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Supporting Information

Graphene wrapped 3,4,9,10-perylenetetracarboxylic dianhydride as high-performance organic cathode for lithium ion batteries

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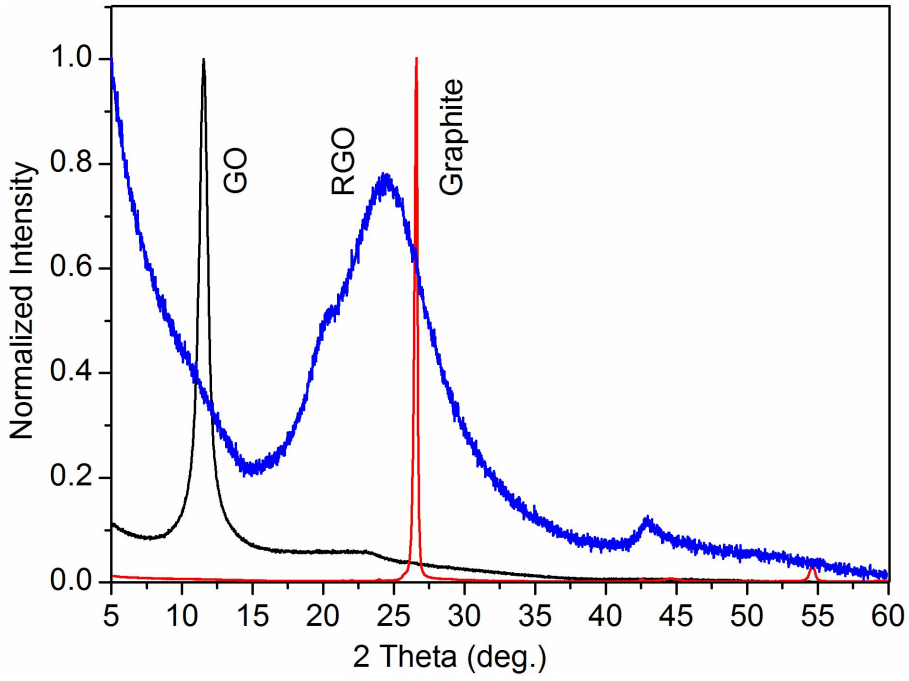

Fig. S1 XRD patterns of natural flake graphite, pre-formed GO and the rGO that prepared by thermal reduction at 400 °C.

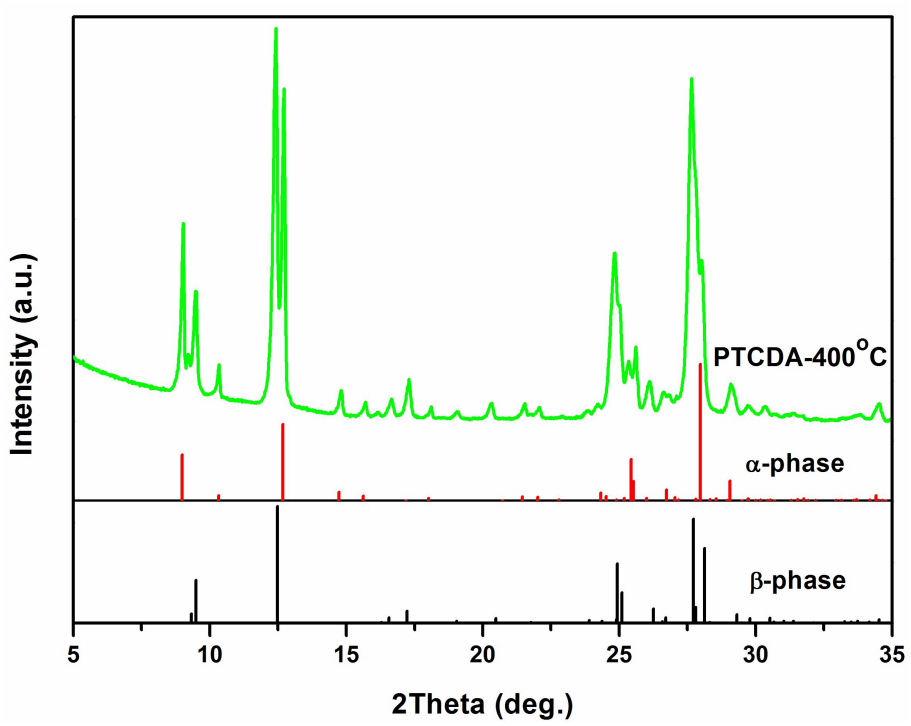

Fig. S2 XRD patterns of 400 °C treated bare PTCDA. The XRD patterns clearly demonstrate the existence of a portion of α phase PTCDA, which also displayed a monoclinic $P2_1/c$ space group. It's evident that the phase transformation occurred at 400 °C and thus give a different XRD patterns for 400 °C treated PTCDA/rGO composite. However, the 400 °C treated bare PTCDA showed no obvious improvement in electrochemical performance compared to pristine PTCDA.

