Electronic Supplementary Material (ESI) for Nanoscale.

Few-layer Mg-deficient borophene nanosheets: I_2 oxidation and ultrasonic delamination from MgB_2

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Supporting Information

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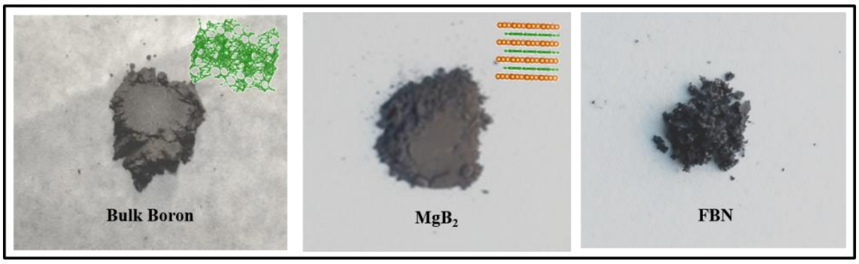


Figure S1. Optical images of bulk boron, MgB_2 and few-layer Mg-deficient borophene nanosheets（FBN）(inserted shows the refined crystal structure) obtained by oxidizing MgB_2 with I_2 in a mixture of CH_3CN and HCl for 14 days at room temperature and subsequently ultrasonic delamination for 2 h in CH_3CN.

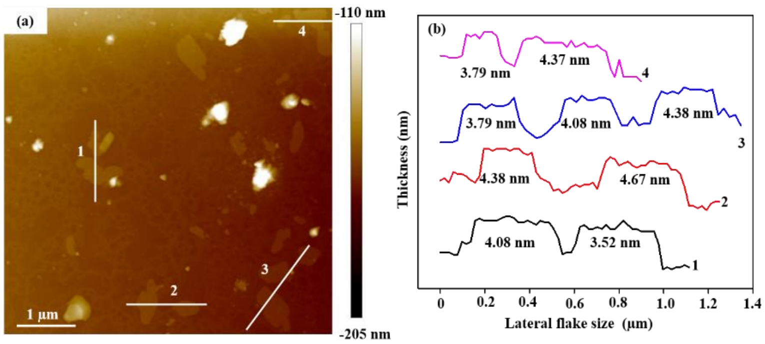
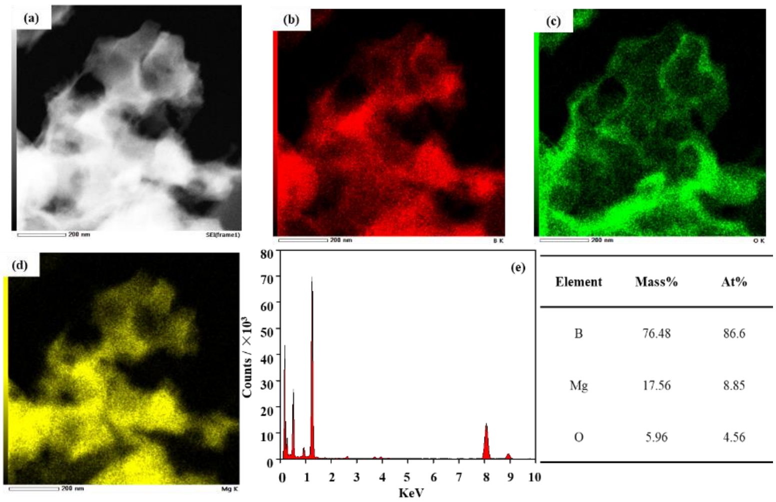


Figure S2. AFM image (a) and the corresponding height profiles (b) of FBN.



Element	Mass%	At%
B	76.48	86.6
Mg	17.56	8.85
O	5.96	4.56

Figure S3. HAADF STEM image (a), the element mapping images (b-d), and the element content statistical diagram (e) of FBN.

