

Supporting Information

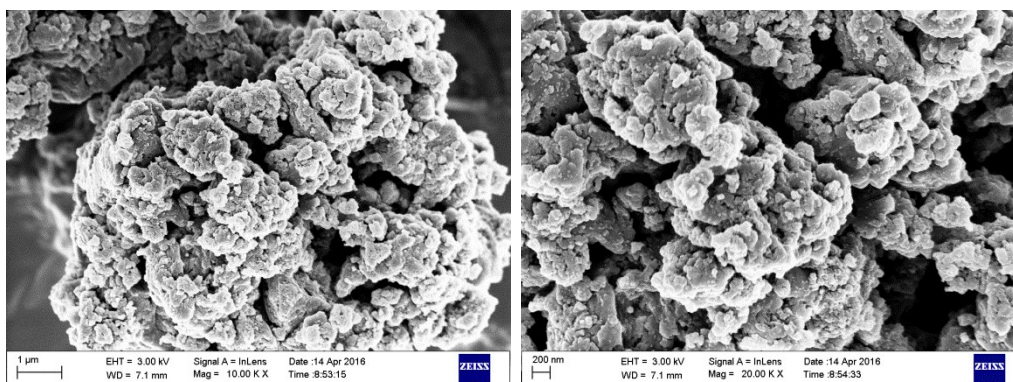
Electrochemical properties of carbonyl substituted phthalocyanines as electrode materials for lithium-ion batteries

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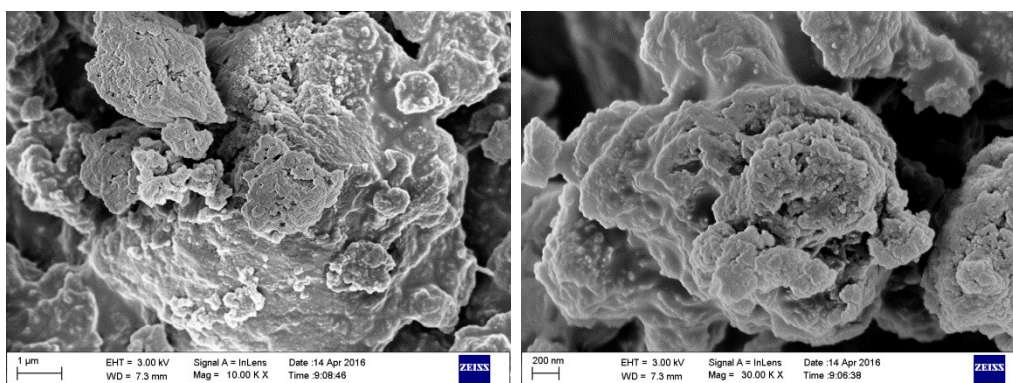
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Figure S1. SEM images of powder samples for **2** (**t-CAL-Pc**). a) before doping I₂; b) after doping I₂

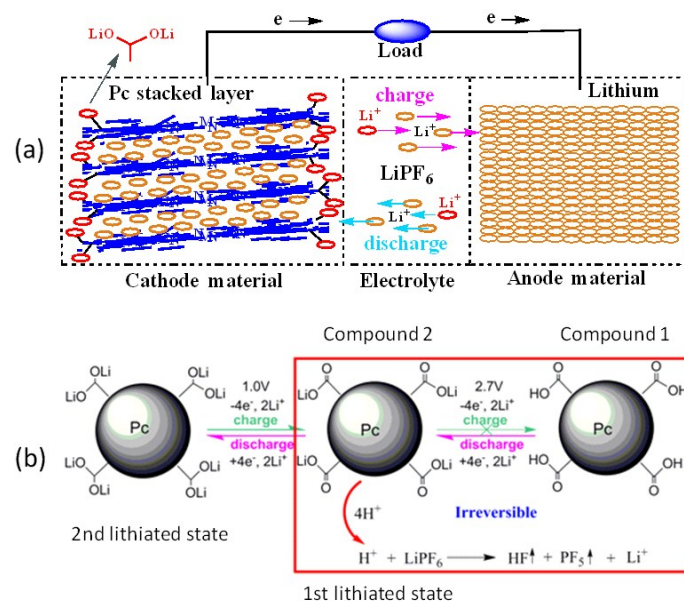


a) Powder sample of compound 2 before doping I₂



b) Powder sample of compound 2 after doping I₂

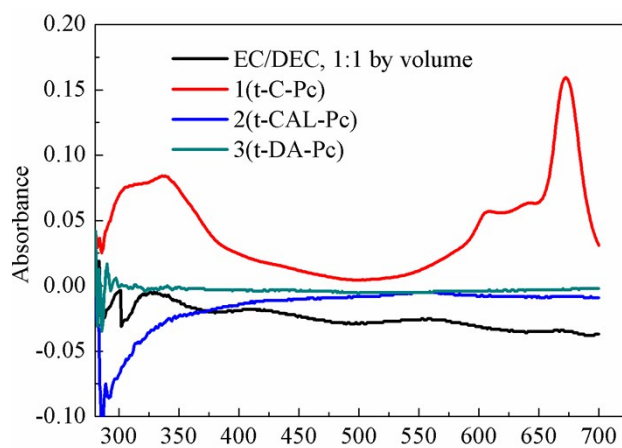
Figure S2. (a) Schematics of Li^+ intercalation process of carbonyl substituted phthalocyanine compounds 1-3; (b) Conversion process of compound 1 into compound 2



(a) For the carbonyl substituted phthalocyanine compounds, the lithiation processes consists of two aspects. One is the lithium intercalation by double bond of carbonyl groups, and the other is the lithium intercalation by the Pc stacked layers. Metallophthalocyanine (MPc) derivatives have stacked layer structures and can promote Li^+ -intercalation, which is also one of the contributions to a higher capacity. This conclusion has been published in our previous work.²¹

(b) This convert process of compound 1 into 2 is corresponding to the electrochemical properties such as CV performance and cycle performance. Firstly, it can be seen from Figure 3a in the manuscript that the symmetry of the CV curves of compound 1 turns to be better with the increase of cycle number, and the shape of the CV curves is more and more close to that of the compound 2. Secondly, it can be also seen from Figure 3b that the rapid capacity decay of the first 20 cycles is precisely the process of transition from compound 1 to compound 2. After 20 cycles the decay rate of capacities is very slow, which is consistent with the capacity decay trend of compound 2. Thirdly, from the curve of the capacity change with cycle numbers in Figure 3c, it can be also seen that the capacity change trend of compound 1 after 20 cycles is very similar with that of compound 2. Therefore, for compound 1, the charge/discharge process during the first 20 cycles is the process of compound 1 convert into compound 2, and the charge/discharge process after the 20 cycles is actually the lithiated process of compound 2.

Figure S3. UV-vis spectra of compounds 1-3 in solvent of EC/DEC (1:1 by volume).



0.05mmol of compound 1-3 is added into 50 mL of solvent (EC/DEC, 1:1 by volume). After placing 5 days, the UV-Vis spectrum test results are as Figure S3. It can be seen that compound **1 (t-C-Pc)** has certain solubility in the electrolyte, while for the compounds **2 (t-CAL-Pc)** and **3 (t-DA-Pc)**, there are almost not dissolved in the electrolyte. The experimental test results are completely consistent with the analysis results discussed in the communication.