

Ensembles of Metastable States Govern Heterogeneous

Accounts of Chemical Research

53, 447-458

DOI: [10.1021/acs.accounts.9b00531](https://doi.org/10.1021/acs.accounts.9b00531)

Citation Report

#	ARTICLE	IF	CITATIONS
1	Effect of Collective Dynamics and Anharmonicity on Entropy in Heterogenous Catalysis: Building the Case for Advanced Molecular Simulations. ACS Catalysis, 2020, 10, 9236-9260.	5.5	63
2	Hydrogen Evolution on Restructured B-Rich WB: Metastable Surface States and Isolated Active Sites. ACS Catalysis, 2020, 10, 13867-13877.	5.5	20
3	Atomically Dispersed Pt-group Catalysts: Reactivity, Uniformity, Structural Evolution, and Paths to Increased Functionality. Journal of Physical Chemistry Letters, 2020, 11, 10114-10123.	2.1	24
4	Reduction of Oxidized Pd/Ag(111) Surfaces by H ₂ : Sensitivity to PdO Island Size and Dispersion. ACS Catalysis, 2020, 10, 10117-10124.	5.5	16
5	Can Fluxionality of Subnanometer Cluster Catalysts Solely Cause Non-Arrhenius Behavior in Catalysis?. Journal of Physical Chemistry C, 2020, 124, 19556-19562.	1.5	8
6	Ab Initio Molecular Dynamics Reveals New Metal-Binding Sites in Atomically Dispersed Pt ₁ /TiO ₂ Catalysts. Journal of Physical Chemistry C, 2020, 124, 24187-24195.	1.5	17
7	Active and Selective Ensembles in Oxide-Derived Copper Catalysts for CO ₂ Reduction. ACS Energy Letters, 2020, 5, 3176-3184.	8.8	71
8	Alloying with Sn Suppresses Sintering of Size-Selected Subnano Pt Clusters on SiO ₂ with and without Adsorbates. Chemistry of Materials, 2020, 32, 8595-8605.	3.2	19
9	Activation of Copper Species on Carbon Nitride for Enhanced Activity in the Arylation of Amines. ACS Catalysis, 2020, 10, 11069-11080.	5.5	29
10	Dynamics of gold clusters on ceria during CO oxidation. Journal of Catalysis, 2020, 392, 39-47.	3.1	20
11	Why Boron Nitride is such a Selective Catalyst for the Oxidative Dehydrogenation of Propane. Angewandte Chemie - International Edition, 2020, 59, 16527-16535.	7.2	75
12	First-principles insight into CO hindered agglomeration of Rh and Pt single atoms on m-ZrO ₂ . Catalysis Science and Technology, 2020, 10, 5847-5855.	2.1	8
13	Reagent-Triggered Isomerization of Fluxional Cluster Catalyst via Dynamic Coupling. Journal of Physical Chemistry Letters, 2020, 11, 3089-3094.	2.1	19
14	Why Boron Nitride is such a Selective Catalyst for the Oxidative Dehydrogenation of Propane. Angewandte Chemie, 2020, 132, 16670-16678.	1.6	7
15	CO ₂ Hydrogenation to Formate and Formic Acid by Bimetallic Palladium-Copper Hydride Clusters. Journal of the American Chemical Society, 2020, 142, 7930-7936.	6.6	79
16	Computational strategies to address the catalytic activity of nanoclusters. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1508.	6.2	5
17	Recent Progress in Using Graphene as an Ultrathin Transparent Support for Transmission Electron Microscopy. Small Structures, 2021, 2, 2000049.	6.9	19
18	Computational Methods in Heterogeneous Catalysis. Chemical Reviews, 2021, 121, 1007-1048.	23.0	198

