Vassiliki-Alexandra Glezakou

List of Publications by Year
in descending order

122 papers	4,877 citations	87723 38 h-index	106150 65 g-index
130 all docs	130 docs citations	130 times ranked	5858 citing authors

#	Article	IF	Citations
1	First-principle investigation on catalytic hydrogenation of benzaldehyde over Pt-group metals. Catalysis Today, 2022, 388-389, 208-215.	2.2	12
2	Ab initio molecular dynamics with enhanced sampling in heterogeneous catalysis. Catalysis Science and Technology, 2022, 12, 12-37.	2.1	29
3	Impact of functional groups on the electrocatalytic hydrogenation of aromatic carbonyls to alcohols. Catalysis Today, 2022, 397-399, 63-68.	2.2	5
4	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
5	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
6	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
7	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
8	Advanced Theory and Simulation to Guide the Development of CO₂ Capture Solvents. ACS Omega, 2022, 7, 12453-12466.	1.6	2
9	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
10	Understanding Metalâ€“Organic Framework Nucleation from a Solution with Evolving Graphs. Journal of the American Chemical Society, 2022, 144, 11099-11109.	6.6	19
11	Hydrogen Bonding Enhances the Electrochemical Hydrogenation of Benzaldehyde in the Aqueous Phase. Angewandte Chemie, 2021, 133, 294-300.	1.6	12
12	Hydrogen Bonding Enhances the Electrochemical Hydrogenation of Benzaldehyde in the Aqueous Phase. Angewandte Chemie - International Edition, 2021, 60, 290-296.	7.2	40
13	Global optimization of chemical cluster structures: Methods, applications, and challenges. International Journal of Quantum Chemistry, 2021, 121, e26553.	1.0	31
14	Progress and challenges in self-healing cementitious materials. Journal of Materials Science, 2021, 56, 201-230.	1.7	34
15	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
16	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
17	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
18	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

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19	Graphene Oxide as a Pb(II) Separation Medium: Has Part of the Story Been Overlooked?. Jacs Au, 2021, 1, 766-776.	3.6	9
20	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
21	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
22	Confinement effects and acid strength in zeolites. Nature Communications, 2021, 12, 2630.	5.8	90
23	Binding and stability of MgO monomers on anatase TiO2(101). Journal of Chemical Physics, 2021, 154, 204703.	1.2	3
24	Surface Density Dependent Catalytic Activity of Single Palladium Atoms Supported on Ceria**. Angewandte Chemie - International Edition, 2021, 60, 22769-22775.	7.2	34
25	Surface Density Dependent Catalytic Activity of Single Palladium Atoms Supported on Ceria**. Angewandte Chemie, 2021, 133, 22951.	1.6	0
26	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
27	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
28	Actinide Molten Salts: A Machine-Learning Potential Molecular Dynamics Study. ACS Applied Materials & Interfaces, 2021, 13, 53398-53408.	4.0	19
29	AMPHIPHILIC WATERâ€LEAN CARBON CAPTURE SOLVENT WETTING BEHAVIOR VIA DECOMPOSITION BY STAINLESSâ€STEEL INTERFACES. ChemSusChem, 2021, 14, 5283-5292.	3.6	1
30	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
31	Mechanism of methanol synthesis on Ni(110). Catalysis Science and Technology, 2021, 11, 3279-3294.	2.1	6
32	Ligand control of low-frequency electron paramagnetic resonance linewidth in Cr(iii) complexes. Dalton Transactions, 2021, 50, 5342-5350.	1.6	5
33	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
34	Electrochemically Tunable Protonâ€Coupled Electron Transfer in Pdâ€Catalyzed Benzaldehyde Hydrogenation. Angewandte Chemie - International Edition, 2020, 59, 1501-1505.	7.2	53
35	Electrochemically Tunable Protonâ€Coupled Electron Transfer in Pdâ€Catalyzed Benzaldehyde Hydrogenation. Angewandte Chemie, 2020, 132, 1517-1521.	1.6	18
36	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

