Federico Calle-Vallejo

List of Publications by Year
in descending order

116 papers	17,950 citations	28274 55 h-index	20961 115 g-index
126 all docs	126 docs citations	126 times ranked	14447 citing authors

#	Article	IF	Citations
1	Universality in Oxygen Evolution Electrocatalysis on Oxide Surfaces. ChemCatChem, 2011, 3, 1159-1165.	3.7	3,208
2	Catalysts and Reaction Pathways for the Electrochemical Reduction of Carbon Dioxide. Journal of Physical Chemistry Letters, 2015, 6, 4073-4082.	4.6	1,524
3	Advances and challenges in understanding the electrocatalytic conversion of carbon dioxide to fuels. Nature Energy, 2019, 4, 732-745.	39.5	1,506
4	Finding optimal surface sites on heterogeneous catalysts by counting nearest neighbors. Science, 2015, 350, 185-189.	12.6	725
5	Theoretical Considerations on the Electroreduction of CO to C₂ Species on Cu(100) Electrodes. Angewandte Chemie - International Edition, 2013, 52, 7282-7285.	13.8	677
6	Introducing structural sensitivity into adsorptionâ€“energy scaling relations by means of coordination numbers. Nature Chemistry, 2015, 7, 403-410.	13.6	600
7	Guidelines for the Rational Design of Ni-Based Double Hydroxide Electrocatalysts for the Oxygen Evolution Reaction. ACS Catalysis, 2015, 5, 5380-5387.	11.2	472
8	Density functional studies of functionalized graphitic materials with late transition metals for oxygen reduction reactions. Physical Chemistry Chemical Physics, 2011, 13, 15639.	2.8	454
9	Tuning the Activity of Pt(111) for Oxygen Electroreduction by Subsurface Alloying. Journal of the American Chemical Society, 2011, 133, 5485-5491.	13.7	447
10	Fast Prediction of Adsorption Properties for Platinum Nanocatalysts with Generalized Coordination Numbers. Angewandte Chemie - International Edition, 2014, 53, 8316-8319.	13.8	366
11	Spectroscopic Observation of a Hydrogenated CO Dimer Intermediate During CO Reduction on Cu(100) Electrodes. Angewandte Chemie - International Edition, 2017, 56, 3621-3624.	13.8	366
12	Identifying active surface phases for metal oxide electrocatalysts: a study of manganese oxide bi-functional catalysts for oxygen reduction and water oxidation catalysis. Physical Chemistry Chemical Physics, 2012, 14, 14010.	2.8	332
13	Structure- and Potential-Dependent Cation Effects on CO Reduction at Copper Single-Crystal Electrodes. Journal of the American Chemical Society, 2017, 139, 16412-16419.	13.7	289
14	Number of outer electrons as descriptor for adsorption processes on transition metals and their oxides. Chemical Science, 2013, 4, 1245.	7.4	273
15	MXenes: New Horizons in Catalysis. ACS Catalysis, 2020, 10, 13487-13503.	11.2	239
16	Physical and Chemical Nature of the Scaling Relations between Adsorption Energies of Atoms on Metal Surfaces. Physical Review Letters, 2012, 108, 116103.	7.8	233
17	Electrochemical water splitting by gold: evidence for an oxide decomposition mechanism. Chemical Science, 2013, 4, 2334.	7.4	229
18	Na-doped ruthenium perovskite electrocatalysts with improved oxygen evolution activity and durability in acidic media. Nature Communications, 2019, 10, 2041.	12.8	227

