Electronic Supplementary Information

Synthesis and characterization of bi-functionalized graphene and expanded graphite using n-butyl lithium and their use for efficient water soluble dye adsorption

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Effect of butyl lithium on E-GPT in absence of carbon dioxide

Briefly, to check the effect of n-BuLi on expanded graphite in absence of carbon dioxide, 25 mg of presonicated E-GPT was taken in a reaction vessel. 4 ml of dry THF (Sigma Aldrich, USA) was added prior to sonication. Then to it, 1 ml of n-BuLi (2.5 M in hexane, Sigma Aldrich, USA) was added drop by drop over a period of 20 mins at a temperature of -78°C using OPERON low temperature reactor. The reaction was at -78°C for 40 mins in an inert dry N₂ atmosphere and it was allowed to rotate at room temperature for 5h. Modified material (N-E-GPT) was filtered using 0.22µm PTFE membrane filter paper under normal room condition and dried in oven for further analysis.

In order to accentuate the changes taken place, Infrared spectroscopy was done in KBr technique as shown in Figure S1.



Figure S1: FTIR spectra of N-E-GPT

Interestingly, the anionic centres generated due to effect of n-BuLi on graphene, scavenged the moisture present in atmosphere leading to hydroxyl functionalized graphite as soon as it was exposed to room condition after completion of reaction. Butyl functionalization also took place

concurrently as expected. However, in the case of M-E-GPT, no peak for hydroxyl group was observed. This suggest that the anionic centres generated due to basicity of n-BuLi over this graphitic materials successfully scavenges all the carbon dioxide during preparation of M-E-GPT.

Survey spectra of XPS



Figure S2: XPS survey of (a) GS, (b) M-GS, (c) E-GPT and (d) M-E-GPT.

Table S1: Absorbance of butyl group and carbonyl group at different time.

Time (mins)	Absorbance Butyl	Absorbance Carbonyl
30	0.60	1.10
60	1.24	1.76
120	1.95	1.97
300	2.8	2.72

Table S2: Absorbance maxima of various CVL sets prepared

Sample	Absorbance Value at 264 nm
CVL	0.777
CV1	0.664
CV2	0.441
CV3	0.278
CV4	0.223