Alejandro A Franco

List of Publications by Year
in descending order

125	4,300	94269 37	128067 60
papers	citations	h-index	g-index

148	148	148	3360
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Artificial Intelligence Applied to Battery Research: Hype or Reality?. Chemical Reviews, 2022, 122, 10899-10969.	23.0	153
2	Towards a Local In situ Xâ€ray Nano Computed Tomography under Realistic Cycling Conditions for Battery Research. Chemistry Methods, 2022, 2, .	1.8	5
3	A Roadmap for Transforming Research to Invent the Batteries of the Future Designed within the European Large Scale Research Initiative BATTERY 2030+. Advanced Energy Materials, 2022, 12, .	10.2	70
4	Perspectives on manufacturing simulations of Li-S battery cathodes. JPhys Energy, 2022, 4, 011002.	2.3	6
5	Towards autonomous high-throughput multiscale modelling of battery interfaces. Energy and Environmental Science, 2022, 15, 579-594.	15.6	17
6	The ARTISTIC Online Calculator: Exploring the Impact of Lithiumâ€Ion Battery Electrode Manufacturing Parameters Interactively Through Your Browser. Batteries and Supercaps, 2022, 5, .	2.4	9
7	Deconvoluting the benefits of porosity distribution in layered electrodes on the electrochemical performance of Li-ion batteries. Energy Storage Materials, 2022, 47, 462-471.	9.5	32
8	Artificial neural network approach for multiphase segmentation of battery electrode nano-CT images. Npj Computational Materials, 2022, 8, .	3.5	20
9	Deconvoluting the impacts of the active material skeleton and the inactive phase morphology on the performance of lithium ion battery electrodes. Energy Storage Materials, 2022, 47, 649-655.	9.5	12
10	Rechargeable Batteries of the Futureâ€”The State of the Art from a BATTERY 2030+ Perspective. Advanced Energy Materials, 2022, 12, .	10.2	124
11	Experimentally Validated Threeâ€Dimensional Modeling of Organicâ€Based Sodiumâ€Ion Battery Electrode Manufacturing. Batteries and Supercaps, 2022, 5, .	2.4	11
12	Designing electrode architectures to facilitate electrolyte infiltration for lithium-ion batteries. Energy Storage Materials, 2022, 49, 268-277.	9.5	29
13	Artificial Intelligence in Electrochemical Energy Storage. Batteries and Supercaps, 2022, 5, .	2.4	2
14	Pore size distribution of carbon black: An approach from a coarse-grained potential. Computational Materials Science, 2022, 209, 111409.	1.4	1
15	Digitalization of Battery Manufacturing: Current Status, Challenges, and Opportunities. Advanced Energy Materials, 2022, 12, .	10.2	51
16	Bridging nano- and microscale X-ray tomography for battery research by leveraging artificial intelligence. Nature Nanotechnology, 2022, 17, 446-459.	15.6	66
17	(Invited) Modelling and Simulation for the Search for New Active Materials for Redox Flow Batteries - Results of the International Project Sonar. ECS Meeting Abstracts, 2022, MA2022-01, 1954-1954.	0.0	0
18	Gaining Insight into the Electrochemical Interface Dynamics in an Organic Redox Flow Battery with a Kinetic Monte Carlo Approach. Small, 2022, 18, .	5.2	1

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19	Understanding the Reaction Steps Involving Polysulfides in 1â€…M LiTFSI in TEGDMEâ€‰:â€‰DOL Using Cyclic Voltammetry Experiments and Modelling. Batteries and Supercaps, 2021, 4, 152-162.	2.4	6
20	Probing and Interpreting the Porosity and Tortuosity Evolution of Li-O₂ Cathodes on Discharge through a Combined Experimental and Theoretical Approach. Journal of Physical Chemistry C, 2021, 125, 4955-4967.	1.5	11
