Batteries & Supercaps

Editorial
doi.org/10.1002/batt.202200149

Chemistry Europe
European Chemical Societies Publishing

www.batteries-supercaps.org

Special Collection

Artificial Intelligence in Electrochemical Energy Storage

Alejandro A. Franco*[a, b, c, d] and Amanda S. Barnard*[e]

The concept of *intelligence* has been defined as a set of processes found in systems, more or less complex, alive or not, which allow these systems to understand, learn or adapt to new situations. Artificial Intelligence (AI) refers to intelligence manifested by machines based on observations while the so-called Machine Learning (ML), a sub-field of AI, refers to a set of computer programs able to improve themselves through experience and use of datasets. Before the advent of ML in the 1950s, scientists needed to know the form of a model before attempting to solve it, whereas ML can devise the form of a model and solve it simultaneously. This represents an acceleration of the scientific method. Since their invention, AI and ML have triggered fascination specially since demonstrated spectacular performances of AI/ML empowered computer programs.

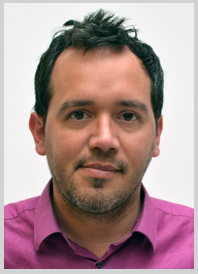
AI and ML are playing a transformative role in scientific research, and in particular in the electrochemical energy storage field, where it can be seen from the continuously increasing number of publications combining experimental characterizations and/or traditional mechanistic (physics-based) models with AI/ML techniques. Scientists and engineers working in the energy storage field, and in particular in the optimization of rechargeable battery technologies, are frequently confronted with multidimensional optimization problems to solve. Battery autonomy, energy density, safety, among other practical properties strongly depend on the materials that are used, on numerous electrode and cell manufacturing process parameters and experimental characterization conditions. Optimizing batteries requires a significant amount of time-consuming and costly trial and error. Due to the powerful capabilities of AI/ML to unravel interdependencies between parameters in large multi-dimensional datasets, they are excellent tools to complement or support traditional research approaches and predict patterns and behavior. Developing AI/ML programs requires time and the training process from data for the so-called supervised techniques can be particularly time consuming, but once they are established, these programs can make reliable predictions or discover parameter correlations in seconds. AI/ML techniques have been used to predict material properties, to predict the influence of manufacturing parameters on battery electrode properties, to analyze electrode tomography images in an automated fashion, to analyze spectra, to generate in seconds virtual materials which look like the real ones, for battery state of health diagnosis, and for predicting battery lifetime, among others.[1] [2]

As we believe that the electrochemical energy storage field is more transdisciplinary than ever, and digitalization plays a crucial role in the acceleration of discoveries and design optimization, with the present special collection, *Batteries & Supercaps* aims to illustrate AI/ML applications across several scales. This collection currently includes 1 Minireview, 4 original research Articles and 1 Concept, but it is still open for contributions from the scientific community. At the materials level, Shao et al. report a review on the use of atomistic scale machine learning to investigate and design electrolytes and interfaces, by introducing a comprehensive overview of technical aspects and applications. Bölle et al. presents a systematic investigation within the framework of Density Functional Theory (DFT) applied to cathode materials for magnesium ion batteries, and a path finder algorithm able to automatically estimate the transition state configuration prior to running computationally expensive Nudged Elastic Band calculations. Jeschke and Johansson show how supervised ML can be applied to classify different lithium–sulfur battery electrolytes a priori based on predicting polysulfide solubility, based on a framework combining DFT and statistical mechanics. At the cell level, Mayilvahanan et al. report an approach to develop interpretable ML models to analyze typical low rate charge curves as the ones generated by using mechanistic models. Kunz et al. present a ML approach able to predict lithium ion battery performance by using training datasets built on cells aged using complex electric vehicle discharge profiles. Finally, El-Bousiydy et al. report a text mining study of the battery scientists' habits while reporting their research in scientific articles, highlighting that many articles do not report important properties such as electrode porosity or electrolyte volume, calling for standardization in data reporting to allow future useful data exploitation by AI/ML algorithms.

