Electronic Supplementary Material (ESI) for Energy Advances.

Van der Waals Gap modulation of Graphene oxide through Mono-Boc ethylenediamine Anchoring for Li-ion Batteries

Sneha Mandal, [1] Vijayamohanan K. Pillai, *[1] Mano Ranjana Ponraj, [2] Thushara Nair, [2] Jebasingh Bhagavathsingh*[2] Stephan L. Grage,[3] Xihong Peng,[4] Jeon Woong Kang,[5] Dorian Liepmann,[6] Arunachala Nadar Mada Kannan,[7] Velmurugan Thavasi,[8] and Venkatasan Renugopalakrishnan[9]

1. Department of Chemistry, Indian Institute of Science Education and Research (IISER), Tirupati, Andhra Pradesh 517507, India.
2. Department of Applied Chemistry, Karunya Institute of Technology and Sciences, Coimbatore, Tamil Nadu 641114, India
3. Karlsruhe Institute of Technology, Institute of Biological Interfaces IBG-2, P.O. Box 3640, 76021 Karlsruhe, Germany
4. College of Integrative Sciences and Arts, Arizona State University, Mesa, AZ 85212, USA.
5. Laser Biomedical Research Centre, G. R. Harrison Spectroscopy Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, United States
6. Dept. of Bioengineering, 80 Hearst Memorial Mining Bldg., University of California, Berkeley, CA 94720
7. The Polytechnic School, Ira A. Fulton Schools of Engineering, Arizona State University, Mesa, AZ 85212, USA
8. Center for Quantum Research and Technology, The University of Oklahoma, 440 W. Brooks Street, Normon, OK 73019, USA
9. Department of Chemistry, Northeastern University, Boston Children's Hospital, Harvard Medical School, Boston, MGB Center for COVID Innovation, MA 02115, USA

Supporting figures:

Figure S1: Digital images of Li-GO-EnBoc electrode fabrication with different concentration of binder (a) 10% (b) 20% and (c) 30%.

A higher percentage of binder has been added to prepare the electrodes as shown in the Figure S1. By varying the percentage of binder, we have optimised the minimum amount of binder required to prepare the thin film electrode.