21	Investigating electrode calendering and its impact on electrochemical performance by means of a new discrete element method model: Towards a digital twin of Li-Ion battery manufacturing. Journal of Power Sources, 2021, 485, 229320.	4.0	118
22	What Can Text Mining Tell Us About Lithiumâ€Ion Battery Researchersâ€™ Habits?. Batteries and Supercaps, 2021, 4, 758-766.	2.4	20
23	Calendering of Li(Ni_{0.33}Mn_{0.33}Co_{0.33})O₂â€Based Cathodes: Analyzing the Link Between Process Parameters and Electrode Properties by Advanced Statistics. Batteries and Supercaps, 2021, 4, 834-844.	2.4	19
24	Understanding the calendering processability of Li(Ni0.33Mn0.33Co0.33)O2-based cathodes. Journal of Power Sources, 2021, 488, 229361.	4.0	48
25	How Machine Learning Will Revolutionize Electrochemical Sciences. ACS Energy Letters, 2021, 6, 1422-1431.	8.8	88
26	Escape from flatland. Nature Machine Intelligence, 2021, 3, 277-278.	8.3	2
27	What Can Text Mining Tell Us About Lithiumâ€Ion Battery Researchersâ€™ Habits?. Batteries and Supercaps, 2021, 4, 689-689.	2.4	3
28	Gaining Insights on Interfacial Dynamics of Methyl Viologen Based Aqueous Organic Redox Flow Battery through a Kinetic Monte Carlo Approach. ECS Meeting Abstracts, 2021, MA2021-01, 429-429.	0.0	0
29	Heterogeneous Solidâ€Electrolyte Interphase in Graphite Electrodes Assessed by 4Dâ€Resolved Computational Simulations. Batteries and Supercaps, 2021, 4, 1457-1463.	2.4	18
30	CHAMPION : Chalmers hierarchical atomic, molecular, polymeric and ionic analysis toolkit. Journal of Computational Chemistry, 2021, 42, 1632-1642.	1.5	3
31	An Invitation to Engage with Computational Modeling: Userâ€Friendly Tool for In Silico Battery Component Generation and Meshing. Batteries and Supercaps, 2021, 4, 1451-1456.	2.4	7
32	Insight on electrolyte infiltration of lithium ion battery electrodes by means of a new three-dimensional-resolved lattice Boltzmann model. Energy Storage Materials, 2021, 38, 80-92.	9.5	61
33	Quantitatively Designing Porous Copper Current Collectors for Lithium Metal Anodes. ACS Applied Energy Materials, 2021, 4, 6454-6465.	2.5	17
34	Machine learning-based assessment of the impact of the manufacturing process on battery electrode heterogeneity. Energy and AI, 2021, 5, 100090.	5.8	31
35	Towards a 3D-resolved model of Si/Graphite composite electrodes from manufacturing simulations. Journal of Power Sources, 2021, 512, 230486.	4.0	17
36	Machine learning 3D-resolved prediction of electrolyte infiltration in battery porous electrodes. Journal of Power Sources, 2021, 511, 230384.	4.0	21

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37	Carbon-Binder Migration: A Three-Dimensional Drying Model for Lithium-ion Battery Electrodes. Energy Storage Materials, 2021, 43, 337-347.	9.5	46
38	Quantitatively Designing Porous Copper Current Collectors for Lithium Metal Anodes. ECS Meeting Abstracts, 2021, MA2021-02, 721-721.	0.0	0
39	A three dimensional kinetic Monte Carlo model for simulating the carbon/sulfur mesostructural evolutions of discharging lithium sulfur batteries. Energy Storage Materials, 2020, 24, 472-485.	9.5	33
40	Artificial Intelligence Investigation of NMC Cathode Manufacturing Parameters Interdependencies. Batteries and Supercaps, 2020, 3, 60-67.	2.4	93
41	Data-driven assessment of electrode calendering process by combining experimental results, in silico mesostructures generation and machine learning. Journal of Power Sources, 2020, 480, 229103.	4.0	70
