Secteur des Sciences et Technologies

Invitation à la soutenance publique de thèse de

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Master en Sciences chimiques à finalité approfondie

Pour l'obtention du grade de Docteur en sciences

« Solid-State Electrochemistry of Organic Battery Materials : Addressing the Redox Potential and Solubility of Quinone Derivatives »

qui se déroulera
le mardi 25 août 2020 à 10h
visioconférence
1348 Louvain-la-Neuve

Jury members :

Prof. Alexandru Vlad (UCLouvain), supervisor
Prof. Jean-François Gohy (UCLouvain), supervisor
Prof. Yann Garcia (UCLouvain), chairperson
Prof. Yaroslav Filinchuk (UCLouvain), secretary
Prof. Sophie Demoustier (UCLouvain)
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In the past decades of human development, the Li-ion battery has established itself as a key technology to manage the storage and consumption of electrical energy, and even more so in the present context of a clean energy transition. Organic electrode materials, which offer the possibility of reduced environmental costs when considering the production and recycling of Li-ion cells, constitute an alternative to commercial inorganic compounds. In particular, since the late 2000's, the search for viable and practical Li-ion organic positive electrode materials has known an increasing interest. This thesis tackles the complex challenge to design organic molecules displaying a high energy density while remaining insoluble in battery electrolytes. Benzoquinone was chosen as starting material, for it presents interesting redox properties – notably a reversible two-electron redox reaction and a very high gravimetric capacity – and can undergo facile molecular modifications.

In a first phase, a benzoquinone derivative bearing two amino groups is investigated in order to establish a new design approach based on intermolecular H-bonding to achieve insolubility of small organic redox molecules in aprotic electrolytes. The robustness of this strategy was assessed by evaluating the solubility and the cycling performances of the hydroquinone derivative in a series of electrolytes with varying dipolar momentum. This allowed to establish the correlation between electrolyte solvent polarity, solubility and cycling stability of the new redox material.

In a second phase, the focus of the thesis was turned towards the issue of increasing the redox potential in quinone derivatives, in order to come up with new organic redox chemistries with a redox process occurring above the air-stability threshold. A novel organic electrode material with its own lithium reservoir was designed, displaying an unusually high redox potential due to a complex intramolecular electrostatic effect. This effect was investigated in depth by combining structural analyses with theoretical calculations.

Finally, the preliminary exploration of a heterocyclic quinone derivative was carried out. This molecule displays a novel organic redox chemistry based on the N-Li bond, which gives the perspective of developing a new class of high-potential organic electrode materials.