# Michail Stamatakis

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 75 papers | 3,226 citations | 26 h-index | 56 g-index |
| 86 ext. papers | 3,886 ext. citations | 6.3 avg, IF | 5.91 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 75 | Coupling the time-warp algorithm with the graph-theoretical kinetic Monte Carlo framework for distributed simulations of heterogeneous catalysts. *Computer Physics Communications*, **2022**, 270, 108148 | 4.2 | 2 |
| 74 | Kinetic Monte Carlo simulations for heterogeneous catalysis: Fundamentals, current status, and challenges.. *Journal of Chemical Physics*, **2022**, 156, 120902 | 3.9 | 3 |
| 73 | Quantum Tunnelling Driven H Formation on Graphene.. *Journal of Physical Chemistry Letters*, **2022**, 3173-3181 | 6.4 | 2 |
| 72 | Tuning the Product Selectivity of Single-Atom Alloys by Active Site Modification. *Surface Science*, **2021**, 717, 121990 | 1.8 | 0 |
| 71 | Surface morphology effects on clathrate hydrate wettability.. *Journal of Colloid and Interface Science*, **2021**, 611, 421-431 | 9.3 | 4 |
| 70 | Periodic Trends in Adsorption Energies around Single-Atom Alloy Active Sites. *Journal of Physical Chemistry Letters*, **2021**, 12, 10060-10067 | 6.4 | 5 |
| 69 | A Novel Modeling Approach to Stochastically Evaluate the Impact of Pore Network Geometry, Chemistry and Topology on Fluid Transport. *Transport in Porous Media*, **2021**, 136, 495-520 | 3.1 | 1 |
| 68 | Directing reaction pathways via in situ control of active site geometries in PdAu single-atom alloy catalysts. *Nature Communications*, **2021**, 12, 1549 | 17.4 | 32 |
| 67 | Mechanistic insights into carbon-carbon coupling on NiAu and PdAu single-atom alloys. *Journal of Chemical Physics*, **2021**, 154, 204701 | 3.9 | 3 |
| 66 | First-principles design of a single-atom alloy propane dehydrogenation catalyst. *Science*, **2021**, 372, 1444-1447 | 33.5 | 62 |
| 65 | The role of oxygenated species in the catalytic self-coupling of MeOH on O pre-covered Au(111). *Faraday Discussions*, **2021**, 229, 251-266 | 3.6 | 4 |
| 64 | DFT benchmark studies on representative species and poisons of methane steam reforming on Ni(111). *Physical Chemistry Chemical Physics*, **2021**, 23, 15601-15612 | 3.6 | 1 |
| 63 | Single-Atom Alloys for the Electrochemical Oxygen Reduction Reaction. *ChemPhysChem*, **2021**, 22, 499-508 | 3.2 | 13 |
| 62 | Correlating Antiagglomerant Performance with Gas Hydrate Cohesion. *ACS Applied Materials & Interfaces*, **2021**, 13, 40002-40012 | 9.5 | 5 |
| 61 | 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*, **2021**, 11, 3681-3696 | 5.5 | 6 |
| 60 | One Decade of Computational Studies on Single-Atom Alloys: Is Design within Reach?. *Accounts of Chemical Research*, **2021**, | 24.3 | 3 |
| 59 | On the behaviour of structure-sensitive reactions on single atom and dilute alloy surfaces. *Catalysis Science and Technology*, **2020**, 10, 5815-5828 | 5.5 | 5 |

