Accelerating the development of new battery materials

Ainhoa Bustinza[1], Maha Ismail[1,2], Iciar Monterrubio[1,2], Oier Arcelus[1], Nebil Katcho[1], Javier García[1], Evaristo Castillo[1], Javier Carrasco[1], Montse Casas-Cabanas[1,3], Marine Reynaud[1]

1. Introduction

Battery innovation relies on developing new electroactive materials. To timely respond to the increasing demand for energy storage solutions, the European Battery 2030+ Initiative targets accelerating by 5-to-10 fold the current rate of battery materials discovery within the next 5-10 years [1]. Taking up this challenge requires disruptive approaches that allow rethinking the traditional experimentation process (based on researcher's chemical intuition and trial-error scheme), which is inherently slow and economically expensive. Indeed, the crystal-chemical space offered by the periodic table for the search for new battery materials is huge and still far from being exhaustively explored.

2. Experimental screening of electrode materials

To accelerate the exploration of broad chemical spaces, our group is developing an autonomous Materials Development Platform, capable of making effective modelling-based predictions, self-driving inorganic synthesis and performing high-throughput characterization experiments. This requires a mind change in our approach to materials research, but also building new lab infrastructures and analytical tools, which include automated high-throughput synthesis modules, automated data analysis programs able to handle large amounts of data, as well as AI-aided experimental planners.

In this presentation, we will present several strategies explored at CIC energiGUNE to speed up the different stages of the development of new materials for Li-ion and Na-ion batteries. Such approaches include:

(i) the use of automated machine-learning-aided screenings of materials databases in search for new families of compounds that can be converted into electroactive materials [2, 3];
(ii) the development of solutions to automatize inorganic syntheses (e.g. co-precipitation, solvothermal, sol-gel; Figure 1) and characterization techniques (e.g. XRD, electrochemistry) [4];

[1] CIC energiGUNE - BRTA, Parque Tecnológico de Álava, C/ Albert Einstein 48, Vitoria-Gasteiz (Spain); mreynaud@cicenergigune.com

[2] Physical Chemistry Department, Pharmacy Faculty, Basque Country University (UPV/EHU), 01006 Vitoria-Gasteiz, Álava Spain.
[3] IKERBASQUE, Basque Foundation for Science, María Díaz de Haro 3, Bilbao, Spain

(iii) the development of analysis tools for automated data treatment and analysis, including a Machine-Learning experimental planner, chemometrics approaches for data analysis of large XAS data sets, or the new FullProfAPP that enables automated Rietveld refinements of large series of data, in particular those generated from operando experiments [4, 5].

Figure 1: Photo of one of the experimental modules for inorganic syntheses developed at CIC energiGUNE

3. Acknowledgments

This work was in particular supported by the Spanish MCIN/AEI/10.13039/501100011033 and ERDF/EU (project ref. PID2019-106519RB-I00, PID2022-140823OB-I00, PhD grant PRE2020-092978), the Basque Government (PhD grants ref. PRE-2021-2-011) and the European Commission (G.A. No 957189).

4. References

1. Roadmap - Battery 2030+ https://battery2030.eu/research/roadmap/
2. Katcho et al. Journal of Applied Crystallography, 52, 2019, pp. 148-157. DOI: 10.1107/S1600576718018484
3. Gallo-Bueno et al. Energy and AI, 2022, 9, pp. 100159 DOI: 10.1016/j.egyai.2022.100159
4. https://cicenergigune.com/en/fullprof-app
5. Fehse et al. Chemistry of Materials, 2022, 34(14), pp. 6529-6540. 10.1021/acs.chemmater.2c01360