

# *Supporting Information*

## **BOROPHENE: A PIEZOCATALYST FOR WATER REMEDICATION**

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## **Experimental Section**

### **Synthesis of borophene**

Borophene was synthesized by using a modified Hummer's method<sup>[29]</sup>. [caution: violent reaction, with possible projection, can occur – reaction should be performed under fume hood with personal protections]. Initially, pure boron powder and potassium permanganate ( $\text{KMnO}_4$ ) were mixed in a proportion of 1:6 and ground for 10 minutes. Simultaneously, an acidic mixture was prepared by mixing ortho-phosphoric acid ( $\text{H}_3\text{PO}_4$ ) and sulfuric acid ( $\text{H}_2\text{SO}_4$ ) in a ratio of 1:9. To control the reaction exothermicity, a precooling procedure was followed by cooling these two mixtures below 5 °C for six hours. When the Boron +  $\text{KMnO}_4$  mixture was poured into the acidic mixture, it immediately ignited and caught flame, eventually turning into dense brown smoke due to an exothermic reaction as shown in Figure S10. The reaction mixture was ultrasonicated for 24 hours at 65°C. After, 200 mL of distilled water was added to quench the reaction, and the mixture was sonicated for another 2 hours. After the completion of the reaction, the product was washed with distilled water (3 times), ethanol (2 times), and 1M HCl (17.5%, 2 times) and dried at 65°C for 12 hours<sup>[30]</sup>. The resultant was thermally reduced to 200 °C for 8 hrs.

### **Piezocatalytic experiments**

The Piezocatalytic activity of borophene was evaluated by monitoring the degradation of selected dyes: methylene blue (10 mg/L, cationic dye), and mixture of dyes [rose Bengal (10 mg/L) + methylene blue (10 mg/L) + rhodamine B (10 mg/L) + methyl orange (10 mg/L)]. Borophene was added to the 40 mL of dye solution to reach 0.5 mg/mL. All the experiments were carried out in 50 mL beaker submerged in an ultrasonicator water bath (120W, 40 kHz). The beaker was kept in the centre of the water bath with constant water level. The temperature of the reaction setup was

maintained at 25°C by flowing cooled water in the water bath. Before conducting piezocatalysis, the adsorption-desorption equilibrium between the catalyst and dye solution was achieved by keeping it in a dark environment for 1 hour. The piezocatalysis experiments were carried out after this step. Upon exposure to ultrasonic vibrations, 2 mL aliquots were collected every minute for the evaluation of the dye concentration by UV-visible spectrophotometry<sup>[22]</sup>.

The degradation efficiency (%) is determined using the main UV-visible absorption peak(s) attributed to the dyes (Methylene Blue: 662 nm; Rhodamine B: 358 and 541 nm; Rose Bengal: 258 and 562 nm; and Methyl Orange: 270 and 464 nm) and using the Beer-Lambert law. The formula is:

$$\text{Degradation efficiency (\%)} = 100 \cdot [C_0 - C_t] / C_0 \quad (1)$$

Where  $C_0$  is the initial concentration, and  $C_t$  is the concentration following an exposure time of (t) minutes. For the mixture of dyes, the degradation efficiency is given as the average degradation efficiency of all dyes.

### **Reusability test for borophene**

After the piezocatalytic degradation of the methylene blue organic dye, the utilized borophene nanosheets were effectively recovered by centrifugation, rinsed three to four times with distilled water, and then dehydrated for two hours in a vacuum oven at 60 °C. This was done to ensure that the nanosheets were free of any moisture. For the purpose of investigating the repeatability of borophene nanosheets, this procedure was carried out six times<sup>[22,25]</sup>.

### **Piezo current Measurement**

The piezo current response was measured by using a three-electrode electrochemical workstation (Biologic EC lab sp-150). In this three-electrode system, borophene acts as a working electrode, platinum wire as a counter electrode, and Ag/AgCl as a reference electrode. 0.1M KOH was used as an electrolyte. For the formation of ink, 20 mg of borophene was added to 1 mL of IPA (isopropyl alcohol), followed by the addition of 20 mL of Nafion as a binder. This mixture was maintained for two hours in an ultrasonic bath.

