Promotion IUF 2016
Rapport d'activité (2016-2021)

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CATÉGORIE : JUNIOR

THÉMATIQUE DE RECHERCHE : MODELISATION MULTI-ECHELLES ET PAR INTELLIGENCE ARTIFICIELLE DE BATTERIES RECHARGEABLES

RÉSUME SCIENTIFIQUE À PROPOS DE LA RÉALISATION DU PROJET DE RECHERCHE IUF (2 pages maximum) :
Avancées majeures / Etat d'achèvement / réorientations éventuelles au cours des 5 ans / Perspectives ouvertes par le travail réalisé

My research activities as a Junior Member of the Institut Universitaire de France (IUF) in the period October 2016 - September 2021, have been focused on the **understanding of the structure-property-function relationships** of composite materials used as electrodes in several types of rechargeable batteries, including lithium ion batteries (LIBs), lithium sulfur batteries (LSBs), lithium air batteries (LABs) and redox flow batteries (RFBs).[1] The numerous materials and parameters involved in these systems and processes makes their understanding very difficult to achieve on the exclusive basis of experimental approaches. This is why **my research activities combined experiments with theory.**

In my research team's work, theory crystallized in the form of **computational models or digital twins**, allowing to simulate the real manufacturing process, electrodes, and devices, and to perform virtual experiments. Once validated by experimental characterizations, such digital twins had strong potential to accelerate the understanding as well as to provide guidelines for the composite material (electrodes) design and optimization. This is because they were designed to reconstruct the history of the real system behavior and to predict its evolution. Given the inherent multiscale complexity of these systems (from materials to processes), my digital twins were often "**multi-scale**",[2] *i.e.* they encompassed **several computational techniques**, each of them addressing through a physics-viewpoint different spatiotemporal scales (*e.g.*

Coarse-Grained Molecular Dynamics, Discrete Element Method, kinetic Monte Carlo, Lattice Boltzmann Method, Finite Element Method). As a complement, we used data-driven methods based on **Artificial Intelligence (AI)/Machine Learning**[3] to unravel **manufacturing parameters interdependencies and make optimal design predictions** from **our own experimental and physics model-generated multidimensional datasets.** We completed these datasets by developing and applying **text mining algorithms** that automatically extract information from large batches of scientific publications. We also developed **Virtual Reality tools** to ease the analysis of experimental and computational results, to assist the experimental researchers and also to disseminate my scientific results in University lectures and in science popularization events.

Since my obtention of my **ERC Consolidator Grant** in 2017,[4] my research activities have been strongly oriented towards the understanding of how industrial-type **manufacturing** parameters impact LIB electrode textural and functional properties and their design optimization. An example of major scientific achievement within this context is our **physics-based computational multiscale model of the entire manufacturing wet process of LIBs**, as far as I know **the first in its kind** in peer-reviewed scientific literature. Such workflow is supported on a computational workflow encompassing physics-based and machine learning models describing the several manufacturing process steps, supported on experimental characterizations using a battery manufacturing plant prototype available in my laboratory. Such process steps involved materials mixing, slurry formulation, coating and drying, calendering, electrolyte impregnation of the assembled cells, and electrochemical performance characterization. Our computational multiscale model is able to predict the influence of manufacturing parameters (*e.g.* slurry formulation, coating gap, and speed, drying rate, calendering pressure) on LIB electrodes texture and performance for a wide spectrum of materials chemistries, paving the way to the acceleration of their optimal design in comparison to traditional trial-and-error approaches.

Besides my ERC Consolidator Grant for my project ARTISTIC, I have obtained several other grants as PI or Work Package or Task leader, as well as in collaboration with industry.[5] An example of that is the BIG MAP European project within the Battery 2030+ umbrella. Within this project I am leading the electrochemistry data storage infrastructure and developing and applying AI approaches to enhance physical models of LIB electrodes.

Within the HELIS European project, I investigated with my team electrochemical reactions and transport processes in LSBs. I was in particular interested on the impact of the **cathode mesostructure** (initial porosity, specific surface area, sulfur loading, sulfur localization, etc.) and **electrolyte volume** on the performance and aging of LSBs. We also studied the operation principles of **Quasi Solid State** LSBs. My approach here encompassed continuum models describing the interplays between transport processes and electrochemical reactions leading to the formation of polysulfides, 4D-resolved kinetic Monte Carlo models (*in house* code "MESSI" coded in Python) able to predict the spatial location of the reaction products upon discharge depending on the operation conditions, and *in house* advanced experimental characterizations. Our physical models simulate discharge and charge operation of electrolyte/carbon electrode interfaces, of electrodes and of full cells. They were also able to simulate electroanalytical experiments (*e.g.* Cyclic Voltammetry) aiming at unraveling the influence of the electrolyte composition on the reaction mechanisms involving polysulfides.

I also investigated with my team electrochemical and transport mechanisms in **Lithium Air Batteries**. This includes **lithium peroxide nucleation** phenomena, lithium peroxide **decomposition** during charge and electrolyte degradation mechanisms. I was also particularly interested on the impact of the **cathode electrode mesostructure** on the **reproducibility**, discharge performance and **rechargeability** of the cells. Our approach encompassed continuum modeling to investigate reaction mechanisms and to propose guidelines for optimized electrode architectures, kinetic Monte Carlo models (Python) to investigate the impact of pores morphology and electrode surface chemistry on the lithium peroxide formation mechanisms, Pore Network Models to assess the impact of the cathode anisotropy on the formation of lithium peroxide and oxygen transport properties, and *in house* electrochemistry experiments.

I studied **Semi-Solid** RFBs containing particles suspensions and RFBs with **organic active molecules**, the latter within the SONAR European project. In the case of SSRFBs we were interested on the interplay between **fluid dynamics**, **particle suspensions dynamics** and **electrochemistry**. We have studied in particular Silicon-based semi-solid electrodes for SSRFBs. Regarding organic-based RFBs, we studied the **electrochemical and aging mechanisms** upon discharge and charge with multiple types of active molecule chemistries. We also investigate electrochemical double layer effects on the reactivity. Our approach encompassed 4D-resolved kinetic Monte Carlo for the simulation of REDOX reactions, aging mechanisms and particle suspensions dynamics, Dissipative Particle Dynamics for investigating particle suspension dynamics, and Discrete Element Method coupled to continuum modeling for the prediction of electrochemical performance. Our activities in this regard were/are carried out in strong link with *in house* experimental characterizations.

My IUF position has been transformative for my career : it gave me the extra time I needed to prepare my ERC project proposal that I finally got accepted in 2017, and it gave me all the freedom I needed to deploy my scientific vision supported on the use of multiple types of computational techniques and on multi, inter and transdisciplinarity, in strong connection with engineering and experimental problems. Lots of networking opportunities arose from my research, resulting in very interesting and productive international scientific collaborations (cristallized in the form of joint publications).

PRODUCTION SCIENTIFIQUE DE LA PÉRIODE 2016-2021 :
Publications scientifiques / Communications orales invitées / Ouvrages / Brevets / Autres réalisations

PUBLICATIONS IN PEER-REVIEWED INTERNATIONAL JOURNALS SINCE THE BEGGINING OF MY IUF POSITION (OCTOBER 2016) (55)

(I underline below the MSc. students, PhD students and postdoc I supervised. The articles where I am corresponding author are indicated with « * »))

The works published in 2022 indicated below have been prepared within the period of my IUF Junior Member position.

[55] Z. Su, T.-T. Nguyen, C. Le Bourlot, F. Cadiou, A. Jamali, V. De Andrade, **A. A.**

Franco, A. Demortière, Towards a Local *In situ* X-ray Nano Computed Tomography under Realistic Cycling Conditions for Battery Research, Chemistry-Methods, in press (2022) https://doi.org/10.1002/cmtd.202100051 (Wiley).

[54] J. Amici, P. Asinari, E. Ayerbe, P. Barboux, P. Bayle-Guillemaud, R. J. Behm, M. Berecibar, E. Berg, A. Bhowmik, S. Bodoardo, I. E. Castelli, I. Cekic-Laskovic, R. Christensen, S. Clark, R. Diehm, R. Dominko, M. Fichtner, **A. A. Franco**, A. Grimaud, N. Guillet, M. Hahlin, S. Hartmann, V. Heiries, K. Hermansson, A. Heuer, S. Jana, L. Jabbour, J. Kallo, A. Latz, H. Lorrmann, O. M. Løvvik, S. Lyonnard, M. Meeus, E. Paillard, S. Perraud, T. Placke, C. Punckt, O. Raccurt, J. Ruhland, E. Sheridan, H. Stein, J.-M. Tarascon, V. Trapp, T. Vegge, M. Weil, W. Wenzel, M. Winter, A. Wolf, K. Edström, A Roadmap for Transforming Research to Invent the Batteries of the Future Designed within the European Large Scale Research Initiative BATTERY 2030+, in press (2022) https://doi.org/10.1002/aenm.202102785 (Wiley).

[53] O. Arcelus, **A.A.Franco***, "Perspectives on manufacturing simulations of Li-S battery cathodes", *J.Phys. Energy*, in press (2022). https://doi.org/10.1088/2515-7655/ac4ac (IOP Sciences).

