

Alejandro A Franco

List of Publications by Year in descending order

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125
papers

4,300
citations

94433

37
h-index

128289

60
g-index

148
all docs

148
docs citations

148
times ranked

3360
citing authors

#	ARTICLE	IF	CITATIONS
1	Boosting Rechargeable Batteries R&D by Multiscale Modeling: Myth or Reality?. Chemical Reviews, 2019, 119, 4569-4627.	47.7	204
2	Multiscale modelling and numerical simulation of rechargeable lithium ion batteries: concepts, methods and challenges. RSC Advances, 2013, 3, 13027.	3.6	200
3	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
4	Artificial Intelligence Applied to Battery Research: Hype or Reality?. Chemical Reviews, 2022, 122, 10899-10969.	47.7	153
5	Rechargeable Batteries of the Future—The State of the Art from a BATTERY 2030+ Perspective. Advanced Energy Materials, 2022, 12, .	19.5	124
6	Investigating electrode calendaring 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.	7.8	118
7	A Multi-Scale Dynamic Mechanistic Model for the Transient Analysis of PEFCs. Fuel Cells, 2007, 7, 99-117.	2.4	107
8	Artificial Intelligence Investigation of NMC Cathode Manufacturing Parameters Interdependencies. Batteries and Supercaps, 2020, 3, 60-67.	4.7	93
9	How Machine Learning Will Revolutionize Electrochemical Sciences. ACS Energy Letters, 2021, 6, 1422-1431.	17.4	88
10	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.	7.8	82
11	Multiscale Model of Carbon Corrosion in a PEFC: Coupling with Electrocatalysis and Impact on Performance Degradation. Journal of the Electrochemical Society, 2008, 155, B367.	2.9	81
12	Transient Multiscale Modeling of Aging Mechanisms in a PEFC Cathode. Journal of the Electrochemical Society, 2007, 154, B712.	2.9	76
13	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.	2.9	72
14	A Comprehensive Model for Non-Aqueous Lithium Air Batteries Involving Different Reaction Mechanisms. Journal of the Electrochemical Society, 2015, 162, A614-A621.	2.9	72
15	Microstructure-Based Modeling of Aging Mechanisms in Catalyst Layers of Polymer Electrolyte Fuel Cells. Journal of Physical Chemistry B, 2011, 115, 8088-8101.	2.6	70
16	Data-driven assessment of electrode calendaring process by combining experimental results, in silico mesostructures generation and machine learning. Journal of Power Sources, 2020, 480, 229103.	7.8	70
17	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, .	19.5	70
18	Impact of carbon monoxide on PEFC catalyst carbon support degradation under current-cycled operating conditions. Electrochimica Acta, 2009, 54, 5267-5279.	5.2	69

