

Supporting information

Chemically Reduced Organic Small Molecule based Lithium Battery with Improved Efficiency

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Theoretical capacity of the molecules was calculated by following the reported procedure.^[1] The formula for theoretical capacity calculation is

$$\text{Theoretical capacity} = (26800n/M)$$

Where n = number of electrons involved

M = molecular weight of the active substance

$$\begin{aligned}\text{Theoretical capacity for Benzoic-PDI} &= (26800 \times 2 / 630) \\ &= 85 \text{ mAh/g}\end{aligned}$$

$$\begin{aligned}\text{Theoretical capacity for Phenyl-PDI} &= (26800 \times 2 / 542) \\ &= 98 \text{ mAh/g}\end{aligned}$$

The volumetric capacity (C_v) of the electrode is calculated by following reported procedure.^[2]

$$C_v (\text{mAh/cm}^3) = C_g (\text{mAh/g}) \times \rho (\text{g/cm}^3)$$

Where C_g = gravimetric capacity of the electrode

ρ = nominal tap density of the electrode which is calculated based on the weight of the active material and geometry of our electrode

TableS1: Volumetric capacity at different C rate

	Volumetric capacity (mAh/cm ³)
1C	76
5C	117
10C	122
20C	65
30C	50

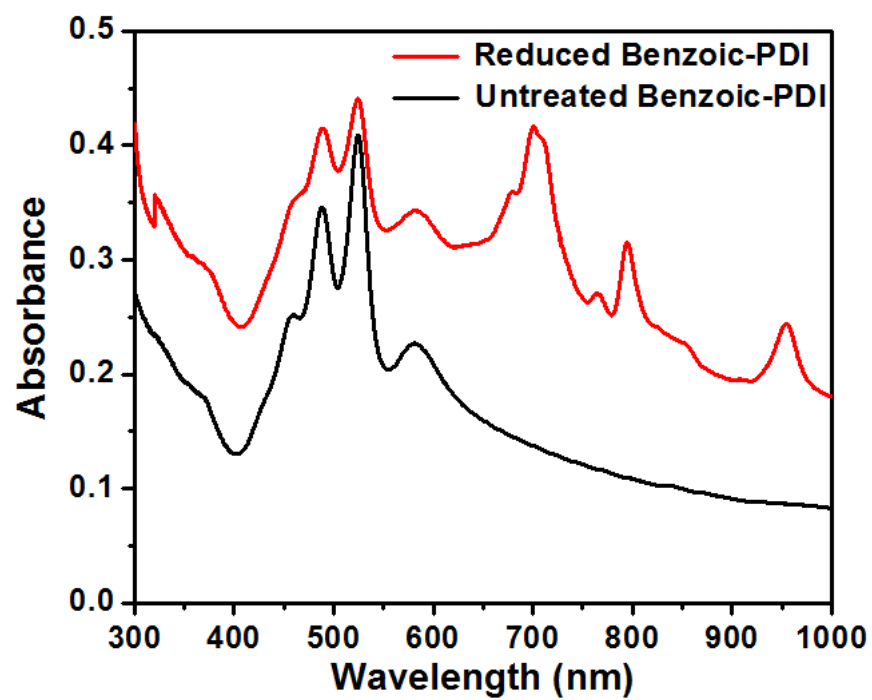


Figure S1. UV- visible absorption spectra of reduced and untreated benzoic-PDI.

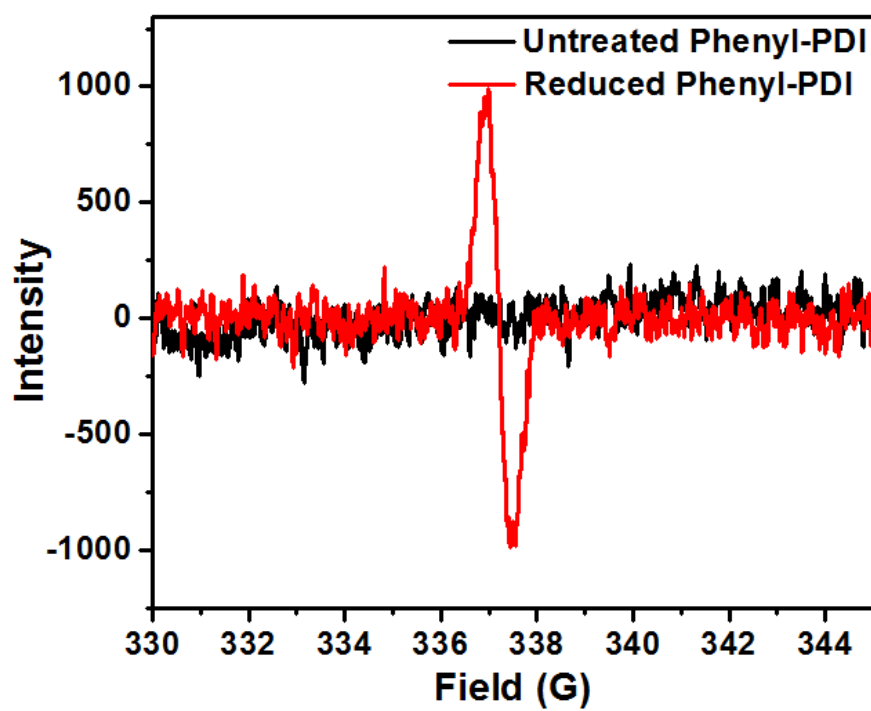


Figure S2. EPR spectra of reduced and untreated Phenyl-PDI.

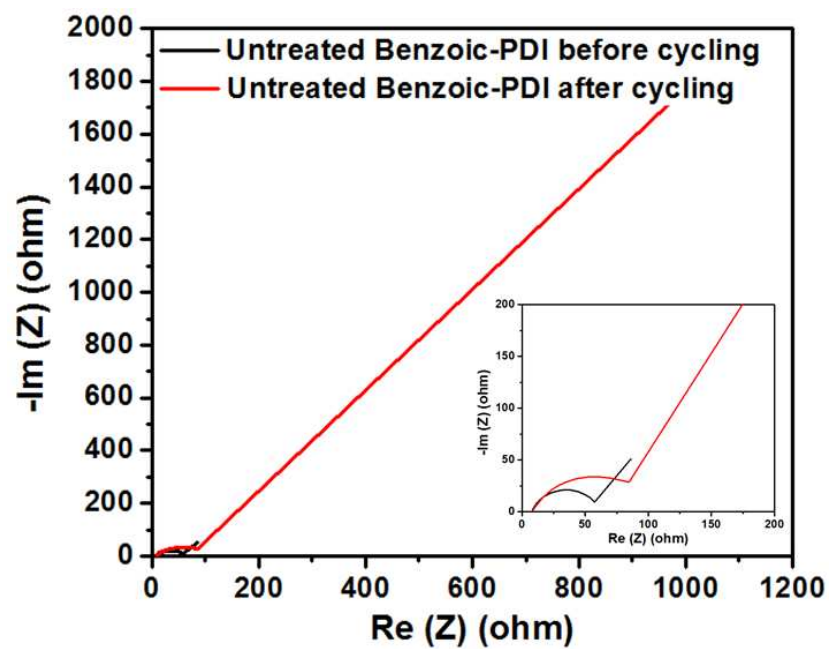


Figure S3. Impedance spectra of untreated Benzoic-PDI before and after 200 charge discharge cycles.

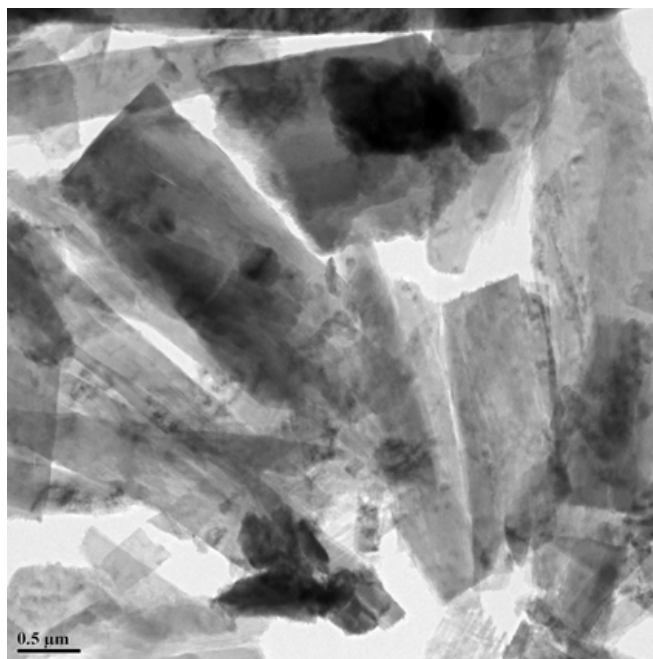


Figure S4. TEM image of untreated Benzoic-PDI.

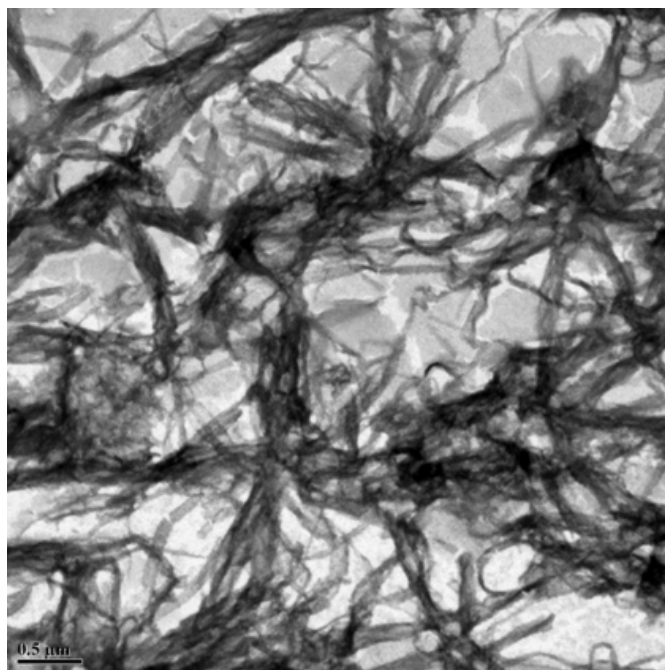


Figure S5. TEM image of reduced Benzoic-PDI.