[a] Prof. Dr. A. A. Franco
Laboratoire de Réactivité et Chimie des Solides (LRCS),
UMR CNRS 7314,
Université de Picardie Jules Verne, Hub de l'Energie,
15, rue Baudelocque, 80039 Amiens Cedex, France
E-mail: alejandro.franco@u-picardie.fr
[b] Prof. Dr. A. A. Franco
Réseau sur le Stockage Electrochimique de l'Energie (RS2E),
FR CNRS 3459, Hub de l'Energie,
15, rue Baudelocque, 80039 Amiens Cedex, France
[c] Prof. Dr. A. A. Franco
ALISTORE-European Research Institute,
FR CNRS 3104, Hub de l'Energie,
15, rue Baudelocque, 80039 Amiens Cedex, France
[d] Prof. Dr. A. A. Franco
Institut Universitaire de France
103 Boulevard Saint Michel, 75005 Paris, France
[e] Prof. Dr. A. S. Barnard
School of Computing
Australian National University
145 Science Road, Acton ACT 2601, Australia
E-mail: Amanda.S.Barnard@anu.edu.au

Special Collection This Editorial is part of a Special Collection on Artificial Intelligence in Electrochemical Energy Storage

Editorial
doi.org/10.1002/batt.202200149
Chemistry Europe
European Chemical Societies Publishing



Alejandro A. Franco is Full Professor at the Université de Picardie Jules Verne (Amiens, France) and Honorary Member of the Institut Universitaire de France (Paris, France). He is the leader of the Theory Open Platform in the ALISTORE European Research Institute. He is an ERC Consolidator Grantee for his project ARTISTIC about the development of a digital twin of the manufacturing process of Lithium-Ion Batteries and he recently won an ERC Proof of Concept Grant. He is also the Chairman of the "Digitalization, Measurement Methods and Quality" Expert Group in the European LiPLANET network. His interests concerns multiscale modeling and artificial intelligence applied to electrochemical energy devices. He won one of the French Prizes on Pedagogy Innovation in 2019 for his use of Virtual Reality to teach battery sciences.

Amanda S. Barnard is Senior Professor in the School of Computing at the Australian National University, where she is both Leader of Computational Science and the Deputy Director. Among other activities, she is the Chair of the Australasian Leadership Computing Grants Scheme, a member of the Expert Panel for the CRP scheme for the National Research Foundation of Singapore, and the Board of Directors for the New Zealand eScience Infrastructure. For her research at the interface of modelling, simulation and machine learning in materials and nanotechnology, she has been awarded in 5 scientific disciplines, and was the 2014 recipient of the Feynman Prize for Nanotechnology (Theory). In 2022, Prof. Barnard was appointed to the Order of Australia, the country's highest honor, for contributions to computational science.

In conclusion, we are now entering exciting times where battery research digitalization, particularly supported on AI and ML, is becoming a reality. It is our responsibility as energy storage scientists to understand this ongoing revolution to realize the full potential of these tools to improve the speed, efficiency, accuracy and utility of the science we do. We would like to acknowledge all the authors for their great works and the reviewers for the careful assessing of the manuscripts. We hope that their works will constitute a source of inspiration for future AI/ML applications in the energy storage field, and beyond. Last but not least, we would like to acknowledge Greta Heydenrych and Rosalba A. Rincón for their initiative, for having invited us to compile this collection and for the organization in 2020 of the journal Virtual Symposium on AI applied to batteries that one of us had the honor to chair. We would like also to congratulate them for their open-mindedness towards disruptive scientific approaches and for performing such an amazing job to make *Batteries & Supercaps* a reference journal in the field in so short time since its creation.

[1] T. Lombardo, M. Duquesnoy, H. El-Bouysidy, F. Årén, A. Gallo-Bueno, P. B. Jørgensen, A. Bhowmik, A. Demortière, E. Ayerbe, F. Alcaide, M. Reynaud, J. Carrasco, A. Grimaud, C. Zhang, T. Vegge, P. Johansson, A. A. Franco, *Chemical Reviews* **2021**, DOI:10.1021/acs.chemrev.1c00108.
[2] A. Mistry, A. A. Franco, S. J. Cooper, S. A. Roberts, V. Viswanathan, *ACS Energy Letters* **2021**, *6*, 1422–1431.

Manuscript received: March 29, 2022
Version of record online: April 5, 2022