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| 58 | A DFT and KMC based study on the mechanism of the water gas shift reaction on the Pd(100) surface. *Physical Chemistry Chemical Physics*, **2020**, 22, 3620-3632 | 3.6 | 18 |
| 57 | Surface facet dependence of competing alloying mechanisms. *Journal of Chemical Physics*, **2020**, 153, 244702 | 3.9 | 6 |
| 56 | Engineering the Surface Architecture of Highly Dilute Alloys: An ab Initio Monte Carlo Approach. *ACS Catalysis*, **2020**, 10, 1224-1236 | 13.1 | 22 |
| 55 | Comparison of Queueing Data-Structures for Kinetic Monte Carlo Simulations of Heterogeneous Catalysts. *Journal of Physical Chemistry A*, **2020**, 124, 7843-7856 | 2.8 | 5 |
| 54 | Toward the accurate modeling of the kinetics of surface reactions using the kinetic Monte Carlo method. *Frontiers of Nanoscience*, **2020**, 17, 95-125 | 0.7 | 3 |
| 53 | Controlling Hydrocarbon (De)Hydrogenation Pathways with Bifunctional PtCu Single-Atom Alloys. *Journal of Physical Chemistry Letters*, **2020**, 11, 8751-8757 | 6.4 | 12 |
| 52 | A Caching Scheme To Accelerate Kinetic Monte Carlo Simulations of Catalytic Reactions. *Journal of Physical Chemistry A*, **2020**, 124, 7140-7154 | 2.8 | 5 |
| 51 | Kinetic Isolation between Turnovers on Au18 Nanoclusters: Formic Acid Decomposition One Molecule at a Time. *ACS Catalysis*, **2019**, 9, 9446-9457 | 13.1 | 10 |
| 50 | Carbon Monoxide Mediated Hydrogen Release from PtCu Single-Atom Alloys: The Punctured Molecular Cork Effect. *Journal of Physical Chemistry C*, **2019**, 123, 10419-10428 | 3.8 | 13 |
| 49 | A Kinetic Monte Carlo Study to Investigate the Effective Permeability and Conductivity of Microfractures within Unconventional Reservoirs **2019**, | | 1 |
| 48 | Estimating permeability in shales and other heterogeneous porous media: Deterministic vs. stochastic investigations. *International Journal of Coal Geology*, **2019**, 205, 140-154 | 5.5 | 15 |
| 47 | 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*, **2019**, 15, 6907-6922 | 5.4 | 13 |
| 46 | CO-Induced Aggregation and Segregation of Highly Dilute Alloys: A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2019**, 123, 9128-9138 | 3.8 | 35 |
| 45 | Efficient and selective carbon-carbon coupling on coke-resistant PdAu single-atom alloys. *Chemical Communications*, **2019**, 55, 15085-15088 | 5.8 | 13 |
| 44 | Elucidating the Stability and Reactivity of Surface Intermediates on Single-Atom Alloy Catalysts. *ACS Catalysis*, **2018**, 8, 5038-5050 | 13.1 | 95 |
| 43 | Pt/Cu single-atom alloys as coke-resistant catalysts for efficient C-H activation. *Nature Chemistry*, **2018**, 10, 325-332 | 17.6 | 308 |
| 42 | Carbon Monoxide Poisoning Resistance and Structural Stability of Single Atom Alloys. *Topics in Catalysis*, **2018**, 61, 428-438 | 2.3 | 75 |
| 41 | On the stochastic modelling of surface reactions through reflected chemical Langevin equations. *Computers and Chemical Engineering*, **2018**, 117, 145-158 | 4 | 3 |

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| 40 | Non-Equilibrium Thermodynamics and Stochastic Dynamics of a Bistable Catalytic Surface Reaction. *Entropy*, **2018**, 20, | 2.8 | 1 |
| 39 | Adlayer structure and lattice size effects on catalytic rates predicted from KMC simulations: NO oxidation on Pt(111). *Journal of Chemical Physics*, **2018**, 149, 184701 | 3.9 | 12 |
| 38 | Lonely Atoms with Special Gifts: Breaking Linear Scaling Relationships in Heterogeneous Catalysis with Single-Atom Alloys. *Journal of Physical Chemistry Letters*, **2018**, 9, 5636-5646 | 6.4 | 127 |
| 37 | MoS monolayer catalyst doped with isolated Co atoms for the hydrodeoxygenation reaction. *Nature Chemistry*, **2017**, 9, 810-816 | 17.6 | 489 |
| 36 | A kinetic Monte Carlo approach to study fluid transport in pore networks. *Journal of Chemical Physics*, **2017**, 147, 134703 | 3.9 | 13 |
| 35 | Beyond mean-field approximations for accurate and computationally efficient models of on-lattice chemical kinetics. *Journal of Chemical Physics*, **2017**, 147, 024105 | 3.9 | 41 |
| 34 | A machine learning approach to graph-theoretical cluster expansions of the energy of adsorbate layers. *Journal of Chemical Physics*, **2017**, 147, 054106 | 3.9 | 23 |
| 33 | Steady-State CO Oxidation on Pd(111): First-Principles Kinetic Monte Carlo Simulations and Microkinetic Analysis. *Topics in Catalysis*, **2017**, 60, 141-151 | 2.3 | 21 |
| 32 | Preparation, Structure, and Surface Chemistry of Ni□Au Single Atom Alloys. *Journal of Physical Chemistry C*, **2016**, 120, 13574-13580 | 3.8 | 60 |
| 31 | Catalyst design from theory to practice: general discussion. *Faraday Discussions*, **2016**, 188, 279-307 | 3.6 | 2 |
| 30 | Controlling Hydrogen Activation, Spillover, and Desorption with Pd-Au Single-Atom Alloys. *Journal of Physical Chemistry Letters*, **2016**, 7, 480-5 | 6.4 | 129 |
| 29 | Rationalizing the Relation between Adlayer Structure and Observed Kinetics in Catalysis. *ACS Catalysis*, **2016**, 6, 2105-2111 | 13.1 | 28 |
| 28 | Innenr□ktitelbild: From Biomass-Derived Furans to Aromatics with Ethanol over Zeolite (Angew. Chem. 42/2016). *Angewandte Chemie*, **2016**, 128, 13545-13545 | 3.6 | |
| 27 | From Biomass-Derived Furans to Aromatics with Ethanol over Zeolite. *Angewandte Chemie - International Edition*, **2016**, 55, 13061-13066 | 16.4 | 73 |
| 26 | From Biomass-Derived Furans to Aromatics with Ethanol over Zeolite. *Angewandte Chemie*, **2016**, 128, 13255-13260 | 3.6 | 26 |
| 25 | Catalysis at the sub-nanoscale: complex CO oxidation chemistry on a few Au atoms. *Catalysis Science and Technology*, **2015**, 5, 134-141 | 5.5 | 23 |
| 24 | Kinetic modelling of heterogeneous catalytic systems. *Journal of Physics Condensed Matter*, **2015**, 27, 013001 | 1.8 | 66 |
| 23 | CO Oxidation on Pd(111): A First-Principles-Based Kinetic Monte Carlo Study. *ACS Catalysis*, **2014**, 4, 2143-2152 | 3.1 | 79 |