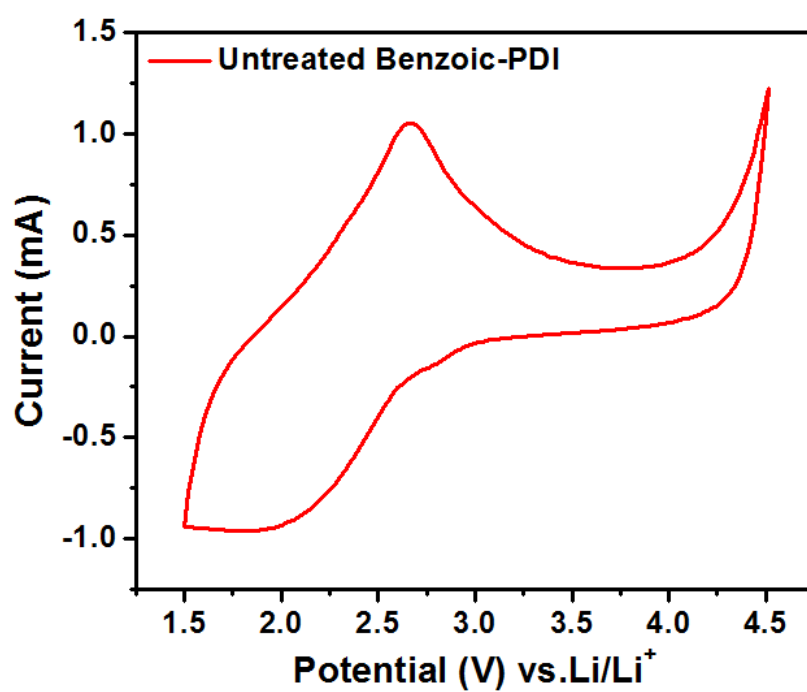


Figure S6. Cyclic voltammetry of untreated Benzoic-PDI

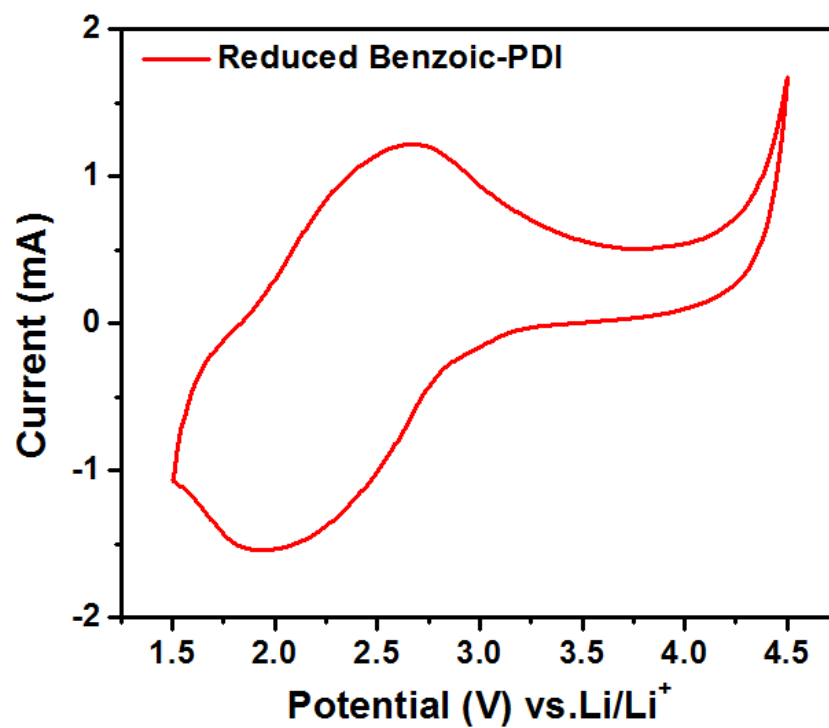


Figure S7. Cyclic voltammetry of reduced Benzoic-PDI.

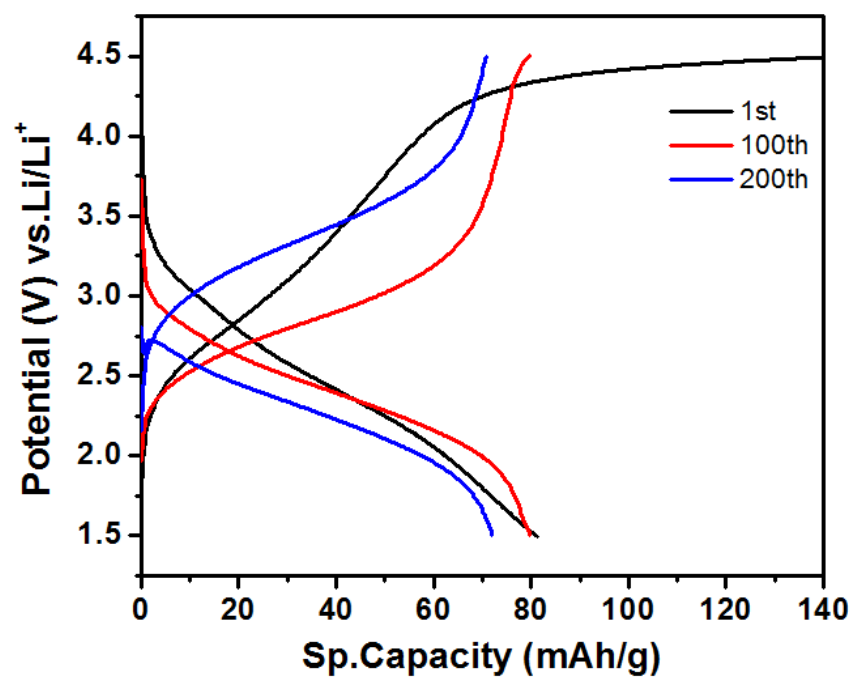


Figure S8. Charge-Discharge curves of reduced Benzoic-PDI at 5 C rate.

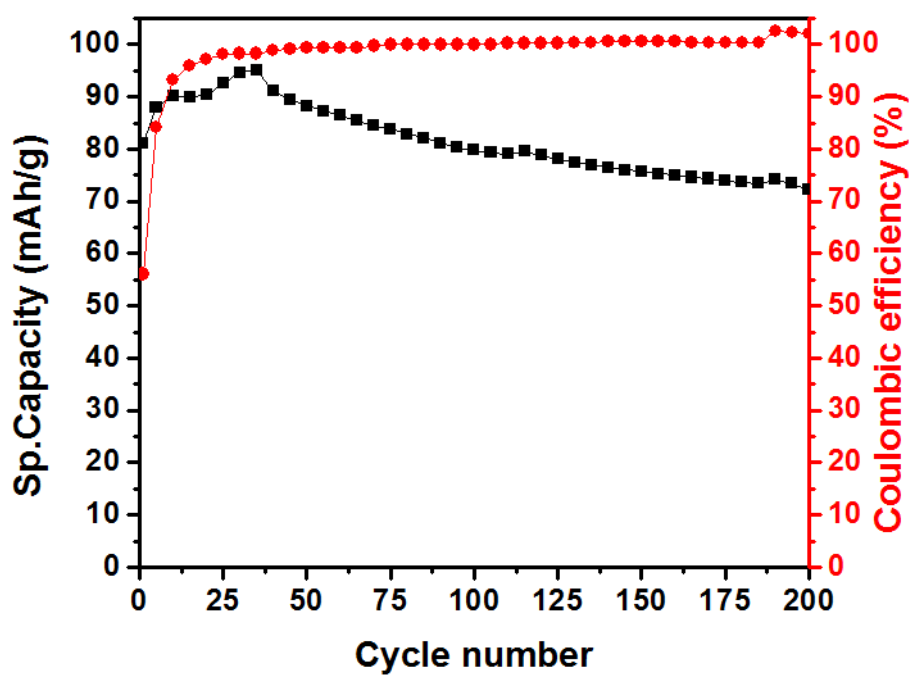


Figure S9. Coulombic efficiency and specific capacity of reduced Benzoic-PDI at 5 C rate as a function of cycle number.

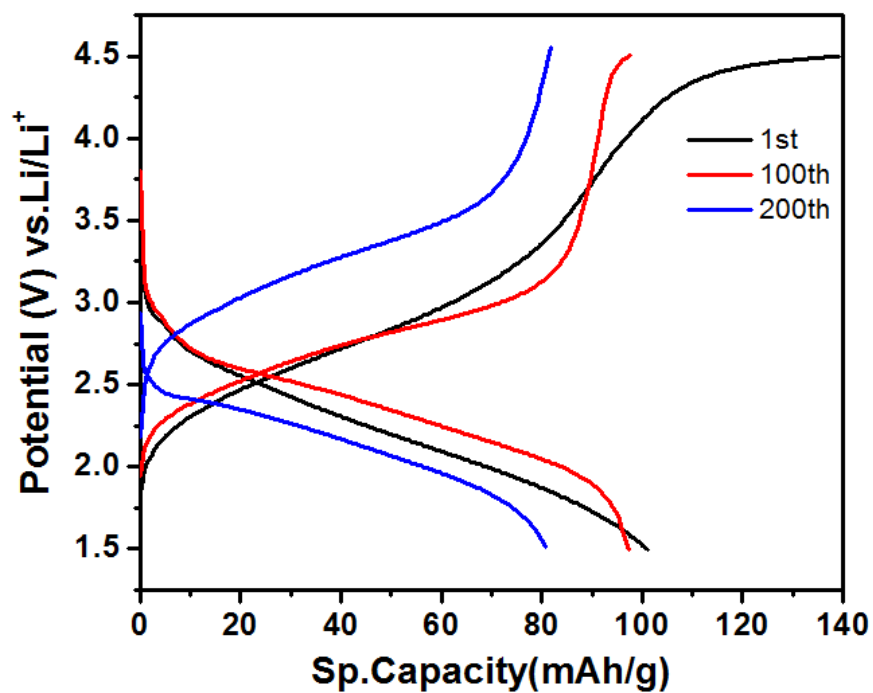


Figure S10. Charge-Discharge curves of reduced Benzoic-PDI at 10 C rate.

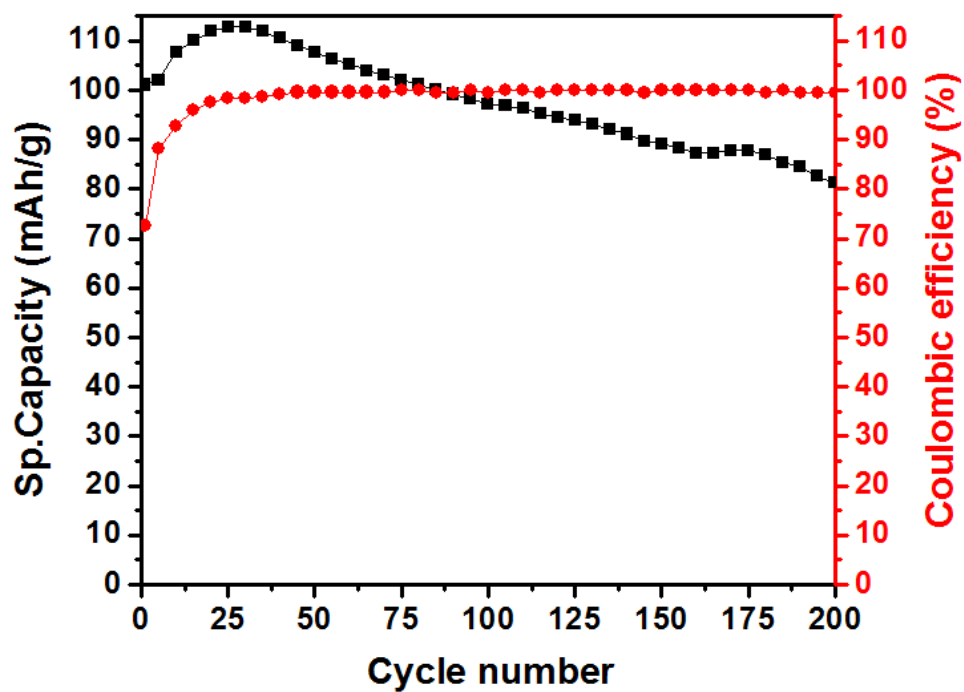


Figure S11. Coulombic efficiency and specific capacity of reduced Benzoic-PDI at 10 C rate as a function of cycle number.