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19	Tailoring the catalytic activity of electrodes with monolayer amounts of foreign metals. Chemical Society Reviews, 2013, 42, 5210.	38.1	202
20	Why Is Bulk Thermochemistry a Good Descriptor for the Electrocatalytic Activity of Transition Metal Oxides?. ACS Catalysis, 2015, 5, 869-873.	11.2	189
21	First-principles computational electrochemistry: Achievements and challenges. Electrochimica Acta, 2012, 84, 3-11.	5.2	180
22	Performance and degradation of Proton Exchange Membrane Fuel Cells: State of the art in modeling from atomistic to system scale. Journal of Power Sources, 2016, 304, 207-233.	7.8	180
23	Why conclusions from platinum model surfaces do not necessarily lead to enhanced nanoparticle catalysts for the oxygen reduction reaction. Chemical Science, 2017, 8, 2283-2289.	7.4	173
24	Bond-Making and Breaking between Carbon, Nitrogen, and Oxygen in Electrocatalysis. Journal of the American Chemical Society, 2014, 136, 15694-15701.	13.7	168
25	Adsorption-Driven Surface Segregation of the Less Reactive Alloy Component. Journal of the American Chemical Society, 2009, 131, 2404-2407.	13.7	160
26	How covalence breaks adsorption-energy scaling relations and solvation restores them. Chemical Science, 2017, 8, 124-130.	7.4	145
27	Enhancing CO₂ Electroreduction to Ethanol on Copperâ€“Silver Composites by Opening an Alternative Catalytic Pathway. ACS Catalysis, 2020, 10, 4059-4069.	11.2	145
28	Structure-sensitive electroreduction of acetaldehyde to ethanol on copper and its mechanistic implications for CO and CO 2 reduction. Catalysis Today, 2016, 262, 90-94.	4.4	132
29	Elucidating the Facet-Dependent Selectivity for CO₂ Electroreduction to Ethanol of Cuâ€“Ag Tandem Catalysts. ACS Catalysis, 2021, 11, 4456-4463.	11.2	130
30	La_{1.5}Sr_{0.5}NiMn_{0.5}Ru_{0.5}O₆Double Perovskite with Enhanced ORR/OER Bifunctional Catalytic Activity. ACS Applied Materials & Interfaces, 2019, 11, 21454-21464.	8.0	129
31	On the behavior of BrÃ¸nsted-Evans-Polanyi relations for transition metal oxides. Journal of Chemical Physics, 2011, 134, 244509.	3.0	128
32	Oxygen reduction and evolution at single-metal active sites: Comparison between functionalized graphitic materials and protoporphyrins. Surface Science, 2013, 607, 47-53.	1.9	121
33	Structure- and Coverage-Sensitive Mechanism of NO Reduction on Platinum Electrodes. ACS Catalysis, 2017, 7, 4660-4667.	11.2	118
34	Does the breaking of adsorption-energy scaling relations guarantee enhanced electrocatalysis?. Current Opinion in Electrochemistry, 2018, 8, 110-117.	4.8	115
35	Spectroscopic Observation of a Hydrogenated CO Dimer Intermediate During CO Reduction on Cu(100) Electrodes. Angewandte Chemie, 2017, 129, 3675-3678.	2.0	112
36	Computational Comparison of Late Transition Metal (100) Surfaces for the Electrocatalytic Reduction of CO to C₂ Species. ACS Energy Letters, 2018, 3, 1062-1067.	17.4	103

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37	Trends in Stability of Perovskite Oxides. Angewandte Chemie - International Edition, 2010, 49, 7699-7701.	13.8	98
38	Theoretical design and experimental implementation of Ag/Au electrodes for the electrochemical reduction of nitrate. Physical Chemistry Chemical Physics, 2013, 15, 3196.	2.8	98
39	Enhanced Electroreduction of Carbon Dioxide to Methanol Using Zinc Dendrites Pulseâ€Deposited on Silver Foam. Angewandte Chemie - International Edition, 2019, 58, 2256-2260.	13.8	98
40	Making the hydrogen evolution reaction in polymer electrolyte membrane electrolysers even faster. Nature Communications, 2016, 7, 10990.	12.8	97
41	Revealing the nature of active sites in electrocatalysis. Chemical Science, 2019, 10, 8060-8075.	7.4	96
42	Structural principles to steer the selectivity of the electrocatalytic reduction of aliphatic ketones on platinum. Nature Catalysis, 2019, 2, 243-250.	34.4	95
43	Design of an Active Site towards Optimal Electrocatalysis: Overlayers, Surface Alloys and Nearâ€Surface Alloys of Cu/Pt(111). Angewandte Chemie - International Edition, 2012, 51, 11845-11848.	13.8	94
44	Generalized trends in the formation energies of perovskite oxides. Physical Chemistry Chemical Physics, 2013, 15, 7526.	2.8	85
45	Importance of Solvation for the Accurate Prediction of Oxygen Reduction Activities of Pt-Based Electrocatalysts. Journal of Physical Chemistry Letters, 2017, 8, 2243-2246.	4.6	85
46	Density functional theory study of adsorption of H2O, H, O, and OH on stepped platinum surfaces. Journal of Chemical Physics, 2014, 140, 134708.	3.0	83
47	Outlining the Scaling-Based and Scaling-Free Optimization of Electrocatalysts. ACS Catalysis, 2019, 9, 4218-4225.	11.2	76
48	A New Type of Scaling Relations to Assess the Accuracy of Computational Predictions of Catalytic Activities Applied to the Oxygen Evolution Reaction. ChemCatChem, 2017, 9, 1261-1268.	3.7	75
49	Structure dependency of the atomic-scale mechanisms of platinum electro-oxidation and dissolution. Nature Catalysis, 2020, 3, 754-761.	34.4	72
50	A Semiempirical Method to Detect and Correct DFT-Based Gas-Phase Errors and Its Application in Electrocatalysis. ACS Catalysis, 2020, 10, 6900-6907.	11.2	71
51	Accounting for Bifurcating Pathways in the Screening for CO₂ Reduction Catalysts. ACS Catalysis, 2017, 7, 7346-7351.	11.2	70
52	A brief review of the computational modeling of CO2 electroreduction on Cu electrodes. Current Opinion in Electrochemistry, 2018, 9, 158-165.	4.8	64
53	On the mechanism of the electrochemical conversion of ammonia to dinitrogen on Pt(1â€¯0â€¯0) in alkaline environment. Journal of Catalysis, 2018, 359, 82-91.	6.2	62
54	Designing water splitting catalysts using rules of thumb: advantages, dangers and alternatives. Physical Chemistry Chemical Physics, 2020, 22, 6797-6803.	2.8	59