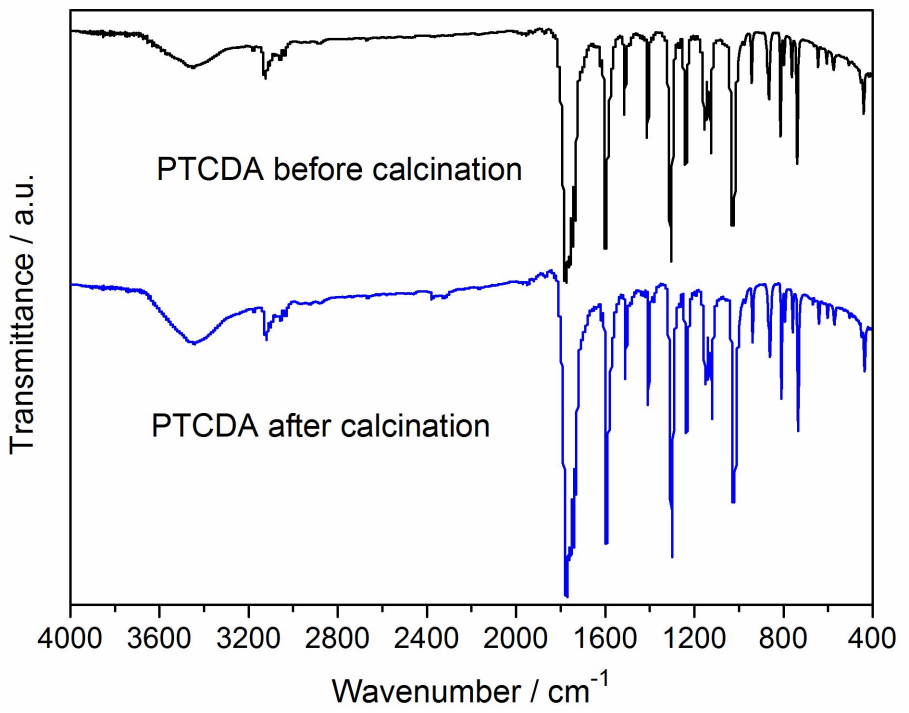

Fig. S3 IR spectra of pristine PTCDA before and after calcination at 400 ºC. The spectra for 400 ºC treated PTCDA show high consistency with pristine PTCDA, indicating the unchanged chemical structure of PTCDA in the PTCDA/rGO composites.

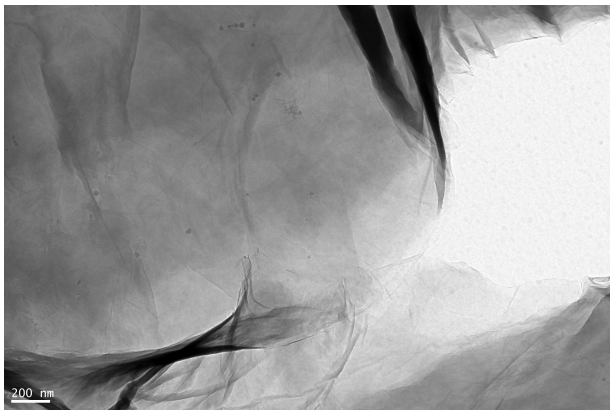

Fig. S4 TEM image of the pre-formed GO nanosheets. It clearly present a sheet-like morphology with multilayer GO nanosheets corrugated together.