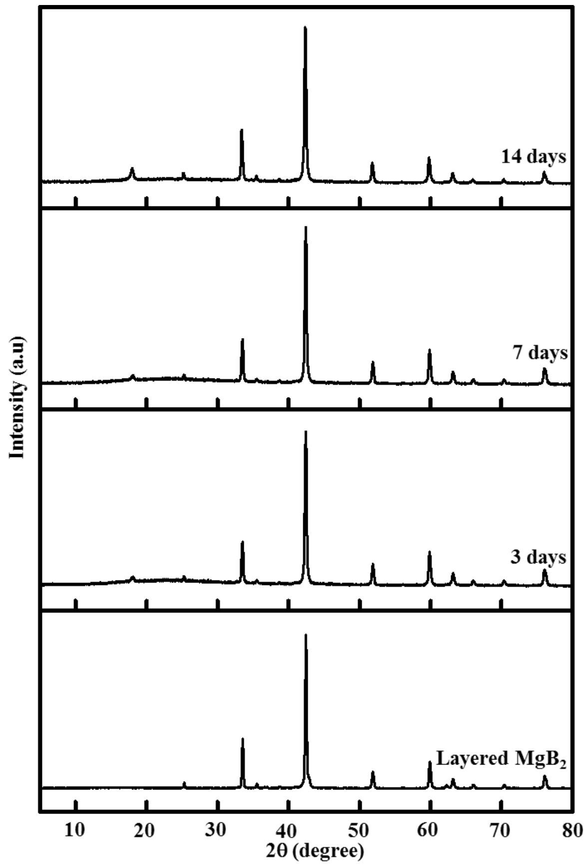


Figure S4. XRD patterns of the obtained materials by oxidizing layered MgB_2 with I_2 in CH_3CN without adding HCl at room temperature in different times.

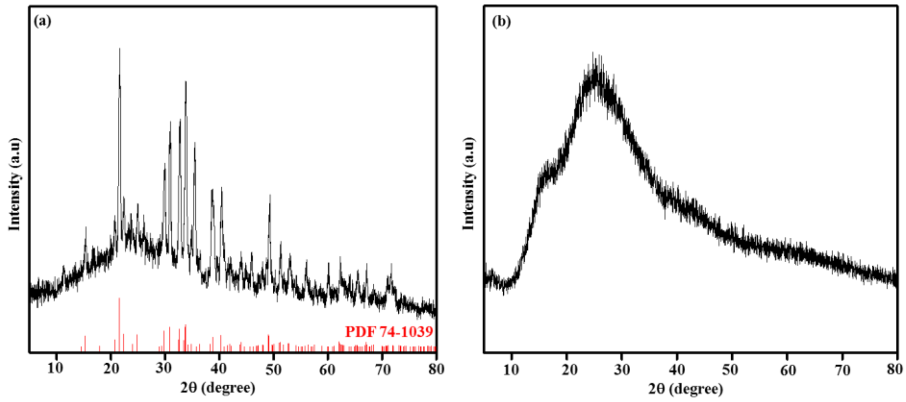


Figure S5. XRD patterns of the obtained materials by treating precursor MgB_2 in a mixture of CH_3CN and HCl (a) and in H_2O (b) without I_2 oxidation.

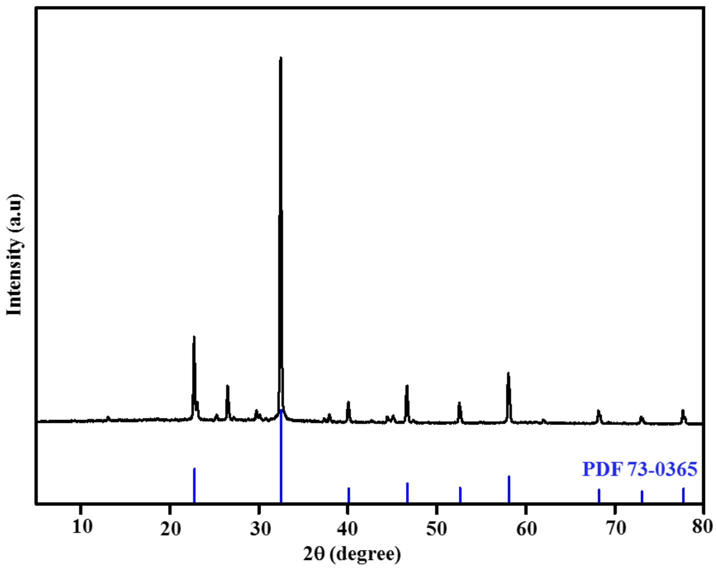


Figure S6. XRD pattern of the obtained material from stirred mixture of CH_3CN and HCl for 14 days at room temperature.

