MICHAIL STAMATAKIS, PhD

Professor of Computational Inorganic Chemistry

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academic url: https://www.chem.ox.ac.uk/people/michail-stamatakis

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

2023 – Present **Professor of Computational Inorganic Chemistry, University of Oxford, UK**

2023 – Present **Tutorial Fellow, Lady Margaret Hall, University of Oxford, UK**

2023 **Academic Visitor at the Department of Chemistry, University of Iceland, Reykjavík, Iceland**

2023 **Academic Visitor at the Theory Department, Fritz Haber Institute of the Max Planck Society, Berlin, Germany**

2022 – 2023 **Professor of Chemical Engineering, University College London, UK**

2018 – 2022 **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**

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

2015 – 2018 **Honorary Research Fellow, Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, UK**

RESEARCH INTERESTS

- Development of multiscale stochastic modelling approaches and parallel algorithms for the simulation of realistic catalyst structures. *Zacros*, a software implementation of these approaches, and *Zacros*-post, the associated post-processing library and GUI, are made available to the scientific community via http://zacros.org/ along with training material.
- 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 (including single-atom alloys) and other materials (e.g., chalcogenides, carbides) 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 the 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**

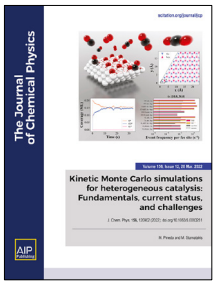
Thesis Title: “Mathematical and Computational Analysis of Signal Transduction Mechanisms in Cellular Networks”.

INVITED JOURNAL ARTICLES

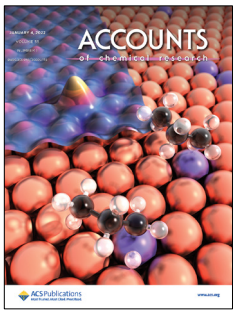
*In the following list, * denotes corresponding authors. Select publications are highlighted with ★.*

Savva, G. D., Benson, R. L., Christidi, I.-A. and **M. Stamatakis*** (2023). "Exact distributed kinetic Monte Carlo simulations for on-lattice chemical kinetics: lessons learnt from medium- and large-scale benchmarks". *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 381(2250): 20220235. *[Invited contribution to the Discussion Meeting issue "Supercomputing simulations of advanced materials" organised and edited by Scott M. Woodley, C. Richard A. Catlow, Nora H De Leeuw and Angelos Michaelides]*.

Savva, G. D., Benson, R. L., Christidi, I.-A. and **M. Stamatakis** (2023). "Large-scale benchmarks of the Time-Warp/Graph-Theoretical Kinetic Monte Carlo approach for distributed on-lattice simulations of catalytic kinetics". *Physical Chemistry Chemical Physics*, 25: 5468-5478. *[Invited contribution to a themed collection on "Computational Modelling as a Tool in Catalytic Science"]*.



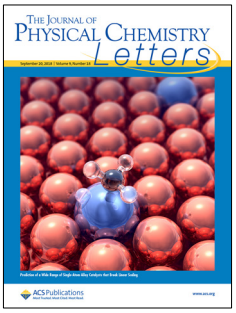
★ Pineda, M. and **M. Stamatakis*** (2022). "Kinetic Monte Carlo simulations for heterogeneous catalysis: Fundamentals, current status and challenges". *The Journal of Chemical Physics*, 156(12): 120902. *[Invited perspective article].* ***[Featured on the front cover of the issue. In the top 25% of all research outputs scored by Altmetric].***



★ Réocreux, R. and **M. Stamatakis*** (2021). "One Decade of Computational Studies on Single-Atom Alloys: Is *In Silico* Design within Reach?". *Accounts of Chemical Research*, 55(1): 87-97. *[Invited perspective article]* ***[Featured on a supplementary cover of the issue. In the top 25% of all research outputs scored by Altmetric].***

Darby, M. T. and **M. Stamatakis*** (2021). "Single-Atom Alloys for the Electrochemical Oxygen Reduction Reaction". *ChemPhysChem*, 22: 499-508. *[Invited contribution to a Special Collection on Single-Atom Catalysis]*.