[52] T. Lombardo, F. Caro, A.C. Ngandjong, J.B. Hoock, M. Duquesnoy, J.C. Delepine, A. Ponchelet, S. Doison, **A.A. Franco***, "The ARTISTIC Online Calculator: Exploring the Impact of Li-ion Battery Electrode Manufacturing Parameters Interactively through your Browser", *Batteries & Supercaps*, in press (2022). https://doi.org/10.1002/batt.202100324 (Wiley).

[51] Z. Deng, V. Kumar, F.T. Bölle, F. Caro, **A.A. Franco***, I.E. Castelli*, P. Canepa*, Z.W. Seh*, "Towards autonomous high-throughput multiscale modelling of battery interfaces", *Energy & Environmental Science*, Advance Article -in press, first published in December 2021- (2022). https://doi.org/10.1039/D1EE02324A (Royal Society of Chemistry).

[50] J. Scharf, M. Chouchane, D. P Finegan, B. Lu, C. Redquest, M.-C. Kim, W. Yao, **A. A Franco**, D. Gostovic, Z. Liu, M. Riccio, F. Zelenka, J.-M. Doux*, Y. S. Meng*, "Bridging Nano and Micro-scale X-ray Tomography for Battery Research by Leveraging Artificial Intelligence", *Nature Nanotechnology*, accepted (2021) (Springer Nature).

[49] M. Fichtner*, K. Edström*, E. Ayerbe, M. Berecibar, A. Bhowmik, I. E. Castellit, S. Clark, R. Dominko, M. Erakca, **A. A. Franco**, A. Grimaud, B. Horstmann, A. Latz, H. Lorrmann, M. Meeus, R. Narayan, F. Pammer, J. Ruhland, H. Stein, T. Vegge, M. Weil, "Rechargeable batteries of the future – The state of the art from a BATTERY 2030+ perspective", *Advanced Energy Materials,* accepted (2021) (Wiley).

[48] E. Ayerbe*, M. Berecibar, S. Clark, **A.A. Franco**, J. Ruhland, "Digitalization of Battery Manufacturing: Current Status, Challenges and Opportunities", *Advanced Energy Materials,* in press (2021) https://doi.org/10.1002/aenm.202102696 (Wiley).

[47] T. Lombardo, M. Duquesnoy, H. El-Bouysidy, F. Aren, A. Gallo-Bueno, P. B. Jorgensen, A. Bhowmik, A. Dermotière, E. Ayerbe, F. Alcaide, M. Reynaud, J. Carrasco, A. Grimaud, C. Zhang, T. Vegge, P. Johansson, **A.A. Franco***, "Artificial

Intelligence Applied to Battery Research: Hype or Reality?", *Chemical Reviews*, in press (2021) https://doi.org/10.1021/acs.chemrev.1c00108 (American Chemical Society).

[46] T. Lombardo, A.C. Ngandjong, A. Belhcen, **A.A. Franco***, "Carbon-Binder Migration: A Three-Dimensional Evaporation Model for Lithium Ion Batteries", *Energy Storage Materials*, 43 (2021) 337 (Elsevier).

[45] C. Liu, O. Arcelus, T. Lombardo, H. Oularbi, **A.A. Franco***, "Towards a 3D-resolved model of Si/Graphite composite electrodes from manufacturing simulations", *Journal of Power Sources*, 512 (2021) 230486 (Elsevier).

[44] A. Shodiev, M. Duquesnoy, O. Arcelus, M. Chouchane, J. Li, **A.A. Franco***, "Machine learning 3D-resolved prediction of electrolyte infiltration in battery porous electrodes", *Journal of Power Sources*, 511 (2021) 230384 (Elsevier).

[43] B. Lu, E. Olivera, J. Scharf, M. Chouchane, C. Fang, M. Ceja, L.E. Pangilinan, S. Zheng, A. Dawson, D. Cheng, W. Bao, O. Arcelus, **A.A. Franco**, X. Li, S.H. Tolbert*, Y. S. Meng*, "Quantitatively Designing Porous Copper Current Collectors for Lithium Metal Anodes", *ACS Applied Energy Materials*, 4 (7) (2021) 6454 (American Chemical Society).

[42] M. Chouchane, **A.A. Franco*,** "An Invitation to Engage with Computational Modeling: User-friendly Tool for In Silico Battery Component Generation and Meshing", *Batteries & Supercaps*, 4 (9) (2021) 1451. Also invited for the Cover Feature of the journal[6] (Wiley).

[41] R. Andersson*, F. Aren, **A.A. Franco**, P. Johansson, "CHAMPION: Chalmers hierarchical atomic, molecular, polymeric and ionic analysis toolkit", *Journal of Computational Chemistry*, 42 (23) (2021) 1632 (Wiley).

[40] M. Duquesnoy, I. Boyano, L. Ganborena, P. Cereijo, E. Ayerbe, **A.A. Franco*,** "Machine Learning-Based Assessment of the Impact of the Manufacturing Process on Battery Electrode Heterogeneity", *Energy and AI*, 5 (2021) 100090 (Elsevier).

[39] M. Chouchane, O. Arcelus, **A.A. Franco***, "Heterogeneous Solid Electrolyte Interphase in Graphite Electrodes Assessed by 4D-Resolved Computational Simulations", *Batteries & Supercaps*, 4 (9) (2021) 1457 (Wiley).

[38] **A.A. Franco***, "Escape from Flatland", *Nature Machine Intelligence* (2021) https://doi.org/10.1038/s42256-021-00334-x (Springer Nature).

[37] Y.-T. Chen, M. Duquesnoy, D.H.S. Tan, J.-M. Doux, H. Yang, G. Deysher, P. Ridley, **A.A. Franco***, Y.S. Meng*, Z. Chen*, "Fabrication of high-quality thin solid-state electrolyte films assisted by machine learning", *ACS Energy Letters*, 6, 4 (2021) 1639 (American Chemical Society).

[36] A. Shodiev, E. Primo, O. Arcelus, M. Chouchane, M. Osenberg, A. Hilger, I. Manke, J. Li, **A.A. Franco***, "Insight on electrolyte infiltration of lithium ion battery electrodes by means of a new three-dimensional-resolved lattice Boltzmann model", *Energy Storage Materials*, 38 (2021) 80 (Elsevier).

[35] H. El-Bousiydy, T. Lombardo, E. N. Primo, M. Duquesnoy, M. Morcrette, P.

Johansson, P. Simon, A. Grimaud, **A.A. Franco***, "What can text mining tell us about lithium-ion battery researchers' habits?", *Batteries & Supercaps*, 4(5) (2021) 758. **Also invited for the Front Cover of the journal in May 2021**[7] (Wiley).

[34] E. Primo, M. Touzin, **A.A. Franco***, "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", *Batteries & Supercaps*, 4(5) (2021) 834 (Wiley).

[33] A. Mistry, **A.A. Franco***, S.A. Roberts, S. Cooper, V. Viswanathan, "How Machine Learning will Revolutionize the Electrochemical Sciences", *ACS Energy Letters*, 6(4) (2021) 1422 (American Chemical Society).

[32] E.N. Primo, M. Chouchane, M. Touzin, P. Vazquez, **A.A. Franco***, "Understanding the calendering processability of $Li(Ni_{0.33}Mn_{0.33}Co_{0.33})O_2$-based cathodes", *Journal of Power Sources*, **488** (2021) 229361 (Elsevier).

[31] A. Ngandjong, T. Lombardo, E. Emiliano, M. Chouchane, A. Shodiev, O. Arcelus, **A.A. Franco***, "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*, **485** (2021) 229320 (Elsevier).

[30] V. Thangavel, A. Mastouri, C. Guéry, M. Morcrette, **A.A. Franco*,** "Understanding the reaction steps involving polysulfides in 1 M LiTFSI in TEGDME:DOL using cyclic voltammetry experiments and modelling", *Batteries & Supercaps*, 4 (1) (2021) 152-162 (Wiley).

[29] R. Andersson, F. Årén, **A.A. Franco**, P. Johansson, "Ion Transport Mechanisms via Time-dependent Local Structure and Dynamics in Highly Concentrated Electrolytes", *Journal of the Electrochemical Society*, **167** (14) (2020) 140537 (Electrochemical Society, IOPScience).

[28] M. Duquesnoy, T. Lombardo, M. Chouchane, E. Primo, **A.A. Franco***, "Data-driven assessment of electrode calendering process by Combining Experimental Results, In Silico Mesostructures Generation and Machine Learning", *Journal of Power Sources*, **480** (2020) 229103 (Elsevier).

[27] A.A. Franco*, J.N. Chotard, E. Loup-Escande, Y. Yin, R. Zhao, A. Rucci, A. Ngandjong, S. Herbulot, B. Beye, J. Ciger, R. Lelong, "Entering the Augmented Era: Immersive and Interactive Virtual Reality for Battery Education and Research", *Batteries & Supercaps,* 3 (11) (2020) 1147-1164. **Also invited cover feature for the journal** (Wiley).[8]

[26] T. Lombardo, J.B. Hoock, E.N. Primo, A.C. Ngandjong, M. Duquesnoy, A.A. Franco*, "Accelerated Optimization Methods for Force-Field Parametrization in Battery Electrode Manufacturing Modeling*" Batteries & Supercaps*, **3** (2020) 721-730 (Wiley).

