Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Data

On the Roles of Graphene Oxide Doping for Enhanced Supercurrent in MgB_2

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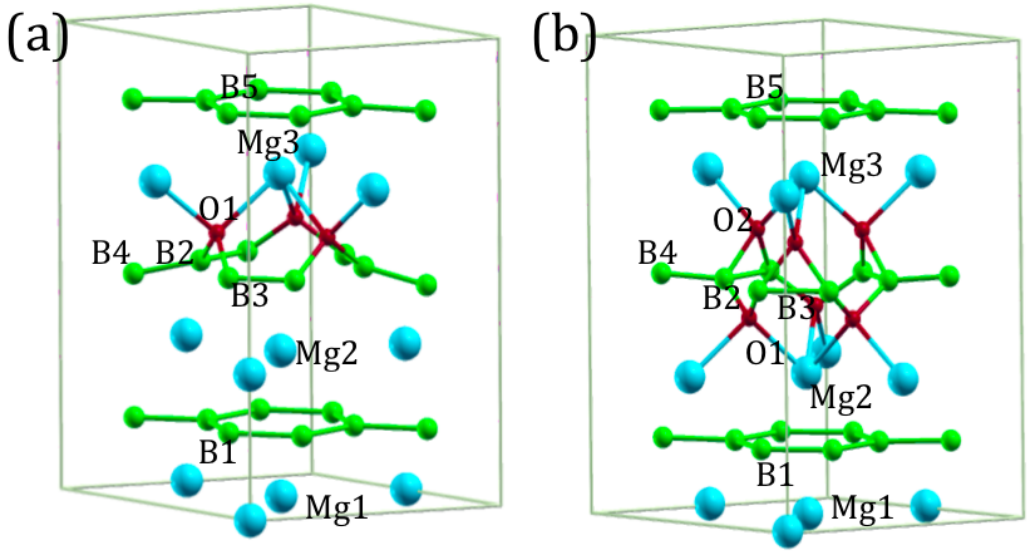
S1 Table 1: The lattice constants, binding energy, formation energy calculated in a 2 x 2 x3 supercell using DFT-GGA.

phases	a (Å)	c (Å)	$E^f_{B\text{-}rich}$ (eV/O)	$E^f_{O\text{-}rich}$ (eV/O)	H^f (eV/atom)
Single O_B	6.16	10.59	2.84	-8.52	0.19
Single O_i	6.17	10.76	2.17	-2.37	0.21
Single-layer Triangle O_i	6.33	10.99	1.44	-3.10	0.37
double-layer Triangle O_i	6.46	11.27	1.13	-3.41	0.61
Bulk MgO	3.01	7.37	-	-	1.01
Bulk MgB_2	3.08	3.51	-	-	0.14
Bulk B_2O_3	4.39	8.75	-	-	0.91

S2. The crystallographic data of the proposed $Mg(B,O)_2$ phases, $MgB_2O_{0.25}$ and $MgB_2O_{0.5}$.



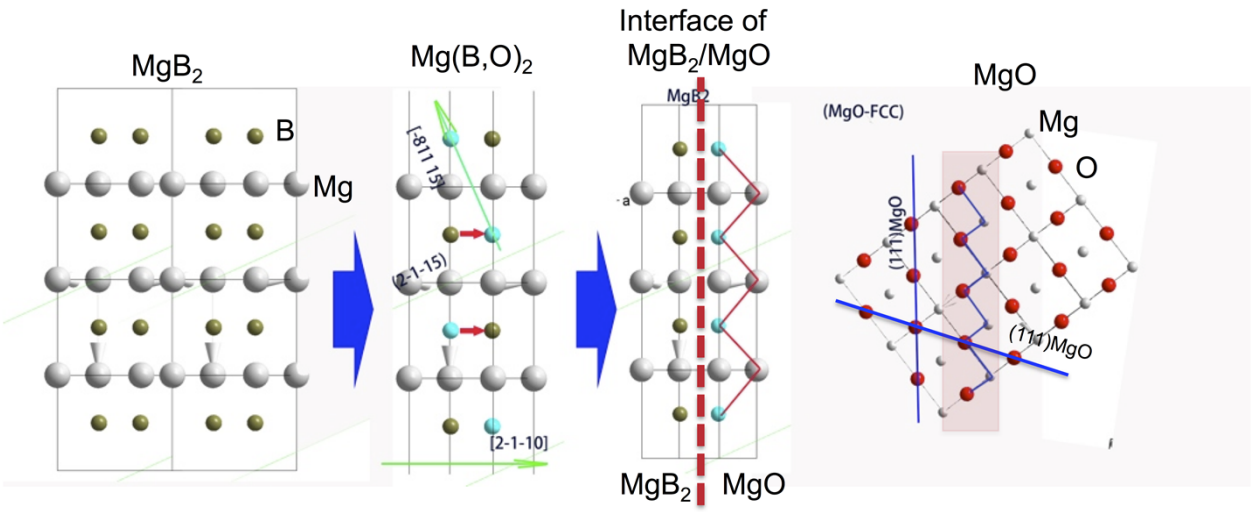
Crystal	$MgB_2O_{0.25}$	$MgB_2O_{0.5}$
Lattice constant (Å)	a = 6.330 c =10.994	a = 6.457 c =11.266
Space group	P31m (No. 157)	P31m (No. 157)
Z value	Z = 12	Z = 12
Atomic position	Mg1: (0.5, 0.5, 0)	Mg1: (0.5, 0.5, 0)
	B1: (0.1672, 0.3323, 0.1581)	B1: (0.1669, 0.3320, 0.1560)
	Mg2: (0.5, 0.5, 0.3082)	Mg2: (0.5, 0.5, 0.2983)
	B2: (0.1284, 0.2785, 0.5046)	O1: (0.2600, 0.5, 0.4206)
	B3: (0.3499, 0.7215, 0.5046)	B2: (0.1202, 0.2847, 0.4909)
	B4: (0.1667, 0.8333, 0.5348)	B3: (0.3356, 0.7153, 0.4909)
	O1: (0.2494, 0.5, 0.5725)	B4: (0.1667, 0.8333, 0.5003)
	Mg3 (0.5, 0.5, 0.6873)	O2: (0.2570, 0.2570, 0.5891)
	B5: (0.1671, 0.3334, 0.8413)	Mg3 (0.5, 0.5, 0.6873)
		B5: (0.1671, 0.3334, 0.8413)
Bond angles	< B2-O1-B3: 110.004^0	< B2-O1-B3: 111.565^0

