Vassiliki-Alexandra Glezakou

List of Publications by Year
in descending order

122 papers	4,877 citations	87843 38 h-index	106281 65 g-index
130 all docs	130 docs citations	130 times ranked	5858 citing authors

#	Article	IF	Citations
1	Dynamic formation of single-atom catalytic active sites on ceria-supported gold nanoparticles. Nature Communications, 2015, 6, 6511.	5.8	370
2	The Role of Reducible Oxideâ€“Metal Cluster Charge Transfer in Catalytic Processes: New Insights on the Catalytic Mechanism of CO Oxidation on Au/TiO₂ from ab Initio Molecular Dynamics. Journal of the American Chemical Society, 2013, 135, 10673-10683.	6.6	308
3	Water-Lean Solvents for Post-Combustion CO₂Capture: Fundamentals, Uncertainties, Opportunities, and Outlook. Chemical Reviews, 2017, 117, 9594-9624.	23.0	249
4	Electrocatalytic Hydrogenation of Biomass-Derived Organics: A Review. Chemical Reviews, 2020, 120, 11370-11419.	23.0	185
5	Ethanol synthesis from syngas over Rh-based/SiO2 catalysts: A combined experimental and theoretical modeling study. Journal of Catalysis, 2010, 271, 325-342.	3.1	174
6	CO Oxidation on Au/TiO₂: Condition-Dependent Active Sites and Mechanistic Pathways. Journal of the American Chemical Society, 2016, 138, 10467-10476.	6.6	159
7	Genesis and Stability of Hydronium Ions in Zeolite Channels. Journal of the American Chemical Society, 2019, 141, 3444-3455.	6.6	119
8	Molecular Simulation Analysis and X-ray Absorption Measurement of Ca2+, K+and Cl-Ions in Solution. Journal of Physical Chemistry B, 2006, 110, 23644-23654.	1.2	115
9	Highly active and stable MgAl2O4-supported Rh and Ir catalysts for methane steam reforming: A combined experimental and theoretical study. Journal of Catalysis, 2014, 316, 11-23.	3.1	104
10	Competitive sorption of CO2 and H2O in 2:1 layer phyllosilicates. Geochimica Et Cosmochimica Acta, 2015, 161, 248-257.	1.6	98
11	Probing equilibrium of molecular and deprotonated water on TiO ₂ (110). Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 1801-1805.	3.3	90
12	Confinement effects and acid strength in zeolites. Nature Communications, 2021, 12, 2630.	5.8	90
13	Theoretical insights into the surface physics and chemistry of redox-active oxides. Nature Reviews Materials, 2020, 5, 460-475.	23.3	89
14	Understanding the Role of Metal and Molecular Structure on the Electrocatalytic Hydrogenation of Oxygenated Organic Compounds. ACS Catalysis, 2019, 9, 9964-9972.	5.5	81
15	Carboxyl intermediate formation via an in situ-generated metastable active site during water-gas shift catalysis. Nature Catalysis, 2019, 2, 916-924.	16.1	79
16	Anharmonicity and Confinement in Zeolites: Structure, Spectroscopy, and Adsorption Free Energy of Ethanol in H-ZSM-5. Journal of Physical Chemistry C, 2016, 120, 7172-7182.	1.5	77
17	A Combined Experimental and Theoretical Study on the Activity and Selectivity of the Electrocatalytic Hydrogenation of Aldehydes. ACS Catalysis, 2018, 8, 7645-7658.	5.5	76
18	Electronic structure, statistical mechanical simulations, and EXAFS spectroscopy of aqueous potassium. Theoretical Chemistry Accounts, 2006, 115, 86-99.	0.5	63

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19	Understanding Heterolytic H₂ Cleavage and Water-Assisted Hydrogen Spillover on Fe₃O₄(001)-Supported Single Palladium Atoms. ACS Catalysis, 2019, 9, 7876-7887.	5.5	63