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19	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. <i>Electrochimica Acta</i> , 2011, 56, 10842-10856.	5.2	68
20	Carbon-Based Electrodes for Lithium Air Batteries: Scientific and Technological Challenges from a Modeling Perspective. <i>ECS Journal of Solid State Science and Technology</i> , 2013, 2, M3084-M3100.	1.8	66
21	Bridging nano- and microscale X-ray tomography for battery research by leveraging artificial intelligence. <i>Nature Nanotechnology</i> , 2022, 17, 446-459.	31.5	66
22	Multi-scale coupling between two dynamical models for PEMFC aging prediction. <i>International Journal of Hydrogen Energy</i> , 2013, 38, 4675-4688.	7.1	64
23	Multiscale Simulation Platform Linking Lithium Ion Battery Electrode Fabrication Process with Performance at the Cell Level. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5966-5972.	4.6	63
24	Insight on electrolyte infiltration of lithium ion battery electrodes by means of a new three-dimensional-resolved lattice Boltzmann model. <i>Energy Storage Materials</i> , 2021, 38, 80-92.	18.0	61
25	A Dynamic Mechanistic Model of an Electrochemical Interface. <i>Journal of the Electrochemical Society</i> , 2006, 153, A1053.	2.9	58
26	4D-resolved physical model for Electrochemical Impedance Spectroscopy of Li(Ni _{1-x} YMn _x Co _y)O ₂ -based cathodes in symmetric cells: Consequences in tortuosity calculations. <i>Journal of Power Sources</i> , 2020, 454, 227871.	7.8	56
27	Diffuse Charge Effects in Fuel Cell Membranes. <i>Journal of the Electrochemical Society</i> , 2009, 156, B225.	2.9	53
28	Fabrication of High-Quality Thin Solid-State Electrolyte Films Assisted by Machine Learning. <i>ACS Energy Letters</i> , 0, , 1639-1648.	17.4	53
29	Morphology of Supported Polymer Electrolyte Ultrathin Films: A Numerical Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 1201-1216.	3.1	52
30	A Microstructurally Resolved Model for Li-S Batteries Assessing the Impact of the Cathode Design on the Discharge Performance. <i>Journal of the Electrochemical Society</i> , 2016, 163, A2817-A2829.	2.9	52
31	Digitalization of Battery Manufacturing: Current Status, Challenges, and Opportunities. <i>Advanced Energy Materials</i> , 2022, 12, .	19.5	51
32	Inhomogeneous Transport in Model Hydrated Polymer Electrolyte Supported Ultrathin Films. <i>ACS Nano</i> , 2013, 7, 6767-6773.	14.6	50
33	Tracking variabilities in the simulation of Lithium Ion Battery electrode fabrication and its impact on electrochemical performance. <i>Electrochimica Acta</i> , 2019, 312, 168-178.	5.2	48
34	Understanding the calendaring processability of Li(Ni _{0.33} Mn _{0.33} Co _{0.33})O ₂ -based cathodes. <i>Journal of Power Sources</i> , 2021, 488, 229361.	7.8	48
35	Pt _[sub x] Co _[sub y] Catalysts Degradation in PEFC Environments: Mechanistic Insights. <i>Journal of the Electrochemical Society</i> , 2009, 156, B410.	2.9	46
36	Carbon-Binder Migration: A Three-Dimensional Drying Model for Lithium-ion Battery Electrodes. <i>Energy Storage Materials</i> , 2021, 43, 337-347.	18.0	46

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37	A Multiscale Model of Electrochemical Double Layers in Energy Conversion and Storage Devices. <i>Journal of the Electrochemical Society</i> , 2014, 161, E3302-E3310.	2.9	45
38	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. <i>Journal of Power Sources</i> , 2011, 196, 2530-2538.	7.8	38
39	Electrode structure effects on the performance of open-cathode proton exchange membrane fuel cells: A multiscale modeling approach. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 9752-9767.	7.1	38
40	A Multiparadigm Modeling Investigation of Membrane Chemical Degradation in PEM Fuel Cells. <i>Journal of the Electrochemical Society</i> , 2016, 163, F59-F70.	2.9	37
41	Stochasticity of Pores Interconnectivity in LiO_2 Batteries and its Impact on the Variations in Electrochemical Performance. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 791-797.	4.6	37
42	Accelerated Optimization Methods for Force-Field Parametrization in Battery Electrode Manufacturing Modeling. <i>Batteries and Supercaps</i> , 2020, 3, 721-730.	4.7	37
43	Mesoscale Effects in the Extraction of the Solid-State Lithium Diffusion Coefficient Values of Battery Active Materials: Physical Insights from 3D Modeling. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 2775-2780.	4.6	35
44	Impact of Li_2O_2 Particle Size on LiO_2 Battery Charge Process: Insights from a Multiscale Modeling Perspective. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3897-3902.	4.6	34
45	A multiscale physical model for the transient analysis of PEM water electrolyzer anodes. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10215.	2.8	33
46	A three dimensional kinetic Monte Carlo model for simulating the carbon/sulfur mesostructural evolutions of discharging lithium sulfur batteries. <i>Energy Storage Materials</i> , 2020, 24, 472-485.	18.0	33
47	Characterization of pore network structure in catalyst layers of polymer electrolyte fuel cells. <i>Journal of Power Sources</i> , 2014, 247, 322-326.	7.8	32
48	A Multi-Paradigm Computational Model of Materials Electrochemical Reactivity for Energy Conversion and Storage. <i>Journal of the Electrochemical Society</i> , 2015, 162, E73-E83.	2.9	32
49	Deconvoluting the benefits of porosity distribution in layered electrodes on the electrochemical performance of Li-ion batteries. <i>Energy Storage Materials</i> , 2022, 47, 462-471.	18.0	32
50	Machine learning-based assessment of the impact of the manufacturing process on battery electrode heterogeneity. <i>Energy and AI</i> , 2021, 5, 100090.	10.6	31
51	Modeling Investigation of the Local Electrochemistry in Lithium- O_2 Batteries: A Kinetic Monte Carlo Approach. <i>Journal of the Electrochemical Society</i> , 2016, 163, A329-A337.	2.9	30
52	Linking the Performances of LiO_2 Batteries to Discharge Rate and Electrode and Electrolyte Properties through the Nucleation Mechanism of Li_2O_2 . <i>Journal of Physical Chemistry C</i> , 2017, 121, 19577-19585.	3.1	30
53	Modeling Chemical Degradation of a Polymer Electrolyte Membrane and its Impact on Fuel Cell Performance. <i>ECS Transactions</i> , 2010, 25, 259-273.	0.5	29
54	Designing electrode architectures to facilitate electrolyte infiltration for lithium-ion batteries. <i>Energy Storage Materials</i> , 2022, 49, 268-277.	18.0	29