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|---|---|---|---|
| 22 | Adsorption Behavior of Noble Metal Clusters and Their Alloys. *Journal of Computational and Theoretical Nanoscience*, **2014**, 11, 511-520 | 0.3 | 9 |
| 21 | Design Principles of Heteroepitaxial Bimetallic Catalysts. *ACS Catalysis*, **2013**, 3, 2248-2255 | 13.1 | 26 |
| 20 | Cell population balance and hybrid modeling of population dynamics for a single gene with feedback. *Computers and Chemical Engineering*, **2013**, 53, 25-34 | 4 | 5 |
| 19 | Controlling a spillover pathway with the molecular cork effect. *Nature Materials*, **2013**, 12, 523-8 | 27 | 88 |
| 18 | Parallel kinetic Monte Carlo simulation framework incorporating accurate models of adsorbate lateral interactions. *Journal of Chemical Physics*, **2013**, 139, 224706 | 3.9 | 91 |
| 17 | Unraveling the Complexity of Catalytic Reactions via Kinetic Monte Carlo Simulation: Current Status and Frontiers. *ACS Catalysis*, **2012**, 2, 2648-2663 | 13.1 | 158 |
| 16 | Multiscale modeling reveals poisoning mechanisms of MgO-supported Au clusters in CO oxidation. *Nano Letters*, **2012**, 12, 3621-6 | 11.5 | 48 |
| 15 | Equivalence of on-Lattice Stochastic Chemical Kinetics with the Well-Mixed Chemical Master Equation in the Limit of Fast Diffusion. *Computers and Chemical Engineering*, **2011**, 35, 2602-2610 | 4 | 38 |
| 14 | Predicting the adsorption behavior in bulk from metal clusters. *Chemical Physics Letters*, **2011**, 518, 99-103 | 2.5 | 12 |
| 13 | A review of multiscale modeling of metal-catalyzed reactions: Mechanism development for complexity and emergent behavior. *Chemical Engineering Science*, **2011**, 66, 4319-4355 | 4.4 | 256 |
| 12 | Deterministic and stochastic population-level simulations of an artificial lac operon genetic network. *BMC Bioinformatics*, **2011**, 12, 301 | 3.6 | 11 |
| 11 | A common repressor pool results in indeterminacy of extrinsic noise. *Chaos*, **2011**, 21, 047523 | 3.3 | 11 |
| 10 | A graph-theoretical kinetic Monte Carlo framework for on-lattice chemical kinetics. *Journal of Chemical Physics*, **2011**, 134, 214115 | 3.9 | 133 |
| 9 | 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*, **2011**, 115, 24750-24762 | 3.8 | 97 |
| 8 | Intrinsic noise and division cycle effects on an abstract biological oscillator. *Chaos*, **2010**, 20, 033118 | 3.3 | 6 |
| 7 | Understanding mixing of Ni and Pt in the Ni/Pt(111) bimetallic catalyst via molecular simulation and experiments. *Journal of Chemical Physics*, **2010**, 133, 224503 | 3.9 | 18 |
| 6 | A mathematical and computational approach for integrating the major sources of cell population heterogeneity. *Journal of Theoretical Biology*, **2010**, 266, 41-61 | 2.3 | 16 |
| 5 | Adaptive coarse-grained Monte Carlo simulation of reaction and diffusion dynamics in heterogeneous plasma membranes. *BMC Bioinformatics*, **2010**, 11, 218 | 3.6 | 8 |

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| 4 | Cell population balance, ensemble and continuum modeling frameworks: Conditional equivalence and hybrid approaches. *Chemical Engineering Science*, **2010**, 65, 1008-1015 | 4.4 | 16 |
| 3 | Comparison of deterministic and stochastic models of the lac operon genetic network. *Biophysical Journal*, **2009**, 96, 887-906 | 2.9 | 46 |
| 2 | Astrocyte signaling in the presence of spatial inhomogeneities. *Chaos*, **2007**, 17, 033123 | 3.3 | 3 |
| 1 | Modeling of ATP-mediated signal transduction and wave propagation in astrocytic cellular networks. *Journal of Theoretical Biology*, **2006**, 241, 649-68 | 2.3 | 30 |