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37	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
38	Single-Step Conversion of Ethanol to n-Butene over Ag-ZrO₂/SiO₂ Catalysts. ACS Catalysis, 2020, 10, 10602-10613.	5.5	34
39	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
40	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
41	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
42	Electrocatalytic Hydrogenation of Biomass-Derived Organics: A Review. Chemical Reviews, 2020, 120, 11370-11419.	23.0	185
43	Subtle changes in hydrogen bond orientation result in glassification of carbon capture solvents. Physical Chemistry Chemical Physics, 2020, 22, 19009-19021.	1.3	3
44	Single-Atom Catalysis: An Analogy between Heterogeneous and Homogeneous Catalysts. ACS Symposium Series, 2020, , 1-15.	0.5	1
45	Molecularâ€Level Overhaul of Î³â€Aminopropyl Aminosilicone/Triethylene Glycol Postâ€Combustion CO₂â€Capture Solvents. ChemSusChem, 2020, 13, 3429-3438.	3.6	16
46	NWPEsSe: An Adaptive-Learning Global Optimization Algorithm for Nanosized Cluster Systems. Journal of Chemical Theory and Computation, 2020, 16, 3947-3958.	2.3	47
47	Theoretical insights into the surface physics and chemistry of redox-active oxides. Nature Reviews Materials, 2020, 5, 460-475.	23.3	89
48	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
49	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
50	How Collective Phenomena Impact CO₂ Reactivity and Speciation in Different Media. Journal of Physical Chemistry A, 2020, 124, 3963-3975.	1.1	11
51	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
52	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
53	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
54	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

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55	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
56	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
57	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
58	Genesis and Stability of Hydronium Ions in Zeolite Channels. Journal of the American Chemical Society, 2019, 141, 3444-3455.	6.6	119
59	Chemical transformations of captured CO2 into cyclic and polymeric carbonates. Journal of CO2 Utilization, 2019, 32, 196-201.	3.3	20
60	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
61	Directed Hydrogen Bond Placement: Low Viscosity Amine Solvents for CO₂ Capture. ACS Sustainable Chemistry and Engineering, 2019, 7, 7535-7542.	3.2	34
62	Molecular Simulation of the Catalytic Regeneration of ⁿBuLi through a Hydrometalation Route. Inorganic Chemistry, 2019, 58, 3033-3040.	1.9	2
63	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
64	The Nature of Hydrogen Adsorption on Platinum in the Aqueous Phase. Angewandte Chemie, 2019, 131, 3565-3570.	1.6	2
65	Impact of pH on Aqueous-Phase Phenol Hydrogenation Catalyzed by Carbon-Supported Pt and Rh. ACS Catalysis, 2019, 9, 1120-1128.	5.5	55
66	The Nature of Hydrogen Adsorption on Platinum in the Aqueous Phase. Angewandte Chemie - International Edition, 2019, 58, 3527-3532.	7.2	62
67	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
68	Formation of Supported Graphene Oxide: Evidence for Enolate Species. Journal of the American Chemical Society, 2018, 140, 5102-5109.	6.6	14
69	Atomic Origins of the Self-Healing Function in Cementâ€“Polymer Composites. ACS Applied Materials & Interfaces, 2018, 10, 3011-3019.	4.0	23
70	Molecular Level Investigation of CH₄ and CO₂ Adsorption in Hydrated Calciumâ€“Montmorillonite. Journal of Physical Chemistry C, 2018, 122, 1125-1134.	1.5	26
71	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
72	Shedding light on black titania. Nature Materials, 2018, 17, 856-857.	13.3	19

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73	Mesoscopic Structure Facilitates Rapid CO₂ Transport and Reactivity in CO₂ Capture Solvents. Journal of Physical Chemistry Letters, 2018, 9, 5765-5771.	2.1	19
74	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
75	Structural Rearrangement of Auâ€“Pd Nanoparticles under Reaction Conditions: An ab Initio Molecular Dynamics Study. ACS Nano, 2017, 11, 1649-1658.	7.3	47
76	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
77	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
78	Water-Lean Solvents for Post-Combustion CO₂Capture: Fundamentals, Uncertainties, Opportunities, and Outlook. Chemical Reviews, 2017, 117, 9594-9624.	23.0	249
79	Polymer-Cement Composites with Self-Healing Ability for Geothermal and Fossil Energy Applications. Chemistry of Materials, 2017, 29, 4708-4718.	3.2	28
80	Phase-Change Aminopyridines as Carbon Dioxide Capture Solvents. Industrial & Engineering Chemistry Research, 2017, 56, 7534-7540.	1.8	14
81	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
82	Integrated Solvent Design for CO2 Capture and Viscosity Tuning. Energy Procedia, 2017, 114, 726-734.	1.8	10
83	Are Water-lean Solvent Systems Viable for Post-Combustion CO2 Capture?. Energy Procedia, 2017, 114, 756-763.	1.8	18
84	Dynamics, Stability, and Adsorption States of Water on Oxidized RuO₂(110). Journal of Physical Chemistry C, 2017, 121, 18505-18515.	1.5	11
85	Heterogeneous catalysis in complex, condensed reaction media. Catalysis Today, 2017, 289, 231-236.	2.2	12
86	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
87	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
88	Structureâ€“property reduced order model for viscosity prediction in single-component CO₂-binding organic liquids. Green Chemistry, 2016, 18, 6004-6011.	4.6	20
89	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
90	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