Wang, Y., Papanikolaou, K. G., Hannagan, R. T., Patel, D. A., Balema, T. A., Cramer, L. A., Kress, P. L., **Stamatakis, M.*** and E. C. H. Sykes* (2020). "Surface facet dependence of competing alloying mechanisms". *The Journal of Chemical Physics*, 153(24): 244702. *[Invited contribution for a Special Collection in Honour of Women in Chemical Physics and Physical Chemistry]*.



★ Darby, M. T., **Stamatakis, M.**, Michaelides, A. and E. C. 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

*In the following list, * denotes corresponding authors and † denotes equally contributing first authors. Select publications are highlighted with ★.*

2024

Schumann, J., **Stamatakis, M.**, Michaelides, A. and R. Réocreux* (2024). "Ten-electron count rule for the binding of adsorbates on single-atom alloy catalysts". *Nature Chemistry*, Accepted.

2023

Li, W., Madan, S. E., Réocreux, R. and **M. Stamatakis*** (2023). "Elucidating the Reactivity of Oxygenates on Single-Atom Alloy Catalysts". *ACS Catalysis*, 13: 15851-15868.

Benson, R. L., Yadavalli, S. S. and **M. Stamatakis*** (2023). "Speeding up the Detection of Adsorbate Lateral Interactions in Graph-Theoretical Kinetic Monte Carlo Simulations". *The Journal of Physical Chemistry A*, 127: 10307-10319.

Hannagan, R. T., Lam, H. Y., Réocreux, R., Wang, Y., Dunbar, A., Lal, V., Çınar, V., Chen. Y., Deshlahra. P., **Stamatakis., M.***, Eagan, N. M.* and E. C. H. Sykes* (2023). "Investigating Spillover Energy as a Descriptor for Single-Atom Alloy Catalyst Design". *The Journal of Physical Chemistry Letters*, 14: 10561-10569.

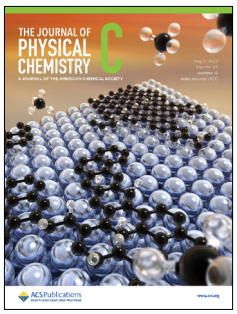
Prats, H.* and **M. Stamatakis** (2023). "Breaking linear scaling relationships with transition metal carbides". *Catalysis Science & Technology*, 13: 4635-4639.

Phan, A., **Stamatakis, M.**, Koh, C. A. and A. Striolo* (2023). "Macroscopic Insights on Clathrate Hydrate Growth from Non-Equilibrium Molecular Dynamics Simulations". *Journal of Colloid and Interface Science*, 649: 185-193.

Prats, H.* and **M. Stamatakis** (2023). "Stability and reactivity of metal nanoclusters supported on transition metal carbides". *Nanoscale Advances*, 5: 3214-3224. ***[Featured on the front cover of the issue].***

Pineda, M.*, Phan, A, Koh, C. A., Striolo, A. and **M. Stamatakis*** (2023). "Stochastic Cellular Automata Modeling of CO_2 Hydrate Growth and Morphology". *Crystal Growth & Design*, 23(6): 4222-4239. ***[Featured on a supplementary cover of the issue].***

★ Yadavalli, S. S., Jones, G., Benson, R. L. and **M. Stamatakis*** (2023). "Assessing the Impact of Adlayer Description Fidelity on Theoretical Predictions of Coking on Ni(111) at Steam Reforming Conditions". *The Journal of Physical Chemistry C*, 127(18): 8591-8606. ***[Featured on a supplementary cover of the issue].***



Ng, B. K. Y., Wong, C. C. Y., Niu, W., Garcia, H. P., Li, Y., Ho, P.-L., Kuo, W. C. H., Taylor, R. A., Taniya, K., Wei, Q., Li, M., **Stamatakis, M.*** and S. C. E. Tsang* (2023). "Molecular Layer-by-layer Re-stacking of MoS_2-In_2Se_3 by Electrostatic means: Assembly of a New Layered Photocatalyst". *Materials Chemistry Frontiers*, 7: 937-945.