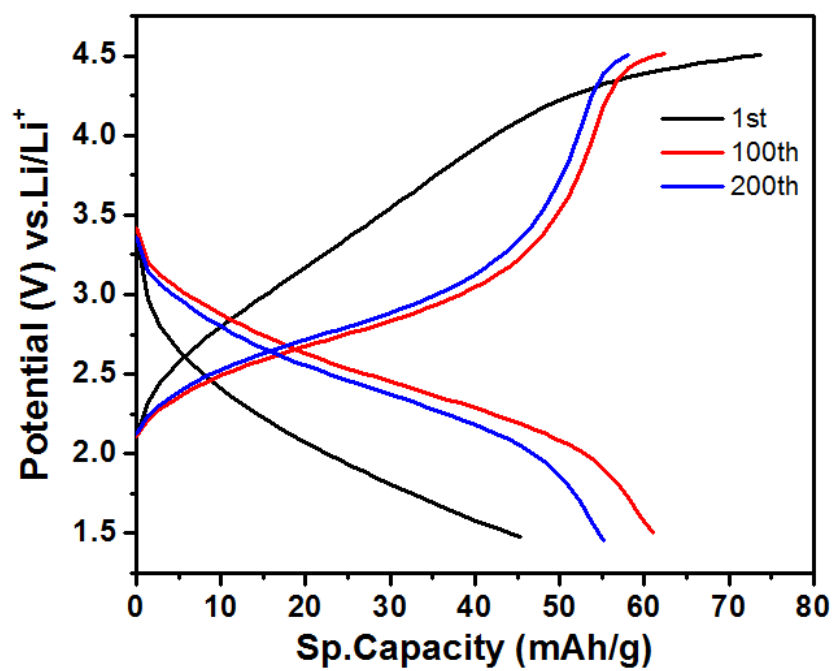


Figure S12. Charge-Discharge curves of reduced Benzoic-PDI at 30 C rate.

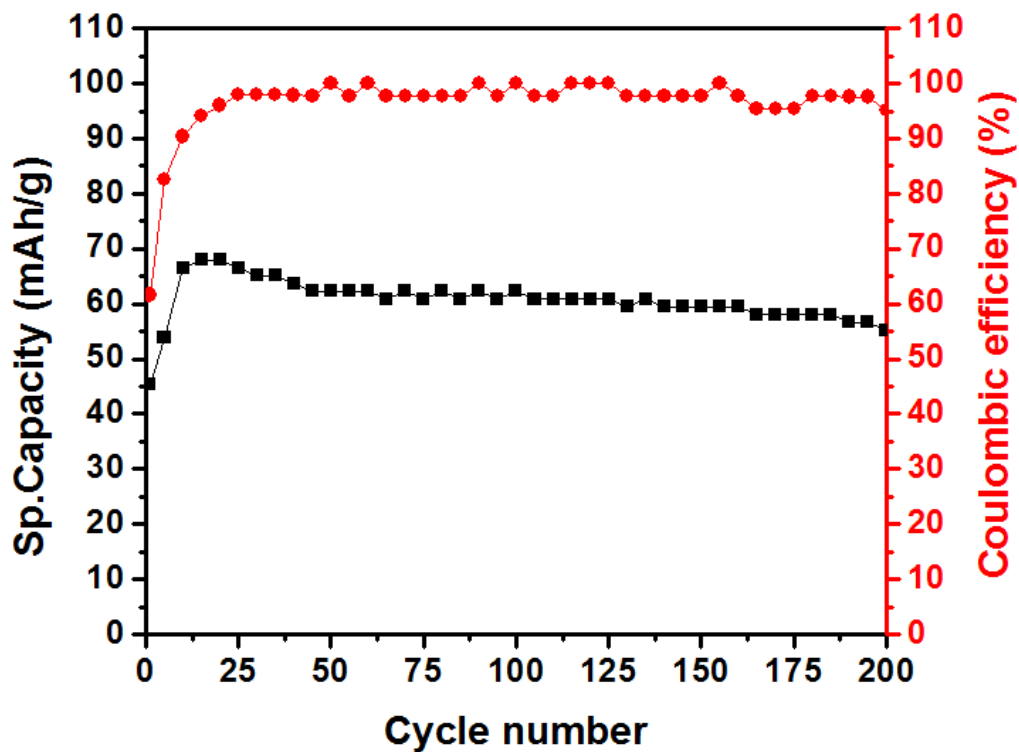


Figure S13. Coulombic efficiency and specific capacity of reduced Benzoic-PDI at 30 C rate as a function of cycle number.

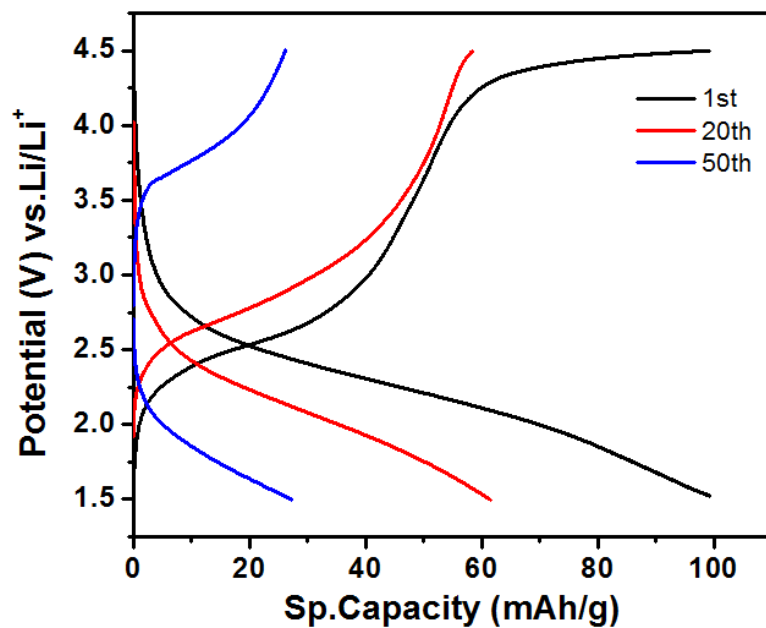


Figure S14. Charge-Discharge curves of untreated Benzoic-PDI at 0.5 C rate.

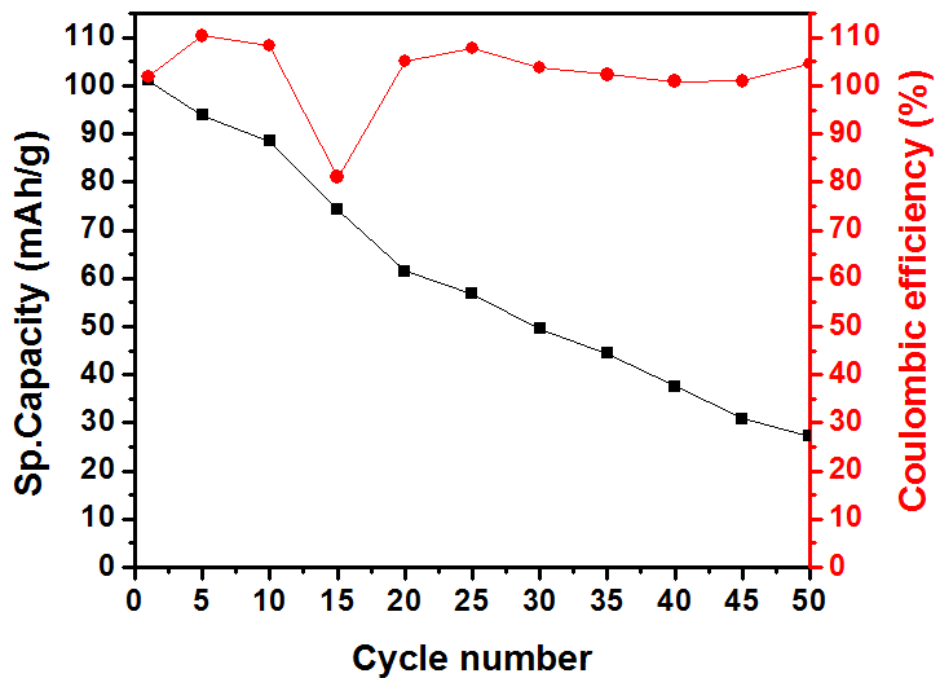


Figure S15. Coulombic efficiency and specific capacity of untreated Benzoic-PDI at 0.5 C rate as a function of cycle number.

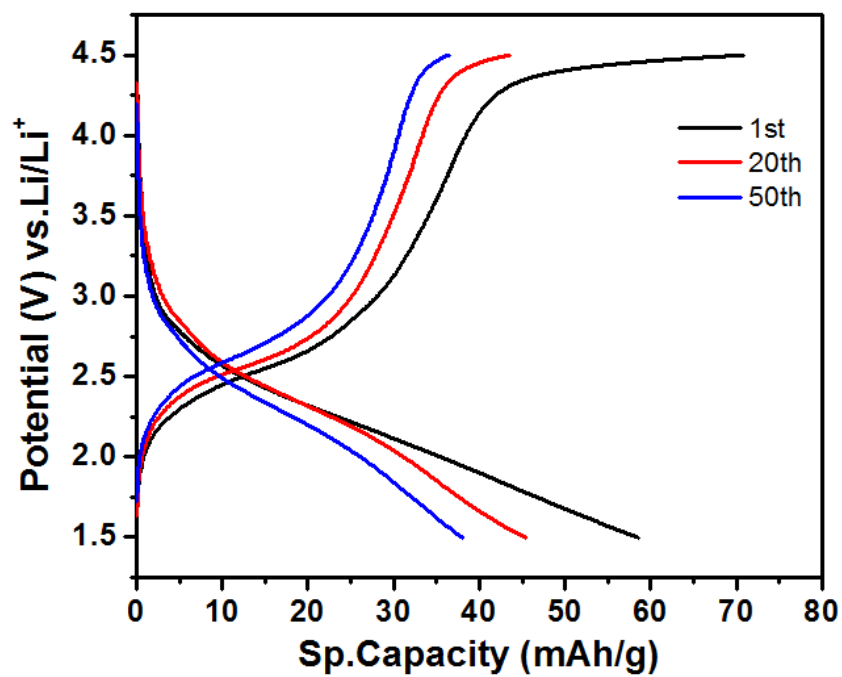


Figure S16. Charge-Discharge curves of untreated Benzoic-PDI at 1 C rate.