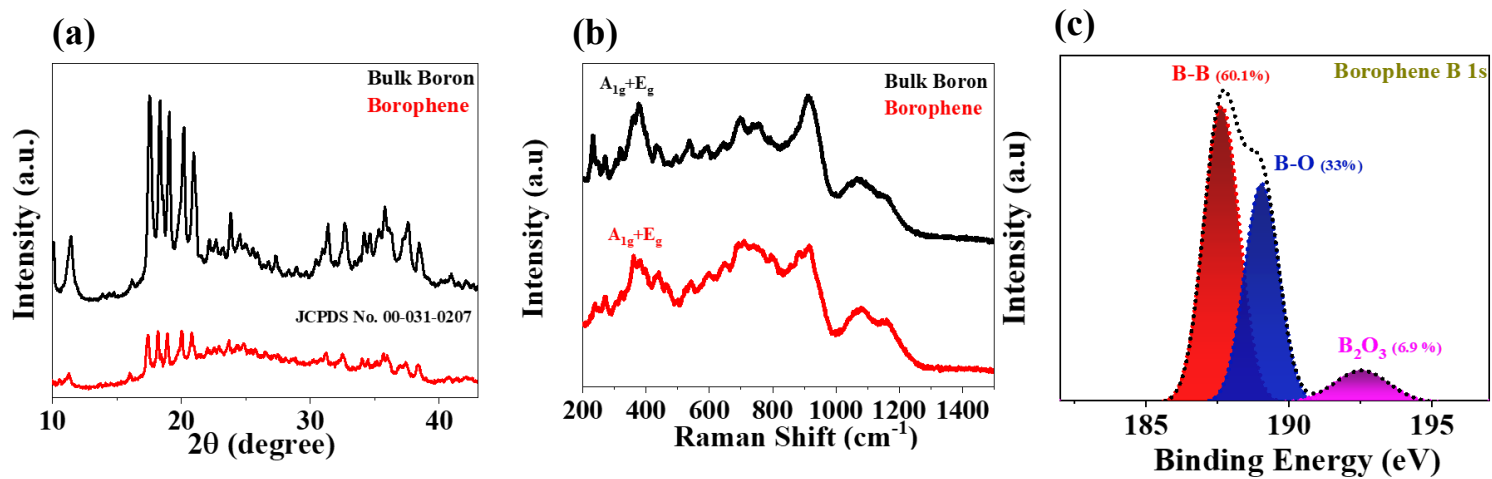
### **Material Characterization**

A Bruker D8 Advanced AXS diffractometer was used to acquire powder X-ray diffraction (PXRD) patterns. A monochromatic irradiation source ( $\lambda = 1.5418 \text{ \AA}$ ) and 40 kV and 30 mA were used to run the diffractometer. The X-ray diffractograms were recorded using a 1 s step time and a 0.02 step size. Transmission electron microscopy (TEM) has been performed with a Thermo Fischer Titan Themis FEG TEM/STEM system operating at 200 kV. The samples were directly observed as a powder or as thin foil (50 nm) fabricated using an ultramicrotome (Leica Ultracut S) after dispersing the material in an epoxy resin and curing at 50 °C. The Bright Field (BF-TEM), the phase contrast high resolution (HR-TEM) imaging and the corresponding selected area diffraction (SAED) pattern have been performed in broad parallel beam TEM mode. High angle annular dark field (HAADF) imaging has been performed in scanning TEM mode with probe size of 500 pm, convergence semi-angle of 20 mrad and probe current of about 50 pA. The camera length has been adjusted in order to have for the HAADF detector inner and outer collection semi-angles between 50 mrad and 100 mrad. High-resolution X-ray Photoelectron Spectra (XPS) were acquired using a Kratos Analytical AXIS UltraDLD spectrometer outfitted with a monochromatic Al K $\alpha$  X-ray laser (1486.6 eV) and a continuous passage energy of 20 eV. Casa XPS was used for spectral decomposition and quantification. A dual beam UV-Vis NIR spectrometer was used to monitor