2022

Schumann, J., **Stamatakis, M.**, Michaelides, A. and R. Réocreux* (2022). "Reactivity of Single-Atom Alloys as Easy as Counting to Ten". *ChemRxiv*. (DOI: 10.26434/chemrxiv-2022-d5hhf)

Xu, R., Kang, L., Papanikolaou, K. G., Wang, B., Marlow, S., He, Q., Zhang, P., Wang, J., Brett, D. J. L., **Stamatakis, M.** and F. R. Wang* (2022). "Improving the ORR performance by enhancing the Pt oxidation resistance". *Journal of Catalysis*, 416: 311-321.

Phan, A., **Stamatakis, M.**, Koh, C. A., and A. Striolo (2022). "Wetting Properties of Clathrate Hydrates in the Presence of Polycyclic Aromatic Compounds: Evidence of Ion-Specific Effects". *The Journal of Physical Chemistry Letters*, 13: 8200-8206.

★ Réocreux, R.*, Sykes, E. C. H., Michaelides, A., and M. Stamatakis* (2022). "Stick or Spill? Scaling Relationships for the Binding Energies of Adsorbates on Single-Atom Alloy Catalysts". *The Journal of Physical Chemistry Letters*, 13: 7314-7319.

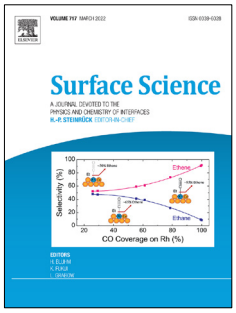
Wang, Y**., Schumann, J.***, Happel, E. E., Çınar, V., Sykes, E. C. H., **Stamatakis, M.**, Michaelides, A., and R. T. Hannagan* (2022). "Observation and Characterization of Dicarbonyls on a RhCu Single-Atom Alloy". *The Journal of Physical Chemistry Letters,* 13(27): 6316-6322.

Peña-Torres, A., Ali, A., **Stamatakis, M.**, and H. Jónsson* (2022). "Indirect Mechanism of Au adatom Diffusion on the Si(100) Surface". *Physical Review B*, 105: 205411.

Han, E., Fang, W., **Stamatakis, M.**, Richardson, J. O., and J. Chen* (2022). "Quantum Tunnelling Driven H_2 Formation on Graphene". *The Journal of Physical Chemistry Letters*, 13: 3173-3181.

Phan, A., Stoner, H. M., **Stamatakis, M.**, Koh, C. A., and A. Striolo* (2022). "Surface Morphology Effects on Clathrate Hydrate Wettability". *Journal of Colloid and Interface Science*, 611: 421-431.

Hannagan, R. T., Wang, Y., Réocreux, R., Schumann, J., **Stamatakis, M.** and E. C. H. Sykes* (2022). "Tuning the Product Selectivity of Single-Atom Alloys by Active Site Modification". *Surface Science*, 717: 121990. ***[Featured on the front cover of the issue].***



★ Prats, H.* and **M. Stamatakis*** (2022). "Atomistic and electronic structure of metal clusters supported on transition metal carbides: implications for catalysis". *Journal of Materials Chemistry A*, 10: 1522-1534.

★ Ravipati, S., Savva, G. D., Christidi, I. A., Guichard, R., Nielsen, J., Réocreux, R. and **M. Stamatakis*** (2022). "Coupling the Time-Warp algorithm with the Graph-Theoretical Kinetic Monte Carlo framework for distributed simulations of heterogeneous catalysts". *Computer Physics Communications*, 270: 108148.

2021

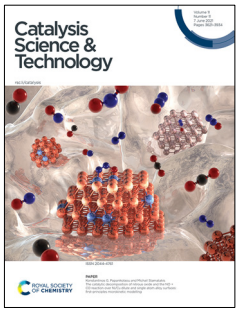
Schumann, J.*, Bao, Y., Hannagan, R. T., Sykes, E. C. H., **Stamatakis, M.** and A. Michaelides* (2021). "Periodic trends in adsorption energies around single-atom alloy active sites". *The Journal of Physical Chemistry Letters*, 12(41): 10060-10067.

Phan, A., **Stamatakis, M.**, Koh, C. A., and A. Striolo (2021). "Correlating Antiagglomerant Performance with Gas Hydrate Cohesion". *ACS Applied Materials & Interfaces*, 13: 40002-40012.