#	ARTICLE	IF	CITATIONS
19	Global Activity Search Uncovers Reaction Induced Concomitant Catalyst Restructuring for Alkane Dissociation on Model Pt Catalysts. <i>ACS Catalysis</i> , 2021, 11, 1877-1885.	5.5	26
20	Fluxional chloro-pyrroleâ€“Pd(ii) complex to cationic Î²-pyrroleâ€“Pd(ii) complex: subtlety in structure-directed bonding mode. <i>New Journal of Chemistry</i> , 2021, 45, 10594-10598.	1.4	1
21	Born to be different: the formation process of Cu nanoparticles tunes the size trend of the activity for CO ₂ to CH ₄ conversion. <i>Nanoscale</i> , 2021, 13, 5857-5867.	2.8	10
22	Theoretical Investigation of Photoinduced Processes in Subnanometer Oxide-Supported Metal Catalysts. <i>Journal of Physical Chemistry C</i> , 2021, 125, 2022-2032.	1.5	4
23	Computationally Guided Searches for Efficient Catalysts through Chemical/Materials Space: Progress and Outlook. <i>Journal of Physical Chemistry C</i> , 2021, 125, 6495-6507.	1.5	4
24	Nanostructure of nickel-promoted indium oxide catalysts drives selectivity in CO ₂ hydrogenation. <i>Nature Communications</i> , 2021, 12, 1960.	5.8	90
25	Theoretical modeling for interfacial catalysis. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1531.	6.2	1
26	When Fluxionality Beats Size Selection: Acceleration of Ostwald Ripening of Subâ€“Nano Clusters. <i>Angewandte Chemie</i> , 2021, 133, 12080-12089.	1.6	3
27	When Fluxionality Beats Size Selection: Acceleration of Ostwald Ripening of Subâ€“Nano Clusters. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 11973-11982.	7.2	13
28	Formaldehyde Selectivity in Methanol Partial Oxidation on Silver: Effect of Reactive Oxygen Species, Surface Reconstruction, and Stability of Intermediates. <i>ACS Catalysis</i> , 2021, 11, 6200-6209.	5.5	14
29	Smart advanced responsive materials, synthesis methods and classifications: from Lab to applications. <i>Journal of Polymer Research</i> , 2021, 28, 1.	1.2	12
30	Thermal Decomposition of Dimethyl Methylphosphonate on Size-Selected Clusters: A Comparative Study between Copper Metal and Cupric Oxide Clusters. <i>Journal of Physical Chemistry C</i> , 2021, 125, 11348-11358.	1.5	7
31	Reversing the Irreversible: Thermodynamic Stabilization of LiAlH ₄ Nanoconfined Within a Nitrogen-Doped Carbon Host. <i>ACS Nano</i> , 2021, 15, 10163-10174.	7.3	24
32	Pulsed Laser in Liquids Made Nanomaterials for Catalysis. <i>Chemical Reviews</i> , 2021, 121, 7568-7637.	23.0	100
33	Operando Surface Studies on Metal-Oxide Interfaces of Bimetal and Mixed Catalysts. <i>ACS Catalysis</i> , 2021, 11, 8645-8677.	5.5	39
34	Nature and identity of the active site via structure-dependent microkinetic modeling: An application to WGS and reverse WGS reactions on Rh. <i>Catalysis Today</i> , 2022, 387, 159-171.	2.2	10
35	Dynamic Interconversion of Metal Active Site Ensembles in Zeolite Catalysis. <i>Annual Review of Chemical and Biomolecular Engineering</i> , 2021, 12, 115-136.	3.3	12
36	Structures and properties of Pd nanoparticles intercalated in layered TiO ₂ : A computational study. <i>Catalysis Today</i> , 2021, , .	2.2	1