20	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
21	The Nature of Hydrogen Adsorption on Platinum in the Aqueous Phase. Angewandte Chemie - International Edition, 2019, 58, 3527-3532.	7.2	62
22	Structure and Dynamics of CO₂ on Rutile TiO₂(110)-1Ã—1. Journal of Physical Chemistry C, 2012, 116, 26322-26334.	1.5	60
23	Spontaneous Activation of CO₂and Possible Corrosion Pathways on the Low-Index Iron Surface Fe(100). Journal of Physical Chemistry C, 2009, 113, 3691-3696.	1.5	58
24	Impact of pH on Aqueous-Phase Phenol Hydrogenation Catalyzed by Carbon-Supported Pt and Rh. ACS Catalysis, 2019, 9, 1120-1128.	5.5	55
25	Environment of Metalâ€“Oâ€“Fe Bonds Enabling High Activity in CO₂ Reduction on Single Metal Atoms and on Supported Nanoparticles. Journal of the American Chemical Society, 2021, 143, 5540-5549.	6.6	54
26	Electrochemically Tunable Protonâ€Coupled Electron Transfer in Pdâ€Catalyzed Benzaldehyde Hydrogenation. Angewandte Chemie - International Edition, 2020, 59, 1501-1505.	7.2	53
27	General Protocol for the Accurate Prediction of Molecular ¹³C/¹H NMR Chemical Shifts via Machine Learning Augmented DFT. Journal of Chemical Information and Modeling, 2020, 60, 3746-3754.	2.5	53
28	Microstructural Response of Variably Hydrated Ca-rich Montmorillonite to Supercritical CO₂. Environmental Science & Technology, 2014, 48, 8612-8619.	4.6	52
29	Structure, dynamics and vibrational spectrum of supercritical CO2/H2O mixtures from ab initio molecular dynamics as a function of water cluster formation. Physical Chemistry Chemical Physics, 2010, 12, 8759.	1.3	51
30	Low-Temperature Oxidation of Methanol to Formaldehyde on a Model Single-Atom Catalyst: Pd Atoms on Fe₃O₄(001). ACS Catalysis, 2019, 9, 10977-10982.	5.5	50
31	Carbon-supported Pt during aqueous phenol hydrogenation with and without applied electrical potential: X-ray absorption and theoretical studies of structure and adsorbates. Journal of Catalysis, 2018, 368, 8-19.	3.1	49
32	Acid/base equilibria in clusters and their role in proton exchange membranes: computational insight. Physical Chemistry Chemical Physics, 2007, 9, 5752.	1.3	48
33	Dimerization Induced Deprotonation of Water on RuO₂(110). Journal of Physical Chemistry Letters, 2014, 5, 3445-3450.	2.1	47
34	Structural Rearrangement of Auâ€“Pd Nanoparticles under Reaction Conditions: An ab Initio Molecular Dynamics Study. ACS Nano, 2017, 11, 1649-1658.	7.3	47
35	NWPEsSe: An Adaptive-Learning Global Optimization Algorithm for Nanosized Cluster Systems. Journal of Chemical Theory and Computation, 2020, 16, 3947-3958.	2.3	47
36	Steam reforming of hydrocarbons from biomass-derived syngas over MgAl2O4-supported transition metals and bimetallic IrNi catalysts. Applied Catalysis B: Environmental, 2016, 184, 142-152.	10.8	46

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37	Norm-Conserving Pseudopotentials and Basis Sets To Explore Lanthanide Chemistry in Complex Environments. Journal of Chemical Theory and Computation, 2019, 15, 5987-5997.	2.3	46
38	Hydrogen Bonding Enhances the Electrochemical Hydrogenation of Benzaldehyde in the Aqueous Phase. Angewandte Chemie - International Edition, 2021, 60, 290-296.	7.2	40
39	Comparative Investigation of Benzene Steam Reforming over Spinel Supported Rh and Ir Catalysts. ACS Catalysis, 2013, 3, 1133-1143.	5.5	39