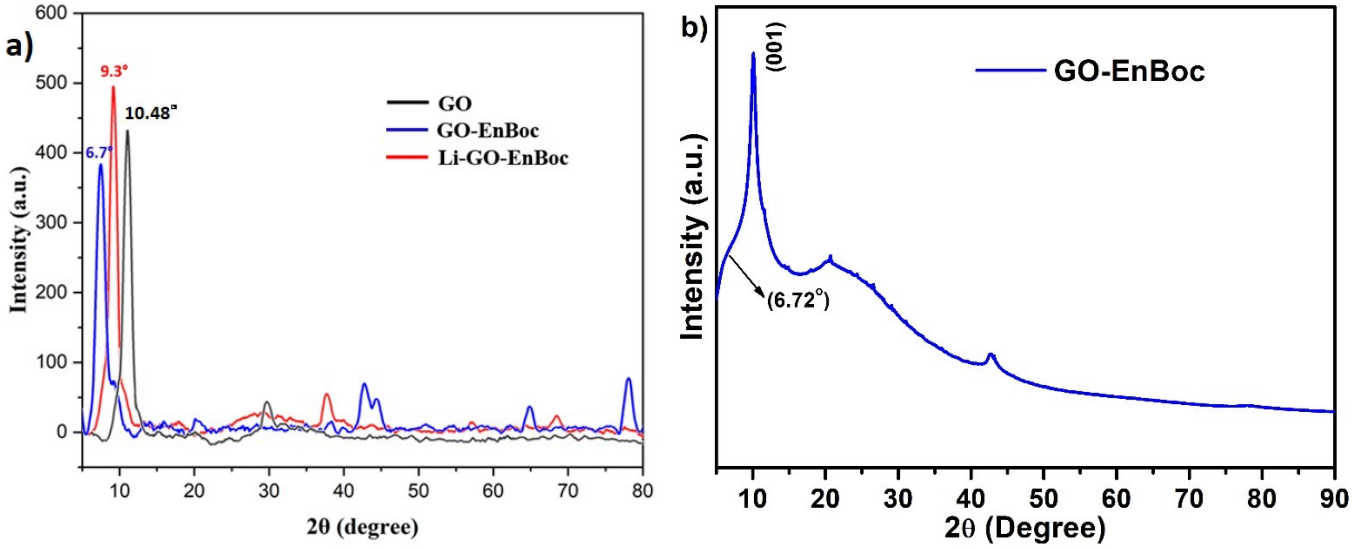


Figure S2: A Comparison of the (a) Powder X-ray Diffraction (XRD) profile of GO, GO-EnBoc, and Li-GO-EnBoc and (b) GO-EnBoc with a scan rate of 0.1° min^{-1}, showing a small hump at 2θ- 6.72°, which probably reflects either the low amount of anchoring or the conformational changes of the EnBoc molecule due to relaxation.

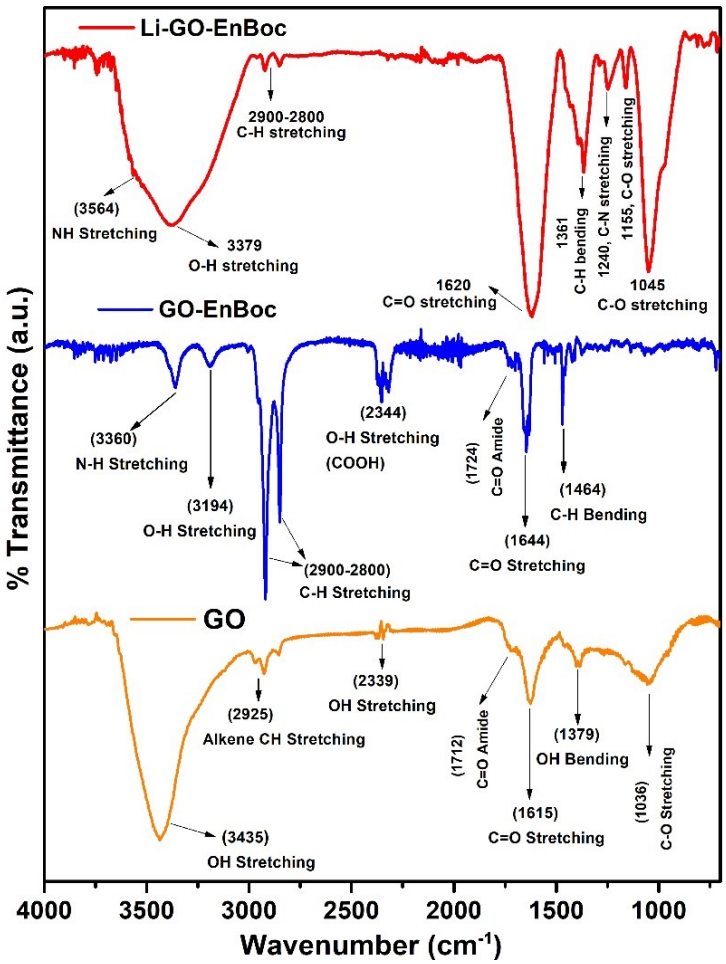
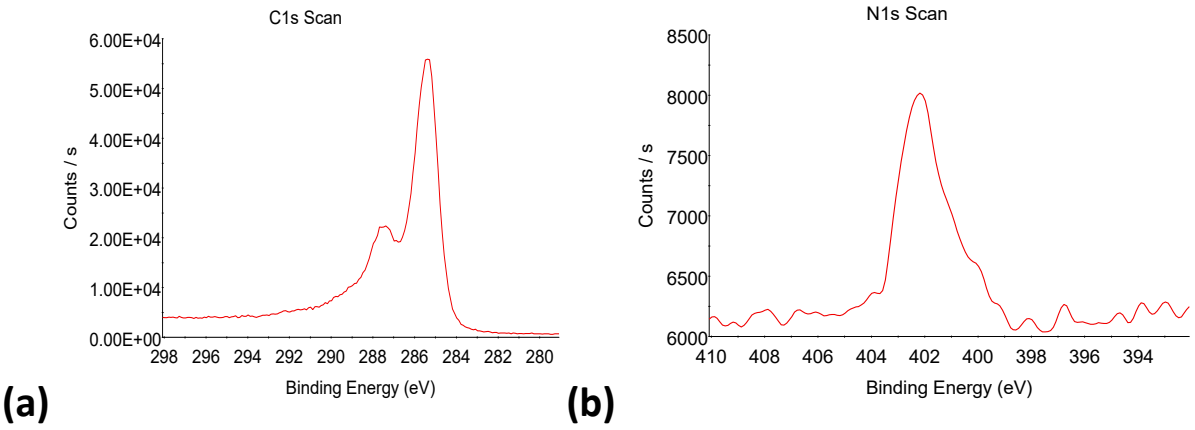
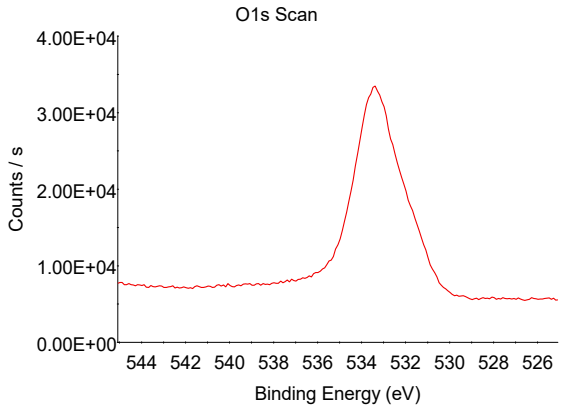