[25] Z. Su, V. De Andrade, S. Cretu, Y. Yin, M. J. Wojcik, **A.A. Franco***, A. Demortière, "X-ray Nanocomputed Tomography in Zernike Phase Contrast for

Studying 3D Morphology of Li–O_2 Battery Electrode", *ACS Appl. Energy Mater.,* **3** (5) (2020) 4093–4102 (American Chemical Society).

[24] M. Chouchane, E.N. Primo, A.A. Franco*, "Mesoscale Effects in the Extraction of Solid-State Lithium Diffusion Coefficient Value of Battery Active Materials: Physical Insights From 3D Modeling", *The Journal of Physical Chemistry Letters*, **11** (2020) 2775-2780 (American Chemical Society).

[23] E. Loup-Escande, S. Herbulot, A. Ngandjong, R. Lelong, G. Loup, **A.A. Franco***, "Effects of a Virtual Reality Game on Learning Performances and Motivation: Example of Nanoviewer in the Field of Energy Storage", *Psychology and Education*, **57**(2) (2020) 111-116 (Psychology and Education).

[22] S. Shodiev, E.N. Primo, M. Chouchane, T. Lombardo, A.C. Ngandjong, A. Rucci, **A.A. Franco***, "4D-resolved physical model for electrochemical impedance spectroscopy of Li ($Ni_{1-x-y}Mn_xCo_y$)O_2-based cathodes in symmetric cells: consequences in tortuosity calculations", *Journal of Power Sources,* **454** (2020) 227871 (invited, special issue in honor to the Nobel Prize of Chemistry 2019) (Elsevier).

[21] V. Thangavel, O.X. Guerrero, M. Quiroga, A.M. Mikala, A. Rucci, **A.A. Franco*,** "A three-dimensional kinetic Monte Carlo model for simulating the carbon/sulfur mesostructural evolutions of discharging lithium sulfur batteries", *Energy Storage Materials*, **24** (2020) 472-485 (Elsevier).

[20] R. Pinto-Cunha, T. Lombardo, E. Primo, **A.A. Franco***, "Artificial Intelligence Investigation of NMC Cathode Manufacturing Parameters Interdependencies", *Batteries & Supercaps*, **3** (2020) 60-67. **Also invited cover feature for the January 2020 issue of the journal** (Wiley)**.**[9]

[19] A.A. Franco*, M. Alfredsson, D. Brandell, C. Frayret, M. Gaberscek, P. Jankowski, A. Rucci, P. Johansson, "Boosting Rechargeable Batteries from Multiscale Modeling: Myth or Reality?", *Chemical Reviews*, **119**, 7 (2019) 4569 (American Chemical Society).

[18] A. Verma, **AA Franco**, P.P. Mukherjee, "Mechanistic Elucidation of Si Particle Morphology on Electrode Performance", *Journal of The Electrochemical Society*, **166** (15) (2019) A3852-A3860 (Electrochemical Society, IOPScience).

[17] M. Chouchane, A. Rucci, T. Lombardo, A.C. Ngandjong, **A.A. Franco***, "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*, **444** (2019) 227285 (Elsevier).

[16] G. Shukla, A.A. Franco*, "Interphases in Electroactive Suspension Systems: Where Chemistry Meets Mesoscale Physics", *Batteries & Supercaps*, **2**(7) (2019) 579. **Also invited front cover for the July 2019 issue of the journal** (Wiley)**.**[10]

[15] A. Torayev, P. Magusin, C. Grey, C. Merlet, **A.A. Franco***, “Text mining assisted review of the literature on Li-O_2 batteries”, *Journal of Physics: Materials*, **2** (2019) 044004 (IOPScience).

[14] M. Chouchane, A. Rucci, **A.A. Franco***, “A Versatile and Efficient Voxelization-Based Meshing Algorithm of Multiple Phases”, *ACS Omega*, **4** (6) (2019) 11141-11144 (Americal Chemical Society).

[13] A. Rucci, A. C. Ngandjong, E. Primo, M. Maiza, **A.A. Franco***, “Tracking variabilities in the simulation of Lithium Ion Battery electrode fabrication and its impact on electrochemical performance”, *Electrochimica Acta*, **312** (2019) 168-178 (Elsevier).

[12] M. Maiza, Y. Mammeri, D.A. Nguyen, N. Legrand, P. Desprez, **A.A. Franco***, “Evaluating the impact of transport inertia on the electrochemical response of lithium ion battery single particle models”, *Journal of Power Sources*, **423** (2019) 263 (Elsevier).

[11] A. Torayev, P.C.M.M. Magusin, C.P. Grey, C. Merlet, **A.A. Franco***, “Importance of Incorporating Explicit 3D-Resolved Electrode Mesostructures in Li–O_2 Battery Models”, *ACS Applied Energy Materials* **1** (11), 6433-6441 (2018) (American Chemical Society).

[10] Y. Yin, **A.A. Franco***, “Unraveling the Operation Mechanisms of Lithium Sulfur Batteries with Ultramicroporous Carbons”, *ACS Applied Energy Materials* **1** (11), 5816-5821 (2018) (American Chemical Society).

[9] G. Shukla, **A.A. Franco***, “Handling Complexity of Semisolid Redox Flow Battery Operation Principles through Mechanistic Simulations”, *The Journal of Physical Chemistry C* **122** (42), 23867-23877 (2018) (American Chemical Society).

[8] C. Gaya, Y. Yin, A. Torayev, Y Mammeri, **A.A. Franco***, Investigation of bi-porous electrodes for lithium oxygen batteries, *Electrochimica Acta* 279, 118-127 (Elsevier).

[7] A. Torayev, A. Rucci, P. Magusin, A. Demortière, V. De Andrade, C. Grey, C. Merlet, **A.A.Franco***, "Stochasticity of Pores Interconnectivity in Lithium Oxygen Batteries and Its Impact on the Variations in Electrochemical Performance ", *J. Phys. Chem. Letters*, **9** (2018) 791 (American Chemical Society).

[6] A. Ngandjong, A. Rucci, M. Maiza, G. Shukla, J. Vazquez-Arenas, **A.A. Franco***, "Towards A Multiscale Simulation Platform Linking Lithium Ion Battery Electrode Fabrication Process With Performance At The Cell Level", *J. Phys. Chem. Letters*, **8** (23) (2017) 5966 (American Chemical Society).

[5] Y. Yin, A. Torayev, C. Gaya, Y. Mammeri, **A.A. Franco***, "Linking the Performances of Li-O_2 Batteries to Discharge Rate, Electrode and Electrolyte Properties through the Nucleation Mechanism of Li_2O_2", *Journal of Physical Chemistry C*, **121** (36) (2017) 19577 (American Chemical Society).

[4] G. Shukla, D. Del Olmo Diaz, V. Thangavel, **A.A. Franco***, "Self-organization of Electroactive Suspensions in Discharging Slurry Batteries: A Mesoscale Modeling Investigation", *ACS Applied Materials and Interfaces*, **9**(21) (2017) 17882 (American Chemical Society).

[3] J.P. Chehab, **A.A. Franco***, Y. Mammeri, "Boundary control of the number of interfaces for the one-dimensional Allen-Cahn equation", *Discrete and Continuous Dynamical Systems - Series S*, **10** (1) (2017) 87 (American Institute of Mathematical Sciences).

[2] Y. Yin, R. Zhao, Y. Deng, **A.A. Franco***, "Compactness of Lithium Peroxide Formed in Li-O_2 Batteries and Its Link To Charge Transport Mechanism: Insights from Stochastic Simulations", *J. Phys. Chem. Letters*, **8**(3) (2017) 599 (American Chemical Society).

[1] V. Thangavel, K.H. Xue, Y. Mammeri, M.A. Quiroga, C. Guery, A. Mastouri, P. Johansson, M. Morcrette, **A.A. Franco***, "A microstructurally resolved model for Li-S batteries assessing the impact of the cathode design on the discharge performance", *J. Electrochem. Soc.*, **163** (13) (2016) A2817 (Electrochemical Society, IOPScience).

OTHER PUBLICATIONS SINCE THE BEGGINING OF MY IUF POSITION (OCTOBER 2016) (1)

(I underline the MSc. students, PhD students and postdoc I supervised. The articles where I am corresponding author are indicated with « * »))

[1] Vera Koester, **A.A. Franco***, "Innovative Computer Games for Battery Education and Research", Chemistry Views, Wiley-VCH (2020) 10.1002/chemv.202000069 (Wiley).

EDITED BOOKS AND JOURNAL SPECIAL ISSUES BY INVITATION SINCE THE BEGGINING OF MY IUF POSITION (OCTOBER 2016) (2)

[2] **A.A. Franco**, invited Ed. of the special issue of the peer-reviewed journal *Batteries & Supercaps* about Artificial Intelligence Applied to Batteries (2020-20221) (Wiley).

[1] **A.A. Franco**, invited Ed. of the special issue of the peer-reviewed journal *Electrochimica Acta* about the 70th Annual Meeting of the International Society of Electrochemistry (Durban, South Africa, 2019) (Elsevier).