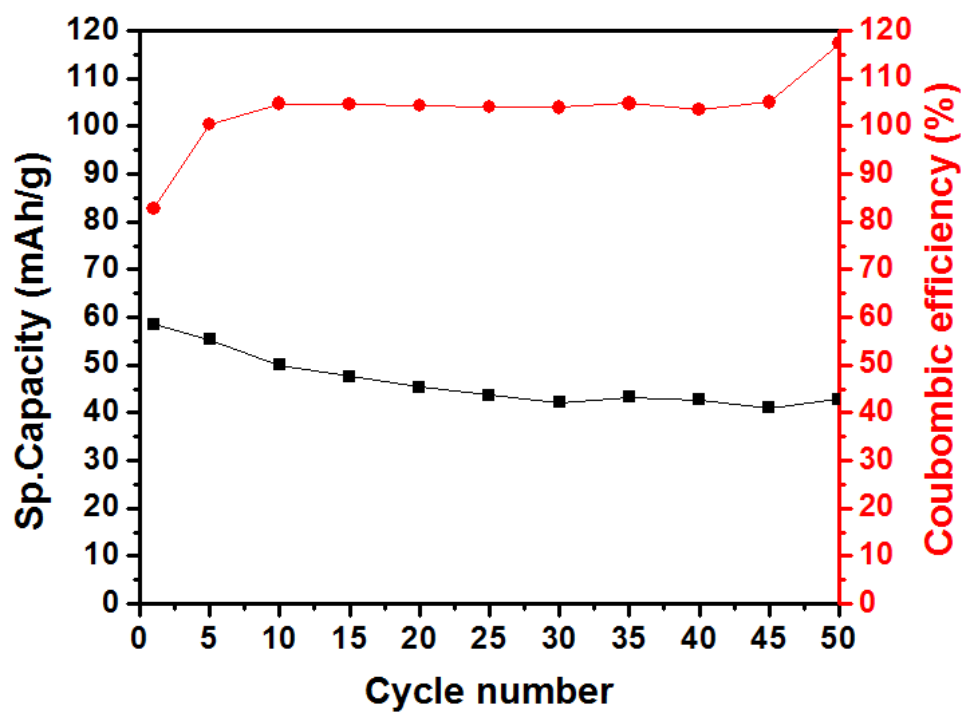


Figure S17. Coulombic efficiency and specific capacity of untreated Benzoic-PDI at 1 C rate as a function of cycle number.

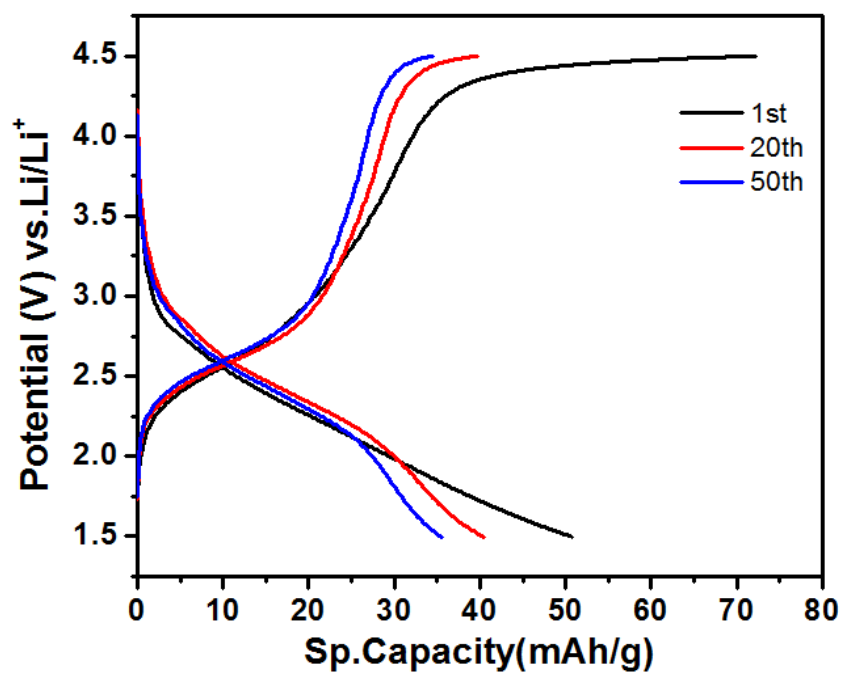


Figure S18. Charge-Discharge curves of untreated Benzoic-PDI at 2 C rate.

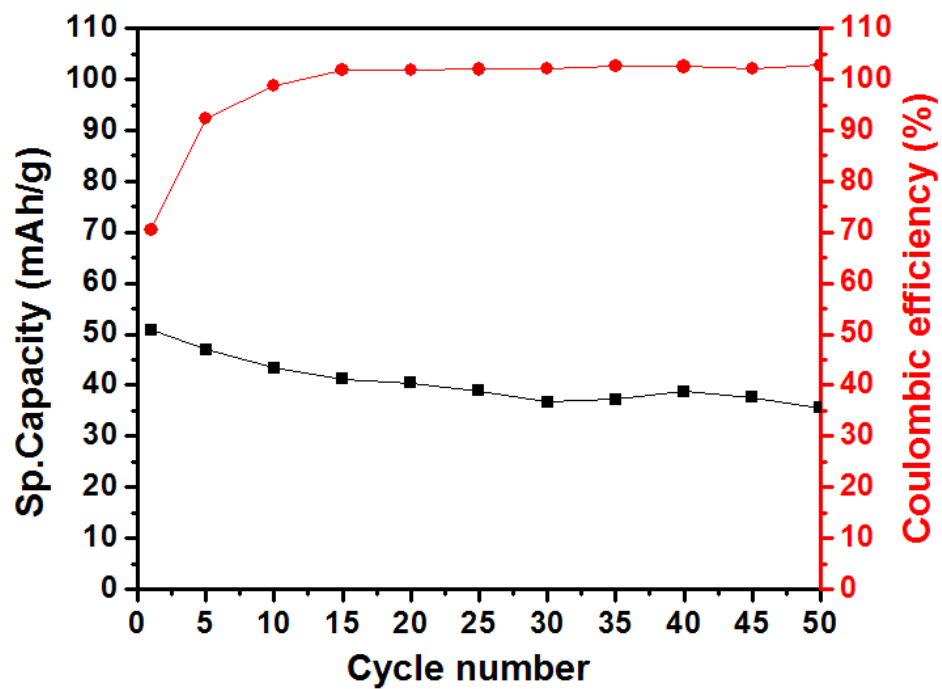


Figure S19. Coulombic efficiency and specific capacity of untreated Benzoic-PDI at 2 C rate as a function of cycle number.

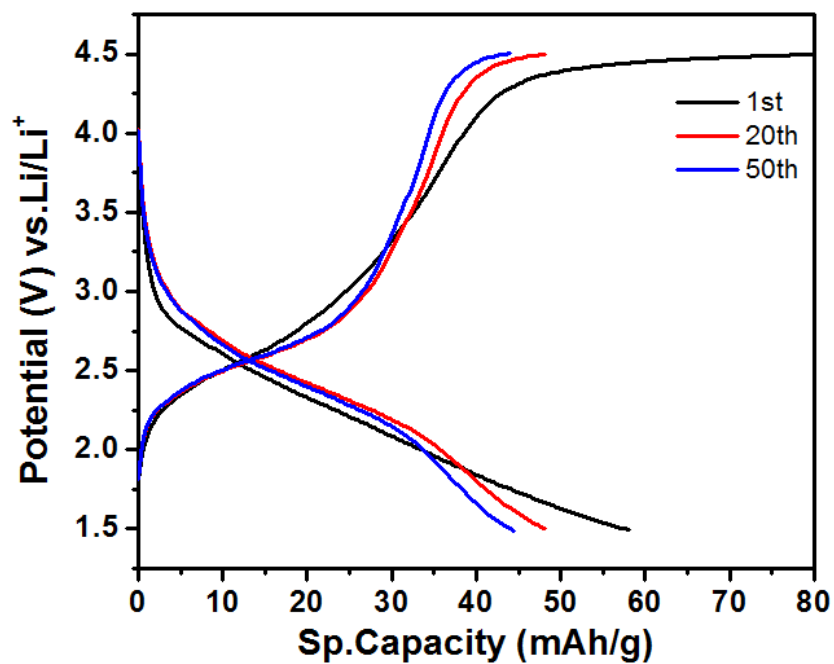


Figure S20. Charge-Discharge curves of untreated Benzoic-PDI at 5 C rate.

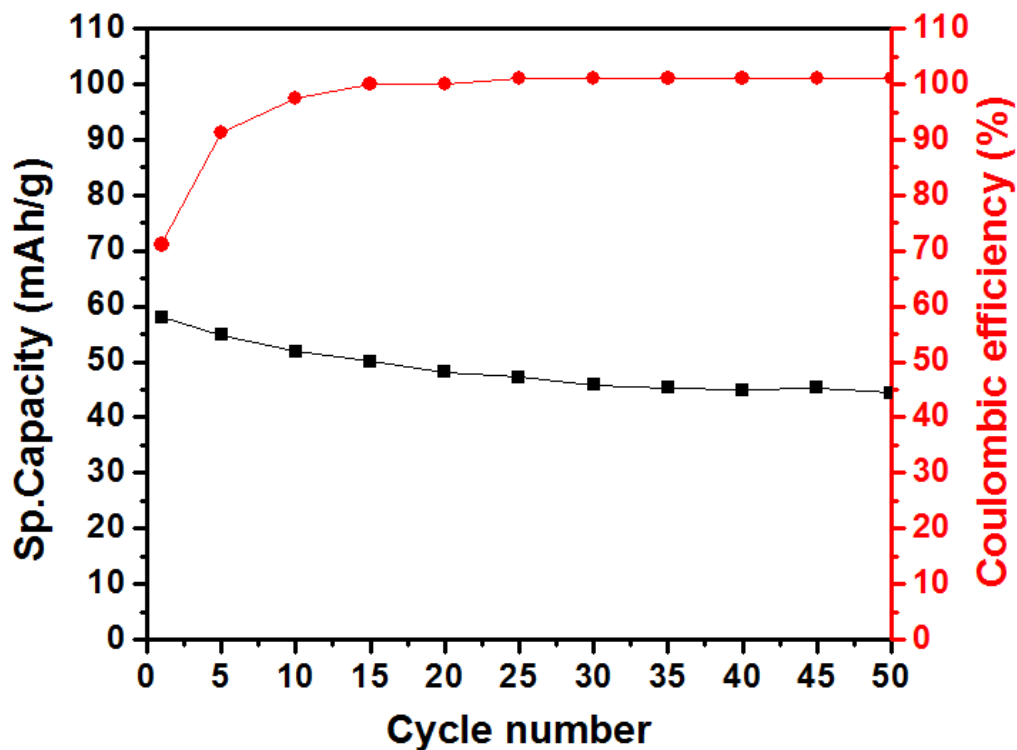


Figure S21. Coulombic efficiency and specific capacity of untreated Benzoic-PDI at 5 C rate as a function of cycle number.