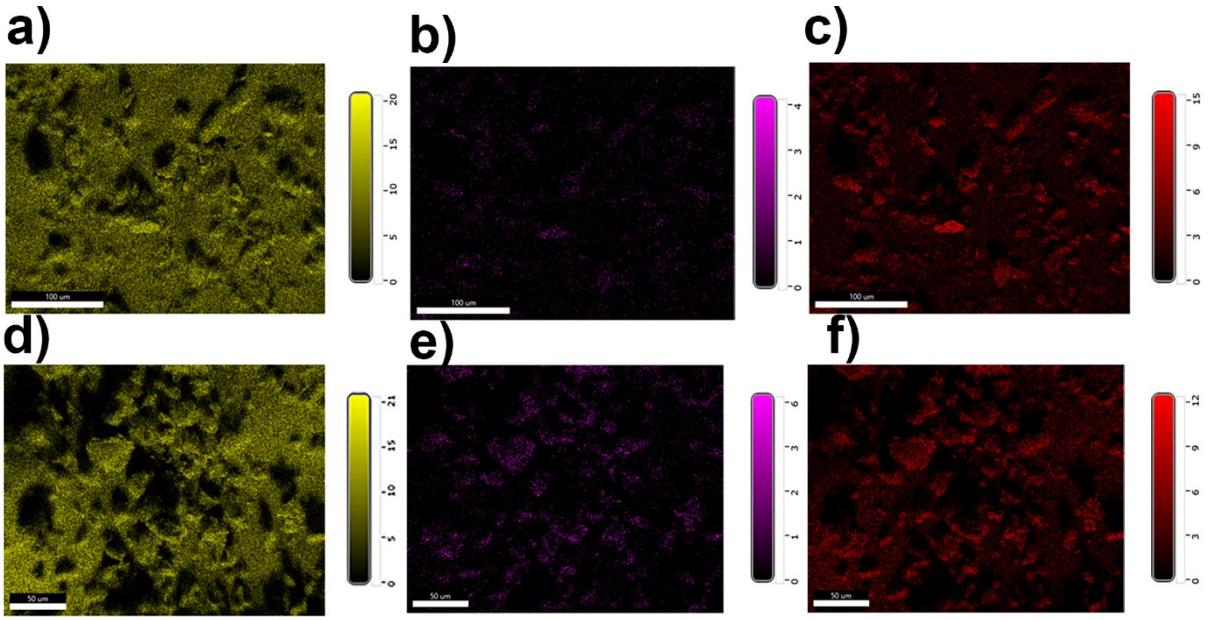
Figure S3: A comparison of the FT-IR spectra of GO, GO-EnBoc and Li-GO-EnBoc to indicate that EnBoc strucitre is intact in the intergallary space but for some minor conformational changes



