Giannis Mpourmpakis

List of Publications by Year
in descending order

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116 papers	5,267 citations	87723 38 h-index	95083 68 g-index
119 all docs	119 docs citations	119 times ranked	6142 citing authors

#	Article	IF	Citations
1	Resolving electrocatalytic imprecision in atomically precise metal nanoclusters. Current Opinion in Chemical Engineering, 2022, 36, 100784.	3.8	6
2	Predicting Segregation Energy in Single Atom Alloys Using Physics and Machine Learning. ACS Omega, 2022, 7, 4471-4481.	1.6	9
3	Structureâ€“Activity Relationships in Lewis Acidâ€“Base Heterogeneous Catalysis. ACS Catalysis, 2022, 12, 4268-4289.	5.5	18
4	The Sensitivity of Metal Oxide Electrocatalysis to Bulk Hydrogen Intercalation: Hydrogen Evolution on Tungsten Oxide. Journal of the American Chemical Society, 2022, 144, 6420-6433.	6.6	32
5	Ligand removal energetics control CO₂ electroreduction selectivity on atomically precise, ligated alloy nanoclusters. Environmental Science: Nano, 2022, 9, 2032-2040.	2.2	4
6	Solvent manipulation of the pre-reduction metalâ€“ligand complex and particle-ligand binding for controlled synthesis of Pd nanoparticles. Nanoscale, 2021, 13, 206-217.	2.8	18
7	Boosting CO₂ Electrochemical Reduction with Atomically Precise Surface Modification on Gold Nanoclusters. Angewandte Chemie - International Edition, 2021, 60, 6351-6356.	7.2	105
8	Designing stable bimetallic nanoclusters via an iterative two-step optimization approach. Molecular Systems Design and Engineering, 2021, 6, 545-557.	1.7	6
9	The role of ligands in atomically precise nanocluster-catalyzed CO₂ electrochemical reduction. Nanoscale, 2021, 13, 2333-2337.	2.8	35
10	Mechanistic understanding of methane-to-methanol conversion on graphene-stabilized single-atom iron centers. Catalysis Science and Technology, 2021, 11, 6390-6400.	2.1	9
11	Boosting CO₂ Electrochemical Reduction with Atomically Precise Surface Modification on Gold Nanoclusters. Angewandte Chemie, 2021, 133, 6421-6426.	1.6	19
12	Correlating structural rules with electronic properties of ligand-protected alloy nanoclusters. Journal of Chemical Physics, 2021, 155, 024303.	1.2	4
13	Hydrogen Evolution Electrocatalyst Design: Turning Inert Gold into Active Catalyst by Atomically Precise Nanochemistry. Journal of the American Chemical Society, 2021, 143, 11102-11108.	6.6	64
14	Predicting ligand removal energetics in thiolate-protected nanoclusters from molecular complexes. Nanoscale, 2021, 13, 2034-2043.	2.8	7
15	CuZrO₃: If it exists it should be a sandwich. Physical Chemistry Chemical Physics, 2021, 23, 23748-23757.	1.3	2
16	A Classification Model to Identify Direct-Acting Mutagenic Polycyclic Aromatic Hydrocarbon Transformation Products. Chemical Research in Toxicology, 2021, 34, 2273-2286.	1.7	3
17	Computational Screening of Lewis Acid Catalysts for the Ene Reaction between Maleic Anhydride and Polyisobutylene. Industrial & Engineering Chemistry Research, 2021, 60, 154-161.	1.8	5
18	Understanding the Single Atom Doping Effects in Oxygen Reduction with Atomically Precise Metal Nanoclusters. Journal of Physical Chemistry C, 2021, 125, 24831-24836.	1.5	7