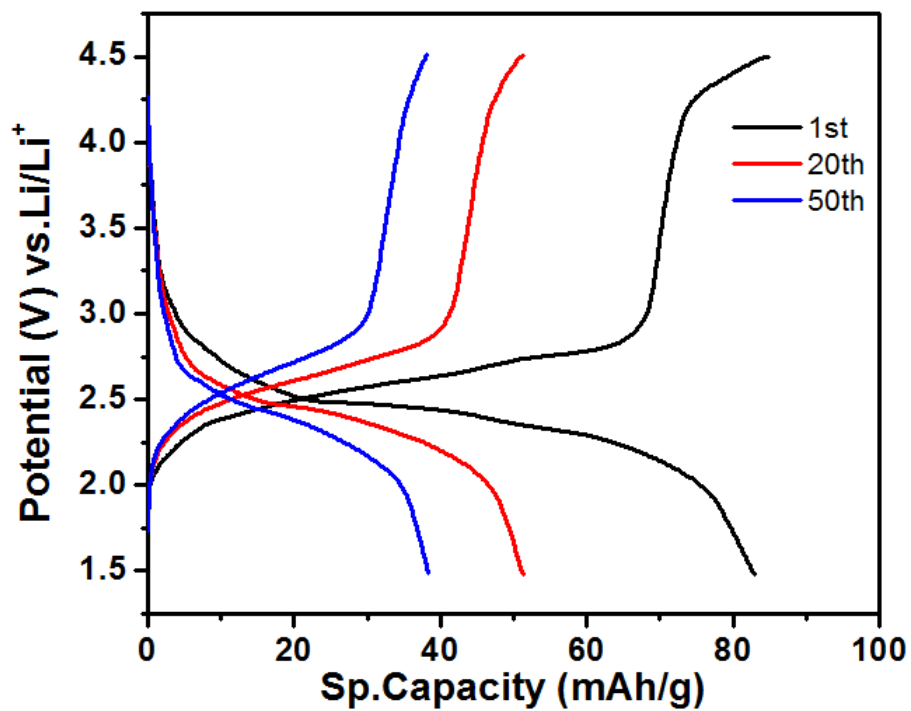


Figure S22. Charge-Discharge curves of reduced Phenyl-PDI at 5 C rate.

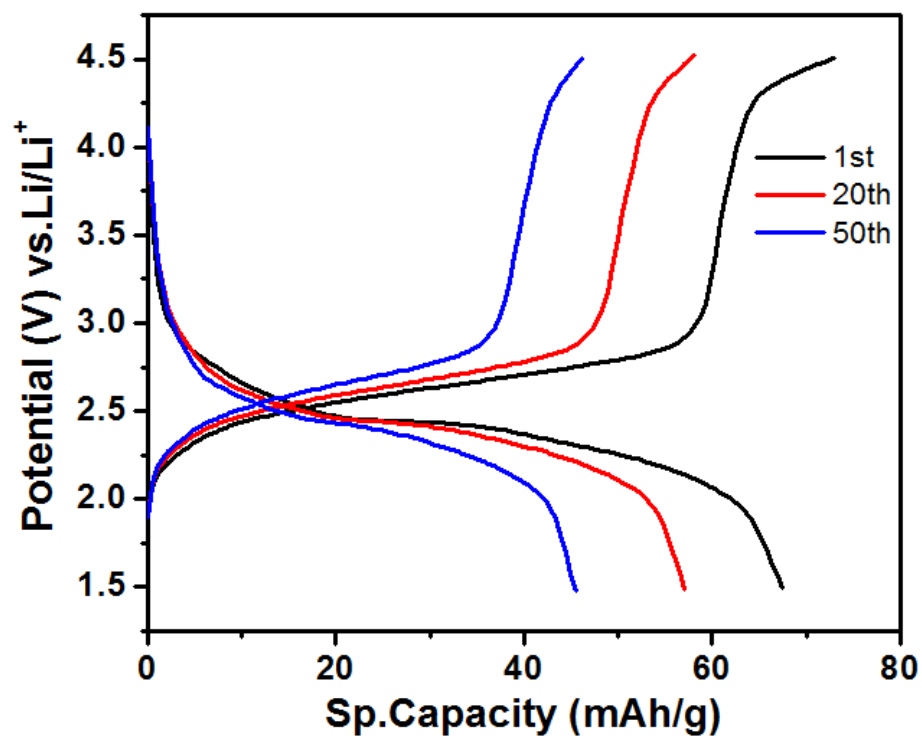


Figure S23. Charge-Discharge curves of reduced Phenyl-PDI at 10 C rate.

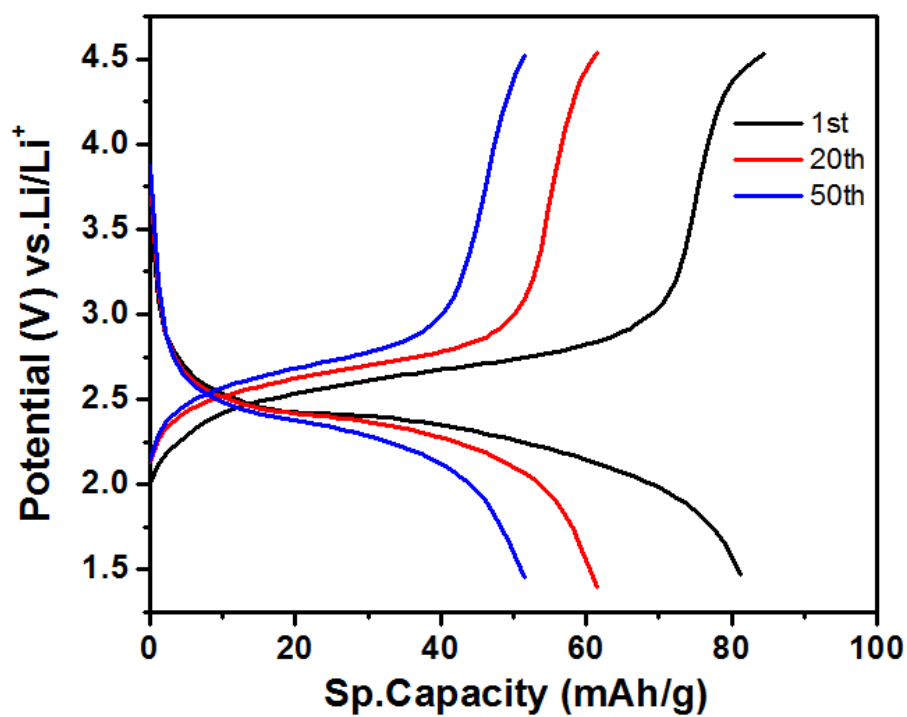


Figure S24. Charge-Discharge curves of reduced Phenyl-PDI at 20 C rate.

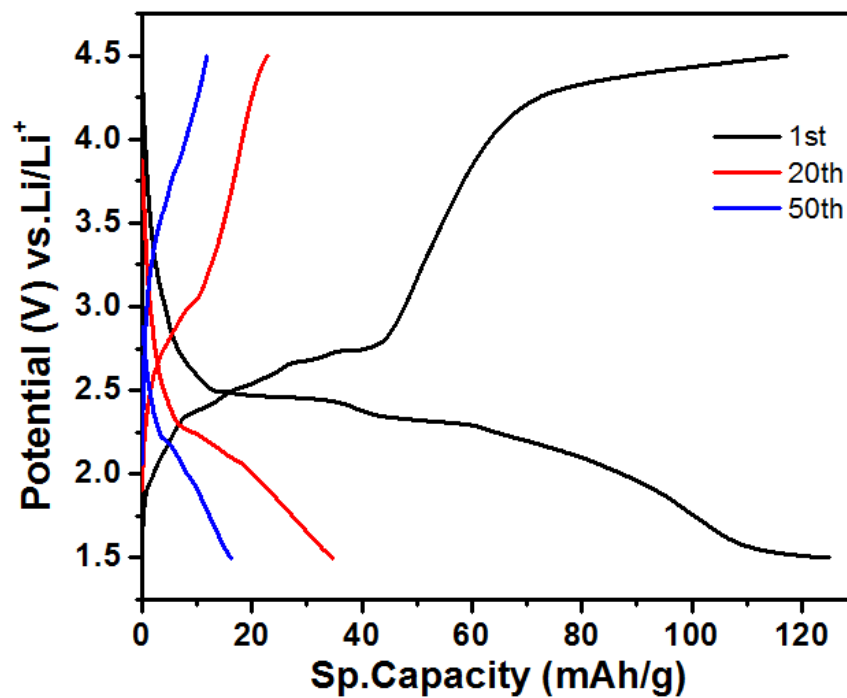


Figure S25. Charge-Discharge curves of untreated Phenyl-PDI at 0.5 C rate.

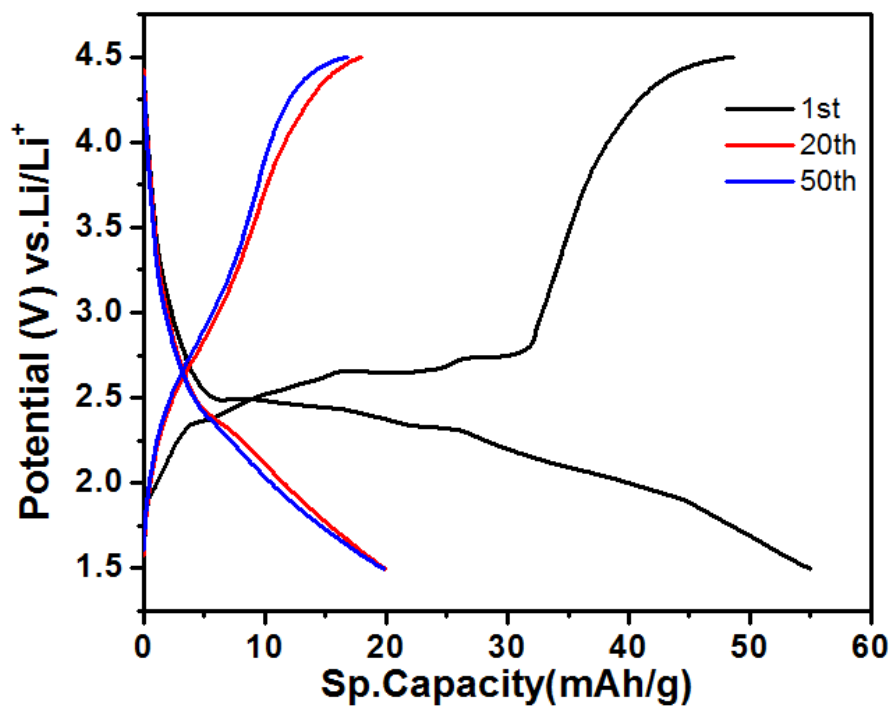


Figure S26. Charge-Discharge curves of untreated Phenyl-PDI at 1 C rate.