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55	Enabling Generalized Coordination Numbers to Describe Strain Effects. ChemSusChem, 2018, 11, 1824-1828.	6.8	57
56	A Step Closer to the Electrochemical Production of Liquid Fuels. Angewandte Chemie - International Edition, 2014, 53, 10858-10860.	13.8	56
57	Affordable Estimation of Solvation Contributions to the Adsorption Energies of Oxygenates on Metal Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 5578-5582.	3.1	54
58	Substantial improvement of electrocatalytic predictions by systematic assessment of solvent effects on adsorption energies. Applied Catalysis B: Environmental, 2020, 276, 119147.	20.2	53
59	Trends in Metal Oxide Stability for Nanorods, Nanotubes, and Surfaces. Journal of Physical Chemistry C, 2011, 115, 2244-2252.	3.1	52
60	Alkali Metal Cation Effects in Structuring Pt, Rh, and Au Surfaces through Cathodic Corrosion. ACS Applied Materials & Interfaces, 2018, 10, 39363-39379.	8.0	50
61	Oxygen Reduction at a Cu-Modified Pt(111) Model Electrocatalyst in Contact with Nafion Polymer. ACS Catalysis, 2014, 4, 3772-3778.	11.2	47
62	Why (1 0 0) Terraces Break and Make Bonds: Oxidation of Dimethyl Ether on Platinum Single-Crystal Electrodes. Journal of the American Chemical Society, 2013, 135, 14329-14338.	13.7	46
63	Nature of Highly Active Electrocatalytic Sites for the Hydrogen Evolution Reaction at Pt Electrodes in Acidic Media. ACS Omega, 2017, 2, 8141-8147.	3.5	46
64	Electrocatalytic Reduction of Nitrate on a Pt Electrode Modified by pâ€Block Metal Adatoms in Acid Solution. ChemCatChem, 2013, 5, 1773-1783.	3.7	45
65	Double-Stranded Water on Stepped Platinum Surfaces. Physical Review Letters, 2016, 116, 136101.	7.8	45
66	Quantitative Coordinationâ€"Activity Relations for the Design of Enhanced Pt Catalysts for CO Electro-oxidation. ACS Catalysis, 2017, 7, 4355-4359.	11.2	45
67	Establishing and Understanding Adsorptionâ€"Energy Scaling Relations with Negative Slopes. Journal of Physical Chemistry Letters, 2016, 7, 5302-5306.	4.6	43
68	Oxygen Reduction Reaction: Rapid Prediction of Mass Activity of Nanostructured Platinum Electrocatalysts. Journal of Physical Chemistry Letters, 2018, 9, 4463-4468.	4.6	43
69	Understanding Adsorption-Induced Effects on Platinum Nanoparticles: An Energy-Decomposition Analysis. Journal of Physical Chemistry Letters, 2014, 5, 3120-3124.	4.6	37
70	Importance of the gas-phase error correction for O2 when using DFT to model the oxygen reduction and evolution reactions. Journal of Electroanalytical Chemistry, 2021, 896, 115178.	3.8	37
71	Interconversions of nitrogen-containing species on Pt(100) and Pt(111) electrodes in acidic solutions containing nitrate. Electrochimica Acta, 2018, 271, 77-83.	5.2	36
72	How oxidation state and lattice distortion influence the oxygen evolution activity in acid of iridium double perovskites. Journal of Materials Chemistry A, 2021, 9, 2980-2990.	10.3	36