#	ARTICLE	IF	CITATIONS
37	Cluster Catalysis with Lattice Oxygen: Tracing Oxygen Transport from a Magnetite (001) Support onto Small Pt Clusters. <i>ACS Catalysis</i> , 2021, 11, 9519-9529.	5.5	14
38	Defying Thermodynamics: Stabilization of Alane Within Covalent Triazine Frameworks for Reversible Hydrogen Storage. <i>Angewandte Chemie</i> , 2021, 133, 26019-26028.	1.6	2
39	Predicted Properties of Active Catalyst Sites on Amorphous Silica: Impact of Silica Preoptimization Protocol. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 12834-12846.	1.8	11
40	Defying Thermodynamics: Stabilization of Alane Within Covalent Triazine Frameworks for Reversible Hydrogen Storage. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 25815-25824.	7.2	11
41	Insights into Coke Formation and Removal under Operating Conditions with a Quantum Nanoreactor Approach. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9413-9421.	2.1	4
42	Exploring Metal Cluster Catalysts Using Swarm Intelligence: Start with Hydrogen Adsorption. <i>Topics in Catalysis</i> , 2022, 65, 215-227.	1.3	2
43	Uranium(VI) reduction at mineral surfaces by Fe(II): Periodic DFT studies of mechanistic aspects and combined action of Fe(II) with humic acid. <i>Surfaces and Interfaces</i> , 2021, 26, 101391.	1.5	3
44	Strong response of Pt clusters to the environment and conditions, formation of metastable states, and simple methods to trace the reversible changes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22718-22732.	1.3	1
45	Manipulating Interfaces of Electrocatalysts Down to Atomic Scales: Fundamentals, Strategies, and Electrocatalytic Applications. <i>Small Methods</i> , 2021, 5, e2001010.	4.6	35
46	Importance learning estimator for the site-averaged turnover frequency of a disordered solid catalyst. <i>Journal of Chemical Physics</i> , 2020, 153, 244120.	1.2	8
47	Atomic level fluxional behavior and activity of CeO ₂ -supported Pt catalysts for CO oxidation. <i>Nature Communications</i> , 2021, 12, 5789.	5.8	53
48	Adsorption and Decomposition of Dimethyl Methylphosphonate on Size-Selected Zirconium Oxide Trimer Clusters. <i>Journal of Physical Chemistry C</i> , 2021, 125, 23688-23698.	1.5	5
49	Nonadiabatic Effects in the Molecular Oxidation of Subnanometric Cu ₅ Clusters. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9143-9150.	1.1	6
50	Unraveling the Nature of Extraframework Catalytic Ensembles in Zeolites: Flexibility and Dynamics of the Copper-Oxo Trimers in Mordenite. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 10906-10913.	2.1	8
51	Dynamics of Heterogeneous Catalytic Processes at Operando Conditions. <i>Jacs Au</i> , 2021, 1, 2100-2120.	3.6	30
52	Understanding the Reaction Dynamics on Heterogeneous Catalysts Using a Simple Stochastic Approach. <i>Journal of Physical Chemistry Letters</i> , 2021, , 11802-11810.	2.1	6
53	Generalizing Performance Equations in Heterogeneous Catalysis from Hybrid Data and Statistical Learning. <i>ACS Catalysis</i> , 2022, 12, 1581-1594.	5.5	6
54	Microscopic mechanisms of cooperative communications within single nanocatalysts. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	5

#	ARTICLE	IF	CITATIONS
55	Enhanced oxygen reduction activity of size-selected platinum subnanocluster catalysts: Pt _n ($n = 3-9$). Catalysis Science and Technology, 2022, 12, 1400-1407.	2.1	6
56	Interpreting the Operando X-ray Absorption Near-Edge Structure of Supported Cu and CuPd Clusters in Conditions of Oxidative Dehydrogenation of Propane: Dynamic Changes in Composition and Size. Journal of Physical Chemistry C, 2022, 126, 1972-1981.	1.5	3
57	Relativistic Effects in Platinum Nanocluster Catalysis: A Statistical Ensemble-Based Analysis. Journal of Physical Chemistry A, 2022, 126, 1345-1359.	1.1	7
58	Modeling surface spin polarization on ceria-supported Pt nanoparticles. Journal of Physics Condensed Matter, 2022, , .	0.7	0
59	Addressing Dynamics at Catalytic Heterogeneous Interfaces with DFT-MD: Anomalous Temperature Distributions from Commonly Used Thermostats. Journal of Physical Chemistry Letters, 2022, 13, 2644-2652.	2.1	12
60	A Review of State of the Art in Phosphine Ligated Gold Clusters and Application in Catalysis. Advanced Science, 2022, 9, e2105692.	5.6	39
61	Data-driven methods to predict the stability metrics of catalytic nanoparticles. Current Opinion in Chemical Engineering, 2022, 36, 100797.	3.8	5
62	Oxidation Dynamics of Supported Catalytic Cu Clusters: Coupling to Fluxionality. ACS Catalysis, 2022, 12, 818-827.	5.5	7
63	Exploring the Stability of Single-Atom Catalysts Using the Density Functional Theory-Based Global Optimization Method: H ₂ Formation on VO _x / γ -Al ₂ O ₃ (100). Journal of Physical Chemistry C, 2022, 126, 6973-6981.	1.5	7
64	Modeling Operando Electrochemical CO ₂ Reduction. Chemical Reviews, 2022, 122, 11085-11130.	23.0	66
65	Theoretical Perspective on Operando Spectroscopy of Fluxional Nanocatalysts. Journal of Physical Chemistry Letters, 2022, 13, 4321-4334.	2.1	7
66	Highly selective electrocatalytic hydrogenation of benzoic acid over Pt/C catalyst supported on carbon fiber. Chemical Engineering Journal, 2022, 445, 136719.	6.6	13
67	Recent advances of amorphous-phase-engineered metal-based catalysts for boosted electrocatalysis. Journal of Materials Science and Technology, 2022, 127, 1-18.	5.6	18
68	Ensemble representation of catalytic interfaces: soloists, orchestras, and everything in-between. Chemical Science, 2022, 13, 8003-8016.	3.7	9
69	Fluxionality of Subnano Clusters Reshapes the Activity Volcano of Electrocatalysis. ChemCatChem, 2022, 14, .	1.8	10
70	Quo vadis multiscale modeling in reaction engineering? – A perspective. Chemical Engineering Research and Design, 2022, 184, 39-58.	2.7	31
71	Single Particle Hopping as an Indicator for Evaluating Electrocatalysts. Nano Letters, 2022, 22, 5495-5502.	4.5	8
72	Simple Model and Spectral Analysis for a Fluxional Catalyst: Intermediate Abundances, Pathway Fluxes, Rates, and Transients. ACS Catalysis, 2022, 12, 8038-8047.	5.5	4

