

Supplementary Information

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

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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.

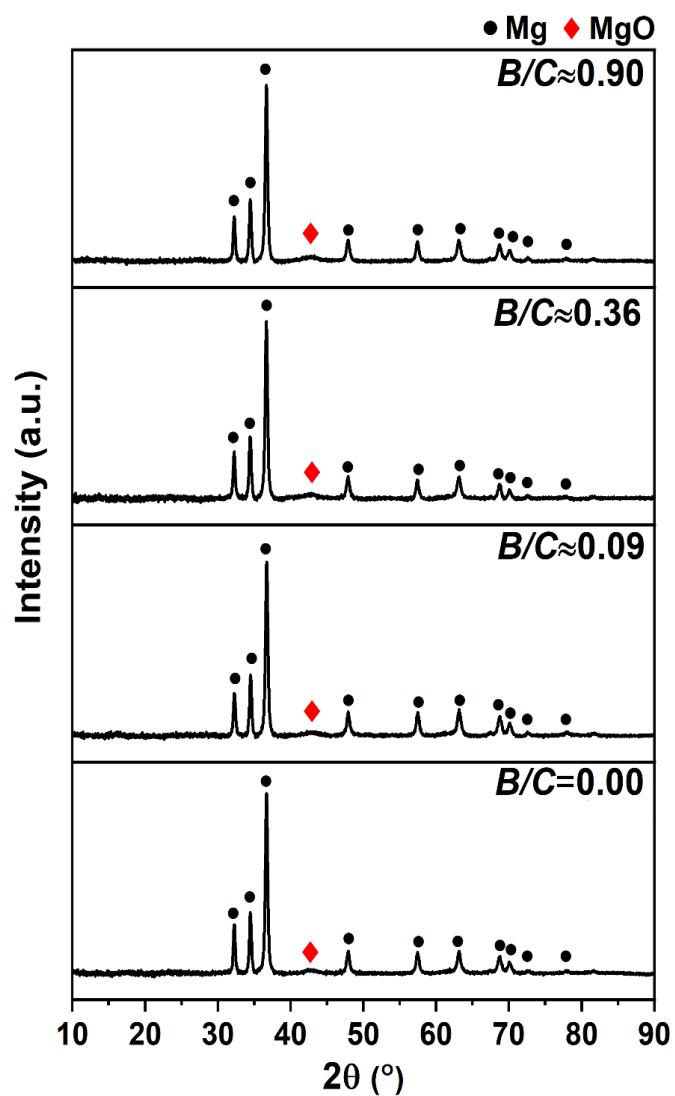


Figure S1. XRD patterns for ball milled Mg-B-erGO nanocomposites at various B/C ratios.

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].

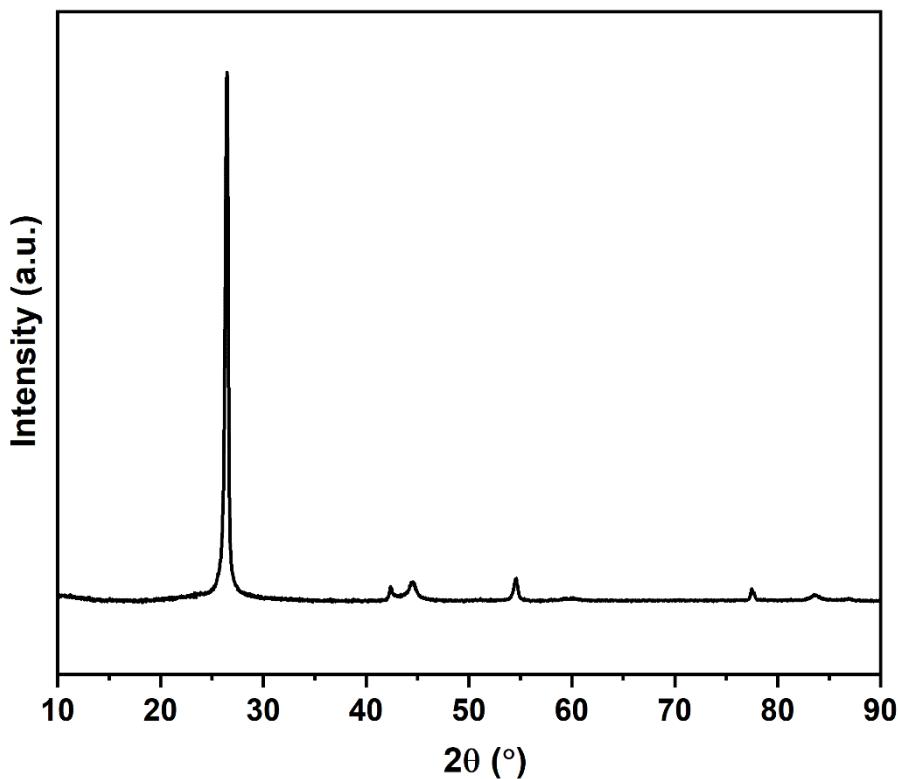


Figure S2. XRD pattern for electrochemical reduced graphene oxide (erGO).