40	Directed Hydrogen Bond Placement: Low Viscosity Amine Solvents for CO₂ Capture. ACS Sustainable Chemistry and Engineering, 2019, 7, 7535-7542.	3.2	34
41	Single-Step Conversion of Ethanol to n-Butene over Ag-ZrO₂/SiO₂ Catalysts. ACS Catalysis, 2020, 10, 10602-10613.	5.5	34
42	Progress and challenges in self-healing cementitious materials. Journal of Materials Science, 2021, 56, 201-230.	1.7	34
43	Surface Density Dependent Catalytic Activity of Single Palladium Atoms Supported on Ceria**. Angewandte Chemie - International Edition, 2021, 60, 22769-22775.	7.2	34
44	Formation Mechanism of the Secondary Building Unit in a Chromium Terephthalate Metalâ€“Organic Framework. Chemistry of Materials, 2014, 26, 6401-6409.	3.2	33
45	Deprotonated Water Dimers: The Building Blocks of Segmented Water Chains on Rutile RuO₂(110). Journal of Physical Chemistry C, 2015, 119, 23552-23558.	1.5	33
46	Dynamic Acid/Base Equilibrium in Single Component Switchable Ionic Liquids and Consequences on Viscosity. Journal of Physical Chemistry Letters, 2016, 7, 1646-1652.	2.1	33
47	Coordination Sphere of Lanthanide Aqua Ions Resolved with Ab Initio Molecular Dynamics and X-ray Absorption Spectroscopy. Inorganic Chemistry, 2021, 60, 3117-3130.	1.9	33
48	Cluster-Models for Uranyl(VI) Adsorption on Î±-Alumina. Journal of Physical Chemistry A, 2011, 115, 1257-1263.	1.1	32
49	Reconciling Work Functions and Adsorption Enthalpies for Implicit Solvent Models: A Pt (111)/Water Interface Case Study. Journal of Chemical Theory and Computation, 2020, 16, 2703-2715.	2.3	32
50	Analysis of Bonding Patterns in the Valence Isoelectronic Series O₃, S₃, SO₂, and OS₂in Terms of Oriented Quasi-Atomic Molecular Orbitals^{â€}. Journal of Physical Chemistry A, 2010, 114, 8923-8931.	1.1	31
51	Global optimization of chemical cluster structures: Methods, applications, and challenges. International Journal of Quantum Chemistry, 2021, 121, e26553.	1.0	31
52	Systematic location of intersecting seams of conical intersection in triatomic molecules: The 1â€‰2Aâ€²â€“2â€‰2Aâ€² conical intersections in BH2. Journal of Chemical Physics, 1998, 108, 5657-5659.	1.2	30
53	Molecular interactions of SO2 with carbonate minerals under co-sequestration conditions: A combined experimental and theoretical study. Geochimica Et Cosmochimica Acta, 2012, 92, 265-274.	1.6	30
54	Ab initio molecular dynamics with enhanced sampling in heterogeneous catalysis. Catalysis Science and Technology, 2022, 12, 12-37.	2.1	29

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55	Polymer-Cement Composites with Self-Healing Ability for Geothermal and Fossil Energy Applications. Chemistry of Materials, 2017, 29, 4708-4718.	3.2	28
56	Structure, dynamics and stability of water/scCO2/mineral interfaces from ab initio molecular dynamics simulations. Scientific Reports, 2015, 5, 14857.	1.6	26
57	Reinventing Design Principles for Developing Lowâ€Viscosity Carbon Dioxideâ€Binding Organic Liquids for Flue Gas Clean Up. ChemSusChem, 2017, 10, 636-642.	3.6	26
58	Molecular Level Investigation of CH₄ and CO₂ Adsorption in Hydrated Calciumâ€“Montmorillonite. Journal of Physical Chemistry C, 2018, 122, 1125-1134.	1.5	26
59	Raman spectrum of supercritical C¹⁸O₂and re-evaluation of the Fermi resonance. Physical Chemistry Chemical Physics, 2012, 14, 2560-2566.	1.3	25
