

Meeting Abstracts

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Derivatives of Naphthoquinone As Potential Electroactive Species for Redox FLOW Batteries

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The generation of energy from renewable sources (solar and wind) is limited by the weather conditions that turn them into intermittent sources. In addition to this, and due to the large amount of energy produced while minimum demand, energy storage technologies are urgently needed. Redox flow batteries (RFBs) are a very attractive technology for large-scale energy storage [1]. Currently RFB systems are mostly based on redox reactions of electroactive metal ions, which are limited by their abundance, low solubility, high cost and toxicity. However, organic species have generated great interest [2]. Quinones are the main organic redox active species that have a key role in the electron transport processes of biological systems depending on molecular aromaticity and their electronic structures [3]; for example, the synthesis of ATP and photosynthesis [4]. However, the synthesis of redox species based on quinone analogs for RFB is associated with the unnecessary factor of human and monetary capital. Therefore, the current computer tools allow great opportunities to screen for valuable quinone species for RFB, as well to optimize resources.

In this work, a chemical system derived from quinones was proposed as possible electroactive species as redox electrolyte for energy storage applications (Figure 1). Computer calculations of the chemical system were carried out to determine the difference in eV between HOMO-LUMO (E_{gap}) in order to predict their electron transfer ability, as well, the relationship towards their redox properties for RFB applications.

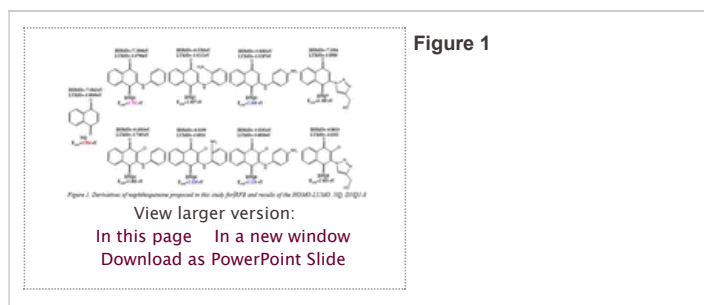
First, the molecules shown in Figure 1 were modeled in the program molden to obtain the z matrices. Then, theoretical calculations were performed by Gaussian v.0.9 using the functional hybrid B3LYP with the base 6-311 + G (d, p) in order to obtain the difference of eV between the HOMO-LUMO of the molecules. Subsequently, the proposed molecules were synthesized by Michael addition of 1,4 (DNQ1-6) using substituted anilines. Here, the synthesis reactions were carried out at 70°C for 12 h. On the other hand, the triazole in the DNQ8 was synthesized by means of a catalyzed 1,3-dipolar addition cycle of Huisgen. Electrochemical Studies were carried out by cyclic and linear voltammetry to evaluate the redox reactions, reversibility and the diffusion coefficients in order to confirm the theoretical calculations of the proposed system.

The theoretical calculations results showed that all materials have a lower E_{gap} compared to their predecessor NQ ($E_{\text{gap}}=3.984\text{eV}$), Figure 1. Therefore, it is possible to say that the DNQ1-8 compounds are suitable as redox electrolyte for flow batteries since at lower E_{gap} higher electrical conductivity, according to the theory of frontier molecular orbitals [5]. Particularly, the DNQ3 and DNQ6 presented the lowest E_{gap} , thus, these compounds could be a very attractive option for a fast electron transfer at the electrode/electrolyte interface in a RFB. All the molecules proposed in Figure 1 were synthesized as describe above. The yields were from 63% to 81%. The molecules synthesized with chlorinated reagents exhibit the highest yield and it was attributed to the presence of a better leaving group. UV-vis studies were performed to

support the correspondence of the E_{gap} by theoretical calculations. For instance, a bathochromic shift of the interactions $\eta \rightarrow \pi^*$ was observed at 480 nm approximately for the DNQ1 as compared to this for the DNQ3 at 540 nm approximately. These preliminary results agreed with the theoretical calculations, higher E_{gap} for the DNQ1 as compared to lower E_{gap} for the DNQ3. Overall, the proposed system seems to be suitable for energy storage applications in RFBs, however, electrochemical studies are being carried out and will be presented at the conference in order to confirm these results.

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