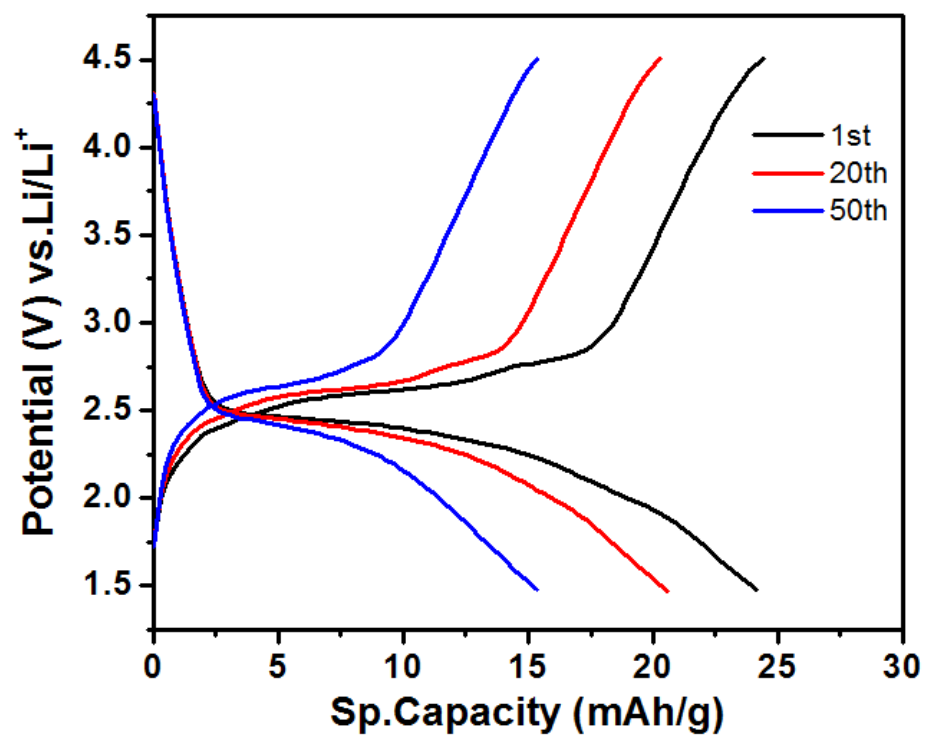


Figure S27. Charge-Discharge curves of untreated Phenyl-PDI at 5 C rate.

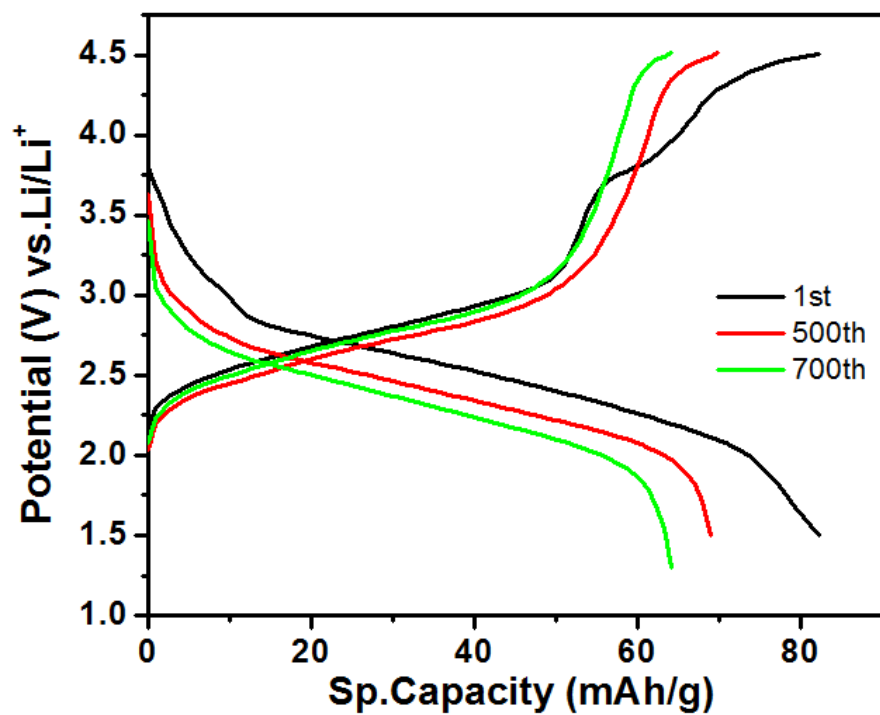


Figure S28. Charge-Discharge curves of reduced Benzoic-PDI at 20C rate.

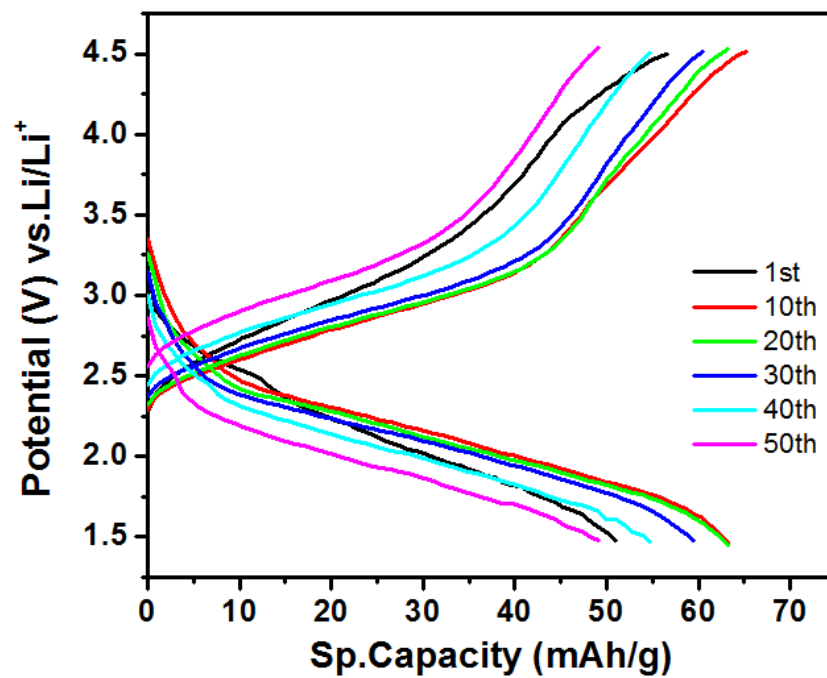


Figure S29. Charge-Discharge curves of reduced Benzoic-PDI at 20C rate of high mass loading (4.5 mg).

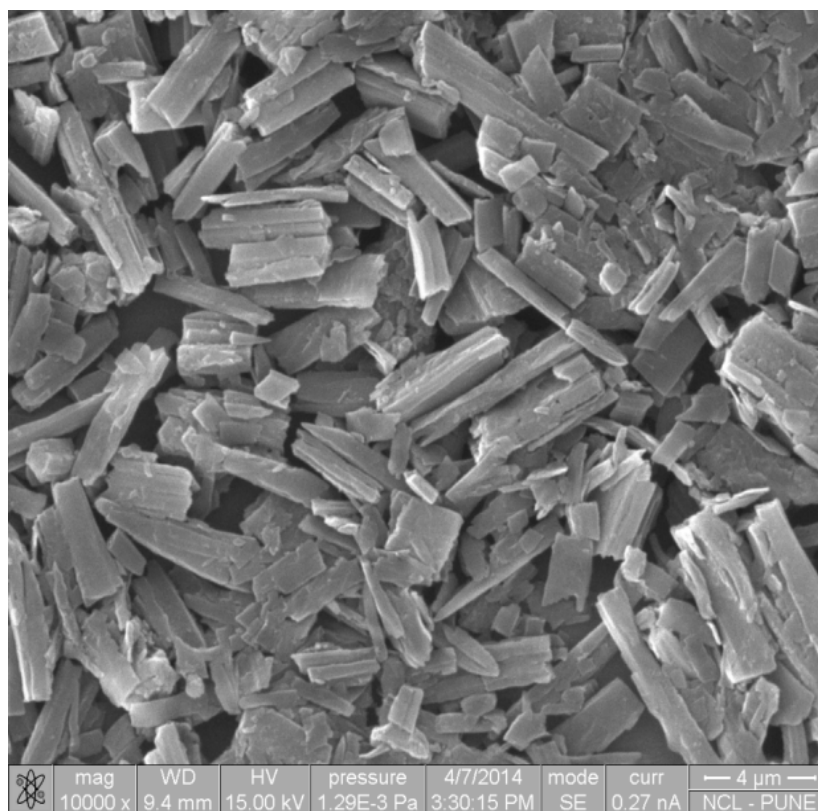


Figure S30. SEM image of untreated Benzoic-PDI.

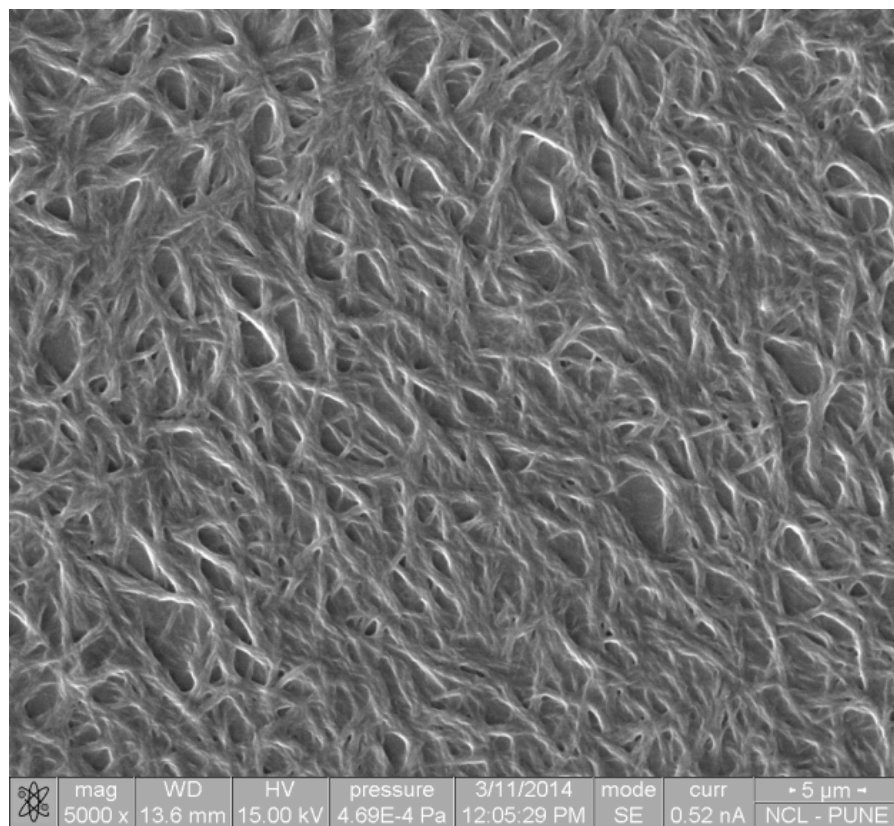


Figure S31. SEM image of reduced Benzoic-PDI.