42	Entering the Augmented Era: Immersive and Interactive Virtual Reality for Battery Education and Research**. Batteries and Supercaps, 2020, 3, 1147-1164.	2.4	6
43	Mesoscale Effects in the Extraction of the Solid-State Lithium Diffusion Coefficient Values of Battery Active Materials: Physical Insights from 3D Modeling. Journal of Physical Chemistry Letters, 2020, 11, 2775-2780.	2.1	35
44	X-ray Nanocomputed Tomography in Zernike Phase Contrast for Studying 3D Morphology of Liâ€“O₂ Battery Electrode. ACS Applied Energy Materials, 2020, 3, 4093-4102.	2.5	28
45	4D-resolved physical model for Electrochemical Impedance Spectroscopy of Li(Ni1-x-yMnxCoy)O2-based cathodes in symmetric cells: Consequences in tortuosity calculations. Journal of Power Sources, 2020, 454, 227871.	4.0	56
46	Accelerated Optimization Methods for Forceâ€Field Parametrization in Battery Electrode Manufacturing Modeling. Batteries and Supercaps, 2020, 3, 721-730.	2.4	37
47	Ion Transport Mechanisms via Time-Dependent Local Structure and Dynamics in Highly Concentrated Electrolytes. Journal of the Electrochemical Society, 2020, 167, 140537.	1.3	19
48	A Versatile and Efficient Voxelization-Based Meshing Algorithm of Multiple Phases. ACS Omega, 2019, 4, 11141-11144.	1.6	22
49	Interphases in Electroactive Suspension Systems: Where Chemistry Meets Mesoscale Physics. Batteries and Supercaps, 2019, 2, 578-578.	2.4	0
50	Text mining assisted review of the literature on Li-O₂ batteries. JPhys Materials, 2019, 2, 044004.	1.8	16
51	Lithium ion battery electrodes predicted from manufacturing simulations: Assessing the impact of the carbon-binder spatial location on the electrochemical performance. Journal of Power Sources, 2019, 444, 227285.	4.0	82
52	Tracking variabilities in the simulation of Lithium Ion Battery electrode fabrication and its impact on electrochemical performance. Electrochimica Acta, 2019, 312, 168-178.	2.6	48
53	Evaluating the impact of transport inertia on the electrochemical response of lithium ion battery single particle models. Journal of Power Sources, 2019, 423, 263-270.	4.0	11
54	Boosting Rechargeable Batteries R&D by Multiscale Modeling: Myth or Reality?. Chemical Reviews, 2019, 119, 4569-4627.	23.0	204

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55	Interphases in Electroactive Suspension Systems: Where Chemistry Meets Mesoscale Physics. Batteries and Supercaps, 2019, 2, 579-590.	2.4	9
56	Mechanistic Elucidation of Si Particle Morphology on Electrode Performance. Journal of the Electrochemical Society, 2019, 166, A3852-A3860.	1.3	7
57	Stochasticity of Pores Interconnectivity in Liâ€“O₂ Batteries and its Impact on the Variations in Electrochemical Performance. Journal of Physical Chemistry Letters, 2018, 9, 791-797.	2.1	37
58	Handling Complexity of Semisolid Redox Flow Battery Operation Principles through Mechanistic Simulations. Journal of Physical Chemistry C, 2018, 122, 23867-23877.	1.5	9
59	Unraveling the Operation Mechanisms of Lithium Sulfur Batteries with Ultramicroporous Carbons. ACS Applied Energy Materials, 2018, 1, 5816-5821.	2.5	17
60	Importance of Incorporating Explicit 3D-Resolved Electrode Mesostructures in Liâ€“O₂ Battery Models. ACS Applied Energy Materials, 2018, 1, 6433-6441.	2.5	14
61	Monte Carlo Modeling of Interfacial Electrochemistry for Energy Applications. , 2018, , 739-751.		2
62	Investigation of bi-porous electrodes for lithium oxygen batteries. Electrochimica Acta, 2018, 279, 118-127.	2.6	23
