# Electrode Materials for Organic Batteries: can Modelling Investigations take part to the Challenge?

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Improvement of success rates for innovation in the research field devoted to the organic battery development mainly relies on the ability to rationally design and fabricate novel functional electrode materials by exploiting the large modularity linked to their intrinsic nature. The emergence of strategies for lead candidates' identification requires an understanding of the incidence of functionalization/modulation of the molecular backbones or change in redox centres,... on electrochemical features for various sets of compounds. This supposes reaching full knowledge of the physical–chemical properties and of the role they are playing in the involved processes. Provided selection criteria and full comprehension can be extracted from such approaches, modelling investigations may play a key role on this emerging area, with the promise of guided research, greener design and faster advances.

A work of prospection can correspond to the initial and most significant milestone in designing advanced materials, especially if differentiation between compounds can be rationalized. Our simulation methodology is thus aimed at defining property-based guidelines within a few sets of modulation. It can be applied to both systematic screening of existing compounds and hypothetical novel candidates, both being modulated through various effects. This should progressively complete the database for the discovery of new/optimized organic electrodes with improved features. Spin density maps, electronic delocalization indices or energy stabilization decomposition, … clearly constitute powerful local indicators that enable to distinguish molecular compounds, especially regarding their ranking in terms of electrochemical features. In particular, fine dissection of these data can give the opportunity to discover subtleties regarding the role played by each parameter within various sets of combined effects of functionalization/heteroatom substitution/nature of backbone, … that could not be disentangled easily otherwise. Recent studies in this area outline lessons originating from the consideration of various families and modifications [see *e.g.* 1–3]. By exploring various invention possibilities, the ultimate goal of such investigations is to help experimentalists engineering a few potentially attracting new compounds.

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[2] C. Frayret, D. Tomerini, C. Gatti, Y. Danten, M. Becuwe, F. Dolhem, P. Poizot, in Proceedings of *CIMTEC 2014, 13th International Conference on Modern Materials and Technologies – 6th Forum on New Materials*, Chapter 3: Batteries, Supercapacitors and Thermoelectrics, *Techna-Group Series Advances in Science and Technology,* June 16 – 19, 2014, Montecatini Terme, Italy, Part A, pp. 146-151.
[3] A.A. Franco, C. Frayret, in: C. Menictas, M. Skyllas-Kazacos, T.M. Lim (Eds.), Advances in batteries for medium– and large–scale energy storage, Woodhead Publishing, 2014, pp. 509–562.