BOOK CHAPTERS BY INVITATION SINCE THE BEGGINING OF MY IUF POSITION (OCTOBER 2016) (3)

(I underline the PhD student I supervised. The chapters where I am corresponding author are indicated with « * »))

[3] J. Yu, **A.A. Franco*,** Mesoscale Modeling and Simulation for Flow Batteries, Fundamentals, book chapter in: "Fundamentals, Characterization Techniques and Modeling of Organic Redox Flow Batteries", Wiley-VCH (2021).

[2] A.A. Franco*, Y. Yin, Monte Carlo Modeling of Interfacial Electrochemistry for Energy Applications, Encyclopedia of Interfacial Chemistry 1st Edition, Elsevier (2017).

[1] A.A. Franco*, Computational Modeling of Lithium-Sulfur Batteries: Myths, Facts and Controversies, in: Li-S Batteries, R. Demir-Cakan (Ed.), World Scientific (Europe) (2017).

PATENT SINCE THE BEGGINING OF MY IUF POSITION (OCTOBER 2016) (1)

[1] A. Torayev, G. Shukla, **A.A. Franco**, Lithium-oxygen battery with electrochemistry-improvement system (2017).

INVITED ORAL COMMUNICATIONS IN CONFERENCES SINCE THE BEGGINING OF MY IUF POSITION (OCTOBER 2016) (50)

The invited lectures in 2022 show/will show results obtained within the period of my IUF Junior Member position.

[50] A.A. Franco, Title: TBA, invited oral presentation at the European Mechanics Society Colloquium - Multiscale mechanics, multiphysics modeling and simulations for energy storage (August 29-31, 2022, Lake of Garda, Italy).

[49] A.A. Franco, Title: TBA, invited oral presentation at the 15th World Congress on Computational Mechanics (WCCM) & 8th Asian-Pacific Congress on Computational Mechanics (APCOM) (July 31-August 5, 2022, Yokohama, Japan).

[48] A.A. Franco, Title: TBA, invited oral presentation at the 11th International Conference on Materials for Advanced Technologies ICMAT 2021 (postponed to 2022 due Covid-19 pandemics, June 19-24, 2022, Singapore).

[47] A.A. Franco, Title: TBA, invited oral presentation, 2022 E-MRS (European Materials Research Society) Spring Meeting & Exhibit (May 30 - June 3, 2022, Strasbourg, France)

[46] A. A. Franco, Title: "Combining machine learning with physical modeling to predict the impact of manufacturing on lithium ion battery electrode properties", invited oral presentation, 14th Pacific Rim Conference on Ceramic and Glass Technology (PACRIM 14) (December 12-17, 2021, Vancouver, Canada).

[45] A.A. Franco, Title: "Digitalization of Lithium–Ion Battery Manufacturing—From Physics-Based Modeling to Artificial Intelligence and Augmented Reality", invited oral presentation, 2021 Materials Research Society Fall Meeting (November 28 – December 8, 2021, Boston, USA).

[44] A.A. Franco, J.N. Chotard, E. Loup-Escande, "Effets de la réalité virtuelle et de la réalité mixte sur l'apprentissage, la motivation et la collaboration d'étudiants dans le domaine de l'énergie", invited keynote, Journées Scientifiques autour des Environments de Simulation Numérique et leurs Apports à la Pédagogie Universitaire, Ministère de l'Enseignement Supérieur, de la Recherche et de l'Innovation (December 3, Lyon, France).

[43] A.A. Franco, Title: "Digital Twins of Battery Manufacturing Processes", invited oral presentation, Workshop "30 years of port Hamiltonian systems and 60th anniversary of Bernhard Maschke" (October 15, 2021, Berlin, Germany, hybrid)

[42] A.A. Franco, Title: "Digital Twins of Battery Manufacturing Processes", invited oral presentation, Workshop on Molecular Simulations and Engineering - MolSimEng 2021 (September 24, 2021, Milano, Italy, hybrid).

[41] A.A. Franco, Title: " Digitalization of battery manufacturing: entering the augmented era", invited oral presentation, Foro Teconologias para el Almacenamiento de Energia 2021 (September 8, 2021, Mexico city, Mexico, online).

[40] A.A. Franco, Title: "Digitalization of Battery Manufacturing through Artificial Intelligence and Multiscale Modeling", invited oral presentation at the virtual MRS-Singapore international conference on "Materials for Humanity (MH21)" (online, July 6-9, 2021).

[39] A.A. Franco, Title: "Digital Twins for Accelerated Battery Manufacturing Optimization", invited oral presentation at the "Emerging 2021" DOC-FAM School - Marie Sklodowska-Curie COFUND (online, June 30, 2021).

[38] A.A. Franco, Title: TBA, invited lecture at the Graphene Flagship's School (postponed due to Covid-19 pandemics, dates to be confirmed).

[37] A.A. Franco, Title: "Artificial Intelligence for Battery Manufacturing Data Mining and Analysis", invited lecture at the DEFACTO Workshop on Digital Approaches In Battery Development" (online, June 8, 2021).

[36] A.A. Franco, Title: "Battery Processes: Modeling at the Coarse-Grained and Continuum Levels", invited keynote lecture at the eSSENCE EMMC e-meeting on "Multiscale Modeling of Materials and Molecules - Physics-based and Data-driven" (online, June 7, 2021).

[35] **A.A. Franco**, Title: "ARTISTIC: Digital Twin of Battery Manufacturing", invited keynote lecture at the German Science Foundation (April 23, 2021, online because of Covid-19 pandemics).

[34] **A.A. Franco**, Title: “Combining Machine Learning and Multiscale Modeling for Accelerated Battery Manufacturing Optimization”, invited oral presentation, Materials Research Society Spring Meeting and Exhibit 2021 (MRS 2021) (April 18-23, 2021, Seattle, USA, online because of Covid-19 pandemics).

[33] **A.A. Franco,** Title: "ARTISTIC: Digital Twin of Lithium Ion Battery Manufacturing", invited lecture at the National Renewable Energy Laboratory (NREL) Machine Learning and Batteries Workshop (March 23, 2021, USA, online because of Covid-19 pandemics).

[32] **A.A. Franco**, Title: “Digital Twin for the Acceleration of the Optimization of Lithium Ion Battery Manufacturing”, invited oral presentation, Electronic Materials and Applications (EMA 2021) (January 19-22, 2021, originally planned in Orlando, USA, online because of Covid-19 pandemics).

[31] **A.A. Franco,** Title: **“**At the Crossroads of Multiscale Modeling, Artificial Intelligence and Virtual Reality in Battery Research”, SACI Young Chemists Symposium, University of Johannesburg, South Africa, November 18, 2020 (Johannesburg, South Africa, online because of Covid-19 pandemics).

[30] **A.A. Franco,** Title: “At the crossroads between battery multiscale modeling, artificial intelligence and virtual reality”, invited oral presentation in the 2nd Virtual *Batteries & Supercaps* journal Symposium (November 12th, 2020, online).**Erreur ! Signet non défini.**

[28-29] **A.A. Franco**, Title: “The ERC ARTISTIC Project: Digital Twin of Battery Manufacturing”, invited lectures to stakeholders within the European Science is Wonderful! 2020 Festival within the Research and Innovation Days, (September 22-24, 2020, online because of Covid-19 pandemics, Europe).

[27] **A.A. Franco**, Title: “Predicting the impact of manufacturing process on electrode texture and battery performance: the ARTISTIC project”, invited oral presentation, IBA 2020 (International Battery Association) meeting (initially planned for March 8-13, 2020 in Bled, Slovenia, but talk postponed for 2022 due to Covid-19 pandemics).

[26] **A.A. Franco**, Title: “Digital Twin of the Manufacturing Process of Rechargeable Batteries: the ARTISTIC Project”, invited oral presentation, 71st Annual Meeting of the International Society of Electrochemistry (September 2, 2020, Belgrade, Serbia, online due to Covid-19 pandemics).

[25] Marc Duquesnoy (representing **A.A. Franco**), “Artificial Intelligence Investigation of NMC Cathode Manufacturing Parameters Interdependencies”, invited oral presentation, Machine Learning for Battery Research Workshop (March 13, 2020, Oxford, United Kingdom).

[24] **A.A. Franco**, "Predicting the influence of manufacturing parameters on lithium ion battery performance: the ARTISTIC project", Keynote, the (2020) TMS 149th Annual Meeting and Exhibition (February 23-27, 2020, San Diego, USA).

[23] **A.A. Franco**, Title: "Multiscale Modeling and Artificial Intelligence as Guidelines of Battery Manufacturing", invited oral presentation, Workshop on Multiscale Modeling for Soft Matter and Materials for Energy (February 20, 2020, Torino, Italy).

[22] **A.A. Franco**, "Artificial Intelligence: Entering into the Augmented Era in Battery R&D", invited oral presentation, Cérémonie de Remise de Prix de la Société Chimique de France, Inter-division Energie (November 28, 2019, Amiens, France).

[21] Alain Ngandjong (in representation of **A.A. Franco**), "The ARTISTIC project: mulitscale simulation platform of battery manufacturing", EIG Concert Japan Symposium (November 7, 2019, Sapporo, Japan).

[20] **A.A. Franco**, "Accelerating Optimization of Lithium Ion Battery Manufacturing through Multiscale Simulations", Keynote, the 236th Meeting of the Electrochemical Society (ECS) (October 13-17, 2019, Atlanta, USA).