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91	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
92	Structure, dynamics and stability of water/scCO2/mineral interfaces from ab initio molecular dynamics simulations. Scientific Reports, 2015, 5, 14857.	1.6	26
93	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
94	Dynamic formation of single-atom catalytic active sites on ceria-supported gold nanoparticles. Nature Communications, 2015, 6, 6511.	5.8	370
95	Use of Solvatochromism to Assay Preferential Solvation of a Prototypic Catalytic Site. Topics in Catalysis, 2015, 58, 258-270.	1.3	2
96	Competitive sorption of CO2 and H2O in 2:1 layer phyllosilicates. Geochimica Et Cosmochimica Acta, 2015, 161, 248-257.	1.6	98
97	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
98	Dimerization Induced Deprotonation of Water on RuO₂(110). Journal of Physical Chemistry Letters, 2014, 5, 3445-3450.	2.1	47
99	Formation Mechanism of the Secondary Building Unit in a Chromium Terephthalate Metalâ€“Organic Framework. Chemistry of Materials, 2014, 26, 6401-6409.	3.2	33
100	Microstructural Response of Variably Hydrated Ca-rich Montmorillonite to Supercritical CO₂. Environmental Science & Technology, 2014, 48, 8612-8619.	4.6	52
101	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
102	Comparative Investigation of Benzene Steam Reforming over Spinel Supported Rh and Ir Catalysts. ACS Catalysis, 2013, 3, 1133-1143.	5.5	39
103	Density Functional Simulations as a Tool To Probe Molecular Interactions in Wet Supercritical CO2. ACS Symposium Series, 2013, , 31-49.	0.5	1
104	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
105	Raman spectrum of supercritical C¹⁸O₂and re-evaluation of the Fermi resonance. Physical Chemistry Chemical Physics, 2012, 14, 2560-2566.	1.3	25
106	Structure and Dynamics of CO₂ on Rutile TiO₂(110)-1Ã—1. Journal of Physical Chemistry C, 2012, 116, 26322-26334.	1.5	60
107	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
108	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

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109	Cluster-Models for Uranyl(VI) Adsorption on Î±-Alumina. Journal of Physical Chemistry A, 2011, 115, 1257-1263.	1.1	32
110	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
111	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
112	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
113	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
114	Acid/base equilibria in clusters and their role in proton exchange membranes: computational insight. Physical Chemistry Chemical Physics, 2007, 9, 5752.	1.3	48
115	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
116	Electronic structure, statistical mechanical simulations, and EXAFS spectroscopy of aqueous potassium. Theoretical Chemistry Accounts, 2006, 115, 86-99.	0.5	63
117	Structure and Thermodynamics of Carbon and Carbon/Silicon Precursors to Nanostructures. Journal of the American Chemical Society, 2002, 124, 6144-6152.	6.6	5
118	Low-Frequency Raman Spectroscopy ofn-Alcohols. LAM Vibration and Crystal Structure. Journal of Physical Chemistry B, 2002, 106, 4405-4411.	1.2	21
119	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
120	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
121	Structure, Bonding, and Heats of Formation of Silatitanacyclobutanes. Journal of Physical Chemistry A, 1997, 101, 8714-8719.	1.1	8
122	Tailored Computational Approaches to Interrogate Heavy Element Chemistry and Structure in Condensed Phase. ACS Symposium Series, 0, , 219-245.	0.5	0