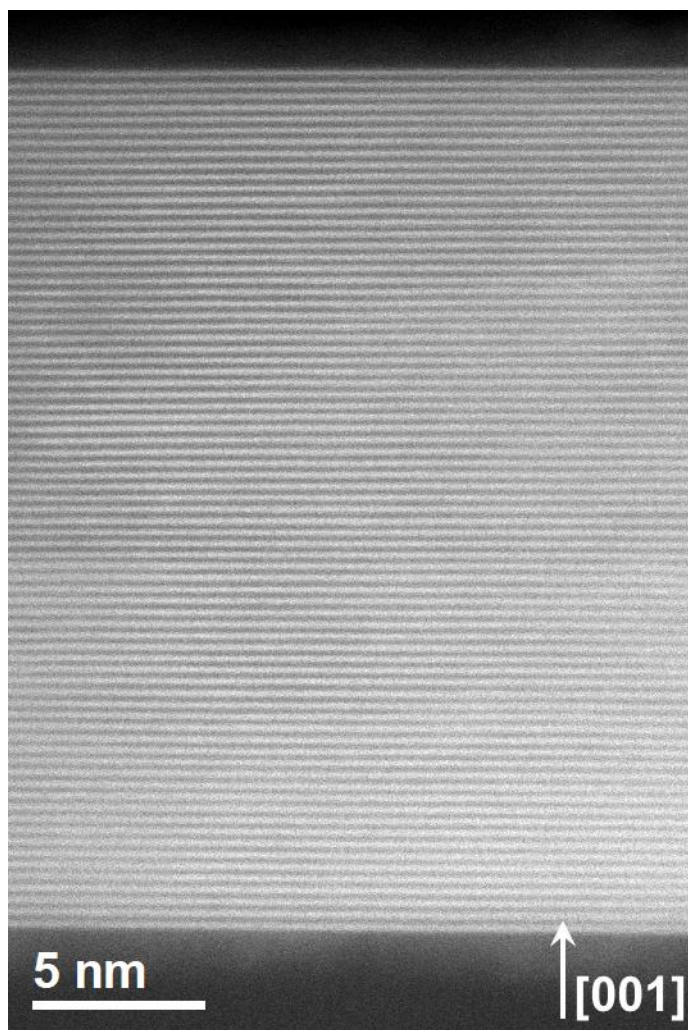
the decrease in the absorbance peak of the pollutants (LAMBDA 750-Perkin Elmer). Using an IRIX STR 500 Raman spectrometer, Raman spectroscopy was used to assess the crystallographic orientation of the produced borophene. The results were collected using a 532 nm Ar ion laser at room temperature (about 1 mW, 50X objective). Fourier Transformation infrared spectroscopy (Perkin Elmer) was used to identify the chemical components and bonds. To identify the lateral size and number of sheets of the borophene sheets, atomic force microscopy (AFM, Bruker) was used. The piezoelectricity was locally probed by using the piezoresponse (PFM) mode of the AFM technique by means of an MFP-3D (Asylum Research/Oxford Instruments, USA) microscope under environment conditions. The dual AC resonance tracking (DART) method<sup>[31]</sup> of the PFM was used for both imaging and spectroscopy modes, and remnant PFM signal (at zero bias) was preferentially recorded when measuring piezoresponse loops in order to promote electromechanical response at the expense of the electrostatic contribution<sup>[32]</sup>. The generation of hydroxyl radicals in the excitation range of 200-800 nm was measured using a fluorescence spectrometer (LS 55 (Perkin Elmer)). A digital scanning oscilloscope (DSO) was used to measure the piezoelectric voltage production.