[19] **A.A. Franco**, "Investigating battery electrode manufacturing through multiscale simulations", invited oral presentation in 2019 European Congress and Exhibition on Advanced Materials and Processes (EUROMAT), Symposium E3: Batteries: From Materials to Cells (September 1-5, 2019, Stockholm, Sweden).

[18] Alain Ngandjong (representing **A.A. Franco**), "Predicting interfaces in battery electrodes from their fabrication process parameters", Keynote at the 3rd International Conference on Applied Surface Science (ICASS 2019) (June 18, 2019, Pisa, Italy).

[17] **A.A. Franco**, "Multiscale Modeling approaches of Rechargeable Batteries", invited oral presentation at the E-CAM Workshop "Electrochemical energy storage: Theory meets industry" (June 12-14, 2019, Paris, France).

[16] **A.A. Franco**, "Multiscale Modeling of Lithium Ion Battery Manufacturing: The ARTISTIC Project", Keynote, Modval 2019 – 16th Symposium on Modeling and Experimental Validation of Electrochemical Energy Technologies (March 12-13, 2019, Braunschweig, Germany).

[15] **A.A. Franco, "**ARTISTIC Project: modeling-driven prediction of optimal rechargeable battery manufacturing parameters", invited oral presentation at the 43rd International Conference and Exposition on Advanced Ceramics and Composites (ICACC 2019) (January 27- February 1, 2019, Daytona Beach, Florida, USA).

[14] **A.A. Franco**, "A Flexible Multiscale Computational Platform for the Simulation of the Battery Fabrication Process", invited oral presentation at the 2018 Materials Research Society Fall Meeting (November 25-30, 2018, Boston, USA).

[13] **A.A. Franco**, "From the self-organization of composite battery materials to their performance in applications: predictive multiscale approaches", invited oral

presentation, 55th Society of Engineering Science (SES) Annual Technical Meeting (October 10-12, 2018, Madrid, Spain).

[12] A.A. Franco, “Multiscale modelling as an optimization tool of the fabrication process and performance of porous electrodes in batteries”, Keynote (sponsored by TOTAL), French Interpore Conference on Porous Media (October 8-10, 2018, Nantes, France).

[11] A.A. Franco, “A Multiscale Simulation Platform of Rechargeable Batteries Linking Fabrication Parameters with Performance at the Cell Level”, invited oral presentation at the 12th International Conference on Ceramic Materials and Components for Energy and Environmental Applications (July 22-27, 2018, Singapore).

[10] A.A. Franco, “ERC Project ARTISTIC: A Computational Platform for the Optimization of Battery Electrode Fabrication Processes”, invited oral presentation, ALISTORE ERI (June 12, 2018, Bohinj, Slovenia).

[9] A.A. Franco, “White and Black Box Computational Approaches for the Prediction of Better Batteries”, invited oral presentation, 6èmes journées AMARENA (May 4, 2018, Amiens, France).

[8] A.A. Franco, "Multiparadigm Computational Approaches to Assess and Optimize Rechargeable Battery Electrodes", invited oral presentation at the (2018) TMS 147th Annual Meeting and Exhibition (March 11-15, 2018, Phoenix, USA).

[7] A.A. Franco, "Combining Multiscale Computational Modeling and Interactive Virtual Reality for Teaching Electrochemical Energy Storage", invited oral presentation at the 68th Meeting of the International Society of Electrochemistry (ISE) (August 27-September 1, 2017, Providence, USA).

[6] A.A. Franco, “Fostering technological breakthroughs in rechargeable batteries through multiscale computational modeling”, invited oral presentation at the XXVI International Materials Research Congress (IMRC 2017) (August 20-26, 2017, Cancun, Mexico).

[5] A.A. Franco, "Catalyzing Batteries Innovation Through Multiscale Computational Modeling", invited lecture at the Heraeus Seminar (August 23-27, 2017, Bad Honnef, Germany).

[4] A.A. Franco, "Dealing with one gogol of batteries: multiscale modeling to the rescue of design and optimization", invited oral presentation in "Power our Future 2017 – The 3rd International Forum on Progress and Trends in Battery and Capacitor Technologies" (July 2-5, 2017, Vitoria-Gasteiz, Spain).

[3] A.A. Franco, "Multiscale computational modeling for the engineering of rechargeable batteries", invited oral presentation in the 2017 Materials Research Society (MRS) Spring Meeting, (April 17-21, 2017, Phoenix, USA).

[2] A.A. Franco, "Mesostructure-performance relationships in rechargeable batteries: challenging the dogma with multiscale computations and immersive

visualization", invited oral presentation in the 20th Topical Meeting of the International Society of Electrochemistry (ISE) (March 19-22, 2017, Buenos Aires, Argentina).

[1] A.A. Franco, "Multiparadigm and multiscale computational modeling of rechargeable batteries: from theory to practice", invited keynote lecture in the MicroEchems/Energy Storage Discussions 2016 (November 6-9, 2016, Hotel Mision La Muralla, Amealco de Bonfil, Mexico).

INVITED SEMINAR AT UNIVERSITIES AND INDUSTRY SINCE THE BEGGINING OF MY IUF POSITION (OCTOBER 2016) (45)

[21] A.A. Franco, Title: "Digitalization Approaches of Battery Manufacturing Processes", invited seminar at Universities of Bochum, Dortmund, and Duisburg-Essen, Germany (online, November 5, 2021).

[20] A.A. Franco, Title: "Digitalization of Battery Manufacturing through Artificial Intelligence and Multiscale Modeling", invited seminar at the Max-Planck-Institut fuer Eisenforschung, Düsseldorf, Germany (online, June 1, 2021).

[19] A.A. Franco, Title: “Digital Twin of Battery Manufacturing”, invited seminar at Chalmers University of Technology, Chalmers Advanced Materials Science Tandem Seminars (online because of Covid-19 pandemics, April 27, 2021).

[18] A.A. Franco, Title “A Digital Twin of Lithium Ion Battery Manufacturing: ARTISTIC", invited seminar at Karlsruhe Institute of Technology, Karlsruhe, Germany (online because of Covid-19 pandemics, May 26, 2021).

[17] A.A. Franco, “Battery Multiscale Modeling Activities at LRCS”, invited seminar at TOTAL Company, online because of Covid-19 pandemics, May 22, 2020.

[16] A.A. Franco, TBA, invited seminar at Uppsala University, Uppsala, Sweden, initially planned for May, 2020, but postponed due to the Covid-19 pandemics.

[15] A.A. Franco, “Manufacturing of Lithium Ion Batteries with the Support of Artificial Intelligence and Multiscale Modeling”, invited seminar at University of California San Diego, San Diego/La Jolla, USA, February 24, 2020.

[14] A.A. Franco, “Manufacturing of Lithium Ion Batteries with the Support of Artificial Intelligence and Multiscale Modeling”, invited seminar at Université de Montréal, Montréal, Canada, February 5, 2020.

[13] A.A. Franco, Title: “Manufacturing of Lithium Ion Batteries with the Support of Multiscale Modeling and Artificial Intelligence”, invited seminar at Oak Ridge National Lab, Oak Ridge, USA, October 18, 2019.

[12] A.A. Franco, “Multiscale modeling of manufacturing and performance of rechargeable batteries”, invited seminar at ENS Lyon, Lyon, France, September 19, 2019 (postponed).

[11] **A.A. Franco**, "Manufacturing lithium ion batteries with the support of multiscale simulations: the ARTISTIC project", invited seminar at CIC Energigune, Vitoria-Gasteiz, Spain, June 21, 2019.

[10] **A.A. Franco**, "ARTISTIC Project: multiscale modeling of lithium ion battery manufacturing", invited seminar at CIDETEC Energy Storage, San Sebastian, Spain, June 18, 2019.

[9] **A.A. Franco**, "ARTISTIC Project: multiscale modeling of lithium ion battery manufacturing", invited seminar at Chalmers University of Technology, Gothenburg, Sweden, May 8, 2019.

[8] **A.A. Franco**, Title: "Catalyzing Innovation in Rechargeable Batteries R&D Through Multiscale Computations", invited seminar at the University of Southampton, Southampton, UK, June 9, 2017.

[7] **A.A. Franco**, Title: "Assessing and Optimizing Rechargeable Batteries through Multiscale Computational Modeling", invited seminar at the Laboratoire d'Electrochimie et de Physicochimie des Materiaux et des Interfaces (LEPMI), Chambery, France, May 11, 2017.

[6] **A.A. Franco**, Title: "Mesostructure-Performance Relationships in Batteries and Fuel Cells: A Computational Multiscale Modeling Perspective", invited seminar at the Universidad Nacional del Sur (UNS), Bahia Blanca, Argentina, March 31, 2017.

[5] **A.A. Franco**, Title: "A Journey Into The Electrochemical Devices World From A Multiscale Modeling Perspective", invited seminar at the Instituto de Fisica de Rosario, Rosario, Argentina, March 23, 2017.

[4] **A.A. Franco**, Title: "Multiscale Simulation Approaches for the Electrochemical Conversion and Storage of Energy", invited seminar at the Laboratoire Amiénois de Mathématique Fondamentale et Appliquée (LAMFA) (January 30, 2017, Amiens, France).