Yadavalli, S. S., Jones, G. and **M. Stamatakis*** (2021). "DFT Benchmark Studies on Representative Species and Poisons of Methane Steam Reforming on Ni(111)". *Physical Chemistry Chemical Physics*, 23: 15601-15612.

★★ Hannagan, R. T.†, Giannakakis, G.†, Réocreux, R.†, Schumann, J., Finzel, J., Wang, Y., Michaelides, A., Deshlahra, P., Christopher, P., Flytzani-Stephanopoulos, M., **Stamatakis, M.*** and E. C. H. Sykes* (2021). "First-principles design of a single-atom–alloy propane dehydrogenation catalyst". *Science*, 372 (6549): 1444-1447. ***[Highlighted in* This Week in Science *by Editor Phil Szuromi. Featured in 14 news stories from 13 outlets. In the top 5% of all research outputs scored by Altmetric].***

Papanikolaou, K. G. and **M. Stamatakis*** (2021). "The Catalytic Decomposition of Nitrous Oxide and the NO + CO Reaction over Ni/Cu Dilute and Single Atom Alloy Surfaces: First-principles Microkinetic Modelling". *Catalysis Science and Technology*, 11: 3681-3696. ***[Featured on the front cover of the issue].***



Anand, M., Beale, A. M., Boronat, M., Bowker, M., ... Réocreux, R., ... **Stamatakis, M.**, et al. (2021). "Advanced approaches: general discussion". *Faraday Discussions*, 229: 378-421.

Anand, M., Baletto, F., Bugaev, A., Catlow, R., ... Réocreux, R., ... **Stamatakis, M.**, et al. (2021). "Theory: general discussion". *Faraday Discussions*, 229: 131-160.

Réocreux, R., Fampiou, I. and **M. Stamatakis*** (2021). "The role of oxygenated species in the catalytic self-coupling of MeOH on O pre-covered Au(111)". *Faraday Discussions*, 229: 251-266.

Kress, P., Romain Réocreux, Hannagan, R., Thuening, T., Boscoboinik, J. A., **Stamatakis, M.*** and E. C. H. Sykes* (2021). "Mechanistic insights into carbon–carbon coupling on NiAu and PdAu single-atom alloys". *The Journal of Chemical Physics*, 154(20): 204701.

★ Ouyang, M., Papanikolaou, K. G., Boubnov, A., Hoffman, A. S., Giannakakis, G., Bare, S. R., **Stamatakis, M.**, Flytzani-Stephanopoulos, M. and E. C. H. Sykes* (2021). "Directing reaction pathways via in situ control of active site geometries in PdAu single-atom alloy catalysts". *Nature Communications*, 12: 1549.

Apostolopoulou, M., **Stamatakis, M.***, Striolo, A.*, Dusterhoft, R., Hull, R and R. Day (2021). "A Novel Modeling Approach to Stochastically Evaluate the Impact of Pore Network Geometry, Chemistry and Topology on Fluid Transport". *Transport in Porous Media*, 136: 495-520.

2020

★ Réocreux, R., Kress, P. L., Hannagan, R. T., Çinar, V., **Stamatakis, M.***, and E. C. H. Sykes* (2020). "Controlling Hydrocarbon (De)Hydrogenation Pathways with Bifunctional PtCu Single-Atom Alloys". *The Journal of Physical Chemistry Letters*, 11(20): 8751-8757.

Savva, G. D. and **M. Stamatakis*** (2020). "Comparison of Queueing Data-Structures for Kinetic Monte Carlo Simulations of Heterogeneous Catalysts". *The Journal of Physical Chemistry A*, 124(38): 7843-7856.

Ravipati, S., Nielsen, J., d'Avezac, M., Hetherington, J. and **M. Stamatakis*** (2020). "A Caching Scheme to Accelerate Kinetic Monte Carlo Simulations of Catalytic Reactions". *The Journal of Physical Chemistry A*, 124(35): 7140-7154.

Papanikolaou, K. G. and **M. Stamatakis*** (2020). "On the behaviour of structure-sensitive reactions on single atom and dilute alloy surfaces". *Catalysis Science & Technology*, 10(17): 5815-5828. ***[Featured on the front cover of the issue. In the top 25% of all research outputs scored by Altmetric].***

Chutia, A.*, Thetford, A., **Stamatakis, M.** and C. R. A. Catlow* (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.