**Table S1-** comparison of different piezocatalytic systems

<b>Piezocatalysts</b>	<b>Pollutants</b>	<b>Reaction time (minutes)</b>	<b>Degradation Efficiency (%)</b>	<b>References</b>
Ba <sub>2</sub> TiMnO <sub>6</sub>	Rhodamine B (5 mg/L)	180	99	[22]
NaNbO <sub>3</sub> nanorods	Rhodamine B (10 mg/L)	80	75	[22]
Bi <sub>2</sub> WO <sub>6</sub>	Methylene Blue (10 mg/L)	35	96	[33]
ZnO nanorods	AO7 (10 mg/L)	100	32	[34]
BaTiO <sub>3</sub> nanowires	Methyl Orange (5mg/L)	160	90	[35]
NaNbO <sub>3</sub> nanorods	Methylene Blue (3mg/L)	190	19	[36]
BiFeO <sub>3</sub> nanowires	Rhodamine B (4 mg/L)	60	60	[37]
LuFeO <sub>3</sub> nanoparticles	Rhodamine B (5 mg/L)	90	30	[38]
<b>Borophene nanosheets</b>	<b>Methylene blue (10 mg/L)</b>	<b>6</b>	<b>97</b>	<b>This work</b>

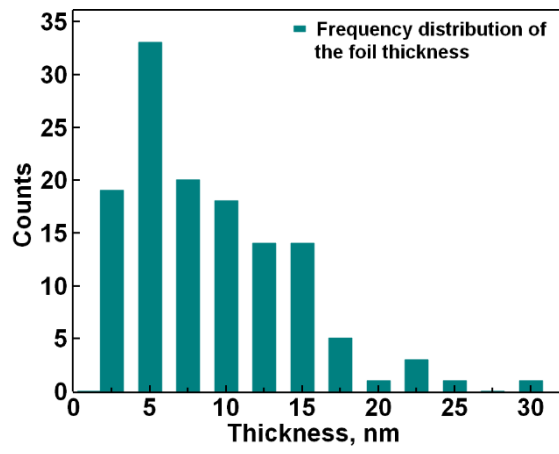


**Figure S1-** (a) XRD pattern of the prepared borophene sheets (b) Raman spectrum of the borophene nanosheets, (c) Binding energy spectra of B 1s.