63	Compactness of the Lithium Peroxide Thin Film Formed in Liâ€“O₂ Batteries and Its Link to the Charge Transport Mechanism: Insights from Stochastic Simulations. Journal of Physical Chemistry Letters, 2017, 8, 599-604.	2.1	26
64	Self-Organization of Electroactive Suspensions in Discharging Slurry Batteries: A Mesoscale Modeling Investigation. ACS Applied Materials & Interfaces, 2017, 9, 17882-17889.	4.0	17
65	Computational Modeling of Lithiumâ€“Sulfur Batteries: Myths, Facts, and Controversies. , 2017, , 335-350.		0
66	Linking the Performances of Liâ€“O2 Batteries to Discharge Rate and Electrode and Electrolyte Properties through the Nucleation Mechanism of Li2O2. Journal of Physical Chemistry C, 2017, 121, 19577-19585.	1.5	30
67	Multiscale Simulation Platform Linking Lithium Ion Battery Electrode Fabrication Process with Performance at the Cell Level. Journal of Physical Chemistry Letters, 2017, 8, 5966-5972.	2.1	63
68	Boundary control of the number of interfaces for the one-dimensional Allen-Cahn equation. Discrete and Continuous Dynamical Systems - Series S, 2017, 10, 87-100.	0.6	1
69	A Microstructurally Resolved Model for Li-S Batteries Assessing the Impact of the Cathode Design on the Discharge Performance. Journal of the Electrochemical Society, 2016, 163, A2817-A2829.	1.3	52
70	Modeling Investigation of the Local Electrochemistry in Lithium-O₂Batteries: A Kinetic Monte Carlo Approach. Journal of the Electrochemical Society, 2016, 163, A329-A337.	1.3	30
71	Structural and surface coverage effects on CO oxidation reaction over carbon-supported Pt nanoparticles studied by quadrupole mass spectrometry and diffuse reflectance FTIR spectroscopy. Physical Chemistry Chemical Physics, 2016, 18, 15278-15288.	1.3	6
72	A multi-scale model of the oxygen reduction reaction on highly active graphene nanosheets in alkaline conditions. Journal of Power Sources, 2016, 328, 492-502.	4.0	14

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73	Impact of Li2O2 Particle Size on Liâ€“O2 Battery Charge Process: Insights from a Multiscale Modeling Perspective. Journal of Physical Chemistry Letters, 2016, 7, 3897-3902.	2.1	34
74	How Does the Surface Structure of Ptâ€“Ni Alloys Control Water and Hydrogen Peroxide Formation?. ACS Catalysis, 2016, 6, 5641-5650.	5.5	9
75	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.	4.0	180
76	A Multiparadigm Modeling Investigation of Membrane Chemical Degradation in PEM Fuel Cells. Journal of the Electrochemical Society, 2016, 163, F59-F70.	1.3	37
77	Fuel Cells and Batteries In Silico Experimentation Through Integrative Multiscale Modeling. Green Energy and Technology, 2016, , 191-233.	0.4	1
78	A Multi-Paradigm Computational Model of Materials Electrochemical Reactivity for Energy Conversion and Storage. Journal of the Electrochemical Society, 2015, 162, E73-E83.	1.3	32
79	Morphology of Supported Polymer Electrolyte Ultrathin Films: A Numerical Study. Journal of Physical Chemistry C, 2015, 119, 1201-1216.	1.5	52
80	A Comprehensive Model for Non-Aqueous Lithium Air Batteries Involving Different Reaction Mechanisms. Journal of the Electrochemical Society, 2015, 162, A614-A621.	1.3	72
81	A Drift-Diffusion Study on Charge Unbalancing Effects in Dye-Sensitized Solar Cells. Journal of the Electrochemical Society, 2015, 162, H753-H758.	1.3	8
82	Coverage-dependent thermodynamic analysis of the formation of water and hydrogen peroxide on a platinum model catalyst. Physical Chemistry Chemical Physics, 2015, 17, 11392-11400.	1.3	20