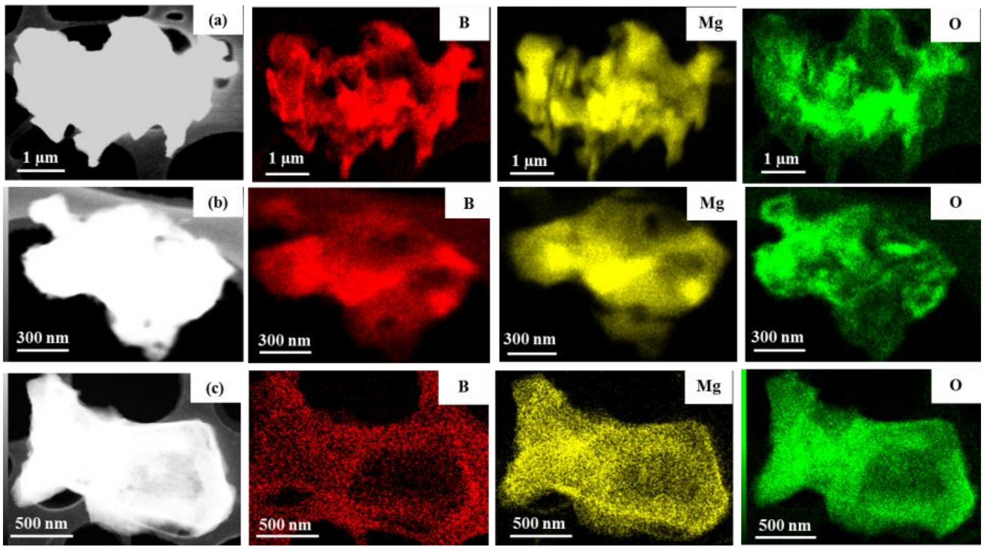


Figure S7. HAADF STEM images and the corresponding element mapping images of the obtained materials by oxidizing MgB_2 with I_2 in a mixture of CH_3CN and HCl for 14 days at room temperature: the oxidized materials (a), washed with water or ethanol (b), and the concentrated supernatant (c).

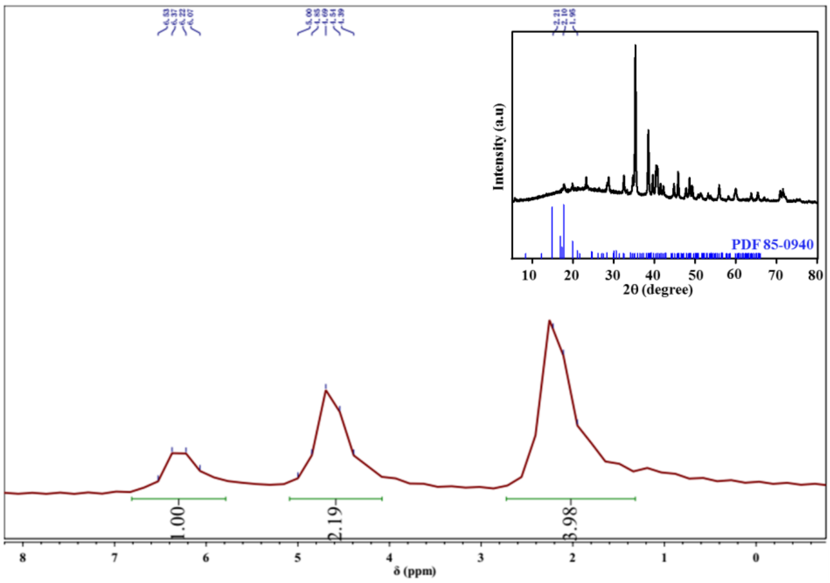


Figure S8. Solid state nuclear magnetic resonance spectrum of the obtained material by oxidizing layered MgB_2 with I_2 and followed by CH_3CN washing (XRD pattern inserted).

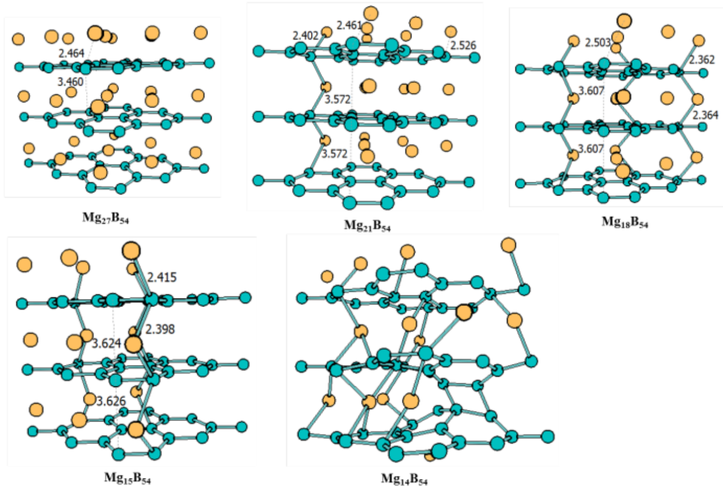


Figure S9. DFT results on the structural change caused by deintercalating Mg atoms from the edge of the model compound $Mg_{27}B_{54}$.