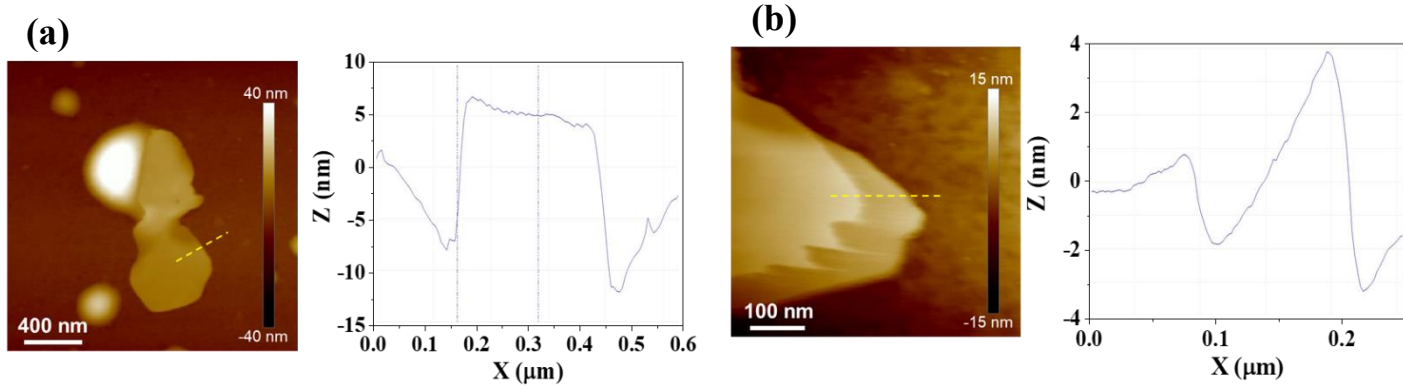


**Figure S2:** HR-TEM image showing an averaged interplanar distance of 0.326 nm.

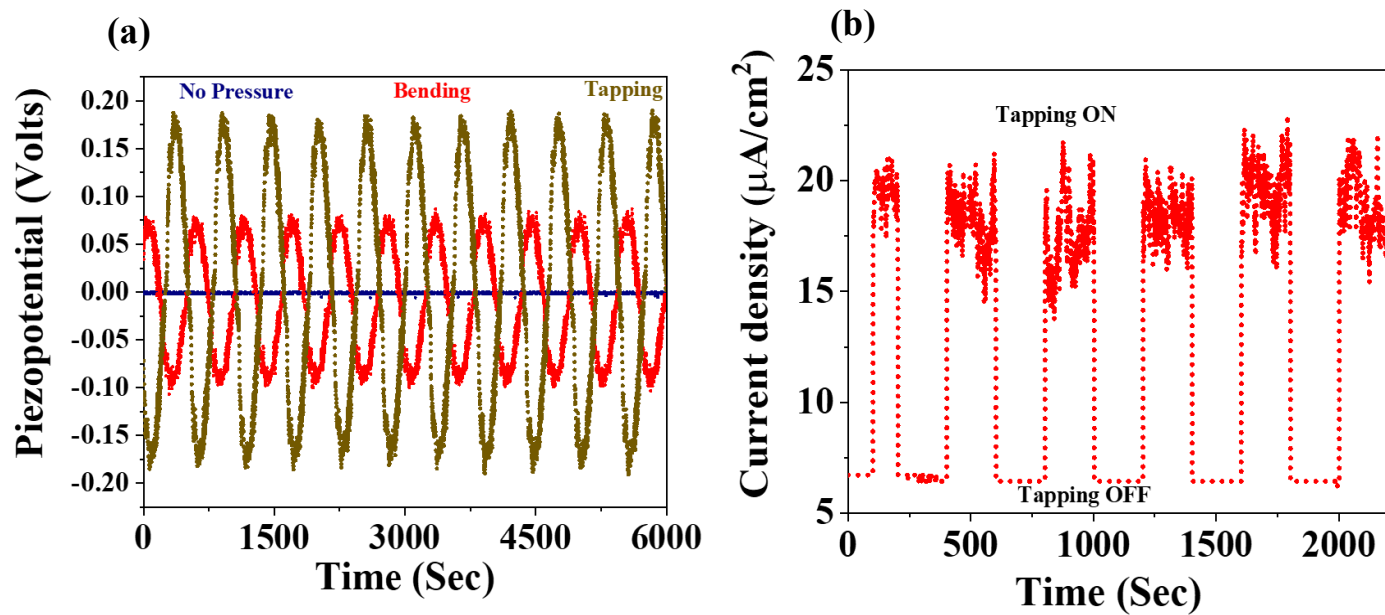




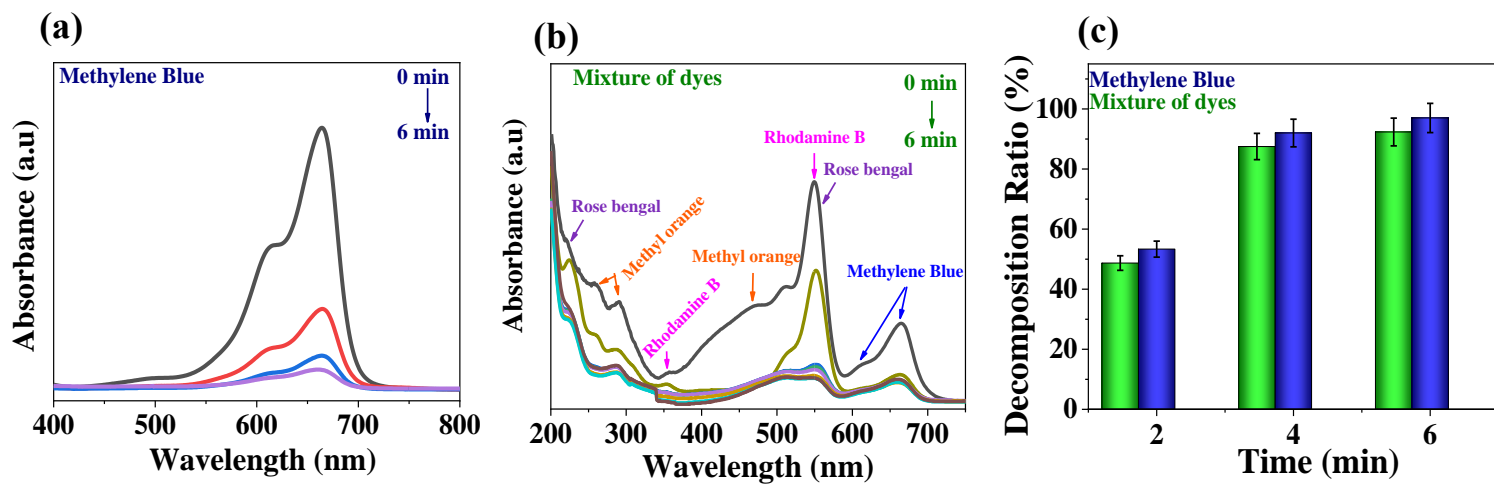
**Figure S3:** Thickness distribution of the prepared borophene sheets.



