competition of the University of Pennsylvania Systems Biology Symposium held in Philadelphia, PA, Jun 23-24.

2008 Scholarship from the Hellenic Professional Society of Texas for excellent scholastic performance during the studies in the Chemical & Biomolecular Engineering Department of Rice University.

2007	One-year sponsored membership in AAAS/Science nominated by the Dean of Engineering Sallie Keller-McNulty in the context of the AAAS/Science Program for Excellence in Science.
2007	Outstanding Teaching Assistant Award by the Chemical & Biomolecular Engineering Department of Rice University in recognition of dedicated service and exceptional efforts serving as a TA in ChBE courses.
2007	Kobayashi Fellowship Award by the Chemical & Biomolecular Engineering Department of Rice University for the best thesis proposal for the academic year 2006 – 2007.
2006	Scholarship from the Georgiou Fr. Zografaki Foundation of Scholarships for distinct performance during academic year 2000 – 2001 in the School of Chemical Engineering of the NTUA.
2006	Award from the Hellenic Association of Chemical Engineers for graduating 1st from the School of Chemical Engineering of the NTUA among the class of 2004.
2005	Award from the Thomaidis Foundation for the best Diploma Thesis on a cross-scientific topic.
2005	Award by the NTUA Rector Prof. Andreas Andreopoulos, for graduating 1st from the School of Chemical Engineering of the NTUA, class of 2004.
2005	Scholarship from the endowment "Leontiou Anagnostou Oikonomidi" for pursuing graduate studies at a non-Hellenic University, in the field of Chemical Engineering.
2003 – 2007	Awards by the Technical Chamber of Greece for ranking 1st during the 2nd, 3rd and 5th year of study in the School of Chemical Engineering at the NTUA.
2001	"Christos Papakyriakopoulos" award for distinction in Mathematics during the 1st and 2nd semester of study at the NTUA.
2001	"Nikolaos Kritikos" award for distinction during the 1st and 2nd semester of study at the NTUA.
2000	Award from the Greek Association of Chemists for ranking 11th in the Panhellenic (national-level) Chemistry student competition held in 1999.
1999	Award from the Greek Mathematical Society for top (rank 1) performance amongst candidates from Lasithiou district in the Panhellenic (national-level) student competition "Thalis" held in 1998 – 1999 school year.
1999 – 2004	Scholarships from the (Hellenic) National Foundation of Scholarships: • for ranking 2nd amongst students who entered through Panhellenic (national-level) exams in the School of Chemical Engineering at the NTUA (1999). • for ranking 4th during the 1st year (1999 – 2000); 2nd during the 3rd year (2001 – 2002); and 1st during the 2nd year (2000 – 2001), 4th year (2002 – 2003) and 5th year (2003 – 2004) of study in the School of Chemical Engineering at the NTUA.

TEACHING EXPERIENCE

Instructor

Chemical Engineering Department, University College London, UK

2018 – Present Developed educational material (lecture slides, coursework), lectured and graded coursework for BENG0091 "Stochastic Calculus and Uncertainty Analysis" (UG level 4th year, in the context of the *Engineering Mathematics* Minor within the *Integrated Engineering Programme*).

2018 – Present Developed educational material (lecture slides), and lectured for PHAS0076 "TYC Materials Modelling" (PhD level; specialty graduate course).

2016 Graded final reports and assessed oral presentations for CENG9001 "Year in Industry" (UG level 4th year).

2014 – 2017 Developed assessment material (coursework and exam questions) and led weekly tutorial sessions for ENGS103P "Mathematical Modelling and Analysis 1" (UG level 1st year within the *Integrated Engineering Programme*).

2013 – Present Mentored students as Reactor Design Expert and graded design project reports for CENG301P "Process Plant Design Project" (UG level 3rd year) [previously also offered with the following module code: CENG3006 "Chemical Engineering Plant Design I" (UG level 3rd year)].