Phase percentages

The phase percentages of Mg and MgO were estimated from Rietveld refinement using FullProf Suite (Version: 7.20)¹ 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

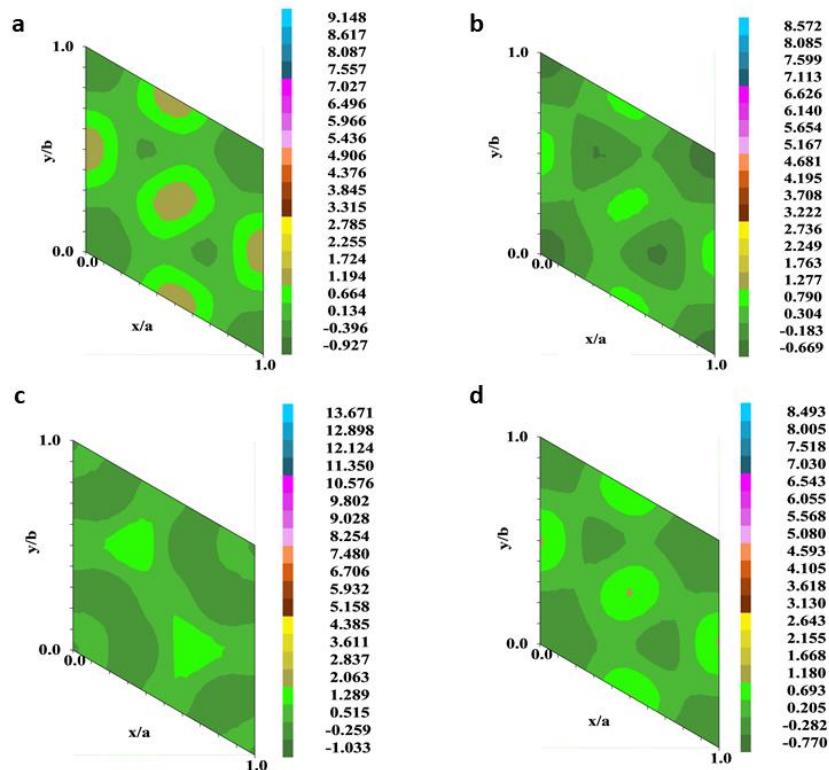


Figure S3. Electron density maps corresponding to (0001) plane of Mg unit cell for ball milled Mg-B-erGO nanocomposites at (a) $B/C=0$, (b) $B/C\approx 0.09$, (c) $B/C\approx 0.36$ and (d) $B/C\approx 0.90$.

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, ~ 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, respectively²⁻⁴. The oxygen functional groups are attached to C while erGO synthesis.

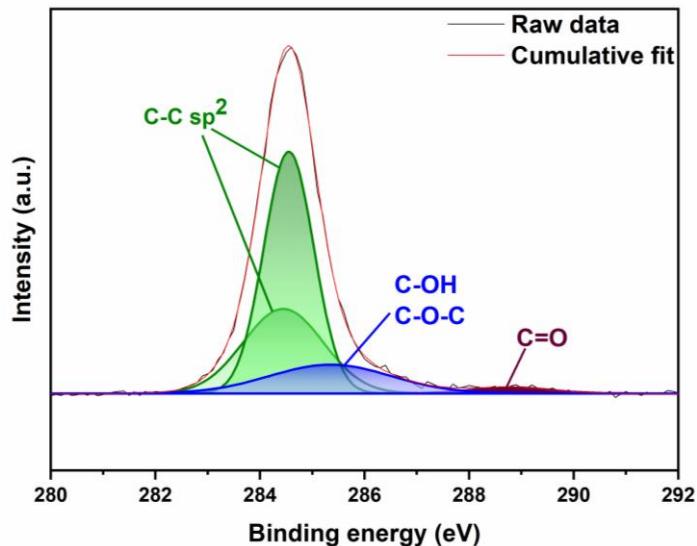


Figure S4. XPS C-1s core-level spectra obtained from erGO.

The B-1s core XPS spectra are shown in Fig. S5. The peaks corresponding to boron substituted carbon, B₄C, C₂-BO, C-BO₂ phases at ~189.1 eV, ~187.7 eV, ~191.4 eV, ~191.8 eV, respectively are absent⁵.

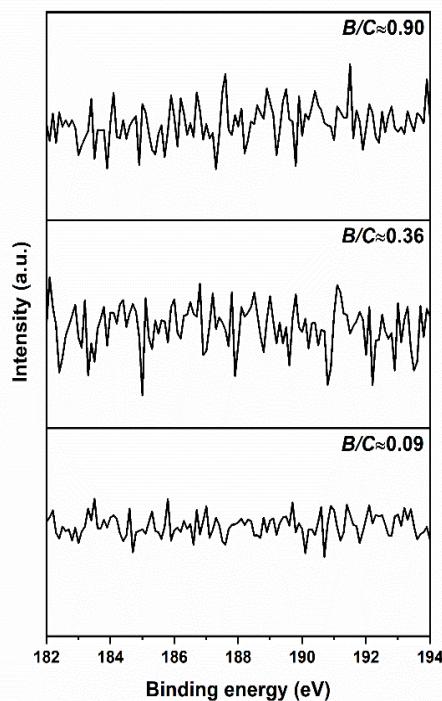


Figure S5. XPS B-1s core spectra for ball milled Mg-B-erGO nanocomposites at various B/C ratios.

References

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