83	Interplay between Reaction Mechanism and Hydroxyl Species for Water Formation on Pt(111). ACS Catalysis, 2015, 5, 1068-1077.	5.5	24
84	Characterization of pore network structure in catalyst layers of polymer electrolyte fuel cells. Journal of Power Sources, 2014, 247, 322-326.	4.0	32
85	A Multiscale Model of Electrochemical Double Layers in Energy Conversion and Storage Devices. Journal of the Electrochemical Society, 2014, 161, E3302-E3310.	1.3	45
86	Electrode structure effects on the performance ofÂopen-cathode proton exchange membrane fuel cells: A multiscale modeling approach. International Journal of Hydrogen Energy, 2014, 39, 9752-9767.	3.8	38
87	Impact of the Cathode Microstructure on the Discharge Performance of Lithium Air Batteries: A Multiscale Model. Journal of the Electrochemical Society, 2014, 161, E3028-E3035.	1.3	72
88	An efficient and cyclic hydrogen evolution reaction mechanism on [Ni(PH2NH2)2]2+ catalysts: a theoretical and multiscale simulation study. RSC Advances, 2014, 4, 5177.	1.7	4
89	Physical Modeling and Numerical Simulation of Direct Alcohol Fuel Cells. , 2014, , 271-319.		1
90	Multiscale Modeling. , 2014, , 1320-1334.		0

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91	Inhomogeneous Transport in Model Hydrated Polymer Electrolyte Supported Ultrathin Films. ACS Nano, 2013, 7, 6767-6773.	7.3	50
92	Study of CO and Hydrogen Interactions on Carbon-Supported Pt Nanoparticles by Quadrupole Mass Spectrometry and Operando Diffuse Reflectance FTIR Spectroscopy. Journal of Physical Chemistry C, 2013, 117, 22756-22767.	1.5	28
93	Multi-scale coupling between two dynamical models for PEMFC aging prediction. International Journal of Hydrogen Energy, 2013, 38, 4675-4688.	3.8	64
94	A multiscale physical model of a polymer electrolyte membrane water electrolyzer. Electrochimica Acta, 2013, 110, 363-374.	2.6	17
95	Multiscale modelling and numerical simulation of rechargeable lithium ion batteries: concepts, methods and challenges. RSC Advances, 2013, 3, 13027.	1.7	200
96	Carbon-Based Electrodes for Lithium Air Batteries: Scientific and Technological Challenges from a Modeling Perspective. ECS Journal of Solid State Science and Technology, 2013, 2, M3084-M3100.	0.9	66
97	Effect of Surface Hydrophilicity on the Formation of Nafion Thin Films Inside PEMFC Catalyst Layers: A Computational Study. ECS Transactions, 2013, 45, 101-108.	0.3	8
98	A multiscale physical model for the transient analysis of PEM water electrolyzer anodes. Physical Chemistry Chemical Physics, 2012, 14, 10215.	1.3	33
99	CO and H₂S Impact on the PEMFC Performance and Durability Under Current Cycling Conditions: A Combined Experimental and Modeling Study. ECS Meeting Abstracts, 2012, MA2012-01, 1495-1495.	0.0	1
100	Microstructure-Based Modeling of Aging Mechanisms in Catalyst Layers of Polymer Electrolyte Fuel Cells. Journal of Physical Chemistry B, 2011, 115, 8088-8101.	1.2	70
101	A multiscale theoretical methodology for the calculation of electrochemical observables from ab initio data: Application to the oxygen reduction reaction in a Pt(111)-based polymer electrolyte membrane fuel cell. Electrochimica Acta, 2011, 56, 10842-10856.	2.6	68
102	XPS investigations of the proton exchange membrane fuel cell active layers aging: Characterization of the mitigating role of an anodic CO contamination on cathode degradation. Journal of Power Sources, 2011, 196, 2530-2538.	4.0	38
