Michail Stamatakis

List of Publications by Year
in descending order

82	4,487	196777 29	116156 66
papers	citations	h-index	g-index

86	86	86	5627
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	3.0	8
2	Atomistic and electronic structure of metal clusters supported on transition metal carbides: implications for catalysis. Journal of Materials Chemistry A, 2022, 10, 1522-1534.	5.2	13
3	Surface morphology effects on clathrate hydrate wettability. Journal of Colloid and Interface Science, 2022, 611, 421-431.	5.0	19
4	Kinetic Monte Carlo simulations for heterogeneous catalysis: Fundamentals, current status, and challenges. Journal of Chemical Physics, 2022, 156, 120902.	1.2	29
5	Quantum Tunnelling Driven H₂ Formation on Graphene. Journal of Physical Chemistry Letters, 2022, 13, 3173-3181.	2.1	10
6	One Decade of Computational Studies on Single-Atom Alloys: Is In Silico Design within Reach?. Accounts of Chemical Research, 2022, 55, 87-97.	7.6	18
7	Indirect mechanism of Au adatom diffusion on the Si(100) surface. Physical Review B, 2022, 105, .	1.1	4
8	Observation and Characterization of Dicarbonyls on a RhCu Single-Atom Alloy. Journal of Physical Chemistry Letters, 2022, 13, 6316-6322.	2.1	2
9	The role of oxygenated species in the catalytic self-coupling of MeOH on O pre-covered Au(111). Faraday Discussions, 2021, 229, 251-266.	1.6	7
10	DFT benchmark studies on representative species and poisons of methane steam reforming on Ni(111). Physical Chemistry Chemical Physics, 2021, 23, 15601-15612.	1.3	4
11	Theory: general discussion. Faraday Discussions, 2021, 229, 131-160.	1.6	0
12	Advanced approaches: general discussion. Faraday Discussions, 2021, 229, 378-421.	1.6	1
13	Singleâ€Atom Alloys for the Electrochemical Oxygen Reduction Reaction. ChemPhysChem, 2021, 22, 499-508.	1.0	20
14	Directing reaction pathways via in situ control of active site geometries in PdAu single-atom alloy catalysts. Nature Communications, 2021, 12, 1549.	5.8	82
15	Mechanistic insights into carbonâ€“carbon coupling on NiAu and PdAu single-atom alloys. Journal of Chemical Physics, 2021, 154, 204701.	1.2	10
16	First-principles design of a single-atomâ€“alloy propane dehydrogenation catalyst. Science, 2021, 372, 1444-1447.	6.0	185
17	Correlating Antiagglomerant Performance with Gas Hydrate Cohesion. ACS Applied Materials & Interfaces, 2021, 13, 40002-40012.	4.0	13
18	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.	2.1	12

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19	Periodic Trends in Adsorption Energies around Single-Atom Alloy Active Sites. Journal of Physical Chemistry Letters, 2021, 12, 10060-10067.	2.1	16
20	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.	1.2	3
21	Tuning the Product Selectivity of Single-Atom Alloys by Active Site Modification. Surface Science, 2021, 717, 121990.	0.8	1
22	Engineering the Surface Architecture of Highly Dilute Alloys: An ab Initio Monte Carlo Approach. ACS Catalysis, 2020, 10, 1224-1236.	5.5	33
23	Comparison of Queueing Data-Structures for Kinetic Monte Carlo Simulations of Heterogeneous Catalysts. Journal of Physical Chemistry A, 2020, 124, 7843-7856.	1.1	8
24	Toward the accurate modeling of the kinetics of surface reactions using the kinetic Monte Carlo method. Frontiers of Nanoscience, 2020, 17, 95-125.	0.3	5
25	Controlling Hydrocarbon (De)Hydrogenation Pathways with Bifunctional PtCu Single-Atom Alloys. Journal of Physical Chemistry Letters, 2020, 11, 8751-8757.	2.1	20
26	A Caching Scheme To Accelerate Kinetic Monte Carlo Simulations of Catalytic Reactions. Journal of Physical Chemistry A, 2020, 124, 7140-7154.	1.1	8
27	On the behaviour of structure-sensitive reactions on single atom and dilute alloy surfaces. Catalysis Science and Technology, 2020, 10, 5815-5828.	2.1	8
28	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.	1.3	22
29	Surface facet dependence of competing alloying mechanisms. Journal of Chemical Physics, 2020, 153, 244702.	1.2	11
30	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.	2.3	21
31	Kinetic Isolation between Turnovers on Au₁₈ Nanoclusters: Formic Acid Decomposition One Molecule at a Time. ACS Catalysis, 2019, 9, 9446-9457.	5.5	20
32	Carbon Monoxide Mediated Hydrogen Release from PtCu Single-Atom Alloys: The Punctured Molecular Cork Effect. Journal of Physical Chemistry C, 2019, 123, 10419-10428.	1.5	19
33	A Kinetic Monte Carlo Study to Investigate the Effective Permeability and Conductivity of Microfractures within Unconventional Reservoirs. , 2019, , .		1
34	Estimating permeability in shales and other heterogeneous porous media: Deterministic vs. stochastic investigations. International Journal of Coal Geology, 2019, 205, 140-154.	1.9	18
35	CO-Induced Aggregation and Segregation of Highly Dilute Alloys: A Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 9128-9138.	1.5	47
36	Efficient and selective carbonâ€“carbon coupling on coke-resistant PdAu single-atom alloys. Chemical Communications, 2019, 55, 15085-15088.	2.2	23

