

## **Supplementary Information**

### **Boron from net charge acceptor to donor and its effect on hydrogen uptake by novel Mg-B-electrochemically synthesized reduced graphene oxide**

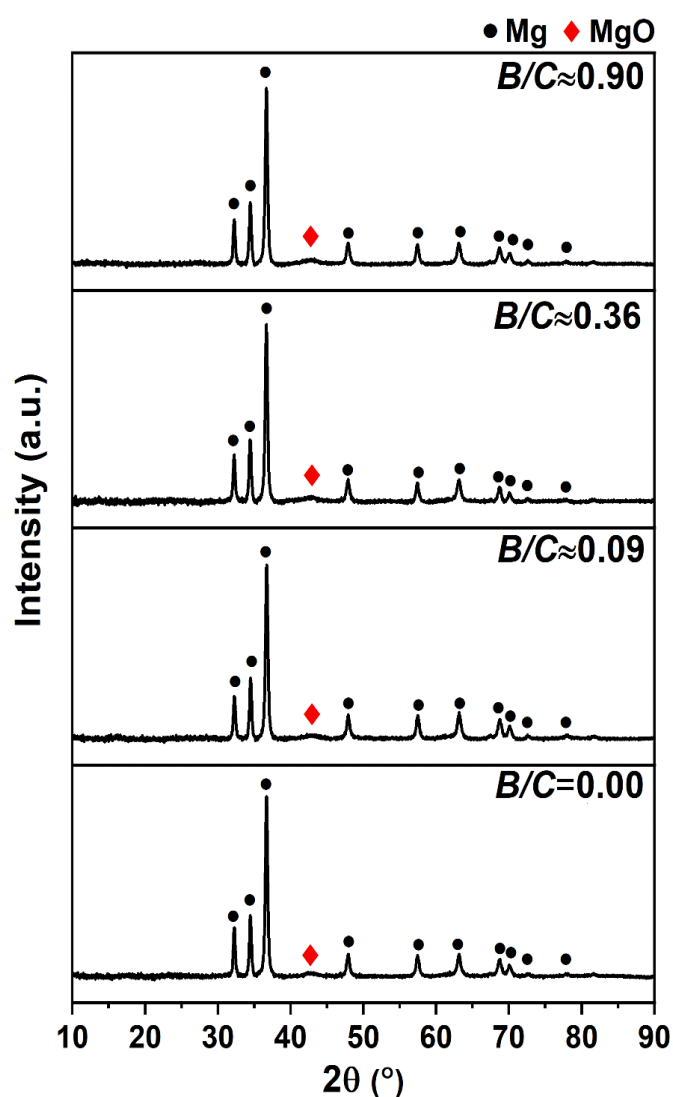
Marla V V Satya Aditya, Srikanta Panda, and Sankara Sarma V Tatiparti\*

Department of Energy Science & Engineering, Indian Institute of Technology Bombay,  
Mumbai 400076, India

**\*Corresponding author E-mail: [sankara@iitb.ac.in](mailto:sankara@iitb.ac.in)**

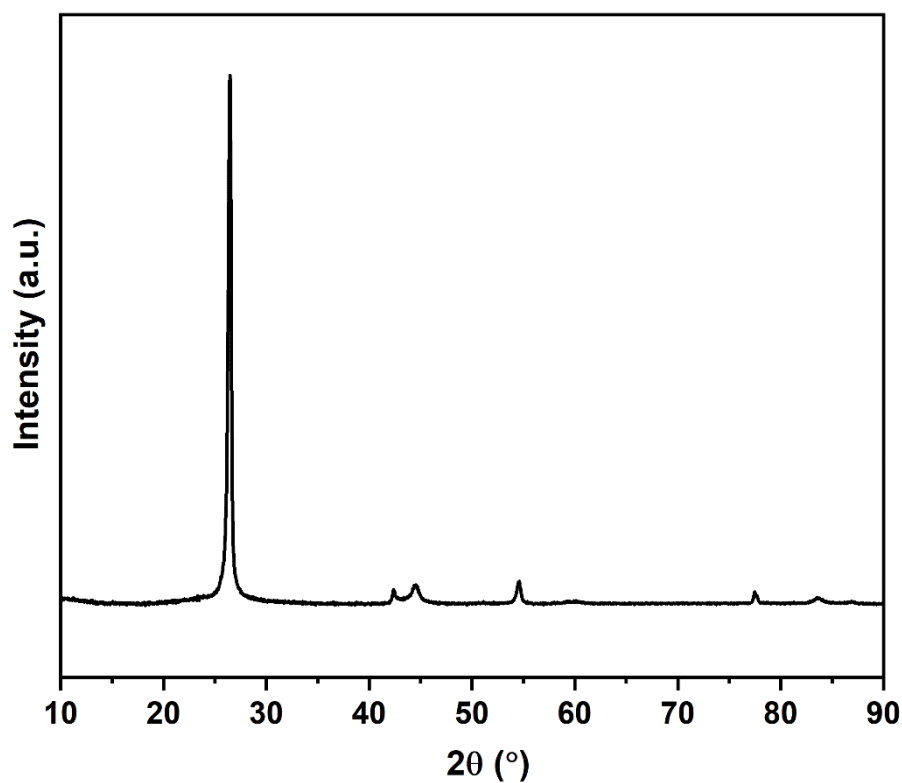
## X-ray diffraction (XRD)

