

Accelerated design of new electrode materials for Li-ion batteries

I. Monterrubio^{1,3}, E. Castillo¹, A. Saracibar^{1,3}, J. Carrasco¹, M. Reynaud¹, M. Casas-Cabanas¹

- 1 *Centre for Cooperative Research on Alternative Energies (CIC energiGUNE), Basque Research and Technology Alliance (BRTA), Alava Technology Park, Albert Einstein 48, 01510 Vitoria-Gasteiz, Spain. * Email: imonterrubio@cicenergigune.com;*
- 2 *Physical Chemistry Department, Pharmacy Faculty, Basque Country University (UPV/EHU), 01006 Vitoria-Gasteiz, Álava Spain.*
- 3 *Inorganic chemistry Department, Science and technology faculty, Basque Country University (UPV/EHU), 48940 Leioa, Bilbao, Spain;*

The global demand for sustainable rechargeable batteries is expected to increase drastically in the next decade as applications continue to take off. Li-ion batteries (LIBs) are the most powerful of the high-capacity rechargeable batteries on the market today, but they have almost reached their energy density limit and, therefore, exploration of new systems and chemistries is mandatory.

Taking up this challenge requires new disruptive approaches and better tools to accelerate the discovery and understanding of new electroactive materials. Several strategies have been proposed by different groups to theoretically identify potential new candidates more efficiently [1–3], but the experimental validation stage often reveals to be the limiting step of the new material discovery process. Several groups are working on different approximations to accelerate the experimental stage differing in the materials, the type of synthesis, the amount of final product, etc. [4–6]

In this work, a novel, validated and reproducible high throughput experimental automated module for the preparation of lab-scale samples of electrode materials will be presented. This module is therefore thought to handle and mix solutions of precursors in appropriate stoichiometries that will be evaporated before the solid-state annealing treatment. This approach enables to build a set-up compatible with a wide range of synthesis routes such as sol-gel, Pechini, co-precipitation-based syntheses, etc, which in turn enable size and morphological control and/or in situ carbon coating of the particles to enhance the ionic conductivity.

References

- [1] A. Jain, G. Hautier, C. J. Moore et al. *Comp. Mater. Sci.*, **2011**, 50(8), 2295–2310.
- [2] G. Rousse, J.M. Tarascon, *Chem. Mater.*, **2013**, 26 (1).
- [3] N. A. Katcho, J. Carrete, M. Reynaud et al., *Appl Crystallogr.*, **2019**, 52, 148-157.
- [4] G. H. Carey, J. R. Dahn, *Comb. Sci.*, **2011**, 13(2), 186–189.
- [5] T. Adhikari, A. Hebert et al. *ACS Comb. Sci.* **2020**, 22, 6, 311–318.
- [6] A. Benayad, D. Diddens et al. *Adv. Energy Mater.* **2021**, 2102678.