Electronic Supplementary Material (ESI) for Energy & Environmental Science

Supporting Information for:

Tailored Redox Functionality of Small Organics For Pseudocapacitive Electrodes

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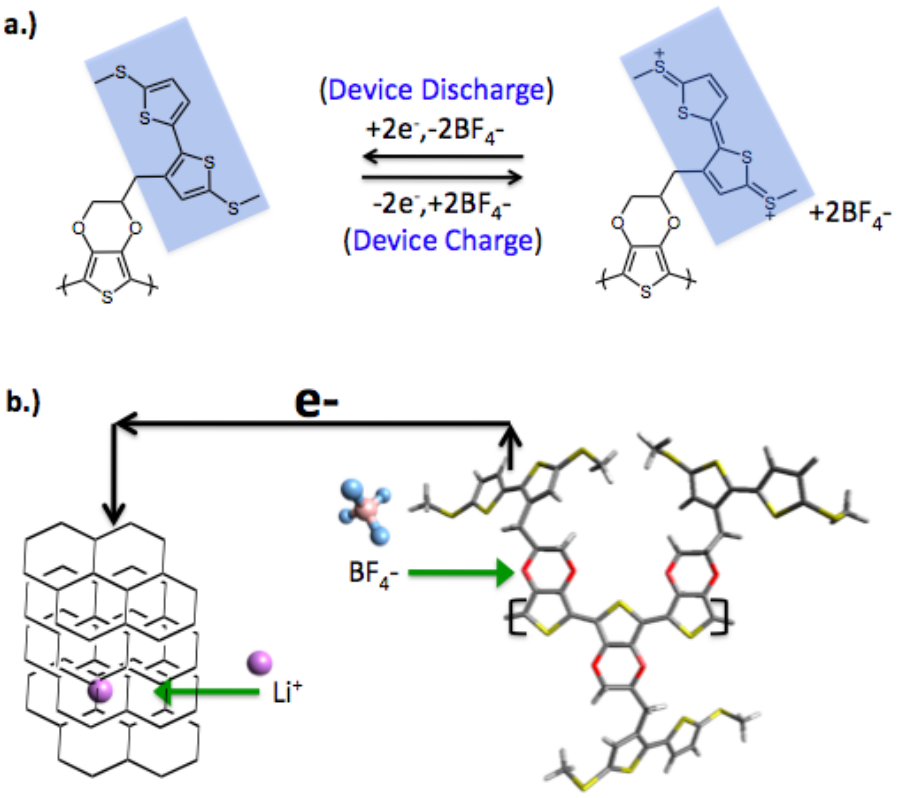

Figure S1. a.) Pendant redox processes during device charging. b.) Schematic of a device based on a graphitic lithium anode and polymer cathode.

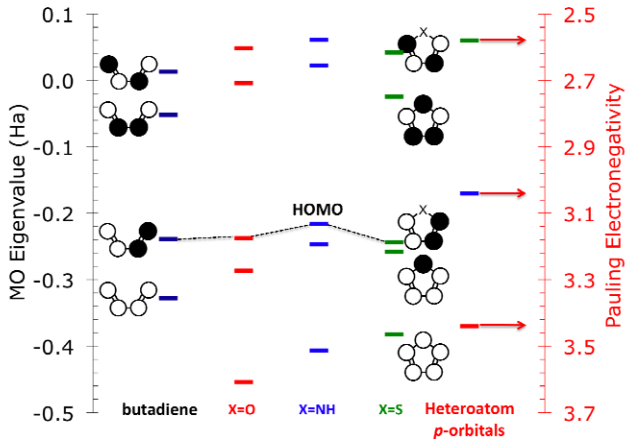

Figure S2. B3LYP/6-31+g(d,p) molecular orbital diagram for π-MOs of 5-member heterocycles. Diagram depicts the interactions of heteroatom p-orbitals with the π-MOs of 1,3-butadiene and resulting combinations. The trend in HOMO levels (NH > O > S) is in good agreement with the shift in oxidation potential, strongly suggesting that the heteroatom provides an almost constant shift in molecules based on the heterocycles, as has been reported elsewhere.

Molecular Test Set Details

The molecular test set consists of 10 molecules for which the experimental 1st oxidation potentials were determined using cyclic voltammetry, the method for which is described in the experimental methods section. Of these molecules, 5, 5'-Bis (methylthio)-2, 2'-bisethylenedioxythiophene, **3**, 5, 5'-Bis(methylthio)-2, 2'-bithiophene, **4**, 5, 5'-Bis(methylthio)-2, 2'-ethylenethiophene, **5**, 5, 5'-Bis(methylthio)-2, 2'-ethylenedithiathiophene, **6**, and 5, 5'-Bis(methylthio)-2, 2'-thiophene, **7**, were synthesized in-house. The remaining molecules, Tetramethylphenylenediamine, **1**, Tetrathiafulvalene, **2**, 1, 4-dimethylthiobenzene, **8**, thianthrene, **9** and 1, 4-dimethoxybenzene, **10** are commercially available.

Complete Reference 38:

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