2013 – Present Coordinated, developed educational material (lecture slides, coursework) and lectured on materials and processes involved in semiconductor device fabrication for CENG0030 "Advanced Materials Processes and Nanotechnology" (UG level 4th year elective) [previously also offered with the following module codes: CENGM05P "Advanced Materials Processes and Nanotechnology" (UG level 4th year elective); CENG3007 "Advanced Materials and Product Engineering" (UG level 3rd year)].

2013 – Present Coordinated, developed educational material (lecture slides, coursework), lectured and graded design project reports for CENG0053 "Process Engineering Modelling & Design" (MSc level) [previously also offered with the following module codes: CENGG01P "Process Systems Modelling & Design" (MSc level); CENGM01P "Process Systems Modelling & Design" (UG level 4th year); CENGM011 "Advanced Process Modelling & Design" (MSc level); CENGG021 "Advanced Process Modelling" (UG level 4th year)].

Chemical & Biomolecular Engineering Department, Rice University, Houston, TX, USA

Fall 2006 Graded and held problem solving sessions for CHBE 301 "Material and Energy Balances". Lectured on the FORTRAN programming language and developed homework problems for CHBE 303 "Computing in Chemical and Biomolecular Engineering".

Fall 2005 Supervised term project for CHBE 301 "Material and Energy Balances". Lectured on the FORTRAN programming language for CHBE 303 "Computing in Chemical and Biomolecular Engineering".

Invited Lecturer

B109: Systems Biology. School of Biomedical Science, Tokyo Medical and Dental University, Tokyo, Japan

Dec 11, 2009 Lecture topic: "Simulating EGFR Dynamics in Cell Membranes: From Simple Models to Multiscale Approaches".

Teaching Assistant

Chemical & Biomolecular Engineering Department, Rice University, Houston, TX

Spring 2007 Maintained course webpage and supervised lab activities for CHBE 305 "Computational Methods in Chemical Engineering".

Spring 2005 Graded homework and supervised computer lab activities for CHBE 305 "Computational Methods in Chemical Engineering".

Fall 2004 Supervised lab modules and graded lab reports for CHBE 443 "Chemical Engineering Laboratory II".

Student Mentor

Chemical Engineering Department, University College London, UK

2012 – present Mentored MEng and MSc students, as well as visiting students performing research in the context of Erasmus placements and other schemes.

Chemical & Biomolecular Engineering Department, Rice University, Houston, TX

2006 – 2007 Mentored undergraduate students performing summer research in the lab of Dr Nikos Mantzaris.

Presentation Coach

Cain Project in Engineering and Professional Communication, Rice University, Houston, TX

2006 – 2007 Provided feedback on undergraduate student presentations to improve content, structure and delivery.

SERVICE – PROFESSIONAL

Professional Affiliations

2017 – Present Founding member of the Early Careers Researchers Forum of the Institution of Chemical Engineers (IChemE)

2016 – Present Fellow of the Higher Education Academy (HEA)

2013 – Present Member of the IChemE - Chartered Scientist (CSci)

2013 – Present Member of the Royal Society of Chemistry (RSC)

2013 – Present Member of the Centre for Process Systems Engineering (CPSE)

2012 – Present Member of the Thomas Young Centre (TYC) - the London Centre for the Theory and Simulation of Materials

2009 – 2010 Member of the Biophysical Society

2007 – 2009 Member of the American Association for the Advancement of Science (AAAS)

2004 – Present Member of the American Institute of Chemical Engineers (AIChE)

Organisation of Professional Meetings

2020 Co-organiser of the "Workshop on Multiscale Computational Catalysis and Materials Science" at the National Institute of Technology (KOSEN), Akashi College, Akashi, Japan.

2019 Co-organiser of session 538 "New Methods and Developments in Computational Catalysis II" at the 2019 AIChE Annual Meeting, Orlando, FL, USA.

2019 Co-organiser and session chair for the "eResearch Domain 3rd Symposium: Computational Sciences for the 21st Century" at UCL, London, UK.

2019 Co-organiser of career and networking event/session "Post-Doctoral Appointment: a Career Crossroad Followed by…?" at ChemEngDay UK 2019.