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55	Study of CO and Hydrogen Interactions on Carbon-Supported Pt Nanoparticles by Quadrupole Mass Spectrometry and Operando Diffuse Reflectance FTIR Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2013, 117, 22756-22767.	3.1	28
56	X-ray Nanocomputed Tomography in Zernike Phase Contrast for Studying 3D Morphology of Li ⁺ O ₂ Battery Electrode. <i>ACS Applied Energy Materials</i> , 2020, 3, 4093-4102.	5.1	28
57	Compactness of the Lithium Peroxide Thin Film Formed in Li ⁺ O ₂ Batteries and Its Link to the Charge Transport Mechanism: Insights from Stochastic Simulations. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 599-604.	4.6	26
58	Interplay between Reaction Mechanism and Hydroxyl Species for Water Formation on Pt(111). <i>ACS Catalysis</i> , 2015, 5, 1068-1077.	11.2	24
59	Metallofullerenes as fuel cell electrocatalysts: A theoretical investigation of adsorbates on C59Pt. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9406.	2.8	23
60	Investigation of bi-porous electrodes for lithium oxygen batteries. <i>Electrochimica Acta</i> , 2018, 279, 118-127.	5.2	23
61	A Versatile and Efficient Voxelization-Based Meshing Algorithm of Multiple Phases. <i>ACS Omega</i> , 2019, 4, 11141-11144.	3.5	22
62	Machine learning 3D-resolved prediction of electrolyte infiltration in battery porous electrodes. <i>Journal of Power Sources</i> , 2021, 511, 230384.	7.8	21
63	Coverage-dependent thermodynamic analysis of the formation of water and hydrogen peroxide on a platinum model catalyst. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 11392-11400.	2.8	20
64	What Can Text Mining Tell Us About Lithium ⁺ Battery Researchers TM Habits?. <i>Batteries and Supercaps</i> , 2021, 4, 758-766.	4.7	20
65	Artificial neural network approach for multiphase segmentation of battery electrode nano-CT images. <i>Npj Computational Materials</i> , 2022, 8, .	8.7	20
66	Calendering of Li(Ni _{0.33} Mn _{0.33} Co _{0.33})O ₂ -Based Cathodes: Analyzing the Link Between Process Parameters and Electrode Properties by Advanced Statistics. <i>Batteries and Supercaps</i> , 2021, 4, 834-844.	4.7	19
67	Ion Transport Mechanisms via Time-Dependent Local Structure and Dynamics in Highly Concentrated Electrolytes. <i>Journal of the Electrochemical Society</i> , 2020, 167, 140537.	2.9	19
68	Heterogeneous Solid ⁺ Electrolyte Interphase in Graphite Electrodes Assessed by 4D ⁺ Resolved Computational Simulations. <i>Batteries and Supercaps</i> , 2021, 4, 1457-1463.	4.7	18
69	New Insights in the Electrocatalytic Proton Reduction and Hydrogen Oxidation by Bioinspired Catalysts: A DFT Investigation. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11861-11867.	2.5	17
70	A multiscale physical model of a polymer electrolyte membrane water electrolyzer. <i>Electrochimica Acta</i> , 2013, 110, 363-374.	5.2	17
71	Self-Organization of Electroactive Suspensions in Discharging Slurry Batteries: A Mesoscale Modeling Investigation. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 17882-17889.	8.0	17
72	Unraveling the Operation Mechanisms of Lithium Sulfur Batteries with Ultramicroporous Carbons. <i>ACS Applied Energy Materials</i> , 2018, 1, 5816-5821.	5.1	17