#	ARTICLE	IF	CITATIONS
73	Applications of in-situ wide spectral range infrared absorption spectroscopy for CO oxidation over Pd/SiO ₂ and Cu/SiO ₂ catalysts. Chinese Journal of Catalysis, 2022, 43, 2001-2009.	6.9	4
74	Data-driven models for ground and excited states for Single Atoms on Ceria. Npj Computational Materials, 2022, 8, .	3.5	5
75	The modulation mechanism of geometric and electronic structures of bimetallic catalysts: Pd ₁₃ Ag (Pd=0) clusters for acetylene semi-hydrogenation. Inorganic Chemistry Frontiers, 2022, 9, 5169-5180.	3.0	1
76	Assessing entropy for catalytic processes at complex reactive interfaces. Annual Reports in Computational Chemistry, 2022, , 3-51.	0.9	1
77	Hydrogen-Induced Restructuring of a Cu(100) Electrode in Electroreduction Conditions. Journal of the American Chemical Society, 2022, 144, 19284-19293.	6.6	20
78	Frustrations of supported catalytic clusters under operando conditions predicted by a simple lattice model. Scientific Reports, 2022, 12, .	1.6	1
79	Mesokinetics as a Tool Bridging the Microscopic-to-Macroscopic Transition to Rationalize Catalyst Design. Accounts of Chemical Research, 2022, 55, 3230-3241.	7.6	3
80	Atom hybridization of metallic elements: Emergence of subnano metallurgy for the post-nanotechnology. Coordination Chemistry Reviews, 2023, 474, 214826.	9.5	3
81	Graphite-Supported Pt _n Cluster Electrocatalysts: Major Change of Active Sites as a Function of the Applied Potential. ACS Catalysis, 2022, 12, 14517-14526.	5.5	13
82	Liquid Fluxional Ga Single Atom Catalysts for Efficient Electrochemical CO ₂ Reduction. Angewandte Chemie - International Edition, 2023, 62, .	7.2	94
83	Liquid Fluxional Ga Single Atom Catalysts for Efficient Electrochemical CO ₂ Reduction. Angewandte Chemie, 2023, 135, .	1.6	13
84	Enhanced stability of sub-nanometric iridium decorated graphitic carbon nitride for H ₂ production upon hydrous hydrazine decomposition. Physical Chemistry Chemical Physics, 2023, 25, 1081-1095.	1.3	2
85	Research progress on the formation, detection methods and application in photocatalytic reduction of CO ₂ of oxygen vacancy. Journal of CO ₂ Utilization, 2023, 67, 102344.	3.3	12
86	â€œMagicâ€•Sinter-Resistant Cluster Sizes of Pt _n Supported on Alumina. Journal of Physical Chemistry Letters, 2022, 13, 11044-11050.	2.1	3
87	Atomistic Insights into the Oxidation of Flat and Stepped Platinum Surfaces Using Large-Scale Machine Learning Potential-Based Grand-Canonical Monte Carlo. ACS Catalysis, 2022, 12, 14812-14824.	5.5	7
88	Atomic-Scale Mechanism of Platinum Catalyst Restructuring under a Pressure of Reactant Gas. Journal of the American Chemical Society, 2023, 145, 392-401.	6.6	9
89	Exploring the Potential Energy Surface of Pt ₆ Sub-Nano Clusters Deposited over Graphene. International Journal of Molecular Sciences, 2023, 24, 870.	1.8	1
90	Single-atom catalysis enabled by high-energy metastable structures. Chemical Science, 2023, 14, 2631-2639.	3.7	5