[3] **A.A. Franco**, Title: "Mesostructure-performance relationships in batteries and fuel cells: challenging the dogma with multiscale computations and immersive visualization", invited seminar at the National Institute of Chemistry Slovenia (NIC), Ljubljana, Slovenia, December 14, 2016.

[2] **A.A. Franco**, Title: "Assessing the World Energy Equation with Mathematical Modeling", invited seminar at the Faculty of Chemistry and Chemical Technology at the University of Ljubljana, Ljubljana, Slovenia, December 14, 2016.

[1] **A.A. Franco**, Title: "Electrochemical Energy Devices from a Multiscale Modeling Perspective", invited seminar at the Universidad Autonoma Metropolitana-Iztapalapa, Mexico, November 10, 2016.

ORAL COMMUNICATION IN THEMATIC DAYS SINCE THE BEGGINING OF MY IUF POSITION (OCTOBER 2016) (10)

[6] **A.A. Franco**, "Modélisation: du matériau au système électrochimique", Atelier A2U/Energie, online because of Covid-19 pandemics, February 5, 2021.

[5] **A.A. Franco**, "White Paper on Artificial Intelligence Applied to Rechargeable Batteries", ALISTORE-European Research Institute, online because of Covid-19 pandemics, December 8, 2020.

[4] **A.A. Franco**, "Application of Artificial Intelligence in Battery Research", ALISTORE-ERI European Network of Research Excellence, CSIC, Barcelona, Spain, December 10, 2019.

[3] **A.A. Franco**, **"Theory vs. Experiment: The Eternal Debate?",** Matinée "Modélisation", Institut de Chimie de Picardie (February 8, 2019, Amiens, France).

[2] **A.A. Franco**, "Multiscale modeling of discharge and charge processes in lithium oxygen batteries", ALISTORE-ERI European Network of Research Excellence, Bath, UK, June 7, 2017.

[1] **A.A. Franco**, "Using Virtual Reality for Teaching and Data Analysis in the field of Energy storage and Conversion", ALISTORE-ERI European Network of Research Excellence, Warsaw University of Technology, Warsaw, Poland, December 13, 2016.

+ 4 oral presentations about prospective energy storage research topics in the LRCS Scientific Days (July every year, -not in 2020 because of Covid-19 pandemics).

INVITED PRESENTATIONS TO THE GENERAL PUBLIC SINCE THE BEGGINING OF MY IUF POSITION (OCTOBER 2016) (23)

[21-23] **A.A. Franco**, "Entering the Augmented Era: Virtual Reality for Battery Education and Research". Three oral presentations and battery virtual reality serious games demonstrations at the "Atelier d'Innovation Pédagogique dans la Médecine" (Workshop on Pedagogy Innovation for Medical Training) at SimuSanté (June 3, 2021, Amiens, France).

[11-20] **A.A. Franco**, several oral presentations (webinars) within the European Science is Wonderful! 2020 Festival within the Research and Innovation Days, following the selection of Prof. Franco's ERC Project "ARTISTIC" to participate in this event (September 22-24, 2020, online because of Covid-19 pandemics, Europe).

[10] **A.A. Franco**, “Faire des meilleures à l’aide de l’intelligence artificielle”, Festival Pint of Science (September 7, 2020, online through YouTube because of Covid-19 pandemics, France).

[9] **A.A. Franco**, “L’Energie: Dompter Cette Force Mystèrieuse à l’aide des Batteries”, Festival Pint of Science (May 20, 2019, Boulogne-Sur-Mer, France)

[8] **A.A. Franco,** “ARTISTIC: Un Nouveau Paradigme dans l’Ingénierie des Batteries”, *Ceremonie de Mise en Lumière* of my ERC Project ARTISTIC, organized in my honour by the CNRS and the UPJV (October 23, 2018, Amiens, France).

[7] **A.A. Franco**, “L’Energie: Dompter Cette Force Mystèrieuse à l’aide des Batteries”, Collège Guy Mareschal (October 18, 2018, Amiens, France).

[6] **A.A. Franco**, “L’Energie: Dompter Cette Force Mystèrieuse à l’aide des Batteries”, Festival Pint of Science (May 16, 2018, Beauvais, France).

[5] **A.A. Franco**, “Projet ERC ARTISTIC : Une Usine Virtuelle des Batteries Lithium-Ion”, *Ceremonie des Créateurs d’Avenir 2018* (February 22, 2018, Amiens, France).

[4] **A.A. Franco**, “L’Intelligence Artificielle et la Réalité Virtuelle comme Outils de Découverte des Batteries du Futur », Conférence Flash Tout Publique Invitée, UFR des Sciences, Université de Picardie Jules Verne (February 19, 2018, Amiens, France).

[3] **A.A. Franco**, “Que La Force Soit Avec Vous“, Association ASTEP (November 9, 2017, Amiens, France).

[2] **A.A. Franco**, "Que La Force Soit Avec Vous", Festival Pint of Science (May 17, 2017, Amiens, France).

[1] **A.A. Franco**,"La modélisation mathématique comme vecteur d'innovation dans le stockage de l'énergie", invited lecture at the ARI Picardie (Picardie Regional Agency for Innovation) within the event "*Témoignages sur la résolution de problèmes industriels par les Mathématiques Appliquées*" (February 10, 2017, Amiens, France).

CONTRIBUTED ORAL COMMUNICATION IN CONFERENCES SINCE THE BEGGINING OF MY IUF POSITION (OCTOBER 2016) (47)

(the presenter is underlined)

[37-47] Several webinar presentations by **A.A. Franco**’s team and himself in the 2nd Battery Manufacturing Days – ARTISTIC Project Webinar Series, organized by A.A. Franco (June 21-25, 2021) (see here).

[28-36] Several webinar presentations by **A.A. Franco**'s team and himself in the 1st Battery Manufacturing Days – ARTISTIC Project Webinar Series, organized by **A.A. Franco** (June 29-July 3, 2020) (see here).

[27] T. Lombardo, R. Pinto Cunha, E. Primo, **A. A. Franco**, "Artificial Intelligence Investigation of NMC Cathode Manufacturing Parameters Interdependencies", oral presentation at the 237th Meeting of the Electrochemical Society (ECS) (May 10-14, 2020, Montréal, Canada, cancelled by the organizers due to the Covid-19 pandemics).

[26] M. Chouchane, A. Rucci, **A.A. Franco, "**Explicit Consideration of Carbon Binder Domains in 3D-Resolved Model to Optimize Fabrication Process", oral presentation at the 2019 Materials Research Society Meeting & Exhibit (MRS) (December 1-6, 2019, Boston, USA).

[25] E. Primo, T. Lombardo, A. C. Ngandjong, M. Touzin, **A. A. Franco**, "Calendering process for thick and thin NMC cathodes: understanding the process parameters effect on the electrode structure and performance", oral presentation at the 70th Annual Meeting of the ISE, Durban, South Africa (August 8, 2019).

[24] A. Ngandjong, E. Primo, T. Lombardo, M. Chouchane, Z. Su, **A. A. Franco**, "Coarse Grained Molecular Simulation of Lithium Ion Electrodes Fabrication: Linking Computations with Experiments", oral presentation at the 70th Annual Meeting of the ISE, Durban, South Africa (August 8, 2019).

[23] A. A. Franco, A. Ngandjong, A. Rucci, E. Primo, A. Shodiyev, M. Chouchane, T. Lombardo, "ARTISTIC: A Predictive Multiscale Simulation Platform of the Fabrication Process of Lithium Ion Batteries", oral presentation at the 70th Annual Meeting of the ISE, Durban, South Africa (August 5, 2019).

[22] H. El-Bousiydy, P. Johansson, **A. A. Franco**, "Digging the scientific literature about NMC active materials using Artificial Intelligence", oral presentation at the 2019 IUPAC World Chemistry Congress, Paris, France (July 8, 2019).

[21] T. Lombardo, A. Ngandjong, E. Primo, J.-B. Hoock, M. Couchane, A. Rucci, A. Shodiyev, **A. A. Franco**, "Human vs. Artificial Intelligence-driven Simulation of the Fabrication Process of Lithium Ion Battery Electrodes", oral presentation at the 2019 IUPAC World Chemistry Congress, Paris, France (July 8, 2019).

[20] A. Ngandjong, A. Rucci, E. Primo, T. Lombardo, M. Chouchane, Z. Su, A. Shodiev, **A. A. Franco**, "Multi-Paradigm Modeling Approach to Simulate the Link between the Fabrication Process and the Performance of Li-Ion Batteries", oral presentation at the 235th Electrochemical Society (ECS) Meeting, Dallas, USA (May 30, 2019).

[19] T. Lombardo, J. B. Hoock, A. Ngandjong, **A. A. Franco**, "Deep Neural Network to guide the Coarse-Grained Molecular Dynamics Parameterization", oral

presentation at the Young Researcher's Workshop on Machine Learning for Materials Science 2019, Helsinki, Finland (May 10, 2019).

[18] **A.A. Franco**, A. Ngandjong, A. Rucci, E. Primo, "Multiscale Simulation of the Fabrication Process of Lithium Ion Battery Electrode", oral presentation at the Americas International Meeting on Electrochemistry and Solid-State Science, Electrochemical Society (September 30-October 4, 2018, Cancun, Mexico).