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37	Elucidating the Stability and Reactivity of Surface Intermediates on Single-Atom Alloy Catalysts. ACS Catalysis, 2018, 8, 5038-5050.	5.5	152
38	Pt/Cu single-atom alloys as coke-resistant catalysts for efficient Câ€“H activation. Nature Chemistry, 2018, 10, 325-332.	6.6	472
39	Carbon Monoxide Poisoning Resistance and Structural Stability of Single Atom Alloys. Topics in Catalysis, 2018, 61, 428-438.	1.3	117
40	Non-Equilibrium Thermodynamics and Stochastic Dynamics of a Bistable Catalytic Surface Reaction. Entropy, 2018, 20, 811.	1.1	1
41	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.	1.2	14
42	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.	2.1	206
43	On the stochastic modelling of surface reactions through reflected chemical Langevin equations. Computers and Chemical Engineering, 2018, 117, 145-158.	2.0	4
44	MoS2 monolayer catalyst doped with isolated Co atoms for the hydrodeoxygenation reaction. Nature Chemistry, 2017, 9, 810-816.	6.6	683
45	A kinetic Monte Carlo approach to study fluid transport in pore networks. Journal of Chemical Physics, 2017, 147, 134703.	1.2	16
46	Beyond mean-field approximations for accurate and computationally efficient models of on-lattice chemical kinetics. Journal of Chemical Physics, 2017, 147, 024105.	1.2	53
47	A machine learning approach to graph-theoretical cluster expansions of the energy of adsorbate layers. Journal of Chemical Physics, 2017, 147, 054106.	1.2	31
48	Steady-State CO Oxidation on Pd(111): First-Principles Kinetic Monte Carlo Simulations and Microkinetic Analysis. Topics in Catalysis, 2017, 60, 141-151.	1.3	26
49	InnenrÃ¼cktitelbild: From Biomassâ€Derived Furans to Aromatics with Ethanol over Zeolite (Angew.) Tj ETQq1 1 0.784314 rgBT /Ove	1.6	0
50	From Biomassâ€Derived Furans to Aromatics with Ethanol over Zeolite. Angewandte Chemie - International Edition, 2016, 55, 13061-13066.	7.2	110
51	From Biomassâ€Derived Furans to Aromatics with Ethanol over Zeolite. Angewandte Chemie, 2016, 128, 13255-13260.	1.6	31
52	Preparation, Structure, and Surface Chemistry of Niâ€“Au Single Atom Alloys. Journal of Physical Chemistry C, 2016, 120, 13574-13580.	1.5	70
53	Catalyst design from theory to practice: general discussion. Faraday Discussions, 2016, 188, 279-307.	1.6	2
54	Bridging model and real catalysts: general discussion. Faraday Discussions, 2016, 188, 565-589.	1.6	3