★ Papanikolaou, K. G., Darby, M. T. and **M. Stamatakis*** (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. In the top 25% of all research outputs scored by Altmetric].***

2019

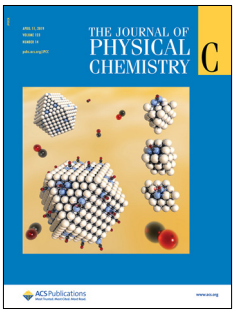
★ Réocreux, R.†, Uhlman, M.†, Thuening, T., Kress, P., Hannagan, R., **Stamatakis, M.*** and E. C. H. Sykes* (2019). "Efficient and Selective Carbon-Carbon Coupling on Coke-Resistant PdAu Single-Atom Alloys". *Chemical Communications*, 55: 15085-15088.

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 Shales and Other Heterogeneous Porous Media: Deterministic vs. Stochastic Investigations". *International Journal of Coal Geology*, 205: 140-154.

2018

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].***

2017

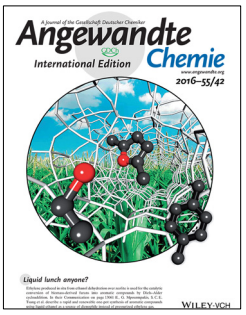
★ Apostolopoulou, M., Day, R., Hull, R., **Stamatakis, M.*** and A. Striolo* (2017). "A kinetic Monte Carlo approach to study fluid transport in pore networks". *The Journal of Chemical Physics*, 147(13): 134703.

Vignola, E., Steinmann, S. N., Vandegehuchte, B. D., Curulla, D., **Stamatakis, M.*** and P. Sautet* (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.

2016



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.

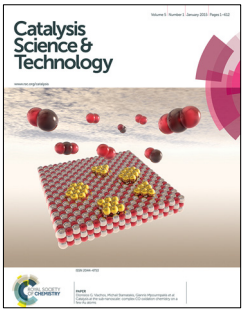
Campbell, C., van Santen, R., **Stamatakis, M.**, Collis, N., Freund, H.-J., Plaisance, C., Sauer, J., Garrett, B., Gross, E., et al. (2016). "Catalyst design from theory to practice: general discussion". *Faraday Discussions*, 188: 279-307.

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.

2015



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].***

2014

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.

2013

★ 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.

2012

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.

2011

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.

2010

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.

2006 – 2009

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

Papanikolaou, K. G. and **M. Stamatakis*** (2020). "Chapter 7: Toward the accurate modeling of the kinetics of surface reactions using the kinetic Monte Carlo method" in Grammatikopoulos, P. (Ed.), "*Computational Modelling of Nanomaterials*", Amsterdam, Netherlands: Elsevier.

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 KEYNOTE LECTURES

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.

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. "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.

INVITED TALKS/ SEMINARS

2023

M. Stamatakis. "Fundamental Understanding and Simulation-Driven Design of Heterogeneous Catalysts". BUA-OXF Partnership in Catalysis Research, Technische Universität Berlin, Berlin, Germany. Nov. 23, 2023.

M. Stamatakis. "A Decade-Long Quest into Understanding and Developing Novel Single-Atom Alloy Catalysts". American Institute of Chemical Engineers Annual Meeting 2023 Annual Meeting. Session 366: In Memoriam of Maria Flytzani-Stephanopoulos. Orlando, FL, USA. Nov. 6, 2023.

M. Stamatakis. "Fundamental Understanding and Simulation-Driven Design of Transition Metal Alloy Catalysts". Inorganic Chemistry Lab, Department of Chemistry, University of Oxford, Oxford, UK, Oct 10, 2023.

M. Stamatakis. "Kinetic Simulations of Heterogeneous Catalysts: Fundamentals, Success Stories & Beyond". Tufts University, Boston, USA, Online Seminar, Oct 3, 2023.

M. Stamatakis. "Coupling the Time-Warp Algorithm with the Graph-Theoretical KMC Approach for Catalysis Simulations on Mega-Lattices and beyond". Theory Department – Fritz Haber Institute, Berlin, Germany, May 4, 2023.

