

## Supporting Information

### Poly-anthraquinone sulfide isomers as electrode materials for extended operating temperatures organic batteries.

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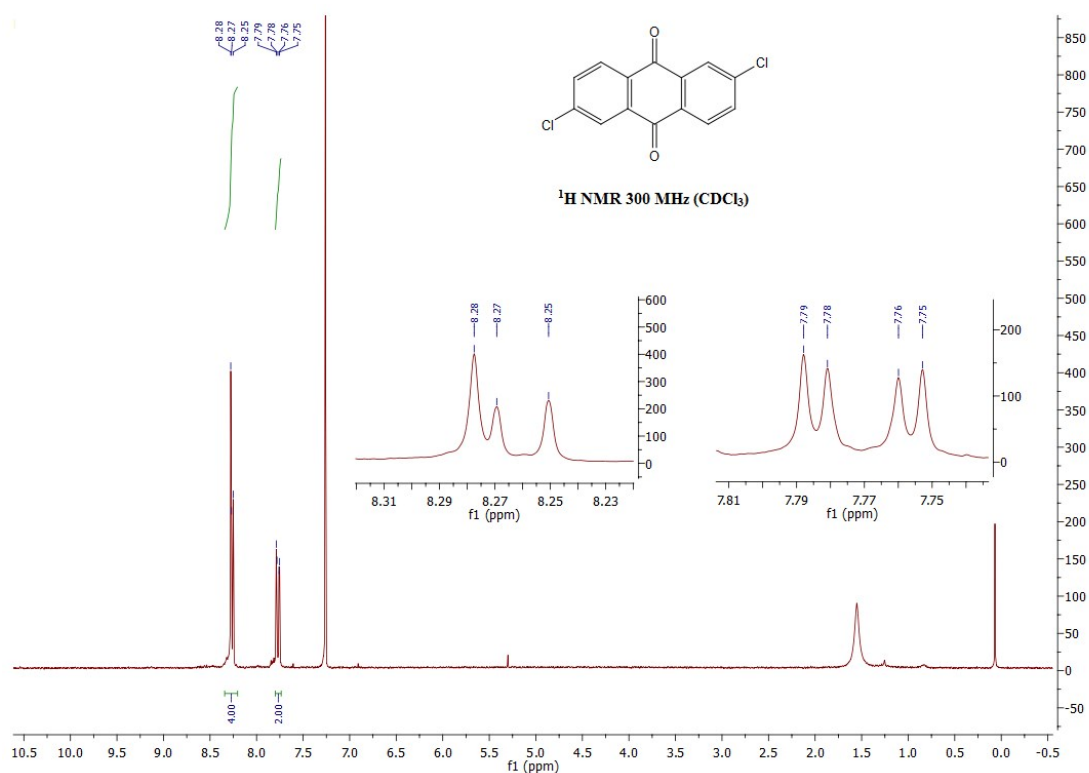
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#### 1. Materials

All chemicals were obtained from commercial sources and used as received unless otherwise noted. 1,5-dichloroanthraquinone (1,5-DCAQ, 96%), 1,8-dichloroanthraquinone (1,8-DCAQ, 97%), 2,6-diaminoanthraquinone (2,6-DAAQ, 97%), Sodium sulfide (Na<sub>2</sub>S), *N*-methyl-2-pyrrolidone (NMP, anhydrous 99.5%), sodium nitrite (NaNO<sub>2</sub>, 99.999%) and Toluene were purchased from Sigma-Aldrich. Cuprous Chloride (CuCl, 99.999%) was ordered from Alfa Aesar. Acetone, CH<sub>2</sub>Cl<sub>2</sub> and HCl were obtained from Carlo Erba. Reactions were monitored by thin-layer chromatography (TLC) analysis using silica gel (60 F254) plates from Merck. The compounds were visualized by longwave (365 nm) or shortwave (254 nm) UV light. Column chromatography was performed using silica gel 60 (230–400 mesh, 0.040–0.063 mm) to purify the product. <sup>1</sup>H liquid NMR were recorded at 300 MHz on Bruker Avance 300 spectrometer in deuterated chloroform (CDCl<sub>3</sub>). Chemical shifts (δ) are expressed in parts per million (ppm) of residual signals from the <sup>1</sup>H isotope solvent (7.26 ppm for CDCl<sub>3</sub>). The coupling constants *J* are expressed in Hz, and the multiplicity of the signals is indicated as follows: s = singlet, brs = broad singlet, d = doublet, t = triplet, dd = doublet of doublets, m = multiplet. Electrospray

ionization high-resolution mass spectrometry experiments were performed with a hybrid tandem quadrupole/time-of flight (Q-TOF) instrument, equipped with a pneumatically assisted electrospray (Zspray) ion source (Micromass, Manchester, UK) operated in positive mode. Melting points were measured using a Kofler bench.