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19	Identification of optimally stable nanocluster geometries via mathematical optimization and density-functional theory. Molecular Systems Design and Engineering, 2020, 5, 232-244.	1.7	10
20	Doping Effect on the Magnetism of Thiolate-Capped 25-Atom Alloy Nanoclusters. Chemistry of Materials, 2020, 32, 9238-9244.	3.2	22
21	Atom-by-Atom Evolution of the Same Ligand-Protected Au₂₁, Au₂₂, Au₂₂Cd₁, and Au₂₄ Nanocluster Series. Journal of the American Chemical Society, 2020, 142, 20426-20433.	6.6	36
22	Heteroatom Tracing Reveals the 30-Atom Auâ€“Ag Bimetallic Nanocluster as a Dimeric Structure. Journal of Physical Chemistry Letters, 2020, 11, 7307-7312.	2.1	9
23	Predicting the Energetics of Hydrogen Intercalation in Metal Oxides Using Acidâ€“Base Properties. ACS Applied Materials & Interfaces, 2020, 12, 44658-44670.	4.0	10
24	Understanding initial zeolite oligomerization steps with first principles calculations. AICHE Journal, 2020, 66, e17107.	1.8	12
25	Monopalladium Substitution in Gold Nanoclusters Enhances CO₂ Electroreduction Activity and Selectivity. ACS Catalysis, 2020, 10, 12011-12016.	5.5	84
26	Improving alkane dehydrogenation activity on Î³-Al₂O₃ through Ga doping. Catalysis Science and Technology, 2020, 10, 7194-7202.	2.1	18
27	Modeling Morphology and Catalytic Activity of Nanoparticle Ensembles Under Reaction Conditions. ACS Catalysis, 2020, 10, 6149-6158.	5.5	38
28	Towards elucidating structure of ligand-protected nanoclusters. Dalton Transactions, 2020, 49, 9191-9202.	1.6	15
29	Rapid Prediction of Bimetallic Mixing Behavior at the Nanoscale. ACS Nano, 2020, 14, 8171-8180.	7.3	17
30	Ligand exchange on Au₃₈(SR)₂₄: substituent site effects of aromatic thiols. Nanoscale, 2020, 12, 9423-9429.	2.8	24
31	Assessing the viability of K-Mo₂C for reverse waterâ€“gas shift scale-up: molecular to laboratory to pilot scale. Energy and Environmental Science, 2020, 13, 2524-2539.	15.6	51
32	Elucidating the stability of ligand-protected Au nanoclusters under electrochemical reduction of CO2. SN Applied Sciences, 2020, 2, 1.	1.5	22
33	Heterometal-Doped M₂₃ (M = Au/Ag/Cd) Nanoclusters with Large Dipole Moments. ACS Nano, 2020, 14, 6599-6606.	7.3	26
34	Understanding the Solubility Behavior of Atomically Precise Gold Nanoclusters. Journal of Physical Chemistry C, 2019, 123, 20006-20012.	1.5	13
35	Predicting Metalâ€“Support Interactions in Oxide-Supported Single-Atom Catalysts. Industrial & Engineering Chemistry Research, 2019, 58, 20236-20246.	1.8	25
36	Unfolding adsorption on metal nanoparticles: Connecting stability with catalysis. Science Advances, 2019, 5, eaax5101.	4.7	66