M. Stamatakis. "Unravelling Complexity in Heterogeneous Catalysis via High-Fidelity Kinetic Monte Carlo Simulation". TACO Colloquium: Taming Complexity in Materials Modeling, Technical University of Vienna, Vienna, Austria. Mar 20, 2023.

M. Stamatakis. "Conquering the Mesoscale in the Simulation of Surfaces and Interfaces via Distributed Lattice-Based Kinetic Monte Carlo". MS381 Stochastic and Multiscale Modeling Approaches for Interfacial Systems - Part I of II, SIAM Conference on Computational Science and Engineering 2023, Amsterdam, The Netherlands. Mar 3, 2023.

M. Stamatakis. "Catalysis *In Silico*: Success Stories and Opportunities for Innovation". Laboratoire de Chimie, École Normale Supérieure de Lyon, France. Jan 29, 2023.

2022

M. Stamatakis. "Rationalising and Predicting the Catalytic Behaviour of Single Atom Alloys via Molecular and Kinetic Modelling", Workshop on Single-Atom Catalysis, "Giulio Natta" Department of Chemistry, Materials and Chemical Engineering, Politecnico di Milano, Milano, Italy, Oct 6, 2022.

Papanikolaou, K., Darby, M. T. and **M. Stamatakis**. "Ensemble Effects and Structure Sensitivity for the CO Oxidation and NO_x Reduction Reactions Catalysed by Dilute Alloys", SMS – Surfaces and materials symposium, York, UK, Jul 23, 2022.

M. Stamatakis. "Next-Generation Kinetic Monte Carlo Approaches for Understanding Catalytic Kinetics at Unprecedented Spatial and Temporal Scales", Software Solutions to the Challenges of Materials Modelling, Satellite meeting by The Royal Society, organised by Prof. Scott Woodley, Prof. Sir Richard Catlow FRS, Prof. Nora H de Leeuw and Prof. Angelos Michaelides FRS, Sedgebrook Hall, Northampton, UK, Jun 9, 2022.

M. Stamatakis. "*In Silico* Design of Single-Atom- and Highly-Dilute-Alloy Catalysts: Success Stories and Opportunities for Innovation", Theory Department – Fritz Haber Institute, Berlin, Germany, Mar 3, 2022.

2021

M. Stamatakis. "Activation and Coupling of C1 Species on Single-Atom Alloy Catalysts". UK-China Newton Researchers Link Workshop: "Catalytic Chemistry and Chemical Technology in C1 Process", Queen's University Belfast, Belfast, UK, Nov 27, 2021.

M. Stamatakis. "Distributed Parallelisation of Kinetic Monte-Carlo Simulations for Heterogeneous Catalysis with the Time-Warp Algorithm". American Chemical Society Fall 2021 National Meeting, Symposium: "Multiscale Modeling in Heterogeneous Catalysis", Virtual, Aug 22, 2021.

M. Stamatakis. "Unraveling the oxidative coupling of methanol on Au(111) using first-principles-based kinetic modelling". American Chemical Society Spring 2021 National Meeting, Symposium: "Elucidations of Mechanisms and Kinetics on Surfaces", Virtual, Apr 7, 2021.

2020

M. Stamatakis. "Highly-Dilute Alloys as Catalysts for Challenging Reactions: New Frontiers and Opportunities for Innovation". Johnson Matthey Modelling Meeting (virtual), Nov 20, 2020.

2019

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.

2018

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 Dilemma". 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.

2017

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.

2016

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. "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.

2015

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.

2014

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.

2013

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.

2012

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.

2008 – 2011

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

2022

Papanikolaou, K., Darby, M. T. and **M. Stamatakis**. "Single-Atom Alloys and Highly Dilute Alloys as Catalysts for Emissions Control", International Conference on Theoretical Aspects of Catalysis (ICTAC), École Normale Supérieure de Lyon, Lyon, France. Jun 16, 2022.

2020

M. Stamatakis. "Algorithm and software development for scalable kinetic Monte Carlo simulations of catalysts". ReaxPro Online Conference (virtual meeting organised in the context of the ReaxPro European Project). Jul 9, 2020.