[17] **A.A. Franco**, A. Torayev, Y. Yin, G. Shukla, M. Maiza, V. Thangavel, A. Rucci, A. Ngandjong, "A Flexible Multiscale Simulation Platform of Rechargeable Batteries", oral presentation at the Americas International Meeting on Electrochemistry and Solid-State Science, Electrochemical Society (September 30-October 4, 2018, Cancun, Mexico).

[16] C. Gaya, Y. Yin, A. Torayev, D. Larcher, C. Surcin, M. Courty, Y. Mammeri, B. Fleutot, M. Morcrette, **A. A. Franco** "Investigation of bi-porous electrodes for lithium oxygen batteries: from modeling to experimental electrodes development", oral presentation at the E-MRS Conference (September 17-20, 2018, Warsaw, Poland).

[15] A. Torayev, P. Magusin, C.P. Grey, C. Merlet, **A.A. Franco**, Role of Pore Mesostructure and Li2O2 growth mechanism on Li-O_2 Battery Performance, oral presentation in the 69th Annual ISE Meeting, September 2-7, 2018, Bologna, Italy.

[14] **A.A. Franco**, A. Ngandjong, A. Rucci, M. Maiza, G. Shukla, E. Primo, Multiscale model predicting the link between electrode fabrication parameters and battery performance, oral presentation in the 69th Annual ISE Meeting, September 2-7, 2018, Bologna, Italy.

[13] **A.A. Franco**, "Impact de la Réalité Virtuelle dans la Transmission de Connaissances en Chimie", Colloque La Transmission, organized by the Institut Universitaire de France (May 28, 2018, Strasbourg, France).

[12] V. Thangavel, A. Mastouri, S. Drvarič Talian, A. Vizintin, R. Dominko, C. Guery, Mathieu Morcrette, **A.A. Franco**, Numerical Models to Deduce the Electrochemistry of Solvated Polysulfides and Li_2S Precipitation Mechanisms, oral presentation in the Li-SM^3, Chicago, United States of America (April 26th 2018).

[11] G. Shukla, O. X. Guerrero-Gutierrez, M. H., Y. Mammeri, A. Salsac, **A. A. Franco**, A Kinetic Monte Carlo Framework for a Discrete Multiphysics description of Semi-Solid Redox Flow Batteries. 15th Symposium on Modeling and Experimental Validation of Electrochemical Energy Devices (ModVal 2018), Aarau, Switzerland. April 12-13, 2018.

[10] C. Gaya, A. Torayev, Y. Yin, C. Surcin, D. Larcher, B. Fleutot, M. Morcrette, **A. A. Franco**, "Impacts of the Electrode Fabrication Process on the Performances of Lithium-Oxygen Batteries", oral presentation at the 68th annual meeting of the International Society of Electrochemistry (August 27 - September 1, 2017, Providence, USA).

[9] M. Maiza, Y. Mammeri, N. Legrand, D. Nguyen, P. Desprez, **A. A. Franco**, "Beyond Newman Model: Microstructurally-resolved Simulations of the Dynamic Responses of Lithium Ion Batteries upon Cycling", oral presentation at the 68th annual meeting of the International Society of Electrochemistry (August 27 - September 1, 2017, Providence, USA).

[8] A. Torayev, P. Magusin, C.P. Grey, C. Merlet, **A.A. Franco**, Importance of Pores Interconnectivity in Cathodes for Li-Oxygen Batteries, the XXVI International Materials Research Congress (August 20-25, 2017, Cancun, México).

[7] S. Malifarge, **A.A. Franco**, B. Delobel, C. Delacourt, “Influence of the Design of High-Energy-Density Graphite Negative Electrodes on the Electrochemical Performance”, oral presentation at the 232nd Meeting of the electrochemical Society, National Harbor, MD, USA, Oct 1-5, 2017.

[6] G. Shukla, D. del Olmo Diaz, V. Thangavel, **A. A. Franco**, "Modeling slurry electrodes for redox flow batteries using kinetic Monte Carlo", oral presentation at the 231st ECS Meeting (New Orleans, USA, May 28 – June 1, 2017).

[5] Y. Yin, C. Gaya, A. Torayev, V. Thangavel, D. Larcher, **A.A. Franco**, "Multi-Scale Modeling and Experimental Characterization of Charge Process of Li-O_2 Batteries: Impacts of Particle Size and Cycling History", oral presentation at the 231st ECS Meeting (New Orleans, USA, May 28 – June 1, 2017).

[4] Y. Yin, R. Zhao, Y. Deng, **A.A. Franco**, "Meso-Scale Model of Li_2O_2 Formation in Li-O_2Batteries: Compactness of Thin Film and Its Link to Charge Transport Mechanism", oral presentation at the 231st ECS Meeting (New Orleans, USA, May 28 – June 1, 2017).

[3] V. Thangavel, M. Morcrette, **A.A. Franco**, Mathematical and Stochastic modelling of Lithium Sulfur batteries, 5th AMARENA days, Amiens, France (May 15th 2017).

[2] V. Thangavel, M. Quiroga, M. Morcrette, **A.A. Franco**, "Microstructurally resolved multiscale models to study the effects of C/S cathode microstructures used in Lithium Sulfur Batteries", oral presentation in the "Lithium Sulfur Batteries: Mechanisms, Modelling and Materials" conference (London, UK, April 27, 2017).

[1] Y. Yin, A. Torayev, C. Gaya, D. Larcher, **A.A. Franco**, "Understanding the role of Li_2O_2 particle size on Li-O2 battery charge process", oral presentation at the 20th Topical Meeting of the International Society of Electrochemistry (ISE) (Buenos Aires, Argentina, March 19-22, 2017).

ENCADREMENT DOCTORAL (Direction de thèses) :

ALREADY DEFENDED PHD THESIS SINCE THE BEGGINING OF MY IUF POSITION (OCTOBER 2016) (12)
Teo Lombardo (2018-2022) Topic: Modeling of the fabrication process of Lithium Ion Battery electrodes – Discrete Particle Approach. Supervision rate: 100%. Co-supervisor: N/A. Publications: **12** (4 x *Batteries & Supercaps*, 5 x *J. Power Sources*, 1 *Chemical Reviews*, 1 *Energy Storage Materials*, 1 submitted). **Second Prize "Young Scientists Artificial Intelligence Workshop" University of Lille, France (2019).**
Mehdi Chouchane (2018-2021) Topic: 3D-resolved modeling of Lithium Ion Battery cycling. Supervision rate: 100%. Co-supervisor: N/A. Publications: **12** (5 x *J. Power Sources*, 1 *ACS Omega*, 1 *J. Phys. Chem. Lett.*, 2 x *Batteries & Supercaps*, 3 submitted). **Current position:** becoming postdoc at **University of Chicago**, USA.
Zeliang Su (2017-2021) Topic: 4D characterization of electrochemical processes in Li-O_2 and Li-S batteries. Supervision rate: 30%. Co-supervisor: Dr. Arnaud Demortiere (LRCS). Publications: **4** (*ACS Applied Energy Materials, Advanced Energy Materials,* 2 submitted). **Current position:** becoming postdoc at **Argonne National Laboratory**, USA.

Abbos Shodiev (2018-2021)

Topic: Modeling of electrolyte filling process of Lithium Ion Battery electrodes.

Supervision rate: 100%.

Co-supervisor: N/A.

Publications: **6** (3 x *J. Power Sources,* 1 *Energy Storage Materials*, 2 submitted).

Current position: research engineer at **SAFT batteries**.

Rasmus Andersson (2016-2020)

Research topic: transport modeling in highly concentrated electrolytes.

Supervision rate: 30%.

Co-supervisor: Patrik Johansson (Chalmers University of Technology, Sweden).

Publications: 3 (1 *Batteries & Supercaps*, 1 *J. Electrochem. Soc.*, 1 *J. Comp. Chem.*).

Current position: Co-founder of the startup **Compular** and technical developer.

Garima Shukla (2015-2019)

Research topic: multiscale modeling of redox flow batteries.

Supervision rate: 70%.

Co-supervisor: Anne-Virginie Salsac (UTC).

Publications: 4 (*ACS Applied Materials and Interfaces*, *J. Phys. Chem. C*, *J. Phys. Chem. Lett., Batteries & Supercaps*).

Current position: founding a start-up about science communication.

Vigneshwaran Thangavel (2015-2019)

Research topic: Multiscale modeling of lithium sulfur batteries.

Supervision rate: 70%.

Co-supervisor: Mathieu Morcrette (LRCS)

Publications: **5** (*J. Electrochem. Soc.*, *J. Phys. Chem. Lett.*, *ACS Applied Materials and Interfaces, Energy Storage Materials, Batteries & Supercaps*).

Current position: postdoc in **Chalmers University of Technology (Sweden).**

Amangeldi Torayev (2016-2019)

Research topic: modeling and experimental characterization of Lithium Air Batteries

Supervision rate: 50%.

Co-supervisor: Clare Grey (University of Cambridge)

Publications: **6** (2 x *J. Phys. Chem. Lett., J. Phys. Chem. C, Electrochim. Acta, ACS Applied Energy Mat., J. Phys.: Mat.*).