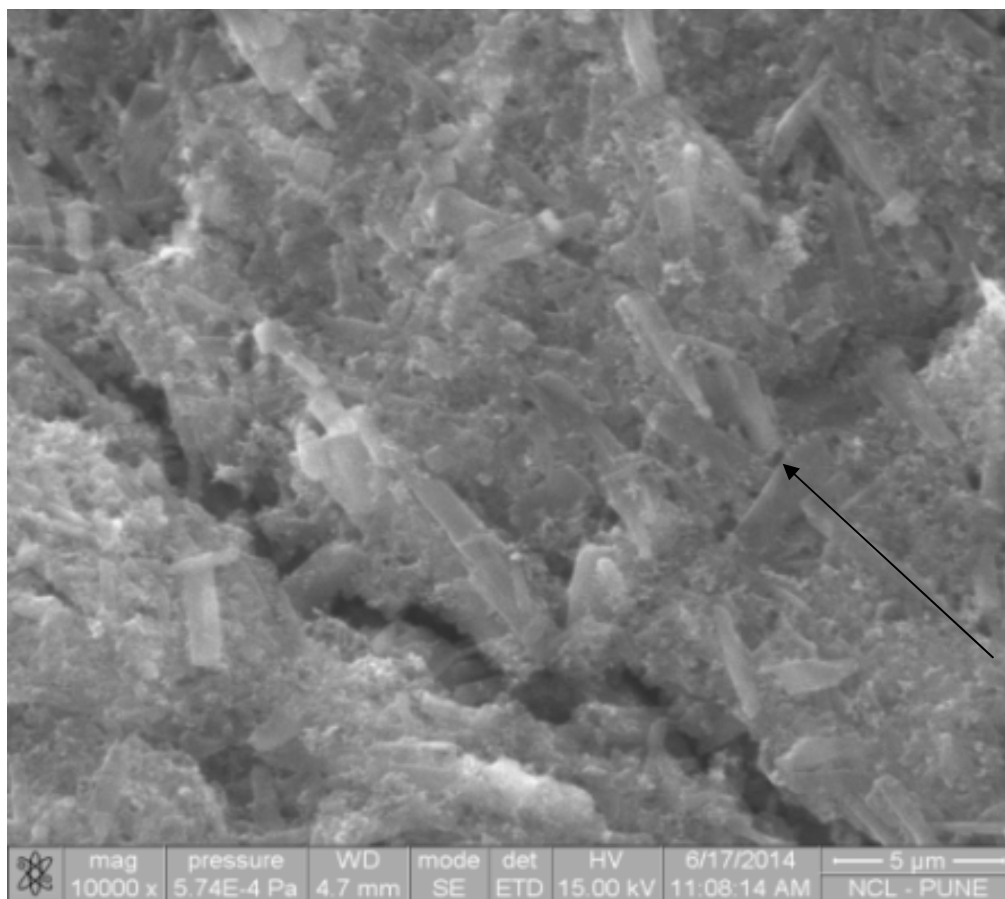


Figure S32. SEM image of untreated Phenyl-PDI before charge discharge cycling.

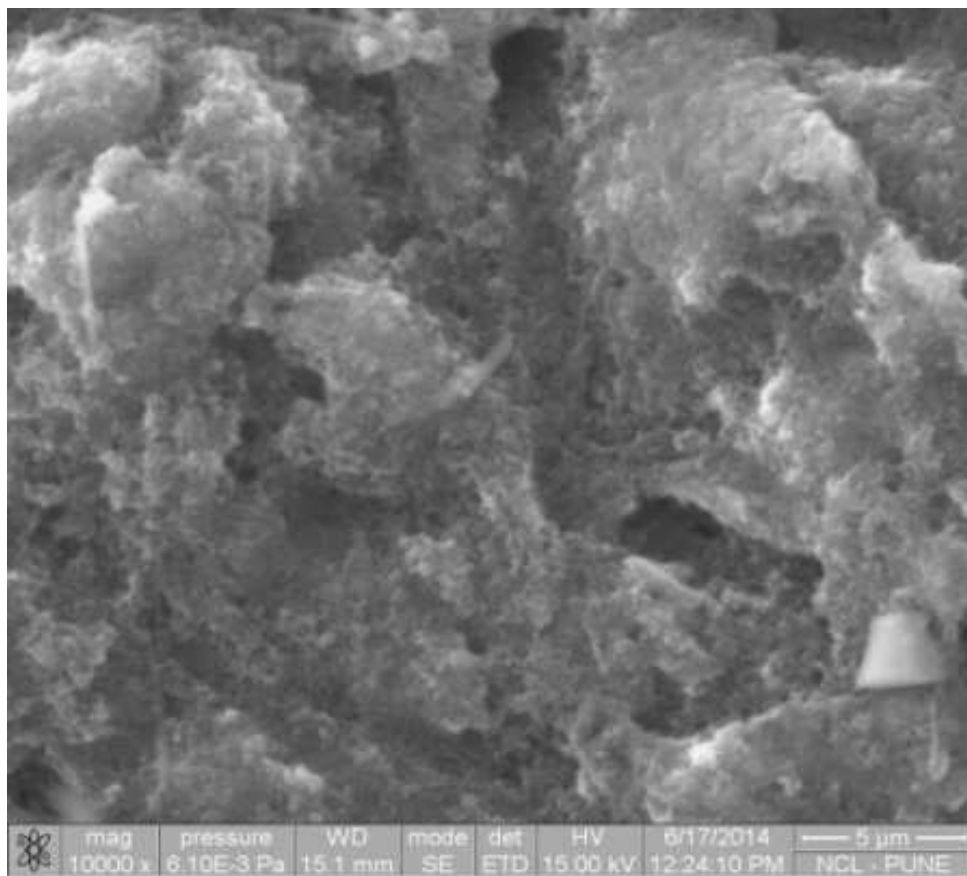


Figure S33. SEM image of untreated Phenyl-PDI after charge discharge cycling.

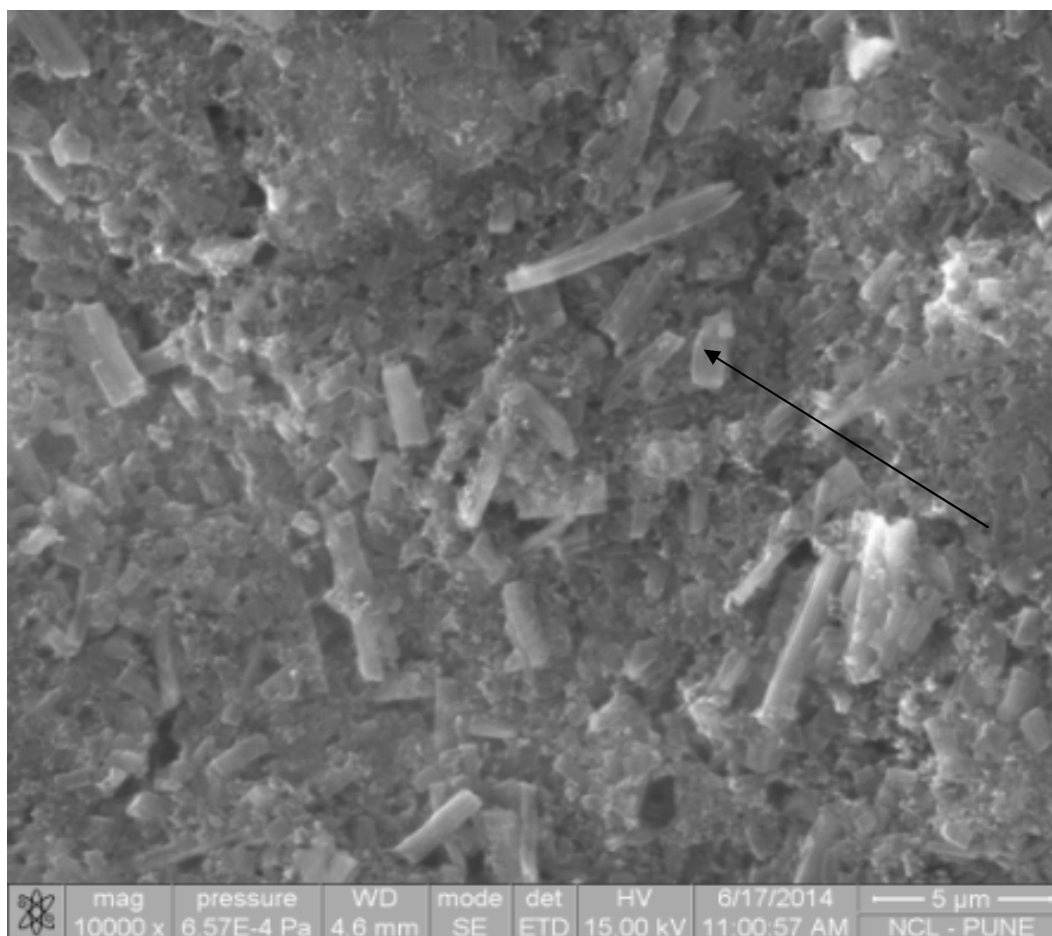


Figure S34. SEM image of untreated Benzoic-PDI before charge discharge cycling.