## 2. NMR spectrum



**Fig. S1:**  $^1\text{H}$  NMR spectrum of 2,6-dichloro-9,10-anthraquinone in  $\text{CDCl}_3$ .

### 3. Thermogravimetric analysis

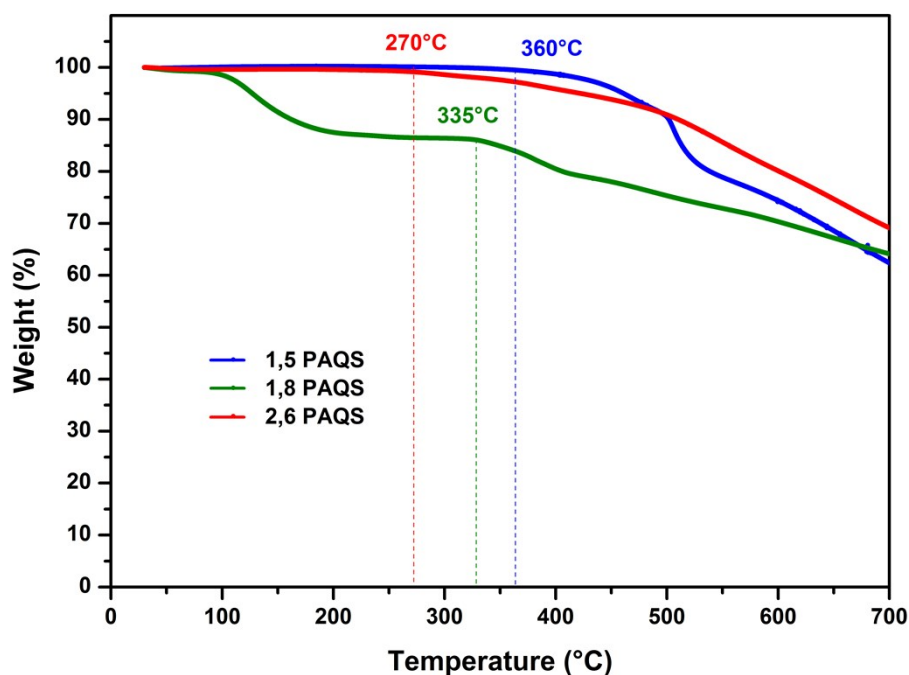


Figure S2. TGA analysis under N<sub>2</sub> atmosphere of PAQS isomers.