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73	Elucidating the Structure of Ethanol-Producing Active Sites at Oxide-Derived Cu Electrocatalysts. ACS Catalysis, 2020, 10, 10488-10494.	11.2	35
74	Theory-Guided Enhancement of CO₂ Reduction to Ethanol on Agâ€“Cu Tandem Catalysts via Particle-Size Effects. ACS Catalysis, 2021, 11, 13330-13336.	11.2	34
75	Initial stages of water solvation of stepped platinum surfaces. Physical Chemistry Chemical Physics, 2016, 18, 3416-3422.	2.8	32
76	Scanning Tunneling Microscopy Evidence for the Dissociation of Carbon Monoxide on Ruthenium Steps. Journal of Physical Chemistry C, 2012, 116, 14350-14359.	3.1	30
77	Selectivity Map for the Late Stages of CO and CO₂ Reduction to C₂ Species on Copper Electrodes. Angewandte Chemie - International Edition, 2021, 60, 10784-10790.	13.8	30
78	The Role of Undercoordinated Sites on Zinc Electrodes for CO₂ Reduction to CO. Advanced Functional Materials, 2022, 32, .	14.9	30
79	How symmetry factors cause potential- and facet-dependent pathway shifts during CO2 reduction to CH4 on Cu electrodes. Applied Catalysis B: Environmental, 2021, 285, 119776.	20.2	28
80	Capturing Solvation Effects at a Liquid/Nanoparticle Interface by Ab Initio Molecular Dynamics: Pt₂₀₁ Immersed in Water. Small, 2016, 12, 5312-5319.	10.0	25
81	Tailoring structural and electronic properties of RuO2 nanotubes: a many-body approach and electronic transport. Physical Chemistry Chemical Physics, 2013, 15, 14715.	2.8	23
82	First-Principles Structural and Electronic Characterization of Ordered SiO₂ Nanowires. Journal of Physical Chemistry C, 2012, 116, 18973-18982.	3.1	22
83	Anisotropic etching of rhodium and gold as the onset of nanoparticle formation by cathodic corrosion. Faraday Discussions, 2016, 193, 207-222.	3.2	21
84	Monitoring the active sites for the hydrogen evolution reaction at model carbon surfaces. Physical Chemistry Chemical Physics, 2021, 23, 10051-10058.	2.8	21
85	Fast Correction of Errors in the DFTâ€Calculated Energies of Gaseous Nitrogenâ€Containing Species. ChemCatChem, 2021, 13, 2508-2516.	3.7	21
86	Impact of Intrinsic Density Functional Theory Errors on the Predictive Power of Nitrogen Cycle Electrocatalysis Models. ACS Catalysis, 2022, 12, 4784-4791.	11.2	20
87	Influence of Van der Waals Interactions on the Solvation Energies of Adsorbates at Ptâ€Based Electrocatalysts. ChemPhysChem, 2019, 20, 2968-2972.	2.1	16
88	Trends in Câ€“O and Nâ€“O bond scission on rutile oxides described using oxygen vacancy formation energies. Chemical Science, 2020, 11, 4119-4124.	7.4	16
89	Revealing the Nature of Active Sites on Ptâ€“Gd and Ptâ€“Pr Alloys during the Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2022, 14, 19604-19613.	8.0	16
90	Role of lattice oxygen content and Ni geometry in the oxygen evolution activity of the Ba-Ni-O system. Journal of Power Sources, 2018, 404, 56-63.	7.8	15