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37	The role of nanoparticle size and ligand coverage in size focusing of colloidal metal nanoparticles. Nanoscale Advances, 2019, 1, 4052-4066.	2.2	61
38	Structureâ€“property relationships on thiolate-protected gold nanoclusters. Nanoscale Advances, 2019, 1, 184-188.	2.2	17
39	Elucidating the optical spectra of [Au₂₅(SR)₁₈]^q nanoclusters. Physical Chemistry Chemical Physics, 2019, 21, 22272-22282.	1.3	12
40	Understanding the Gas Phase Chemistry of Alkanes with First-Principles Calculations. Journal of Chemical & Engineering Data, 2018, 63, 2430-2437.	1.0	1
41	Design of Copperâ€Based Bimetallic Nanoparticles for Carbon Dioxide Adsorption and Activation. ChemSusChem, 2018, 11, 1169-1178.	3.6	27
42	Design of highly selective ethanol dehydration nanocatalysts for ethylene production. Nanoscale, 2018, 10, 4004-4009.	2.8	10
43	Mechanistic Studies on the Michael Addition of Amines and Hydrazines To Nitrostyrenes: Nitroalkane Elimination via a Retro-aza-Henry-Type Process. Journal of Organic Chemistry, 2018, 83, 1176-1184.	1.7	28
44	Direct Catalytic Conversion of Biomass-Derived Furan and Ethanol to Ethylbenzene. ACS Catalysis, 2018, 8, 1843-1850.	5.5	41
45	Influence of Atomic-Level Morphology on Catalysis: The Case of Sphere and Rod-Like Gold Nanoclusters for CO₂ Electroreduction. ACS Catalysis, 2018, 8, 4996-5001.	5.5	142
46	Size-, Shape-, and Composition-Dependent Model for Metal Nanoparticle Stability Prediction. Nano Letters, 2018, 18, 2696-2704.	4.5	63
47	Understanding Alkane Dehydrogenation through Alcohol Dehydration on Î³-Al₂O₃. Industrial & Engineering Chemistry Research, 2018, 57, 16657-16663.	1.8	15
48	Computational Study of Methane Activation on Î³-Al₂O₃. ACS Omega, 2018, 3, 18242-18250.	1.6	30
49	Structureâ€“Activity Relationships in Alkane Dehydrogenation on Î³-Al₂O₃: Site-Dependent Reactions. ACS Catalysis, 2018, 8, 11570-11578.	5.5	75
50	Rethinking Heterometal Doping in Ligand-Protected Metal Nanoclusters. Journal of Physical Chemistry Letters, 2018, 9, 6773-6778.	2.1	29
51	Elucidating the active sites for CO₂ electroreduction on ligand-protected Au₂₅ nanoclusters. Catalysis Science and Technology, 2018, 8, 3795-3805.	2.1	76
52	Factors Differentiating the Effectiveness of Polyprotic Acids as Inhibitors of Calcium Oxalate Crystallization in Kidney Stone Disease. Crystal Growth and Design, 2018, 18, 5617-5627.	1.4	22
53	Carboranes: the strongest BrÃ¸nsted acids in alcohol dehydration. Catalysis Science and Technology, 2017, 7, 2001-2011.	2.1	15
54	Potassiumâ€Promoted Molybdenum Carbide as a Highly Active and Selective Catalyst for CO₂ Conversion to CO. ChemSusChem, 2017, 10, 2408-2415.	3.6	65

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55	CO₂ activation on Cu-based Zr-decorated nanoparticles. Catalysis Science and Technology, 2017, 7, 2245-2251.	2.1	26
56	Site-selective substitution of gold atoms in the Au24(SR)20 nanocluster by silver. Journal of Colloid and Interface Science, 2017, 505, 1202-1207.	5.0	24
57	Molecular â€œsurgeryâ€•on a 23-gold-atom nanoparticle. Science Advances, 2017, 3, e1603193.	4.7	121
58	Computational Insights into Adsorption of C4 Hydrocarbons in Cation-Exchanged ZSM-12 Zeolites. Industrial & Engineering Chemistry Research, 2017, 56, 7062-7069.	1.8	11
59	Elucidating the role of oxygen coverage in CO₂ reduction on Mo₂C. Catalysis Science and Technology, 2017, 7, 5521-5529.	2.1	23
60	Reconstructing the Surface of Gold Nanoclusters by Cadmium Doping. Journal of the American Chemical Society, 2017, 139, 17779-17782.	6.6	84
61	Thermodynamic stability of ligand-protected metal nanoclusters. Nature Communications, 2017, 8, 15988.	5.8	99
62	CO2 activation on bimetallic CuNi nanoparticles. Progress in Natural Science: Materials International, 2016, 26, 487-492.	1.8	50
63	InnenrÃ¼cktitelbild: From Biomassâ€Derived Furans to Aromatics with Ethanol over Zeolite (Angew.) Tj ETQq1 1 0.784314 rgBT /Ove	1.6	0
64	From Biomassâ€Derived Furans to Aromatics with Ethanol over Zeolite. Angewandte Chemie - International Edition, 2016, 55, 13061-13066.	7.2	110
65	From Biomassâ€Derived Furans to Aromatics with Ethanol over Zeolite. Angewandte Chemie, 2016, 128, 13255-13260.	1.6	31
66	Molecular modifiers reveal a mechanism of pathological crystal growth inhibition. Nature, 2016, 536, 446-450.	13.7	156
67	Description and Role of Bimetallic Prenucleation Species in the Formation of Small Nanoparticle Alloys. Journal of the American Chemical Society, 2015, 137, 15852-15858.	6.6	40
68	DFT-driven multi-site microkinetic modeling of ethanol conversion to ethylene and diethyl ether on Î³-Al2O3(1 1 1). Journal of Catalysis, 2015, 323, 121-131.	3.1	54
69	Au₁₃: CO Adsorbs, Nanoparticle Responds. Journal of Physical Chemistry C, 2015, 119, 18196-18202.	1.5	15
70	Understanding the Importance of Carbenium Ions in the Conversion of Biomass-Derived Alcohols with First-Principles Calculations. Journal of Physical Chemistry C, 2015, 119, 16139-16147.	1.5	18
71	Structure-activity relationships in the production of olefins from alcohols and ethers: a first-principles theoretical study. Catalysis Science and Technology, 2015, 5, 4547-4555.	2.1	23
72	Catalyst Design Based on Morphology- and Environment-Dependent Adsorption on Metal Nanoparticles. ACS Catalysis, 2015, 5, 6296-6301.	5.5	49