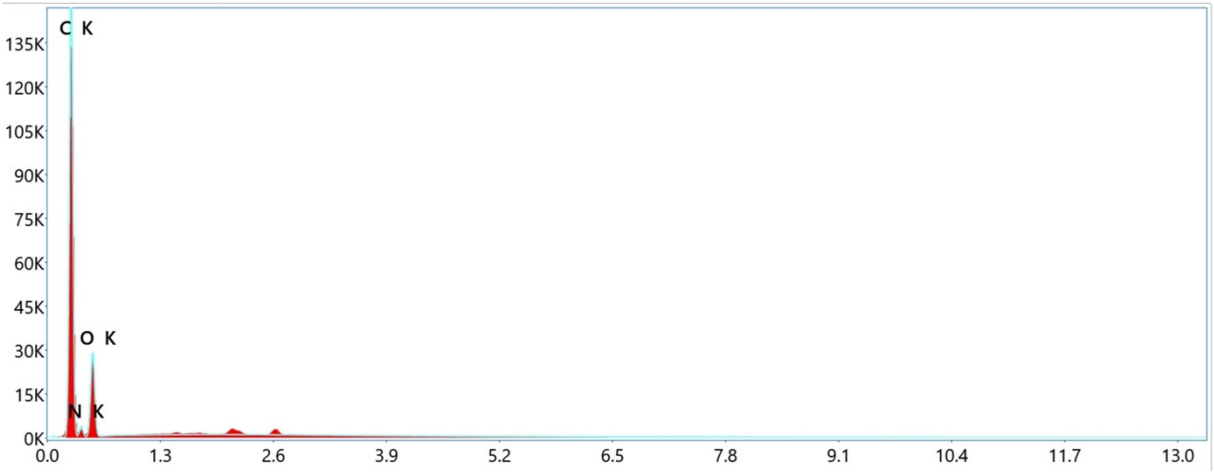


(c)

Figure S4: X-ray Photoelectron Spectra (XPS) of (a) C 1s, (b) N 1s and (c) O 1s core level of GO-EnBoc to reveal the elemental composition and oxidations states



g)



h)

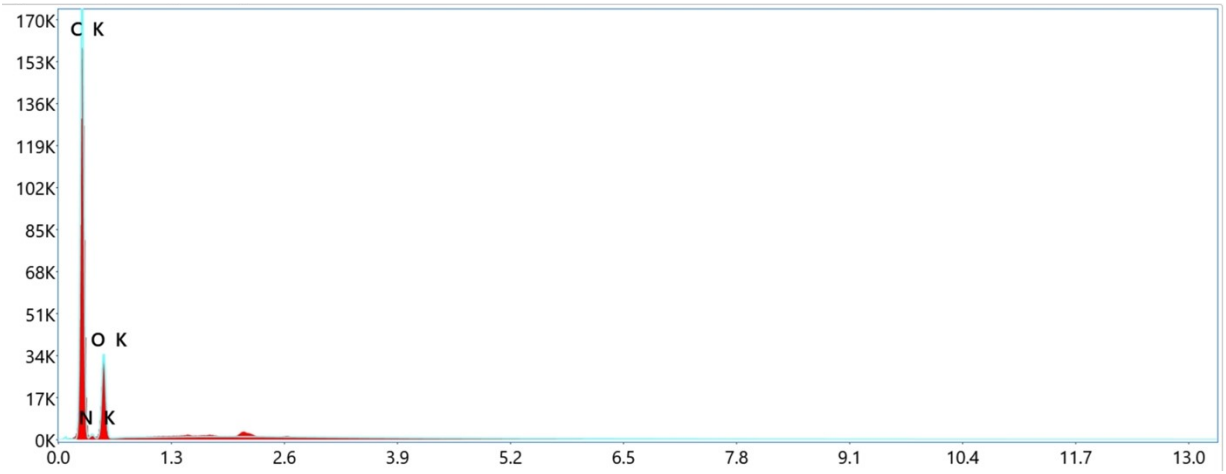


Figure S5: Elemental mapping images of (a,b,c) Li-GO-EnBoc and (d,e,f) GO-EnBoc electrode respectively, (a & d) carbon, (b & e) nitrogen and (c & f) oxygen and the corresponding energy dispersive X-ray (EDX) spectrum of (g) GO-EnBoc and (h) Li-GO-EnBoc.