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55	Controlling Hydrogen Activation, Spillover, and Desorption with Pdâ€“Au Single-Atom Alloys. Journal of Physical Chemistry Letters, 2016, 7, 480-485.	2.1	169
56	Rationalizing the Relation between Adlayer Structure and Observed Kinetics in Catalysis. ACS Catalysis, 2016, 6, 2105-2111.	5.5	33
57	Kinetic modelling of heterogeneous catalytic systems. Journal of Physics Condensed Matter, 2015, 27, 013001.	0.7	85
58	Catalysis at the sub-nanoscale: complex CO oxidation chemistry on a few Au atoms. Catalysis Science and Technology, 2015, 5, 134-141.	2.1	25
59	Adsorption Behavior of Noble Metal Clusters and Their Alloys. Journal of Computational and Theoretical Nanoscience, 2014, 11, 511-520.	0.4	10
60	CO Oxidation on Pd(111): A First-Principles-Based Kinetic Monte Carlo Study. ACS Catalysis, 2014, 4, 2143-2152.	5.5	94
61	Design Principles of Heteroepitaxial Bimetallic Catalysts. ACS Catalysis, 2013, 3, 2248-2255.	5.5	31
62	Cell population balance and hybrid modeling of population dynamics for a single gene with feedback. Computers and Chemical Engineering, 2013, 53, 25-34.	2.0	5
63	Controlling a spillover pathway with the molecular cork effect. Nature Materials, 2013, 12, 523-528.	13.3	119
64	Parallel kinetic Monte Carlo simulation framework incorporating accurate models of adsorbate lateral interactions. Journal of Chemical Physics, 2013, 139, 224706.	1.2	122
65	Unraveling the Complexity of Catalytic Reactions via Kinetic Monte Carlo Simulation: Current Status and Frontiers. ACS Catalysis, 2012, 2, 2648-2663.	5.5	195
66	Multiscale Modeling Reveals Poisoning Mechanisms of MgO-Supported Au Clusters in CO Oxidation. Nano Letters, 2012, 12, 3621-3626.	4.5	52
67	A common repressor pool results in indeterminacy of extrinsic noise. Chaos, 2011, 21, 047523.	1.0	11
68	A graph-theoretical kinetic Monte Carlo framework for on-lattice chemical kinetics. Journal of Chemical Physics, 2011, 134, 214115.	1.2	171
69	First-Principles-Based Kinetic Monte Carlo Simulation of the Structure Sensitivity of the Waterâ€“Gas Shift Reaction on Platinum Surfaces. Journal of Physical Chemistry C, 2011, 115, 24750-24762.	1.5	108
70	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.	2.0	46
71	Predicting the adsorption behavior in bulk from metal clusters. Chemical Physics Letters, 2011, 518, 99-103.	1.2	12
72	A review of multiscale modeling of metal-catalyzed reactions: Mechanism development for complexity and emergent behavior. Chemical Engineering Science, 2011, 66, 4319-4355.	1.9	306

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73	Deterministic and stochastic population-level simulations of an artificial lac operon genetic network. BMC Bioinformatics, 2011, 12, 301.	1.2	13
74	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.	1.2	18
75	A mathematical and computational approach for integrating the major sources of cell population heterogeneity. Journal of Theoretical Biology, 2010, 266, 41-61.	0.8	19
76	Adaptive coarse-grained Monte Carlo simulation of reaction and diffusion dynamics in heterogeneous plasma membranes. BMC Bioinformatics, 2010, 11, 218.	1.2	10
77	Cell population balance, ensemble and continuum modeling frameworks: Conditional equivalence and hybrid approaches. Chemical Engineering Science, 2010, 65, 1008-1015.	1.9	18
78	Intrinsic noise and division cycle effects on an abstract biological oscillator. Chaos, 2010, 20, 033118.	1.0	6
79	Comparison of Deterministic and Stochastic Models of the lac Operon Genetic Network. Biophysical Journal, 2009, 96, 887-906.	0.2	53
80	A Mathematical and Computational Approach for Integrating the Major Sources of Cell Population Heterogeneity. Biophysical Journal, 2009, 96, 307a.	0.2	0
81	Astrocyte signaling in the presence of spatial inhomogeneities. Chaos, 2007, 17, 033123.	1.0	3
82	Modeling of ATP-mediated signal transduction and wave propagation in astrocytic cellular networks. Journal of Theoretical Biology, 2006, 241, 649-668.	0.8	39