60	Atomic Origins of the Self-Healing Function in Cementâ€“Polymer Composites. ACS Applied Materials & Interfaces, 2018, 10, 3011-3019.	4.0	23
61	Molecular Level Understanding of the Free Energy Landscape in Early Stages of Metalâ€“Organic Framework Nucleation. Journal of the American Chemical Society, 2019, 141, 6073-6081.	6.6	23
62	Ab initio molecular dynamics assessment of thermodynamic and transport properties in (K,Li)Cl and (K,) Tj ETQq0 0 0 rgBT /Overlock 10	2.3	23
63	Insights into the physical and chemical properties of a cement-polymer composite developed for geothermal wellbore applications. Cement and Concrete Composites, 2019, 97, 279-287.	4.6	22
64	Influence of Ag metal dispersion on the thermal conversion of ethanol to butadiene over Ag-ZrO2/SiO2 catalysts. Journal of Catalysis, 2020, 386, 30-38.	3.1	22
65	Low-Frequency Raman Spectroscopy ofn-Alcohols. LAM Vibration and Crystal Structure. Journal of Physical Chemistry B, 2002, 106, 4405-4411.	1.2	21
66	Activity of Cuâ€“Alâ€“Oxo Extra-Framework Clusters for Selective Methane Oxidation on Cu-Exchanged Zeolites. Jacs Au, 2021, 1, 1412-1421.	3.6	21
67	Structureâ€“property reduced order model for viscosity prediction in single-component CO₂-binding organic liquids. Green Chemistry, 2016, 18, 6004-6011.	4.6	20
68	Chemical transformations of captured CO2 into cyclic and polymeric carbonates. Journal of CO2 Utilization, 2019, 32, 196-201.	3.3	20
69	Shedding light on black titania. Nature Materials, 2018, 17, 856-857.	13.3	19
70	Mesoscopic Structure Facilitates Rapid CO₂ Transport and Reactivity in CO₂ Capture Solvents. Journal of Physical Chemistry Letters, 2018, 9, 5765-5771.	2.1	19
71	Norm-Conserving Pseudopotentials and Basis Sets to Explore Actinide Chemistry in Complex Environments. Journal of Chemical Theory and Computation, 2021, 17, 3360-3371.	2.3	19
72	Actinide Molten Salts: A Machine-Learning Potential Molecular Dynamics Study. ACS Applied Materials & Interfaces, 2021, 13, 53398-53408.	4.0	19

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73	Understanding Metalâ€“Organic Framework Nucleation from a Solution with Evolving Graphs. Journal of the American Chemical Society, 2022, 144, 11099-11109.	6.6	19
74	Are Water-lean Solvent Systems Viable for Post-Combustion CO2 Capture?. Energy Procedia, 2017, 114, 756-763.	1.8	18
75	Electrochemically Tunable Protonâ€Coupled Electron Transfer in Pdâ€Catalyzed Benzaldehyde Hydrogenation. Angewandte Chemie, 2020, 132, 1517-1521.	1.6	18
76	Diffusion and Surface Segregation of Interstitial Ti Defects Induced by Electronic Metalâ€“Support Interactions on a Au/TiO₂ Nanocatalyst. ACS Catalysis, 2022, 12, 4455-4464.	5.5	17
77	Impact of Nonadiabatic Charge Transfer on the Rate of Redox Chemistry of Carbon Oxides on Rutile TiO₂(110) Surface. ACS Catalysis, 2015, 5, 1764-1771.	5.5	16
78	Molecularâ€Level Overhaul of Î³â€Aminopropyl Aminosilicone/Triethylene Glycol Postâ€Combustion CO₂â€Capture Solvents. ChemSusChem, 2020, 13, 3429-3438.	3.6	16
79	Phase-Change Aminopyridines as Carbon Dioxide Capture Solvents. Industrial & Engineering Chemistry Research, 2017, 56, 7534-7540.	1.8	14
80	Formation of Supported Graphene Oxide: Evidence for Enolate Species. Journal of the American Chemical Society, 2018, 140, 5102-5109.	6.6	14
81	The Role of Ir in Ternary Rh-Based Catalysts for Syngas Conversion to C2 + Oxygenates. Topics in Catalysis, 2012, 55, 595-600.	1.3	13
