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The quest of performant redox-active organic compounds for battery electrodes: contribution from computational modelling

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PURPOSE OF THE ABSTRACT

The rising worldwide consumption of energy is currently initiating new behaviours and will go on promoting the search for innovation and breakthrough in the area of electrical energy storage set-ups. This will involve, in the long run, the development of batteries that are both more sustainable and sufficiently efficient to meet the demand of new electrical devices. The potential advent of organic-based electrodes would constitute a step toward this direction. In this area, fancy ways of discovering new materials precisely targeted towards applications optimization with departure from standards mainly relies on the conjunction of synthesis feasibility and subsequent obtention of satisfying features especially (but not solely) of electrochemical nature. To this respect, a high-stability combined with a low-solubility in the electrolyte along with sufficiently low/redox potential (according to the type of electrode (i.e. negative/positive)), high capacity (in link with the effective use of the maximum number of available redox centres or/and how they behave in terms of redox potential), reversibility (cycling ability) are desirable. To this usual way of considering this equation adds the question of electron conduction requirement in view of departing from the massive use of carbon additives to circumvent the traditional insulating character of organic-based electrodes, which surely tarnish the image of this kind of materials, especially when compared with their inorganic counterparts. To overcome this issue, a key strategy would be to directly engineer conductive backbones. Within this context, computational modelling not only enables to satisfy green chemistry principles but also contributes to complement the characterization of experimental works or even to initiate the search for guidelines allowing advances towards breakthroughs in the field.

FIGURES

FIGURE 1

FIGURE 2

KEYWORDS

Organic batteries | Molecular DFT

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