The hexagonal bulk B_2O_3 is calculated using the low-pressure phase with a $P3_1$ space group, [1]. The calculated lattice constants are a = 4.39 Å, c = 8.75 Å and the bandgap is 6.25 eV under the GGA.

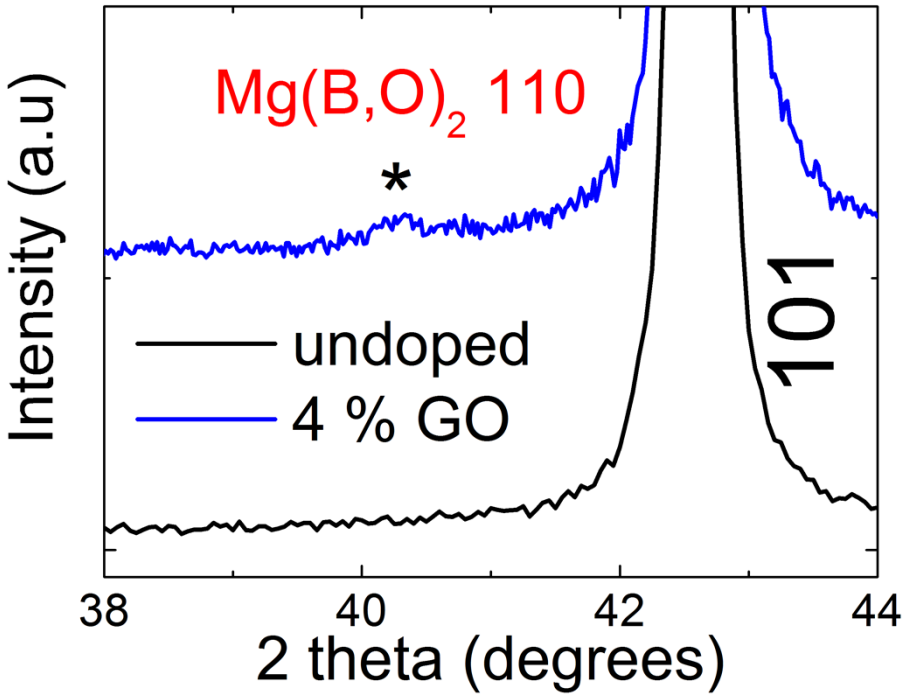
[1]; D. Li and W. Y. Ching, Phys. Rev. B **54**, 13616 (1996).

S3 Phase separation of $Mg(B,O)_2$ to nanoccrystalline MgO and MgB_2

The spherical precipitates have essentially the same crystal structure as the parent phase as seen in the sample, which suggests that the phase separation commonly occurs with a high interconnectivity of the two phases to minimize the strain and is an isotropic effect. As there is a good lattice match between (001)MgB_2//(111)MgO where a small in-plan mismatch (<3 %) will be an ideal interface for phase separation of $Mg(B,O)_2$ to MgB_2 and MgO. A schematic diagram illustrates the phase separation of MgBO phase to MgB_2 and MgO. Grey circles represent Mg atoms; yellow ones represent boron and blue ones represent oxygen.



S4 Evidence of $Mg(B,O)_2$ phase in the MgB_2 in the X-ray diffraction (with the X-ray index table for $Mg(B,O)_2$



X-ray table for $Mg(B,O)_2$

2 theta (deg)	*d*-spacing	Intensity (%)	*hkl*
32.64	2.7412	51.2	110
41.09	2.1950	100.0	101
49.86	1.8323	48.0	001
58.25	1.5826	47.0	100
73.75	1.2837	14.17	201
80.05	1.1977	12.88	103