82	Electro-reduction of organics on metal cathodes: A multiscale-modeling study of benzaldehyde on Au (111). Catalysis Today, 2020, 350, 39-46.	2.2	13
83	Heterogeneous catalysis in complex, condensed reaction media. Catalysis Today, 2017, 289, 231-236.	2.2	12
84	Structure and Stability of the Ionic Liquid Clusters [EMIM]_n[BF₄]_{n+1}^{â€“} (n = 1â€“9): Implications for Electrochemical Separations. Journal of Physical Chemistry Letters, 2020, 11, 6844-6851.	2.1	12
85	First-principle investigation on catalytic hydrogenation of benzaldehyde over Pt-group metals. Catalysis Today, 2022, 388-389, 208-215.	2.2	12
86	Selective acetylene hydrogenation over single metal atoms supported on Fe3O4(001): A first-principle study. Journal of Chemical Physics, 2020, 152, 154703.	1.2	12
87	Hydrogen Bonding Enhances the Electrochemical Hydrogenation of Benzaldehyde in the Aqueous Phase. Angewandte Chemie, 2021, 133, 294-300.	1.6	12
88	Dynamics, Stability, and Adsorption States of Water on Oxidized RuO₂(110). Journal of Physical Chemistry C, 2017, 121, 18505-18515.	1.5	11
89	How Collective Phenomena Impact CO₂ Reactivity and Speciation in Different Media. Journal of Physical Chemistry A, 2020, 124, 3963-3975.	1.1	11
90	Integrated Solvent Design for CO2 Capture and Viscosity Tuning. Energy Procedia, 2017, 114, 726-734.	1.8	10

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91	Creating self-assembled arrays of mono-oxo (MoO ₃) ₁ species on TiO ₂ (101) via deposition and decomposition of (MoO ₃) _n oligomers. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	10
92	Light Makes a Surface Banana-Bond Split: Photodesorption of Molecular Hydrogen from RuO2(110). Journal of the American Chemical Society, 2016, 138, 8714-8717.	6.6	9
93	Polymer-cement composites with adhesion and re-adhesion (healing) to casing capability for geothermal wellbore applications. Cement and Concrete Composites, 2020, 107, 103490.	4.6	9
94	Graphene Oxide as a Pb(II) Separation Medium: Has Part of the Story Been Overlooked?. Jacs Au, 2021, 1, 766-776.	3.6	9
95	Mechanistic Understanding of Catalytic Conversion of Ethanol to 1-Butene over 2D-Pillared MFI Zeolite. Journal of Physical Chemistry C, 2020, 124, 28437-28447.	1.5	9
96	Structure, Bonding, and Heats of Formation of Silatitanacyclobutanes. Journal of Physical Chemistry A, 1997, 101, 8714-8719.	1.1	8
97	On the Role of Enthalpic and Entropic Contributions to the Conformational Free Energy Landscape of MILâ€101(Cr) Secondary Building Units. Advanced Theory and Simulations, 2020, 3, 2000092.	1.3	7
98	Understanding Adsorption of Organics on Pt(111) in the Aqueous Phase: Insights from DFT Based Implicit Solvent and Statistical Thermodynamics Models. Journal of Chemical Theory and Computation, 2022, 18, 1849-1861.	2.3	7
99	Mechanism of methanol synthesis on Ni(110). Catalysis Science and Technology, 2021, 11, 3279-3294.	2.1	6
100	Tuning the Charge and Hydrophobicity of Graphene Oxide Membranes by Functionalization with Ionic Liquids at Epoxide Sites. ACS Applied Materials & Interfaces, 2022, 14, 19031-19042.	4.0	6
101	Structure and Thermodynamics of Carbon and Carbon/Silicon Precursors to Nanostructures. Journal of the American Chemical Society, 2002, 124, 6144-6152.	6.6	5