XRD patterns of magnesium (Mg)-boron (B)-electrochemically synthesized reduced graphene oxide (erGO) nanocomposites are shown in Fig. S1. The peaks at  $\sim 32.2^\circ$ ,  $\sim 34.4^\circ$ ,  $\sim 36.6^\circ$ ,  $\sim 47.8^\circ$ ,  $\sim 57.4^\circ$ ,  $\sim 63.1^\circ$ ,  $\sim 67.3^\circ$ ,  $\sim 68.6^\circ$ ,  $\sim 70.2^\circ$ ,  $\sim 72.5^\circ$ ,  $\sim 77.8^\circ$  and  $\sim 81.5^\circ$  correspond to hexagonal close packed structure (hcp) of Mg phase [ICSD code: 76748]. The minor peak at  $\sim 42.8^\circ$  corresponds to MgO [ICSD code: 104845]. Peaks corresponding to erGO are not seen.



**Figure S1.** XRD patterns for ball milled Mg-B-erGO nanocomposites at various  $B/C$  ratios.

XRD pattern of erGO is shown in Fig. S2. Peaks corresponding to  $\sim 26.56^\circ$ ,  $\sim 42.39^\circ$ ,  $\sim 44.56^\circ$ ,  $\sim 54.48^\circ$ , and  $\sim 77.61^\circ$  correspond to carbon [ICSD code: 31170].



**Figure S2.** XRD pattern for electrochemical reduced graphene oxide (erGO).

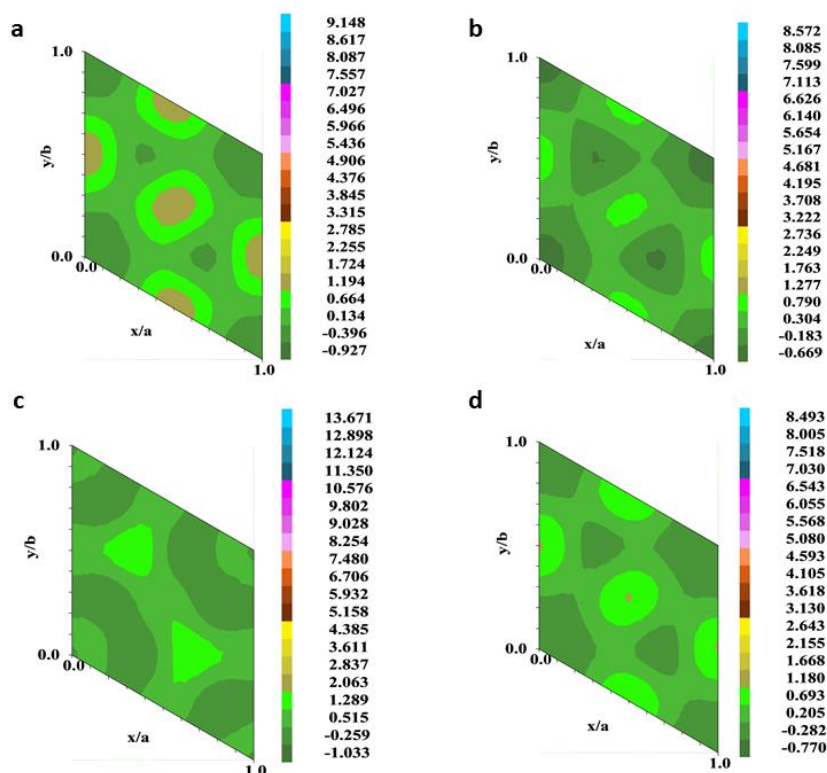
### Phase percentages

The phase percentages of Mg and MgO were estimated from Rietveld refinement using FullProf Suite (Version: 7.20)<sup>1</sup> and shown in Table S1.