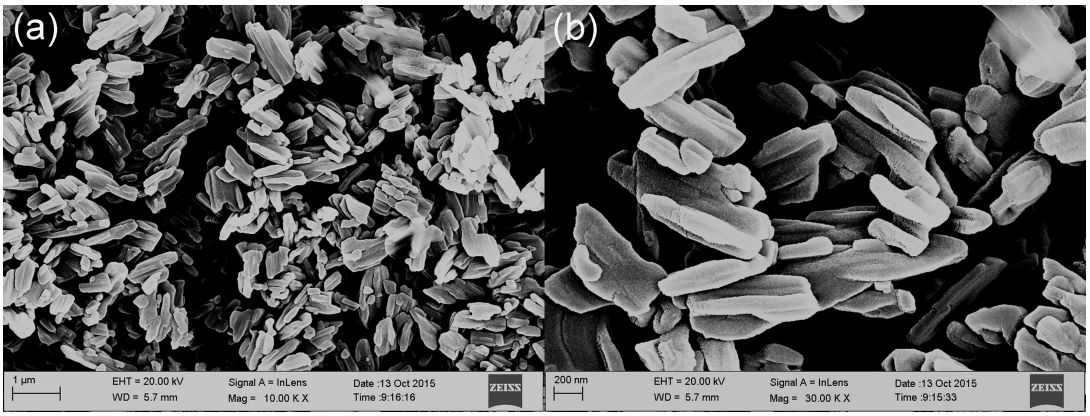

Fig. S5 SEM images of the pristine PTCDA particles. The rod-like pristine PTCDA particles are about 1 μm in length and 200 nm in diameter, and adjacent PTCDA particles are loosely stacked together.

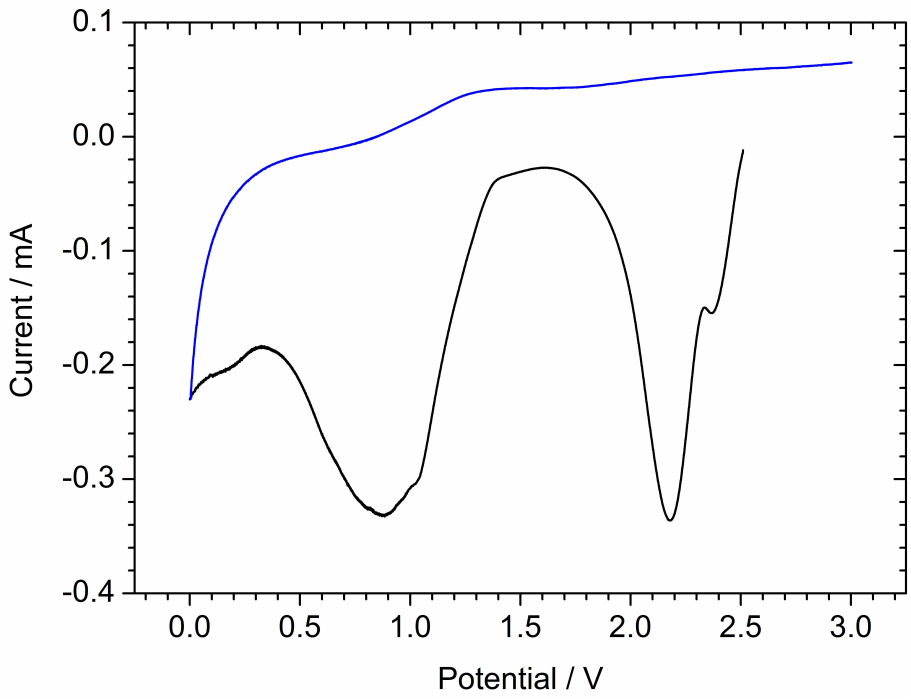

Fig. S6 CV curves of PTCDA electrode in the potential range of 0.01-3 V at a scan rate of 0.1 mV S^{-1}. The black and blue curves are CV profiles of the initial half cycle of discharge and the subsequent charge half cycle, respectively. Obvious cathodic peaks can be observed in the initial half cycle, which are corresponding to lithium enolization reaction at the carbonyl oxygens and the electrochemical reaction of lithium insertion on the unsaturated carbons of C_6 rings. In addition, only few weak anodic peaks can be observed in the following charge half cycle, confirming the irreversibility of the electrochemical behavior in this low potential range.