2018 Co-organiser of IChemE Catalysis Special Interest Group event titled "Kinetic and Transport Modelling and Experiments in Catalytic Systems".

2018 Lead organiser of Computational Catalysis sessions and chair of session 402 "Computational Catalysis I: Fundamentals" at the 2018 AIChE Annual Meeting, Pittsburgh, PA, USA.

2017 Co-organiser and co-chair of session 578 "Computational Catalysis I: Fundamentals" at the 2017 AIChE Annual Meeting, Minneapolis, MN, USA.

2016 Co-organiser and chair of session 399 "Computational Catalysis I: Fundamental Metal Catalysis"; co-organiser and co-chair of session 578 "Computational Catalysis IV: Metal Oxides, Sulfides, Phosphides, Zeolites, Etc." at the 2016 AIChE Annual Meeting, San Francisco, CA, USA.

2016 Session chair at the UK Catalysis Conference 2016, Loughborough, UK.

2015 Co-organiser and chair of session 392 "Computational Catalysis III" at the 2015 AIChE Annual Meeting, Salt Lake, UT, USA.

2014 Co-organiser and chair of session 245 "Computational Catalysis III: Reaction Environment and Coverage Effects" at the 2014 AIChE Annual Meeting, Atlanta, GA, USA.

2014 Co-organiser of the 2014 Recent Appointees in Materials Modelling Meeting, London, UK.

2013 Co-organiser and chair of session 434 "Multiscale Modeling" at the 2013 AIChE Annual Meeting, San Francisco, CA, USA.

Reviewer for Funding Institutions

Agency for Science, Technology and Research (A*STAR) in Singapore

German Research Foundation (Deutsche Forschungsgemeinschaft, DFG)

Natural Sciences and Engineering Research Council of Canada (NSERC)

Polish National Science Centre (Narodowe Centrum Nauki, NCN)

Swiss National Supercomputing Center (Centro Svizzero di Calcolo Scientifico, CSCS)

UK Research and Innovation (UKRI) [formerly Research Councils UK (RCUK)]

USA Department of Energy (DoE)

Reviewer for Professional Journals

ACS Catalysis

ACS Nano

ACS Sustainable Chemistry & Engineering

Advanced Functional Materials

AIChE Journal

Angewandte Chemie

Applied Surface Science

Biofabrication

Biophysical Journal

BMC Bioinformatics

Catalysis Science & Technology

Chemical Engineering and Processing: Process Intensification

Chemical Engineering Journal

Chemical Engineering Research and Design

Computer Physics Communications

Computers & Chemical Engineering

IEEE Life Sciences Letters

Industrial & Engineering Chemistry Research

Journal of Catalysis

Journal of Chemical & Engineering Data

Journal of Computational Physics

Journal of Mathematical Biology

Journal of Molecular Catalysis A: Chemical

Journal of Molecular Liquids

Journal of Multiscale Modeling & Simulation (SIAM)

Journal of Physical Chemistry

Journal of Physics and Chemistry of Solids

Journal of the Royal Society Interface

Langmuir

Molecular Catalysis A

Nature Catalysis

Nature Communications

Physical Chemistry Chemical Physics

Physical Review E

Physical Review Letters

PLoS One

Proceedings of the National Academy of Sciences (PNAS)

Science Advances

Surface Science

The Journal of Chemical Physics

SERVICE – UNIVERSITY

2018 – Present	Non professorial member of the UCL Academic Board
2013 – Present	Member of the Departmental Seminars Committee (2013), the Staff-Student Consultative Committee (2012-2013), Head of the Publicity and Recruitment Committee (2014-Present), and Departmental Librarian (2012-Present) at UCL Chemical Engineering
2012 – Present	Member of the Researcher Development Working Group (2012-2014), the Research Software Development Resource Allocation Group (2012-present) and the Computational Resource Allocation Group (2014-present) at UCL
2007 – 2009	Member of the executive committee of BCM-Rice Consulting and Entrepreneurial Corps