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	SiC Nanotubes:â€‰A Novel Material for Hydrogen Storage. Nano Letters, 2006, 6, 1581-1583.	4.5	334
2	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
3	Carbon Nanoscrolls:Â A Promising Material for Hydrogen Storage. Nano Letters, 2007, 7, 1893-1897.	4.5	270
4	DFT Study of Furfural Conversion to Furan, Furfuryl Alcohol, and 2-Methylfuran on Pd(111). ACS Catalysis, 2012, 2, 2496-2504.	5.5	232
5	Mechanistic Study of Alcohol Dehydration on Î³-Al₂O₃. ACS Catalysis, 2012, 2, 1846-1853.	5.5	199
6	Molecular modifiers reveal a mechanism of pathological crystal growth inhibition. Nature, 2016, 536, 446-450.	13.7	156
7	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
8	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
9	Molecular â€œsurgeryâ€•on a 23-gold-atom nanoparticle. Science Advances, 2017, 3, e1603193.	4.7	121
10	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
11	From Biomassâ€Derived Furans to Aromatics with Ethanol over Zeolite. Angewandte Chemie - International Edition, 2016, 55, 13061-13066.	7.2	110
12	Boosting CO₂ Electrochemical Reduction with Atomically Precise Surface Modification on Gold Nanoclusters. Angewandte Chemie - International Edition, 2021, 60, 6351-6356.	7.2	105
13	Structureâ€“activity relationships on metal-oxides: alcohol dehydration. Catalysis Science and Technology, 2014, 4, 3861-3869.	2.1	100
14	Thermodynamic stability of ligand-protected metal nanoclusters. Nature Communications, 2017, 8, 15988.	5.8	99
15	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
16	Identification of Descriptors for the CO Interaction with Metal Nanoparticles. Nano Letters, 2010, 10, 1041-1045.	4.5	91
17	Fe encapsulation by silicon clusters:Ab initioelectronic structure calculations. Physical Review B, 2003, 68, .	1.1	86
18	Reconstructing the Surface of Gold Nanoclusters by Cadmium Doping. Journal of the American Chemical Society, 2017, 139, 17779-17782.	6.6	84

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19	Monopalladium Substitution in Gold Nanoclusters Enhances CO₂ Electroreduction Activity and Selectivity. ACS Catalysis, 2020, 10, 12011-12016.	5.5	84
20	Determination of Proton Affinities and Acidity Constants of Sugars. Journal of Physical Chemistry A, 2013, 117, 5211-5219.	1.1	81
21	Elucidating the active sites for CO₂ electroreduction on ligand-protected Au₂₅ nanoclusters. Catalysis Science and Technology, 2018, 8, 3795-3805.	2.1	76
22	Structureâ€“Activity Relationships in Alkane Dehydrogenation on Î³-Al₂O₃: Site-Dependent Reactions. ACS Catalysis, 2018, 8, 11570-11578.	5.5	75
23	Unfolding adsorption on metal nanoparticles: Connecting stability with catalysis. Science Advances, 2019, 5, eaax5101.	4.7	66
24	Potassiumâ€Promoted Molybdenum Carbide as a Highly Active and Selective Catalyst for CO₂ Conversion to CO. ChemSusChem, 2017, 10, 2408-2415.	3.6	65
25	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
26	Size-, Shape-, and Composition-Dependent Model for Metal Nanoparticle Stability Prediction. Nano Letters, 2018, 18, 2696-2704.	4.5	63
27	The role of nanoparticle size and ligand coverage in size focusing of colloidal metal nanoparticles. Nanoscale Advances, 2019, 1, 4052-4066.	2.2	61
28	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
29	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
30	Multiscale Modeling Reveals Poisoning Mechanisms of MgO-Supported Au Clusters in CO Oxidation. Nano Letters, 2012, 12, 3621-3626.	4.5	52
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	CO2 activation on bimetallic CuNi nanoparticles. Progress in Natural Science: Materials International, 2016, 26, 487-492.	1.8	50
33	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
34	Catalyst Design Based on Morphology- and Environment-Dependent Adsorption on Metal Nanoparticles. ACS Catalysis, 2015, 5, 6296-6301.	5.5	49
35	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
36	Role of Co in enhancing the magnetism of small Fe clusters. Physical Review B, 2005, 72, .	1.1	43