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91	Toward Efficient Tandem Electroreduction of CO₂ to Methanol using Anodized Titanium. ACS Catalysis, 2021, 11, 8467-8475.	11.2	13
92	Evaluation of the Electrochemical Stability of Model Cu-Pt(111) Near-Surface Alloy Catalysts. Electrochimica Acta, 2015, 179, 469-474.	5.2	12
93	Fast identification of optimal pure platinum nanoparticle shapes and sizes for efficient oxygen electroreduction. Nanoscale Advances, 2019, 1, 2901-2909.	4.6	12
94	Quantifying Local and Cooperative Components in the Ferroelectric Distortion of BaTiO₃: Learning from the Off-Center Motion in the MnCl₆^{5â€“} Complex Formed in KCl:Mn⁺. Inorganic Chemistry, 2014, 53, 6534-6543.	4.0	11
95	Different promoting roles of ruthenium for the oxidation of primary and secondary alcohols on PtRu electrocatalysts. Journal of Catalysis, 2021, 400, 166-172.	6.2	11
96	The bifunctional volcano plot: thermodynamic limits for single-atom catalysts for oxygen reduction and evolution. Journal of Materials Chemistry A, 2022, 10, 5937-5941.	10.3	11
97	On the shifting peak of volcano plots for oxygen reduction and evolution. Electrochimica Acta, 2022, 426, 140799.	5.2	11
98	Identifying the time-dependent predominance regimes of step and terrace sites for the Fischerâ€“Tropsch synthesis on ruthenium based catalysts. Catalysis Science and Technology, 2016, 6, 6495-6503.	4.1	10
99	Electrochemical formation and surface characterisation of Cu2â^'xTe thin films with adjustable content of Cu. RSC Advances, 2013, 3, 21648.	3.6	8
100	Enhanced Electroreduction of Carbon Dioxide to Methanol Using Zinc Dendrites Pulseâ€Deposited on Silver Foam. Angewandte Chemie, 2019, 131, 2278-2282.	2.0	7
101	Interplaying coordination and ligand effects to break or make adsorptionâ€energy scaling relations. Exploration, 2022, 2, .	11.0	7
102	Structure-sensitive scaling relations among carbon-containing species and their possible impact on CO2 electroreduction. Journal of Catalysis, 2021, 395, 136-142.	6.2	6
103	Gasâ€phase errors affect DFTâ€based electrocatalysis models of oxygen reduction to hydrogen peroxide. ChemElectroChem, 2022, 9, .	3.4	6
104	Finding Key Factors for Efficient Water and Methanol Activation at Metals, Oxides, MXenes, and Metal/Oxide Interfaces. ACS Catalysis, 2022, 12, 1237-1246.	11.2	5
105	Computational-experimental study of the onset potentials for CO2 reduction on polycrystalline and oxide-derived copper electrodes. Electrochimica Acta, 2021, 380, 138247.	5.2	4
106	Selectivity Map for the Late Stages of CO and CO 2 Reduction to C 2 Species on Copper Electrodes. Angewandte Chemie, 2021, 133, 10879-10885.	2.0	3
107	Gasâ€Phase Errors Affect DFTâ€Based Electrocatalysis Models of Oxygen Reduction to Hydrogen Peroxide. ChemElectroChem, 2022, 9, .	3.4	2
108	Metallicity enhancement in coreâ€“shell SiO2@RuO2nanowires. RSC Advances, 2014, 4, 34696-34700.	3.6	1

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109	Theoretical Study of the Structural Stability and the Electronic Properties of Al_mH_n Clusters. Journal of Computational and Theoretical Nanoscience, 2011, 8, 609-615.	0.4	0
110	Tailoring the electronic structure of graphene for catalytic and nanoelectronic applications. , 2011, , .		0
111	InnenrÃ¼cktitelbild: Theoretical Considerations on the Electroreduction of CO to C2Species on Cu(100) Electrodes (Angew. Chem. 28/2013). Angewandte Chemie, 2013, 125, 7463-7463.	2.0	0
112	How Au Outperforms Pt in the Catalytic Reduction of Methane Towards Ethane and Molecular Hydrogen. Topics in Catalysis, 2018, 61, 1290-1299.	2.8	0
113	Primary Vs. Secondary Alcohols Electrooxidation: Mechanistic Insights. ECS Meeting Abstracts, 2021, MA2021-01, 1870-1870.	0.0	0
114	(Invited) Structure-Activity Relationships for CO and CO2 Electroreduction to C2 Species on Copper. ECS Meeting Abstracts, 2017, , .	0.0	0
115	Tandem Electrochemical Conversion of CO₂ to Liquid Fuels and Chemical Feedstocks. ECS Meeting Abstracts, 2022, MA2022-01, 1615-1615.	0.0	0
116	(Digital Presentation) High-Resolution Imaging of Active Sites Under Reaction Conditions for Carbon-Based Electrocatalysis. ECS Meeting Abstracts, 2022, MA2022-01, 627-627.	0.0	0