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73	Quantitatively Designing Porous Copper Current Collectors for Lithium Metal Anodes. ACS Applied Energy Materials, 2021, 4, 6454-6465.	5.1	17
74	Towards a 3D-resolved model of Si/Graphite composite electrodes from manufacturing simulations. Journal of Power Sources, 2021, 512, 230486.	7.8	17
75	Towards autonomous high-throughput multiscale modelling of battery interfaces. Energy and Environmental Science, 2022, 15, 579-594.	30.8	17
76	Text mining assisted review of the literature on Li-O ₂ batteries. JPhys Materials, 2019, 2, 044004.	4.2	16
77	Multi-scale simulation of fuel cells: From the cell to the system. Solid State Ionics, 2011, 192, 615-618.	2.7	15
78	Carbon Catalyst-Support Corrosion in Polymer Electrolyte Fuel Cells: Mechanistic Insights. ECS Transactions, 2008, 13, 35-55.	0.5	14
79	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.	7.8	14
80	Importance of Incorporating Explicit 3D-Resolved Electrode Mesostuctures in Li-O ₂ Battery Models. ACS Applied Energy Materials, 2018, 1, 6433-6441.	5.1	14
81	Multi-scale Modeling-based Prediction of PEM Fuel Cells MEA Durability under Automotive Operating Conditions. ECS Transactions, 2009, 25, 65-79.	0.5	13
82	CO Impact on the Stability Properties of PtCo Nanoparticles in PEM Fuel Cell Anodes: Mechanistic Insights. Journal of the Electrochemical Society, 2011, 158, B1358.	2.9	13
83	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.	18.0	12
84	Mechanistic Investigations of NO ₂ Impact on ORR in PEM Fuel Cells: a Coupled Experimental and Multi-scale Modeling Approach. ECS Transactions, 2009, 25, 1595-1604.	0.5	11
85	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.	7.8	11
86	Probing and Interpreting the Porosity and Tortuosity Evolution of Li-O ₂ Cathodes on Discharge through a Combined Experimental and Theoretical Approach. Journal of Physical Chemistry C, 2021, 125, 4955-4967.	3.1	11
87	Experimentally Validated Three-Dimensional Modeling of Organic-Based Sodium-Ion Battery Electrode Manufacturing. Batteries and Supercaps, 2022, 5, .	4.7	11
88	Transient Multi-Scale Modelling of Ageing Mechanisms in a Polymer Electrolyte Fuel Cell: An Irreversible Thermodynamics Approach. ECS Transactions, 2007, 6, 1-23.	0.5	10
89	Towards a Multiscale Modeling Methodology for the Prediction of the Electro-Activity of PEM Fuel Cell Catalysts. ECS Transactions, 2010, 25, 167-173.	0.5	9
90	Pt _x Co _y Catalysts Degradation in PEFC Environments: Mechanistic Insights. Journal of the Electrochemical Society, 2010, 157, B943.	2.9	9