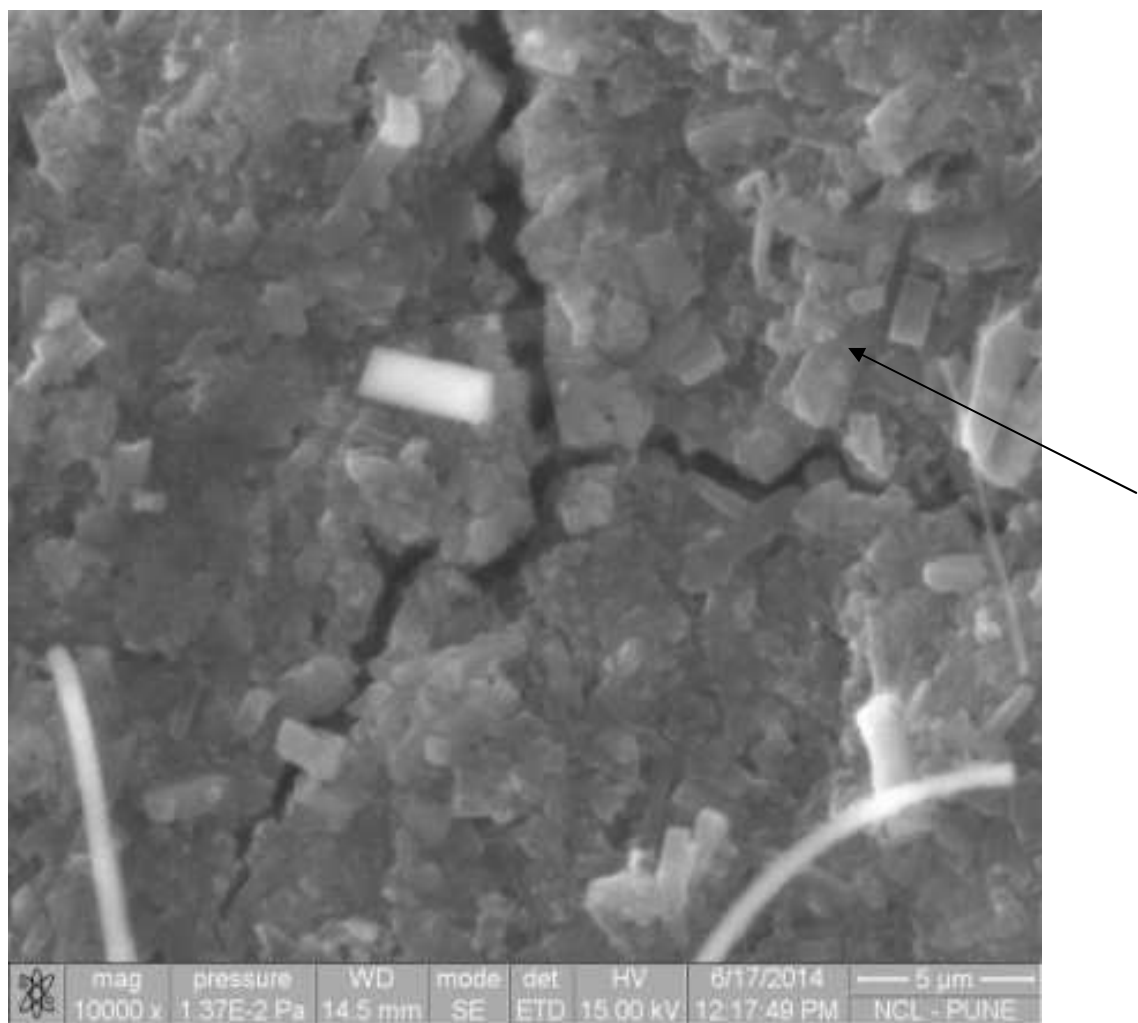


Figure S35. SEM image of untreated Benzoic-PDI after charge discharge cycling.

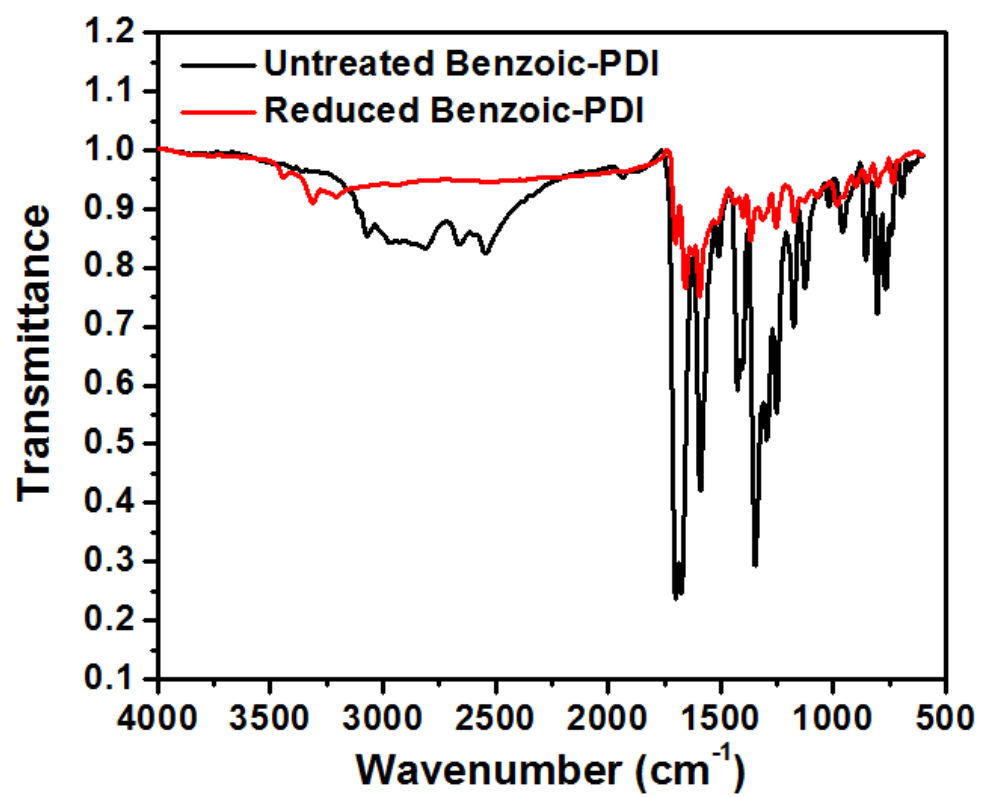


Figure S36. FTIR of untreated and reduced Benzoic-PDI.

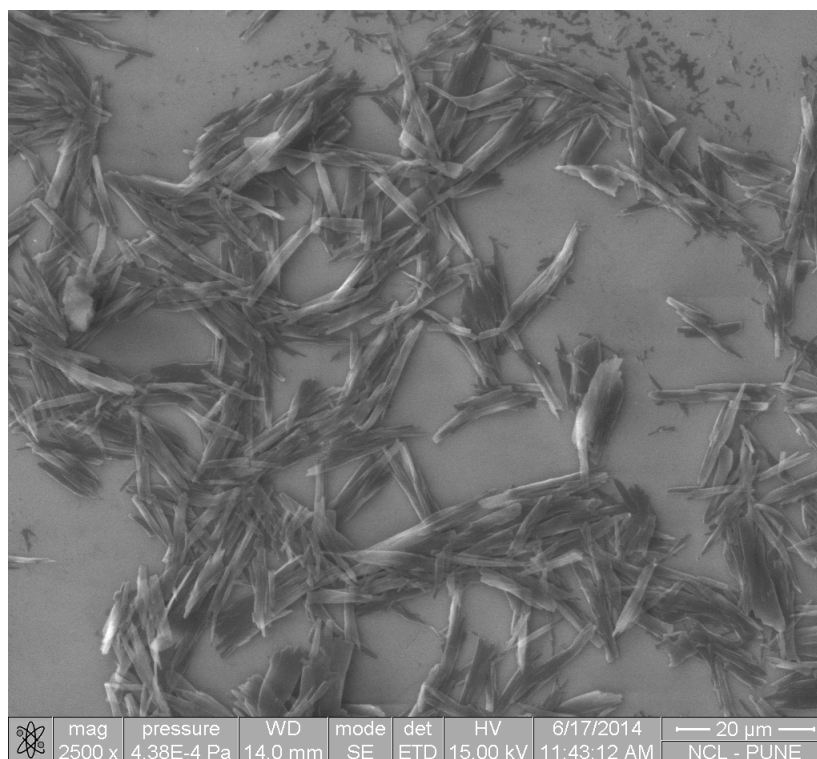


Figure S37. SEM image of untreated Phenyl-PDI.

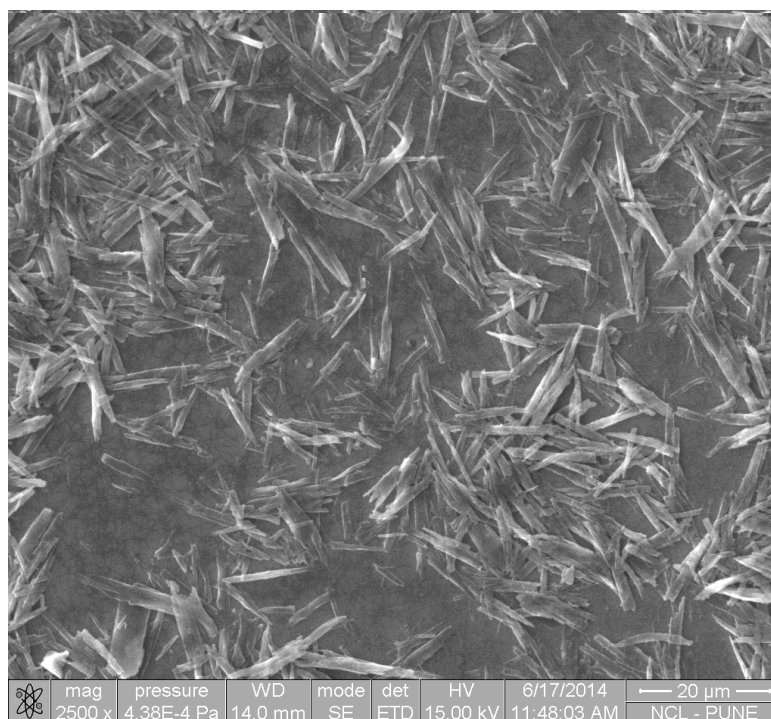


Figure S38. SEM image of reduced Phenyl-PDI.

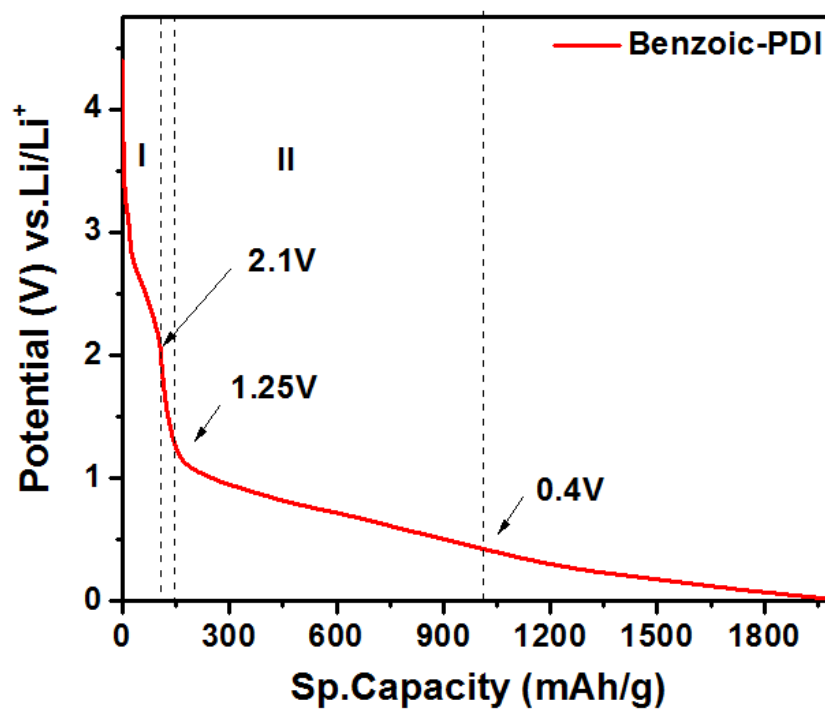


Figure S39. Deep discharge of Benzoic-PDI.



Figure S40. Photograph of interdigitated microelectrodes used for the conductivity measurements.

References

- [1] Han, C.; Li, Z.; Li, W.-J.; Chou, S.-L.; Dou, S.-X. *J. Mater. Chem. A*, **2014**, 2, 11683.
- [2] Wang, B.; Li, X.; Qiu, T.; Luo, B.; Ning, J.; Li, J.; Zhang, X.; Liang, M.; Zhi, L. *Nano Lett.* **2013**, 13, 5578.