2019

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.

2018

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.

2017

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.

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.

2016

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.

2015

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.

2014

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.

2013

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.

2012

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.

2011

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.

2010

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.

2009

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.

2008

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.

2004-2007

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

2022 "Preventing Catalyst Poisoning in Methane Valorisation Chemistries". 42 months. £78,000. Impact Studentship sponsored by Johnson Matthey PLC.

2021 "*Transition Metal Carbides as Efficient Catalysts for Methane Partial Oxidation*". 24 months. €212,934. Project ID: 891756. Sponsored by the European Commission (Horizon 2020).

2020 "*Zacros* Software Package Development: Towards Petascale Kinetic Monte Carlo Simulations with the Time-Warp Algorithm". 12 months. £102,763. Project ID: ARCHER2-eCSE01-13. Sponsored by the Edinburgh Parallel Computing Centre through subcontracting from the Engineering and Physical Sciences Research Council, UK.

2018 "Computational Design of Poisoning-Resistant Catalysts for Methane-Steam Reforming". 42 months. £66,000. 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

2023 Friedrich Wilhelm Bessel Research Award by the Alexander von Humboldt Foundation. *(The Alexander von Humboldt Foundation bestows Friedrich Wilhelm Bessel Research Awards annually to 20 internationally renowned scientists from outside Germany. The prize is regarded as one of the most prestigious German research awards to foreign scientists).*

2022 Faraday Division Horizon Prize by the Royal Society of Chemistry "*for the development of single-atom alloys, a new class of catalysts that play a prominent role in the energy and sustainability fields*".

2020 Fellow of the Royal Society of Chemistry (FRSC).

2016 Fellow of the Higher Education Academy (FHEA).

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

College Tutor

Lady Margaret Hall, University College London, UK

2023 – Present Developed material for and held tutorial sessions for Chemistry students (UG level 1st – 3rd year).

Instructor

Chemical Engineering Department, University College London, UK

2018 – 2023 Developed educational material (lecture slides, video lectures, 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 – 2023 Developed educational material (lecture slides, video lectures), 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 – 2023 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 – 2023 Coordinated, developed educational material (lecture slides, video lectures, coursework, quizzes) 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 – 2023 Coordinated, developed educational material (lecture slides, video lectures, coursework, final project, quizzes), 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 and Researcher Mentor

Chemical Engineering Department, University College London, UK

2012 – 2023 Mentored MEng, MSc and PhD students, Post-Doctoral Research Associates and Fellows, 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

2020 – 2021	Member of the Early Career Advisory Board of ACS Catalysis
2020 – Present	Fellow of the Royal Society of Chemistry (FRSC)
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 – 2020	Member of the Royal Society of Chemistry (RSC)
2013 – 2023	Member of the Centre for Process Systems Engineering (CPSE)
2012 – 2023	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

2023	Lead organiser of Workshop “KMC as a Tool for Understanding Catalytic Function”, at the Fritz Haber Institute, Berlin, Germany.
2020	Co-organiser of virtual Workshop on “Theory, Applications, and Tools for Multiscale Kinetic Modeling”, with Prof. Matteo Maestri (Politecnico di Milano) and Prof. Dionisios G. Vlachos (University of Delaware).
2020	Lead organiser of the “ReaxPro Online Conference”, a virtual meeting in the context of the ReaxPro European Project.
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

Czech Science Foundation (Grantová agentura České republiky, GAČR)

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 Applied Materials & Interfaces

ACS Catalysis

ACS Nano

ACS Sustainable Chemistry & Engineering

Advanced Functional Materials

AIChE Journal

Angewandte Chemie

Applied Catalysis B: Environmental

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

Nature Catalysis

Nature Chemistry

Nature Communications

Physical Chemistry Chemical Physics

Physical Review E

Physical Review Letters

PLoS One

Proceedings of the National Academy of Sciences (PNAS)

Proceedings of the Royal Society A

Science

Science Advances

Surface Science

The Journal of Chemical Physics

SERVICE – UNIVERSITY

University College London, UK

2020 – 2023	Departmental Graduate (PhD) Tutor
2018 – 2023	Non professorial member of the UCL Academic Board
2013 – 2023	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 – 2023	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