#	ARTICLE	IF	CITATIONS
91	Mechanistic Insights into Molecular Crystalline Organometallic Heterogeneous Catalysis through Parahydrogen-Based Nuclear Magnetic Resonance Studies. <i>Journal of the American Chemical Society</i> , 2023, 145, 2619-2629.	6.6	1
92	Local supermetastable active structure via electrochemical reconstruction toward electrooxidation process. <i>Chem Catalysis</i> , 2023, 3, 100501.	2.9	3
93	Studying, Promoting, Exploiting, and Predicting Catalyst Dynamics: the Next Frontier in Heterogeneous Catalysis. <i>Journal of Physical Chemistry C</i> , 2023, 127, 2127-2146.	1.5	6
94	Highly dispersed 1Ånm PtPd bimetallic clusters for formic acid electrooxidation through a CO-free mechanism. <i>Journal of Energy Chemistry</i> , 2023, 78, 554-564.	7.1	12
95	Recent advances of computational studies on bioethanol to light olefin reactions using zeolite and metal oxide catalysts. <i>Chemical Engineering Science</i> , 2023, 270, 118532.	1.9	2
96	Ptâ€‰%:â€‰%Ge Ratio as a Lever of Activity and Selectivity Control of Supported PtGe Clusters in Thermal Dehydrogenation**. <i>ChemCatChem</i> , 2023, 15, .	1.8	1
97	Electrocatalytic Hydrogen Evolution at Full Atomic Utilization over ITO-Supported Sub-nano-Pt_{<i>n</i>} Clusters: High, Size-Dependent Activity Controlled by Fluxional Pt Hydride Species. <i>Journal of the American Chemical Society</i> , 2023, 145, 5834-5845.	6.6	15
98	Promoterâ€‰“Poison Partnership Protects Platinum Performance in Coked Cluster Catalysts. <i>Journal of Physical Chemistry C</i> , 2023, 127, 5376-5384.	1.5	0
99	Hydrogen Evolution on Electrodeâ€‰Supported Pt_{<i>n</i>} Clusters: Ensemble of Hydride States Governs the Size Dependent Reactivity. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	0
100	Hydrogen Evolution on Electrodeâ€‰Supported Pt_{<i>n</i>} Clusters: Ensemble of Hydride States Governs the Size Dependent Reactivity. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	4
101	Protein Dynamics and Enzymatic Catalysis. <i>Journal of Physical Chemistry B</i> , 2023, 127, 2649-2660.	1.2	11
102	Adsorption of Molecules on Defective CeO₂ for Advanced Catalysis. <i>ACS Catalysis</i> , 2023, 13, 4629-4645.	5.5	15
103	Influence of framework Al density in chabazite zeolites on copper ion mobility and reactivity during NOx selective catalytic reduction with NH3. <i>Nature Catalysis</i> , 2023, 6, 276-285.	16.1	23
104	Ultrathin TiO_x Nanosheets Rich in Tetracoordinated Ti Sites for Propane Dehydrogenation. <i>ACS Catalysis</i> , 2023, 13, 6104-6113.	5.5	2
105	Mechanism of Stoichiometrically Governed Titanium Oxide Brownian Tree Formation on Stepped Au(111). <i>Journal of Physical Chemistry C</i> , 0, , .	1.5	1
106	Boosting heterogeneous catalyst discovery by structurally constrained deep learning models. <i>Materials Today Chemistry</i> , 2023, 30, 101541.	1.7	0
118	Ultra-small Moâ€‰Pt subnanoparticles enable CO₂ hydrogenation at room temperature and atmospheric pressure. <i>Chemical Communications</i> , 2023, 59, 11947-11950.	2.2	0