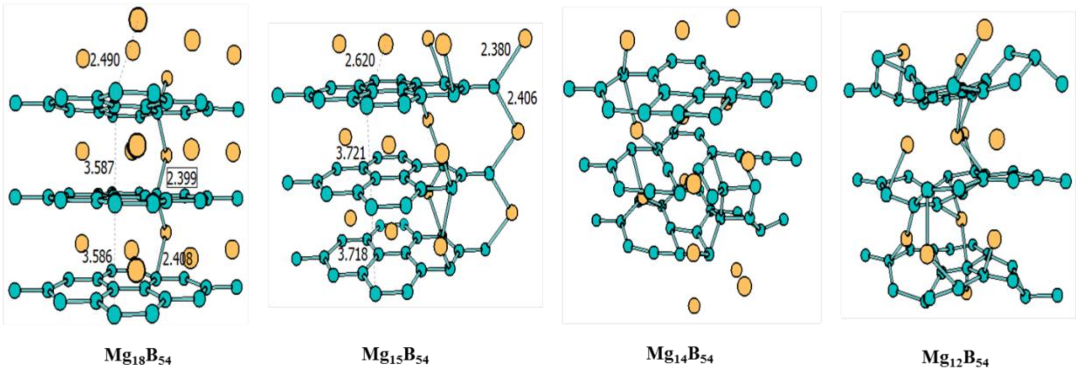


Figure S10. DFT results on the structural change caused by deintercalating Mg atoms from the random directions of the model compound $Mg_{27}B_{54}$.

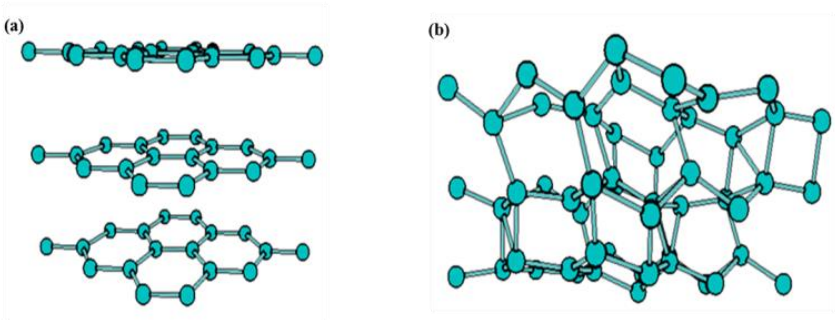


Figure S11. Comparison of ideal state B_{54} structure (a) and the simulated optimized B_{54} structure by deintercalating Mg atoms step by step from the model compound $Mg_{27}B_{54}$.

Table S1. Elemental analysis results of the obtained materials by oxidizing layered MgB_2 with I_2 in the mixture of CH_3CN and different acids for 14 days at room temperature.

sample	ICP-AES value（mg/L)		Stoichiometric ratio
	Mg	B	Mg:B
Layered MgB_2	1.177	1.125	$Mg_{0.92}B_2$
oxalic acid	1.087	1.178	$Mg_{0.82}B_2$
salicylic acid	1.085	1.152	$Mg_{0.84}B_2$
concentrated sulfuric acid	0.998	1.141	$Mg_{0.77}B_2$
50% sulfuric acid	0.533	0.912	$Mg_{0.52}B_2$
hydrochloric acid	0.146	0.589	$Mg_{0.22}B_2$

Table S2. Elemental analysis results of the obtained materials by oxidizing layered MgB_2 with I_2 in a mixture of CH_3CN and HCl for 14 days at room temperature: the oxidized materials, washed with water or ethanol, and the concentrated supernatant.

Element	At % After oxidation	At % After washing	At % Concentrated supernatant
B	73.96	81.23	3.45
Mg	20.80	13.56	24.63
O	5.24	5.21	71.92