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37	Direct Catalytic Conversion of Biomass-Derived Furan and Ethanol to Ethylbenzene. ACS Catalysis, 2018, 8, 1843-1850.	5.5	41
38	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
39	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
40	Modeling Morphology and Catalytic Activity of Nanoparticle Ensembles Under Reaction Conditions. ACS Catalysis, 2020, 10, 6149-6158.	5.5	38
41	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
42	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
43	The role of ligands in atomically precise nanocluster-catalyzed CO₂ electrochemical reduction. Nanoscale, 2021, 13, 2333-2337.	2.8	35
44	Informatics guided discovery of surface structure-chemistry relationships in catalytic nanoparticles. Journal of Chemical Physics, 2014, 140, 094705.	1.2	34
45	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
46	Magnetic enhancement and magnetic reduction in binary clusters of transition metal atoms. Journal of Chemical Physics, 2004, 120, 11901-11904.	1.2	31
47	What Controls Au Nanoparticle Dispersity during Growth?. Nano Letters, 2010, 10, 3408-3413.	4.5	31
48	From Biomassâ€Derived Furans to Aromatics with Ethanol over Zeolite. Angewandte Chemie, 2016, 128, 13255-13260.	1.6	31
49	Computational Study of Methane Activation on Î³-Al₂O₃. ACS Omega, 2018, 3, 18242-18250.	1.6	30
50	Rethinking Heterometal Doping in Ligand-Protected Metal Nanoclusters. Journal of Physical Chemistry Letters, 2018, 9, 6773-6778.	2.1	29
51	Growth Mechanisms of Metal Nanoparticles via First Principles. Physical Review Letters, 2009, 102, 155505.	2.9	28
52	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
53	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
54	Design of Copperâ€Based Bimetallic Nanoparticles for Carbon Dioxide Adsorption and Activation. ChemSusChem, 2018, 11, 1169-1178.	3.6	27

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55	Liquid-phase dehydration of propylene glycol using solid-acid catalysts. Applied Catalysis A: General, 2012, 449, 59-68.	2.2	26
56	CO₂ activation on Cu-based Zr-decorated nanoparticles. Catalysis Science and Technology, 2017, 7, 2245-2251.	2.1	26
57	Heterometal-Doped M₂₃ (M = Au/Ag/Cd) Nanoclusters with Large Dipole Moments. ACS Nano, 2020, 14, 6599-6606.	7.3	26
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	Predicting Metalâ€“Support Interactions in Oxide-Supported Single-Atom Catalysts. Industrial & Engineering Chemistry Research, 2019, 58, 20236-20246.	1.8	25
60	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
61	Ligand exchange on Au₃₈(SR)₂₄: substituent site effects of aromatic thiols. Nanoscale, 2020, 12, 9423-9429.	2.8	24
62	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
63	Elucidating the role of oxygen coverage in CO₂ reduction on Mo₂C. Catalysis Science and Technology, 2017, 7, 5521-5529.	2.1	23
64	Surface Conductivity of Hydrogenated Diamond Films. Physical Review Letters, 2008, 100, 106801.	2.9	22
65	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
66	Doping Effect on the Magnetism of Thiolate-Capped 25-Atom Alloy Nanoclusters. Chemistry of Materials, 2020, 32, 9238-9244.	3.2	22
67	Elucidating the stability of ligand-protected Au nanoclusters under electrochemical reduction of CO2. SN Applied Sciences, 2020, 2, 1.	1.5	22
68	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
69	Carbon-nanotube tips with edge made of a transition metal. Applied Physics Letters, 2005, 87, 193105.	1.5	19
70	Boosting CO₂ Electrochemical Reduction with Atomically Precise Surface Modification on Gold Nanoclusters. Angewandte Chemie, 2021, 133, 6421-6426.	1.6	19
71	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
72	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

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73	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
74	Improving alkane dehydrogenation activity on Î³-Al₂O₃ through Ga doping. Catalysis Science and Technology, 2020, 10, 7194-7202.	2.1	18
75	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
76	Structureâ€“Activity Relationships in Lewis Acidâ€“Base Heterogeneous Catalysis. ACS Catalysis, 2022, 12, 4268-4289.	5.5	18
77	Ene Hydroperoxidation of Isobutenylarenes within Dye-Exchanged Zeolite Naâ˜Y:Â Control of Site Selectivity by Cationâ˜Arene Interactions. Journal of Organic Chemistry, 2003, 68, 2839-2843.	1.7	17
78	Structureâ€“property relationships on thiolate-protected gold nanoclusters. Nanoscale Advances, 2019, 1, 184-188.	2.2	17
79	Rapid Prediction of Bimetallic Mixing Behavior at the Nanoscale. ACS Nano, 2020, 14, 8171-8180.	7.3	17
80	A Multi Scale Theoretical Study of Li⁺ Interaction with Carbon Nanotubes. Journal of Nanoscience and Nanotechnology, 2006, 6, 3731-3735.	0.9	16
81	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
82	Au₁₃: CO Adsorbs, Nanoparticle Responds. Journal of Physical Chemistry C, 2015, 119, 18196-18202.	1.5	15
83	Carboranes: the strongest BrÃ¸nsted acids in alcohol dehydration. Catalysis Science and Technology, 2017, 7, 2001-2011.	2.1	15
84	Understanding Alkane Dehydrogenation through Alcohol Dehydration on Î³-Al₂O₃. Industrial & Engineering Chemistry Research, 2018, 57, 16657-16663.	1.8	15
85	Towards elucidating structure of ligand-protected nanoclusters. Dalton Transactions, 2020, 49, 9191-9202.	1.6	15
86	Understanding the Solubility Behavior of Atomically Precise Gold Nanoclusters. Journal of Physical Chemistry C, 2019, 123, 20006-20012.	1.5	13
87	Predicting the adsorption behavior in bulk from metal clusters. Chemical Physics Letters, 2011, 518, 99-103.	1.2	12
88	Elucidating the optical spectra of [Au₂₅(SR)₁₈]^q nanoclusters. Physical Chemistry Chemical Physics, 2019, 21, 22272-22282.	1.3	12
89	Understanding initial zeolite oligomerization steps with first principles calculations. AICHE Journal, 2020, 66, e17107.	1.8	12
90	Computational Insights into Adsorption of C4 Hydrocarbons in Cation-Exchanged ZSM-12 Zeolites. Industrial & Engineering Chemistry Research, 2017, 56, 7062-7069.	1.8	11