Table S1- GO-EnBoc

Element	Weight %	MDL	Atomic %	Net Int.
C - K	73.6	0.01	78.2	2332.4
N - K	6.2	0.09	5.7	56.1
O - K	20.2	0.03	16.1	484.5

Table S2- Li-GO-EnBoc

Element	Weight %	MDL	Atomic %	Net Int.
C - K	76.3	0.01	80.9	2774.7
N - K	3.0	0.09	2.7	29.3
O - K	20.7	0.03	16.4	579.3

Table S1 and S2: Comparison of the weight and atomic percentage of the elements present in GO-Enboc and Li-GO-EnBoc respectively.

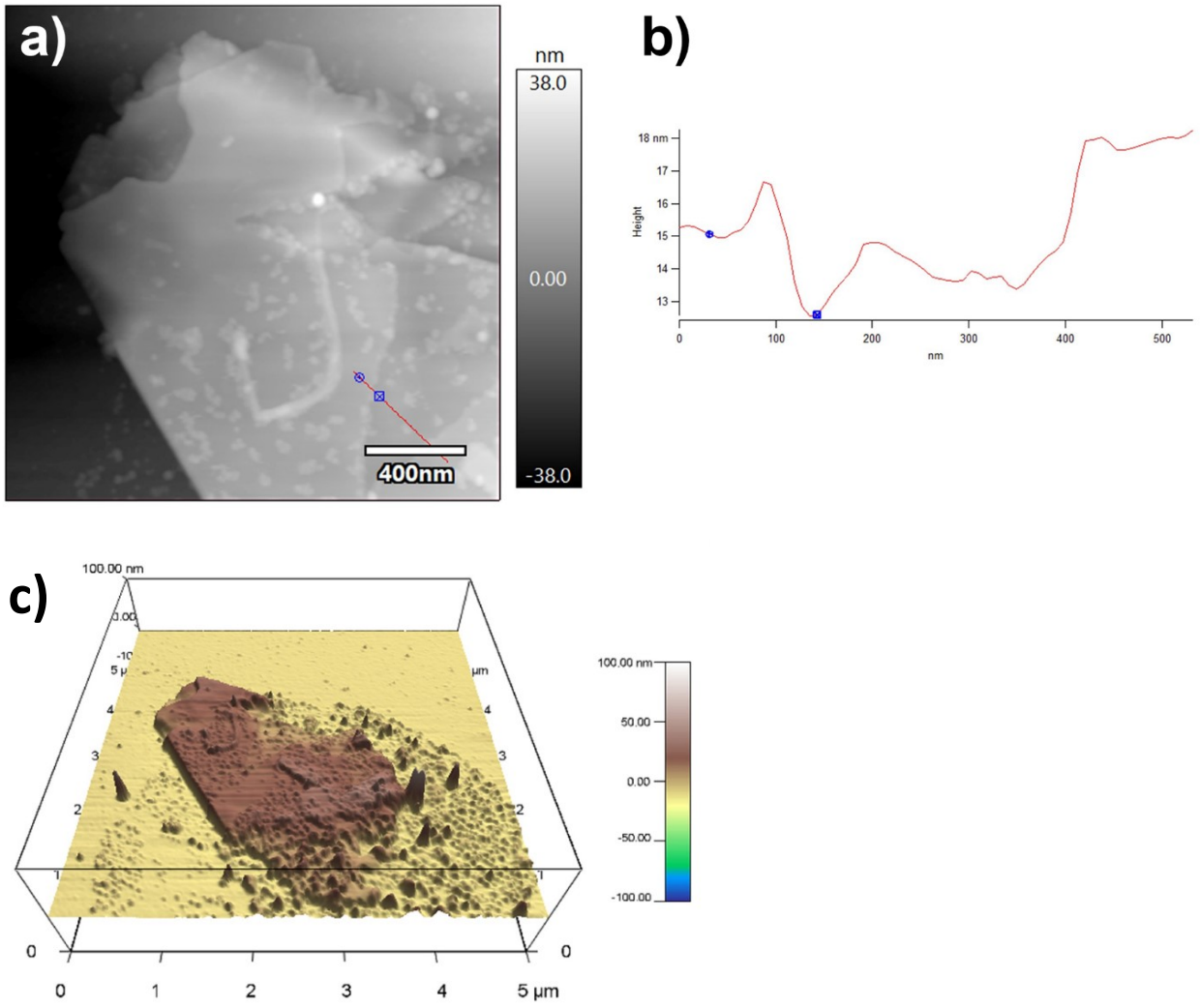


Figure S6: AFM image of (a) Li-GO-EnBoc (b) height profile and (c) Three-dimensional image.