### 4. Electrodes solubility in electrolytes

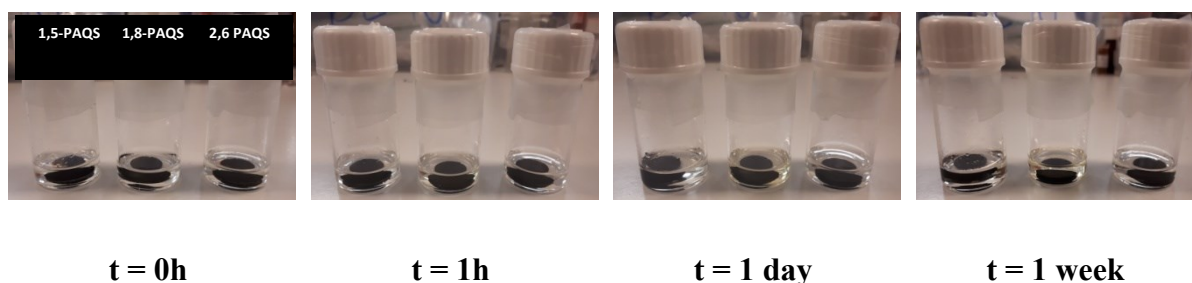
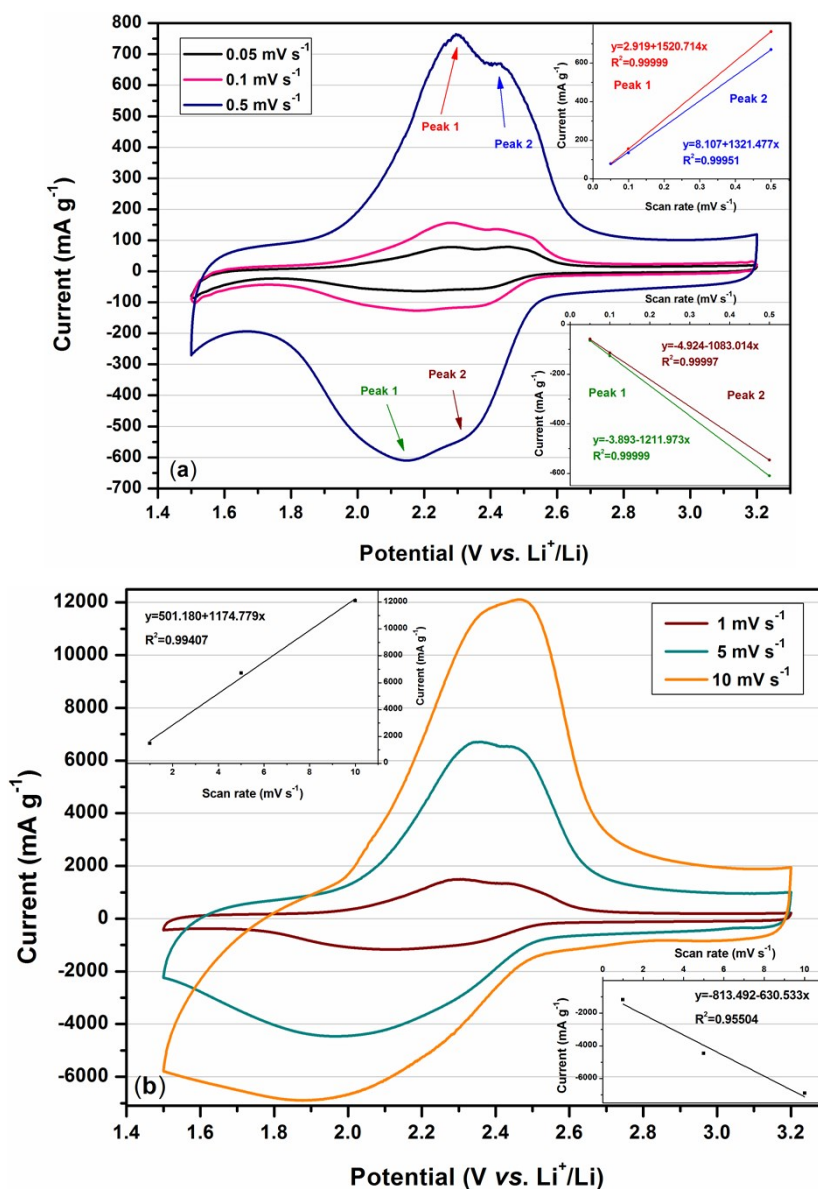


Figure S3. Pictures showing the dissolution behavior of PAQS electrode materials in 1M LiTFSI DOL/DME, (1:1 v/v) during a week.

### 5. CV curves analysis

In Fig. S4, typical curves of 2,6-PAQS at different scan rates are plotted. As it is highlighted in insets, fitting curves have very high correlation coefficient ( $R^2 > 0.999$ ) for slow scan rates obviously because of quite well defined two peaks in both cathodic and anodic parts of the CV (Fig. S4a). For faster scan rates (Fig. S4b), high currents added to peaks which started to fusion and become broad especially on the cathodic part leading to a lack of precision during the

determination of the peak position and finally lower  $R^2$  but still superior to 0.95, so it indicates that, scan rates and current peaks are linked through a linear relation. Those data demonstrate that the 2,6-PAQS redox reaction is a surface process whose kinetics are mainly determined by the charge transfer which is a property highly related to amorphous polymer electrodes.<sup>1,2</sup>



**Fig. S4:** Typical CV curves of 2,6-PAQS at different scan rates (0.05, 0.1, 0.5 mV s<sup>-1</sup> (a); 1, 5, 10 mV s<sup>-1</sup> (b)). The insets show the linear relation of cathodic or anodic peak current vs. scan rate.

## 6. References

1. Z. Song, Y. Qian, M. L. Gordin, D. Tang, T. Xu, M. Otani, H. Zhan, H. Zhou and D. Wang, *Angew. Chem. Int. Ed.*, 2015, **54**, 13947-13951.
2. A. Ahmad, A. Imani, L. Mao, R. Iqbal, H. Zhang, Z. A. Ghazi, R. Ahmad, A. A. Khan, L. Xie, C.-M. Chen, Z. Zhang and Z. Wei, *Adv. Mater. Technol.*, 2019, **4**, 1900617.