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91	Symmetry-Switching Molecular Fe(O₂)_n⁺ Clusters. Journal of Physical Chemistry A, 2011, 115, 7456-7460.	1.1	10
92	Adsorption Behavior of Noble Metal Clusters and Their Alloys. Journal of Computational and Theoretical Nanoscience, 2014, 11, 511-520.	0.4	10
93	Design of highly selective ethanol dehydration nanocatalysts for ethylene production. Nanoscale, 2018, 10, 4004-4009.	2.8	10
94	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
95	Predicting the Energetics of Hydrogen Intercalation in Metal Oxides Using Acidâ€“Base Properties. ACS Applied Materials & Interfaces, 2020, 12, 44658-44670.	4.0	10
96	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
97	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
98	Predicting Segregation Energy in Single Atom Alloys Using Physics and Machine Learning. ACS Omega, 2022, 7, 4471-4481.	1.6	9
99	Importance of multi-reference configuration interaction for 3Î£uâ¯â†X3Î£gâ¯ transitions of linear HC7H. Chemical Physics Letters, 2002, 356, 398-402.	1.2	8
100	Computational-based catalyst design for thermochemical transformations. MRS Bulletin, 2011, 36, 211-215.	1.7	7
101	Predicting ligand removal energetics in thiolate-protected nanoclusters from molecular complexes. Nanoscale, 2021, 13, 2034-2043.	2.8	7
102	Hydrogen Storage in Carbon Nanotubes: A Multi-Scale Theoretical Study. Journal of Nanoscience and Nanotechnology, 2006, 6, 87-90.	0.9	7
103	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
104	Assessing the Density Functional Theory in the Hydrogen Storage Problem. Journal of Nanoscience and Nanotechnology, 2008, 8, 3091-3096.	0.9	6
105	Designing stable bimetallic nanoclusters via an iterative two-step optimization approach. Molecular Systems Design and Engineering, 2021, 6, 545-557.	1.7	6
106	Resolving electrocatalytic imprecision in atomically precise metal nanoclusters. Current Opinion in Chemical Engineering, 2022, 36, 100784.	3.8	6
107	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
108	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

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109	Correlating structural rules with electronic properties of ligand-protected alloy nanoclusters. Journal of Chemical Physics, 2021, 155, 024303.	1.2	4
110	Ligand removal energetics control CO₂ electroreduction selectivity on atomically precise, ligated alloy nanoclusters. Environmental Science: Nano, 2022, 9, 2032-2040.	2.2	4
111	A Classification Model to Identify Direct-Acting Mutagenic Polycyclic Aromatic Hydrocarbon Transformation Products. Chemical Research in Toxicology, 2021, 34, 2273-2286.	1.7	3
112	State-specific RKKY interaction in small magnetic clusters. Physical Review B, 2004, 70, .	1.1	2
113	CuZrO₃: If it exists it should be a sandwich. Physical Chemistry Chemical Physics, 2021, 23, 23748-23757.	1.3	2
114	Understanding the Gas Phase Chemistry of Alkanes with First-Principles Calculations. Journal of Chemical & Engineering Data, 2018, 63, 2430-2437.	1.0	1
115	InnenrÃ¼cktitelbild: From Biomassâ€Derived Furans to Aromatics with Ethanol over Zeolite (Angew.) Tj ETQq1 1 0.784314 rgBT /Ove	1.6	0
116	Hydrogen storage in carbon nanotubes: a multi-scale theoretical study. Journal of Nanoscience and Nanotechnology, 2006, 6, 87-90.	0.9	0