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73	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
74	Adsorption Behavior of Noble Metal Clusters and Their Alloys. Journal of Computational and Theoretical Nanoscience, 2014, 11, 511-520.	0.4	10
75	Informatics guided discovery of surface structure-chemistry relationships in catalytic nanoparticles. Journal of Chemical Physics, 2014, 140, 094705.	1.2	34
76	Understanding the Stability and Electronic and Adsorption Properties of Subnanometer Group XI Monometallic and Bimetallic Catalysts. Journal of Physical Chemistry C, 2014, 118, 18521-18528.	1.5	16
77	Structureâ€“activity relationships on metal-oxides: alcohol dehydration. Catalysis Science and Technology, 2014, 4, 3861-3869.	2.1	100
78	Density Functional Theory-Computed Mechanisms of Ethylene and Diethyl Ether Formation from Ethanol on Î³-Al₂O₃(100). ACS Catalysis, 2013, 3, 1965-1975.	5.5	130
79	Effect of oxide supports in stabilizing desirable Ptâ€“Ni bimetallic structures for hydrogenation and reforming reactions. Physical Chemistry Chemical Physics, 2013, 15, 12156.	1.3	21
80	Determination of Proton Affinities and Acidity Constants of Sugars. Journal of Physical Chemistry A, 2013, 117, 5211-5219.	1.1	81
81	Uâ€calculation of the LSDAâ€‰+â€‰U functional using the hybrid B3LYP and HSE functionals. Physica Status Solidi (B): Basic Research, 2013, 250, 356-363.	0.7	35
82	Liquid-phase dehydration of propylene glycol using solid-acid catalysts. Applied Catalysis A: General, 2012, 449, 59-68.	2.2	26
83	Mechanistic Study of Alcohol Dehydration on Î³-Al₂O₃. ACS Catalysis, 2012, 2, 1846-1853.	5.5	199
84	Multiscale Modeling Reveals Poisoning Mechanisms of MgO-Supported Au Clusters in CO Oxidation. Nano Letters, 2012, 12, 3621-3626.	4.5	52
85	DFT Study of Furfural Conversion to Furan, Furfuryl Alcohol, and 2-Methylfuran on Pd(111). ACS Catalysis, 2012, 2, 2496-2504.	5.5	232
86	A Combined DFT and Statistical Mechanics Study for the CO Oxidation on the Au₁₀^{â€“1} Cluster. Journal of Physical Chemistry C, 2011, 115, 20192-20200.	1.5	28
87	Symmetry-Switching Molecular Fe(O₂)_n⁺ Clusters. Journal of Physical Chemistry A, 2011, 115, 7456-7460.	1.1	10
88	Computational-based catalyst design for thermochemical transformations. MRS Bulletin, 2011, 36, 211-215.	1.7	7
89	Predicting the adsorption behavior in bulk from metal clusters. Chemical Physics Letters, 2011, 518, 99-103.	1.2	12
90	Identification of Descriptors for the CO Interaction with Metal Nanoparticles. Nano Letters, 2010, 10, 1041-1045.	4.5	91