**Table S1.** Phase percentages of Mg and MgO in the ball milled Mg-B-erGO nanocomposites for various *B/C* ratios.

<i>B/C</i> ratio	Mg (%)	MgO (%)	Convergence ( $\chi^2$ )
0.00	89.21	10.79	2.42
0.09	79.86	20.14	3.11
0.36	84.91	15.09	2.58
0.90	82.80	17.20	3.73

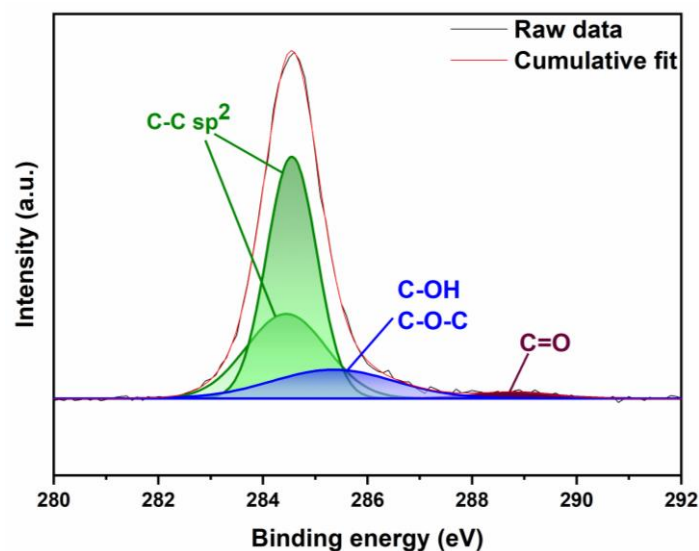
## Electron density maps



**Figure S3.** Electron density maps corresponding to (0001) plane of Mg unit cell for ball milled Mg-B-erGO nanocomposites at (a)  $B/C=0$ , (b)  $B/C \approx 0.09$ , (c)  $B/C \approx 0.36$  and (d)  $B/C \approx 0.90$ .

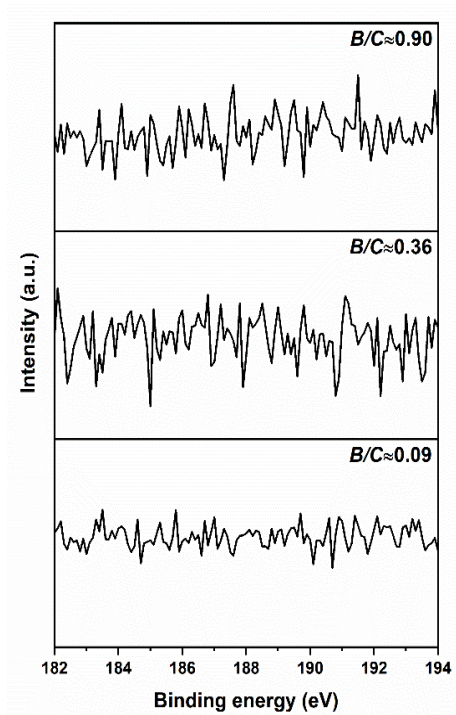
## X-ray photoelectron spectroscopy (XPS)

The C-1s core XPS spectra obtained from erGO are shown in Fig. S4. Peaks observed at binding energies  $\sim 284.44 - 284.55$  eV,  $\sim 285.35$  eV and  $288.8$  eV correspond to  $sp^2$  hybridized C-C, C-OH (alkoxy), C-O-C (epoxy), and C=O (carbonyl) functional groups, respectively<sup>2-4</sup>. The oxygen functional groups are attached to C while erGO synthesis.



**Figure S4.** XPS C-1s core-level spectra obtained from erGO.

The B-1s core XPS spectra are shown in Fig. S5. The peaks corresponding to boron substituted carbon, B<sub>4</sub>C, C<sub>2</sub>-BO, C-BO<sub>2</sub> phases at ~189.1 eV, ~187.7 eV, ~191.4 eV, ~191.8 eV, respectively are absent<sup>5</sup>.



**Figure S5.** XPS B-1s core spectra for ball milled Mg-B-erGO nanocomposites at various  $B/C$  ratios.

## References

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4. Kovtun, A. *et al.* Accurate chemical analysis of oxygenated graphene-based materials using X-ray photoelectron spectroscopy. *Carbon* **143**, 268–275 (2019).
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