103	Multi-scale simulation of fuel cells: From the cell to the system. Solid State Ionics, 2011, 192, 615-618.	1.3	15
104	CO Impact on the Stability Properties of PtxCoy Nanoparticles in PEM Fuel Cell Anodes: Mechanistic Insights. Journal of the Electrochemical Society, 2011, 158, B1358.	1.3	13
105	Modeling Chemical Degradation of a Polymer Electrolyte Membrane and its Impact on Fuel Cell Performance. ECS Transactions, 2010, 25, 259-273.	0.3	29
106	Fullerene-Based Materials as Catalysts for Fuel Cells. ECS Transactions, 2010, 25, 1-6.	0.3	7
107	Towards a Multiscale Modeling Methodology for the Prediction of the Electro-Activity of PEM Fuel Cell Catalysts. ECS Transactions, 2010, 25, 167-173.	0.3	9
108	New Insights in the Electrocatalytic Proton Reduction and Hydrogen Oxidation by Bioinspired Catalysts: A DFT Investigation. Journal of Physical Chemistry A, 2010, 114, 11861-11867.	1.1	17

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109	Pt[sub x]Co[sub y] Catalysts Degradation in PEFC Environments: Mechanistic Insights. Journal of the Electrochemical Society, 2010, 157, B943.	1.3	9
110	Metallofullerenes as fuel cell electrocatalysts: A theoretical investigation of adsorbates on C59Pt. Physical Chemistry Chemical Physics, 2010, 12, 9406.	1.3	23
111	Multi-scale Modeling-based Prediction of PEM Fuel Cells MEA Durability under Automotive Operating Conditions. ECS Transactions, 2009, 25, 65-79.	0.3	13
112	CO Induced Reconstruction of PtxCoy Electrocatalytic Nanoparticles in a PEM Fuel Cell Anode under Transportation Operating Conditions. ECS Transactions, 2009, 25, 275-292.	0.3	6
113	Diffuse Charge Effects in Fuel Cell Membranes. Journal of the Electrochemical Society, 2009, 156, B225.	1.3	53
114	Mechanistic Investigations of NO₂ Impact on ORR in PEM Fuel Cells: a Coupled Experimental and Multi-scale Modeling Approach. ECS Transactions, 2009, 25, 1595-1604.	0.3	11
115	Impact of carbon monoxide on PEFC catalyst carbon support degradation under current-cycled operating conditions. Electrochimica Acta, 2009, 54, 5267-5279.	2.6	69
116	Pt[sub x]Co[sub y] Catalysts Degradation in PEFC Environments: Mechanistic Insights. Journal of the Electrochemical Society, 2009, 156, B410.	1.3	46
117	Multiscale Model of Carbon Corrosion in a PEFC: Coupling with Electrocatalysis and Impact on Performance Degradation. Journal of the Electrochemical Society, 2008, 155, B367.	1.3	81
118	Transient Multi-Scale Modeling of PtxCoy Catalysts Degradation in PEFC Environments. ECS Transactions, 2008, 13, 29-66.	0.3	7
119	Carbon Catalyst-Support Corrosion in Polymer Electrolyte Fuel Cells: Mechanistic Insights. ECS Transactions, 2008, 13, 35-55.	0.3	14
120	Transient Multi-Scale Modelling of Ageing Mechanisms in a Polymer Electrolyte Fuel Cell: An Irreversible Thermodynamics Approach. ECS Transactions, 2007, 6, 1-23.	0.3	10
121	Transient Multiscale Modeling of Aging Mechanisms in a PEFC Cathode. Journal of the Electrochemical Society, 2007, 154, B712.	1.3	76
122	A Multi-Scale Dynamic Mechanistic Model for the Transient Analysis of PEFCs. Fuel Cells, 2007, 7, 99-117.	1.5	107
123	A Dynamic Mechanistic Model of an Electrochemical Interface. Journal of the Electrochemical Society, 2006, 153, A1053.	1.3	58
124	Fabrication of High-Quality Thin Solid-State Electrolyte Films Assisted by Machine Learning. ACS Energy Letters, 0, , 1639-1648.	8.8	53
125	Innovative Computer Games for Battery Education and Research. ChemistryViews, 0, , .	0.0	0