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91	What Controls Au Nanoparticle Dispersity during Growth?. Nano Letters, 2010, 10, 3408-3413.	4.5	31
92	Growth Mechanisms of Metal Nanoparticles via First Principles. Physical Review Letters, 2009, 102, 155505.	2.9	28
93	Correlating Particle Size and Shape of Supported Ru/Î³-Al₂O₃ Catalysts with NH₃ Decomposition Activity. Journal of the American Chemical Society, 2009, 131, 12230-12239.	6.6	279
94	The Effects of the MgO Support and Alkali Doping on the CO Interaction with Au. Journal of Physical Chemistry C, 2009, 113, 7329-7335.	1.5	18
95	Insights into the Early Stages of Metal Nanoparticle Formation via First-Principle Calculations: the Roles of Citrate and Water. Langmuir, 2008, 24, 7465-7473.	1.6	49
96	Surface Conductivity of Hydrogenated Diamond Films. Physical Review Letters, 2008, 100, 106801.	2.9	22
97	Assessing the Density Functional Theory in the Hydrogen Storage Problem. Journal of Nanoscience and Nanotechnology, 2008, 8, 3091-3096.	0.9	6
98	Enhancement of the Ionization-Potential of K and Rb upon Chemisorption on a C60Molecule. Journal of Physical Chemistry C, 2007, 111, 6593-6596.	1.5	5
99	Carbon Nanoscrolls:Â A Promising Material for Hydrogen Storage. Nano Letters, 2007, 7, 1893-1897.	4.5	270
100	Effect of curvature and chirality for hydrogen storage in single-walled carbon nanotubes: A Combined ab initio and Monte Carlo investigation. Journal of Chemical Physics, 2007, 126, 144704.	1.2	45
101	Why boron nitride nanotubes are preferable to carbon nanotubes for hydrogen storage?An ab initio theoretical study. Catalysis Today, 2007, 120, 341-345.	2.2	120
102	SiC Nanotubes:â€‰ A Novel Material for Hydrogen Storage. Nano Letters, 2006, 6, 1581-1583.	4.5	334
103	Haeckelites: A promising anode material for lithium batteries application. An ab initio and molecular dynamics theoretical study. Applied Physics Letters, 2006, 89, 233125.	1.5	18
104	A Multi Scale Theoretical Study of Li⁺ Interaction with Carbon Nanotubes. Journal of Nanoscience and Nanotechnology, 2006, 6, 3731-3735.	0.9	16
105	Why alkali metals preferably bind on structural defects of carbon nanotubes: A theoretical study by first principles. Journal of Chemical Physics, 2006, 125, 204707.	1.2	40
106	Hydrogen Storage in Carbon Nanotubes: A Multi-Scale Theoretical Study. Journal of Nanoscience and Nanotechnology, 2006, 6, 87-90.	0.9	7
107	Hydrogen storage in carbon nanotubes: a multi-scale theoretical study. Journal of Nanoscience and Nanotechnology, 2006, 6, 87-90.	0.9	0
108	Carbon-nanotube tips with edge made of a transition metal. Applied Physics Letters, 2005, 87, 193105.	1.5	19

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109	Role of Co in enhancing the magnetism of small Fe clusters. Physical Review B, 2005, 72, .	1.1	43
110	Magnetic enhancement and magnetic reduction in binary clusters of transition metal atoms. Journal of Chemical Physics, 2004, 120, 11901-11904.	1.2	31
111	State-specific RKKY interaction in small magnetic clusters. Physical Review B, 2004, 70, .	1.1	2
112	Ene Hydroperoxidation of Isobutenylarenes within Dye-Exchanged Zeolite Naâˆ’Y:Â Control of Site Selectivity by Cationâˆ’Arene Interactions. Journal of Organic Chemistry, 2003, 68, 2839-2843.	1.7	17
113	Fe encapsulation by silicon clusters:Ab initioelectronic structure calculations. Physical Review B, 2003, 68, .	1.1	86
114	Understanding the structure of metal encapsulated Si cages and nanotubes: Role of symmetry and d-band filling. Journal of Chemical Physics, 2003, 119, 7498-7502.	1.2	56
115	Stabilization of Si-based cage clusters and nanotubes by encapsulation of transition metal atoms. New Journal of Physics, 2002, 4, 78-78.	1.2	92
116	Importance of multi-reference configuration interaction for 3Î£uâˆ’â†X3Î£gâˆ’ transitions of linear HC7H. Chemical Physics Letters, 2002, 356, 398-402.	1.2	8