Current position: Postdoctoral researcher at **Oxford University (UK).**

Caroline Gaya (2016-2019)

Research topic: design, characterization, and modeling of lithium-air batteries for aircraft

applications (in collaboration with IRT Saint Exupery).

Supervision rate: 100%

Publications: **3** (*J. Phys. Chem. Lett.*, *J. Phys. Chem. C*, *Electrochim. Acta*) + **1** submitted.

Finalist of the competition Ma thèse en 180 Secondes of the Région Hauts de France

Current position: permanent research engineer at **Zodiac Aerospace/Safran.**

Mariem Maiza (2015-2018)

Research topic: multiphysics modeling of lithium-ion batteries (in collaboration with

SAFT Batteries).

Supervision rate: 50%.

Co-supervisors: Philippe Desprez, Nathalie Legrand, Dihn Nguyen (SAFT Batteries)

Publications: **3** (*J. Phys. Chem. Lett., J. Power Sources, Electrochim. Acta*).

Current position: Postdoctoral researcher at **Groupe Renault.**

Yinghui Yin (2014-2017)

Research topic: Coupled Modeling/Experimental Investigation of Lithium-Air Batteries.

Supervision rate: 50%.

Co-supervisor: Dominique Larcher (UPJV)

Publications: **5** (*J. Electrochem. Soc.*, 2 x *J. Phys. Chem. Lett.*, *J. Phys. Chem. C*, *Electrochim. Acta*)

Recipient of the Région Hauts de France Prize for the best PhD thesis

Recipient of the Université de Picardie Jules Verne Prize for the best PhD thesis

Current position: Permanent research engineer at **SAFT Batteries.**

Simon Malifarge (2014-2017)

Research topic: modeling of high energy density negative electrodes in lithium-ion batteries (in collaboration with Renault).

Supervision rate: 30%

Co-supervisor: Charles Delacourt.(LRCS)

Publications: **3** (3 x *J. Electrochem. Soc.*)

Current position: research engineer at **Groupe Renault.**

ONGOING PHD THESIS STARTED WITHIN THE PERIOD OF MY IUF POSITION (8)

Mohammed El-Abdali (2021-2024)

Topic: Physics-based modeling of the manufacturing process of solid-state batteries.

Supervision rate: 50%.

Co-supervisor: Dr. Vincent Seznec (LRCS).

Publications: N/A.

Antonio Carnevali (2021-2024)

Topic: Machine learning-based discovery of materials for batteries applied to Internet of Things.

Supervision rate: 50%.

Co-supervisor: Dr. Rosa Palacin (CSIC, Barcelona, Spain).

Publications: N/A.

Chaoyue Liu (2020-2023)

Topic: Modeling-based Optimization of Battery Manufacturing.

Supervision rate: 100%.

Co-supervisor: N/A.

Publications: **1** (1 *J. Power Sources*).

Jiahui Xu (2020-2023)

Topic: Multi-fidelity Modeling of Battery Manufacturing.

Supervision rate: 70%.

Co-supervisor: Dr. Arnaud Demortière (LRCS).

Publications: **1** (1 submitted).

Jia Yu (2020-2023)

Topic: Modeling of Organic Redox Flow Batteries.

Supervision rate: 100%.

Co-supervisor: N/A.

Publications: **2** (2 submitted).

Marc Duquesnoy (2019-2023)

Topic: Application of Machine Learning Models to Assess Battery Big Data

Supervision rate: 50% (he worked under my supervision as Big Data engineer in 2019-2020 at 100% of supervision by myself and he started his PhD thesis in October 2020 funded by ALISTORE-ERI).

Co-supervisor: Since October 2020, Elixabete Ayerbe (CIDETEC Energy Storage, San Sebastian, Spain) and UMICORE company.

Publications: **9** (3 x *Batteries & Supercaps*, 2 x *Journal of Power Sources*, 1 *ACS Energy Letters*, 1 *Energy & AI*, 1 *Chemical Reviews*, 1 submitted).

Fanny Lambert (2019-2022)

Topic: Multiscale Modeling of Organic-Based Lithium and Sodium Ion Batteries.

Supervision rate: 50%.

Co-supervisor: Assistant Prof. Christine Frayret (LRCS).

Publications: **2** (*Physical Chemistry Chemical Physics,* 1 submitted).

Hassna El-Bousiydy (2018-2022)

Topic: Text Mining of Battery Litterature.

Supervision rate: 50%.

Co-supervisor: Prof. Patrik Johansson (Chalmers University of Technology, Sweden).

Publications: **2** (*Batteries & Supercaps,* 1 *Chem. Rev.*).

AUTRES AVANCÉES SIGNIFICATIVES AU COURS DE LA PÉRIODE :

I am convinced that the research we do is not useful if it is not shared with others, and especially with young people who are the future of our society. Part of my teaching vision was recently published in my interview with *Chemistry Views* (Chemistry Europe).[11] During my IUF Junior Member position, I developed a teaching program and science popularization approach of **excellence** to disseminate my research activities, with a **highly innovative** character through the methodologies employed.

I have developed and implemented **immersive and interactive Virtual Reality (VR) serious games** for energy technologies teaching (see photo).[12] My six-years-experience with VR technology has shown that students develop a better understanding of how these technologies work and how they are made of and they feel more engaged and motivated to learn complex concepts. They also develop collaborative skills because students not playing usually encourage the ones wearing the VR headsets. VR provides also an interactive way to learn computational modeling because access to the computational models is made through a metaphor of visualization and interaction in an informed virtual environment, that is based on knowledge-based models. I also developed **Mixed Reality serious games**. This is a new concept I created based on the real-time interaction between real objects and a virtual environment. An illustrative example is the so-called "Smart Grid" serious game I published in Ref. [12]. In this game, one of the students drives an electric vehicle in the VR environment, while others interact with 3D-printed small-scale windmills, solar panels among other objects affecting the energy production, distribution, and consumption in the VR environment. These serious games help students to better understand concepts or explore new aspects in addition to those that I present in my lectures. I have been also strongly involved in science popularization events using these VR serious games, such as Pint of Science (see list above and Ref. [13]).

PRIX ET DISTINCTIONS SCIENTIFIQUES OBTENUS AU COURS DE LA PÉRIODE (indiquer les dates) :

2016-2021	**Junior Member of the Institut Universitaire de France (IUF)**
2017-present	**Member of the Direction Committee** of the LRCS, Amiens, France
2018-present	**ERC Consolidator Grantee (European Research Council)**
2019-present	**Full Professor (1st class -PR1-)**, UPJV/LRCS, Amiens, France)
2019	**Recipient of the National Award for Pedagogy Innovation** (PEPS 2019) for my work on the development and use of Virtual Reality for energy storage education

2019-present	**Invited Member of the Scientific Council of the French Institute IFP Energies Nouvelles**
2020-present	**Advisory Editorial Board Member** of ***Batteries & Supercaps*** (Chemistry Europe, Wiley)
2021-present	**Chairman** of the Expert Group "Digitalization, Measurement Methods and Quality" in the **LiPLANET Battery Manufacturing European Network**
2021-2026	**Prime d'Encadrement Doctoral et de Recherche (PEDR)**

AUTRES OBSERVATIONS :

I would like to thank the IUF for having supported me for these amazing 5 years. I will always be very grateful. More information about my activities can be found in my research website.[1]

Acceptez-vous la mise en ligne de ce document sur le site internet de l'IUF : OUI (EN VERSION PDF).

REFERENCES USED ABOVE AS HYPERLINKS

1. My research team website: https://www.modeling-electrochemistry.com/ (accessed on October, 2021).

2. Franco, A.A., Rucci, A., Brandell, D., Frayret, C., Gaberscek, M., Jankowski, P. and Johansson, P., 2019. Boosting rechargeable batteries R&D by multiscale modeling: myth or reality?. *Chemical Reviews*, *119*(7), pp.4569-4627.

3. Lombardo, T., Duquesnoy, M., El-Bouysidy, H., …, Franco, A.A. 2021. Artificial Intelligence Applied to Battery Research: Hype or Reality?, *Chemical Reviews*, https://doi.org/10.1021/acs.chemrev.1c00108 (2021).

4. Website of my ERC-funded project "ARTISTIC": https://www.erc-artistic.eu/ (accessed on October, 2021).

5. https://www.modeling-electrochemistry.com/projects
(accessed on January 2022).

6. https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/batt.202100202 (accessed on October 2021).

7. https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/batt.202100077
(accessed on October 2021).

8. https://chemistry-europe.onlinelibrary.wiley.com/doi/full/10.1002/batt.202000233
(accessed October 2021).

[9]. https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/batt.201900208 (accessed October 2021).

[10]. https://onlinelibrary.wiley.com/doi/abs/10.1002/batt.201900085 (accessed on October 2021).

[11]. Koester, V., Franco, A.A. 2020. Innovative Computer Games for Battery Education and Research, *Chemistry Views*, Wiley-VCH (2020). 10.1002/chemv.202000069.

[12]. Franco, A.A. *et al.* 2020. Entering the Augmented Era: Immersive and Interactive Virtual Reality for Battery Education and Research. *Batteries & Supercaps*, *3*(11), pp.1147-1164.

[13]. https://www.modeling-electrochemistry.com/teaching (accessed on October 2021).