102	Ligand control of low-frequency electron paramagnetic resonance linewidth in Cr(iii) complexes. Dalton Transactions, 2021, 50, 5342-5350.	1.6	5
103	Impact of functional groups on the electrocatalytic hydrogenation of aromatic carbonyls to alcohols. Catalysis Today, 2022, 397-399, 63-68.	2.2	5
104	Functionalization of Electrodes with Tunable [EMIM]_x[Cl]_{x+1}^{â€“} Ionic Liquid Clusters for Electrochemical Separations. Chemistry of Materials, 2022, 34, 2612-2623.	3.2	5
105	Impact of Cr and Co on 99Tc retention in magnetite: A combined study of ab initio molecular dynamics and experiments. Journal of Hazardous Materials, 2020, 387, 121721.	6.5	3
106	Subtle changes in hydrogen bond orientation result in glassification of carbon capture solvents. Physical Chemistry Chemical Physics, 2020, 22, 19009-19021.	1.3	3
107	Molecular dynamics simulations of a hydrophilic MIL-160-based membrane demonstrate pressure-dependent selective uptake of industrially relevant greenhouse gases. Materials Advances, 2021, 2, 5922-5934.	2.6	3
108	Binding and stability of MgO monomers on anatase TiO2(101). Journal of Chemical Physics, 2021, 154, 204703.	1.2	3

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109	Use of Solvatochromism to Assay Preferential Solvation of a Prototypic Catalytic Site. Topics in Catalysis, 2015, 58, 258-270.	1.3	2
110	Trends in Homolytic Bond Dissociation Energies of Five- and Six-Coordinate Hydrides of Group 9 Transition Metals: Co, Rh, Ir. Journal of Physical Chemistry A, 2017, 121, 1993-2000.	1.1	2
111	Molecular Simulation of the Catalytic Regeneration of ⁿBuLi through a Hydrometalation Route. Inorganic Chemistry, 2019, 58, 3033-3040.	1.9	2
112	The Nature of Hydrogen Adsorption on Platinum in the Aqueous Phase. Angewandte Chemie, 2019, 131, 3565-3570.	1.6	2
113	The role of sub-surface hydrogen on CO2 reduction and dynamics on Ni(110): An ab initio molecular dynamics study. Journal of Chemical Physics, 2021, 155, 044702.	1.2	2
114	Advanced Theory and Simulation to Guide the Development of CO₂ Capture Solvents. ACS Omega, 2022, 7, 12453-12466.	1.6	2
115	Properties of polyvinylchloride in solution: an hydrodynamic and vibrational spectroscopy study. Journal of Polymer Science, Part B: Polymer Physics, 1999, 37, 1351-1356.	2.4	1
116	Density Functional Simulations as a Tool To Probe Molecular Interactions in Wet Supercritical CO2. ACS Symposium Series, 2013, , 31-49.	0.5	1
117	Single-Atom Catalysis: An Analogy between Heterogeneous and Homogeneous Catalysts. ACS Symposium Series, 2020, , 1-15.	0.5	1
118	AMPHIPHILIC WATERâ€LEAN CARBON CAPTURE SOLVENT WETTING BEHAVIOR VIA DECOMPOSITION BY STAINLESSâ€STEEL INTERFACES. ChemSusChem, 2021, 14, 5283-5292.	3.6	1
119	Computational and Experimental Study for the Denitrification of Biomass-Derived Hydrothermal Liquefaction Oil. ACS Sustainable Chemistry and Engineering, 2021, 9, 13406-13413.	3.2	1
120	Surface Density Dependent Catalytic Activity of Single Palladium Atoms Supported on Ceria**. Angewandte Chemie, 2021, 133, 22951.	1.6	0
121	Determining the Adsorption Energetics of 2,3-Butanediol on RuO2(110): Coupling First-Principles Calculations With Global Optimizers. Frontiers in Energy Research, 2022, 9, .	1.2	0
122	Tailored Computational Approaches to Interrogate Heavy Element Chemistry and Structure in Condensed Phase. ACS Symposium Series, 0, , 219-245.	0.5	0