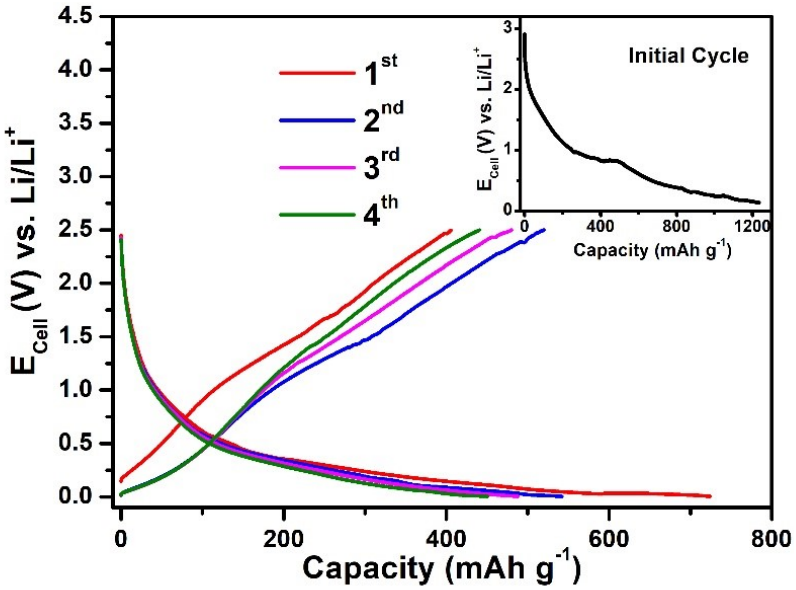


Figure S7: Charge-discharge profiles for GO-EnBoc electrode cycled at 25 mA g^{-1} between 2.5 and 0.005 V vs Li/Li^+ in a 1 M solution of $LiPF_6$ in a 1:1 (*v/v*) mixture of ethylene carbonate (EC) and dimethyl carbonate (DMC) as the electrolyte.

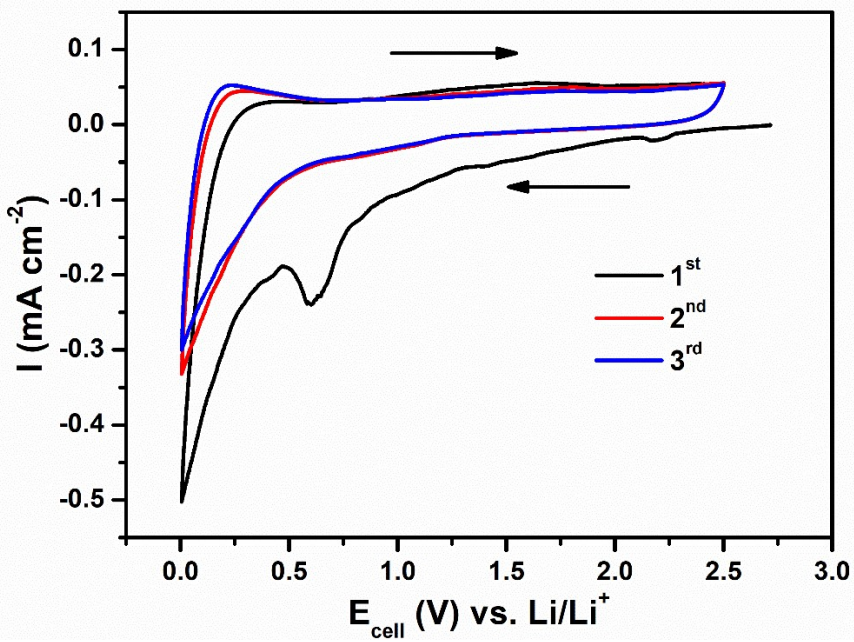


Figure S8: Cyclic voltammograms of GO-EnBoc electrode in a 1 M solution of $LiPF_6$ electrolyte with Li as counter and reference electrode at a scan rate of 0.1 mV s^{-1}.