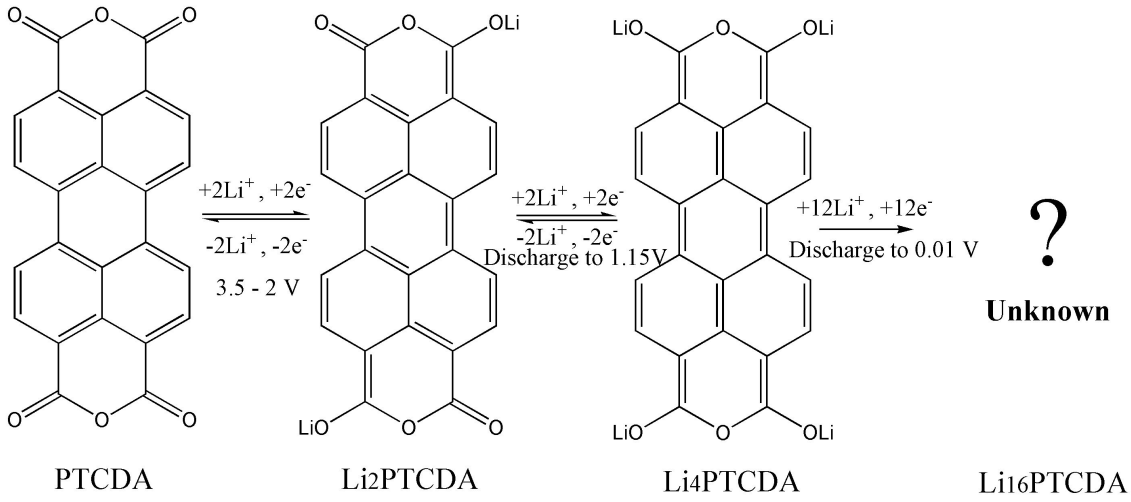

Fig. S7 Schematic illustration for the proposed electrochemical reactions during Li-ion insertion/deinsertion in PTCDA. And the PTCDA electrode exhibit a multi-step Li insertion process when deep discharged to 0.01 V. About 12 Li ions are gradually incorporated by the unsaturated carbons of C_6 aromatic rings in the potential range of 1.15-0.01 V, resulting in the formation of Li_{16}PTCDA, but the exactly molecular structure is unknown.

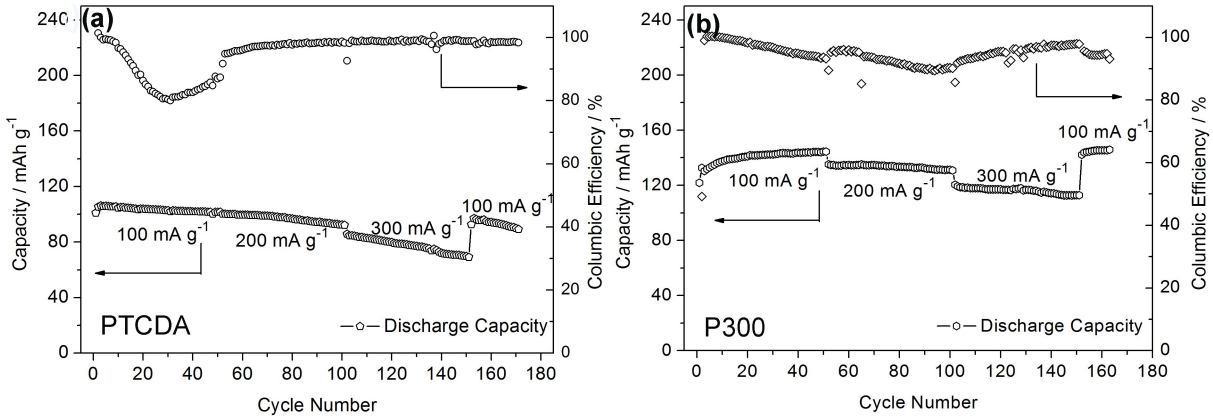

Fig. S8 Rate capabilities of (a) pristine PTCDA and (b) P300. The rate performance of bare PTCDA was significantly improved by rGO wrapping.

Table S1 Comparison of the electrochemical performances of rGO wrapped PTCDA with other organic cathodes that are relevant to PTCDA.

Electrode material	Theoretical capacity [mAh g^{-1}]	Current rate [mA g^{-1}]	Discharge potential [V vs Li/Li^+]	Capacity 1st cycle [mAh g^{-1}]	Capacity retention [%] (cycle number)	Capacity [mAh g^{-1}] (cycling rate)	Ref.
PTCDA/rGO	273	100	2.5, 2.35	138	123% (200)	130 (1.83C), 100 (3.66C)	
Sulfide PTCDA	273	100	2.4	131	113% (250)	N/A	7
UP	116	50	2.43	80	162% (50)	90 (1.7C)	9
EDP	106	50	sloping curve	85	88.2% (50)	20 (0.95C)	9
HP	197	50	2.7, 2.3	130	84.6% (50)	100 (1C)	9
Reduced benzoic-PDI	85	425	sloping curve	90	88% (200)	100 (20C), 68 (30C)	10
PTCDA/CNT	273	100	2.4	122	74% (300)	120 (1C), 115 (2C)	11
PI/CNT	N/A	100	sloping curve	115	93% (300)	N/A	11