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91	How Does the Surface Structure of Pt–Ni Alloys Control Water and Hydrogen Peroxide Formation?. ACS Catalysis, 2016, 6, 5641-5650.	11.2	9
92	Handling Complexity of Semisolid Redox Flow Battery Operation Principles through Mechanistic Simulations. Journal of Physical Chemistry C, 2018, 122, 23867-23877.	3.1	9
93	Interphases in Electroactive Suspension Systems: Where Chemistry Meets Mesoscale Physics. Batteries and Supercaps, 2019, 2, 579-590.	4.7	9
94	The ARTISTIC Online Calculator: Exploring the Impact of Lithium–Ion Battery Electrode Manufacturing Parameters Interactively Through Your Browser. Batteries and Supercaps, 2022, 5, .	4.7	9
95	Effect of Surface Hydrophilicity on the Formation of Nafion Thin Films Inside PEMFC Catalyst Layers: A Computational Study. ECS Transactions, 2013, 45, 101-108.	0.5	8
96	A Drift-Diffusion Study on Charge Unbalancing Effects in Dye-Sensitized Solar Cells. Journal of the Electrochemical Society, 2015, 162, H753-H758.	2.9	8
97	Transient Multi-Scale Modeling of Pt _x Co _y Catalysts Degradation in PEFC Environments. ECS Transactions, 2008, 13, 29-66.	0.5	7
98	Fullerene-Based Materials as Catalysts for Fuel Cells. ECS Transactions, 2010, 25, 1-6.	0.5	7
99	Mechanistic Elucidation of Si Particle Morphology on Electrode Performance. Journal of the Electrochemical Society, 2019, 166, A3852-A3860.	2.9	7
100	An Invitation to Engage with Computational Modeling: User–Friendly Tool for In Silico Battery Component Generation and Meshing. Batteries and Supercaps, 2021, 4, 1451-1456.	4.7	7
101	CO Induced Reconstruction of Pt _x Co _y Electrocatalytic Nanoparticles in a PEM Fuel Cell Anode under Transportation Operating Conditions. ECS Transactions, 2009, 25, 275-292.	0.5	6
102	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.	2.8	6
103	Entering the Augmented Era: Immersive and Interactive Virtual Reality for Battery Education and Research**. Batteries and Supercaps, 2020, 3, 1147-1164.	4.7	6
104	Understanding the Reaction Steps Involving Polysulfides in 1 M LiTFSI in TEGDME:DOL Using Cyclic Voltammetry Experiments and Modelling. Batteries and Supercaps, 2021, 4, 152-162.	4.7	6
105	Perspectives on manufacturing simulations of Li-S battery cathodes. JPhys Energy, 2022, 4, 011002.	5.3	6
106	Towards a Local <i>In situ</i> X-ray Nano Computed Tomography under Realistic Cycling Conditions for Battery Research. Chemistry Methods, 2022, 2, .	3.8	5
107	An efficient and cyclic hydrogen evolution reaction mechanism on [Ni(PH ₂ NH ₂) ₂] ²⁺ catalysts: a theoretical and multiscale simulation study. RSC Advances, 2014, 4, 5177.	3.6	4
108	What Can Text Mining Tell Us About Lithium–Ion Battery Researchers’ Habits?. Batteries and Supercaps, 2021, 4, 689-689.	4.7	3

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109	CHAMPION : Chalmers hierarchical atomic, molecular, polymeric and ionic analysis toolkit. Journal of Computational Chemistry, 2021, 42, 1632-1642.	3.3	3
110	Monte Carlo Modeling of Interfacial Electrochemistry for Energy Applications. , 2018, , 739-751.		2
111	Escape from flatland. Nature Machine Intelligence, 2021, 3, 277-278.	16.0	2
112	Artificial Intelligence in Electrochemical Energy Storage. Batteries and Supercaps, 2022, 5, .	4.7	2
113	CO and H ₂ S 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
114	Fuel Cells and Batteries In Silico Experimentation Through Integrative Multiscale Modeling. Green Energy and Technology, 2016, , 191-233.	0.6	1
115	Physical Modeling and Numerical Simulation of Direct Alcohol Fuel Cells. , 2014, , 271-319.		1
116	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.	1.1	1
117	Pore size distribution of carbon black: An approach from a coarse-grained potential. Computational Materials Science, 2022, 209, 111409.	3.0	1
118	Gaining Insight into the Electrochemical Interface Dynamics in an Organic Redox Flow Battery with a Kinetic Monte Carlo Approach. Small, 2022, 18, .	10.0	1
119	Computational Modeling of Lithium-Sulfur Batteries: Myths, Facts, and Controversies. , 2017, , 335-350.		0
120	Interphases in Electroactive Suspension Systems: Where Chemistry Meets Mesoscale Physics. Batteries and Supercaps, 2019, 2, 578-578.	4.7	0
121	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
122	Multiscale Modeling. , 2014, , 1320-1334.		0
123	Innovative Computer Games for Battery Education and Research. ChemistryViews, 0, , .	0.0	0
124	Quantitatively Designing Porous Copper Current Collectors for Lithium Metal Anodes. ECS Meeting Abstracts, 2021, MA2021-02, 721-721.	0.0	0
125	(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