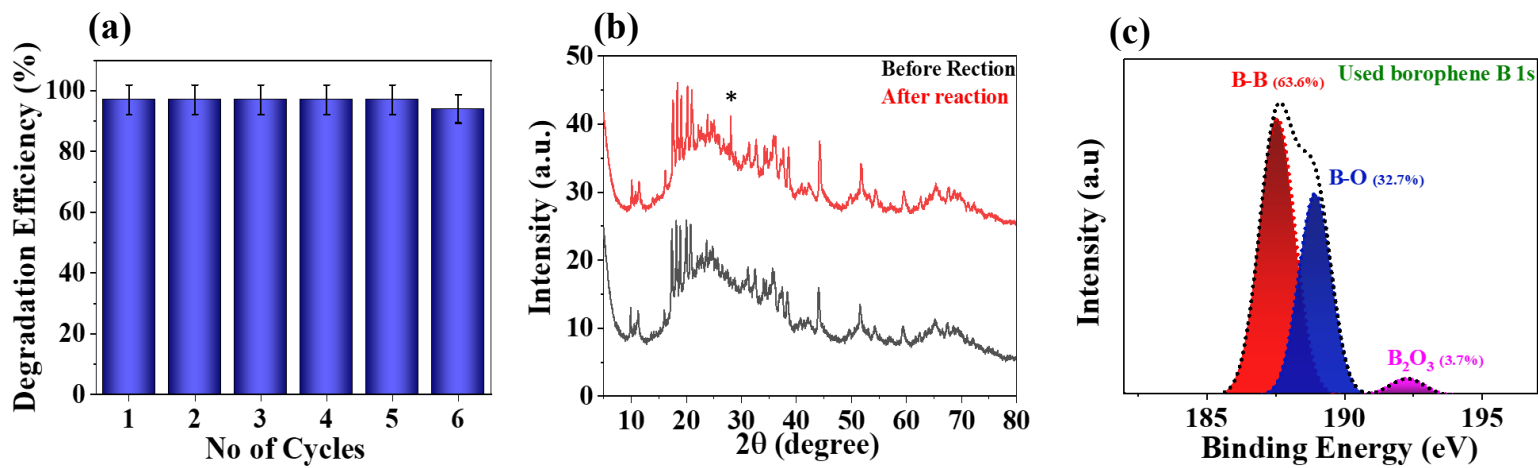
**Figure S4:** (a-b) AFM images of the borophene sheets.



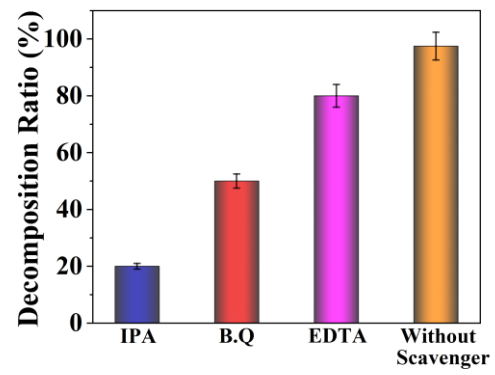
**Figure S5:** (a) Formation of piezo potential, (b) piezo current response.



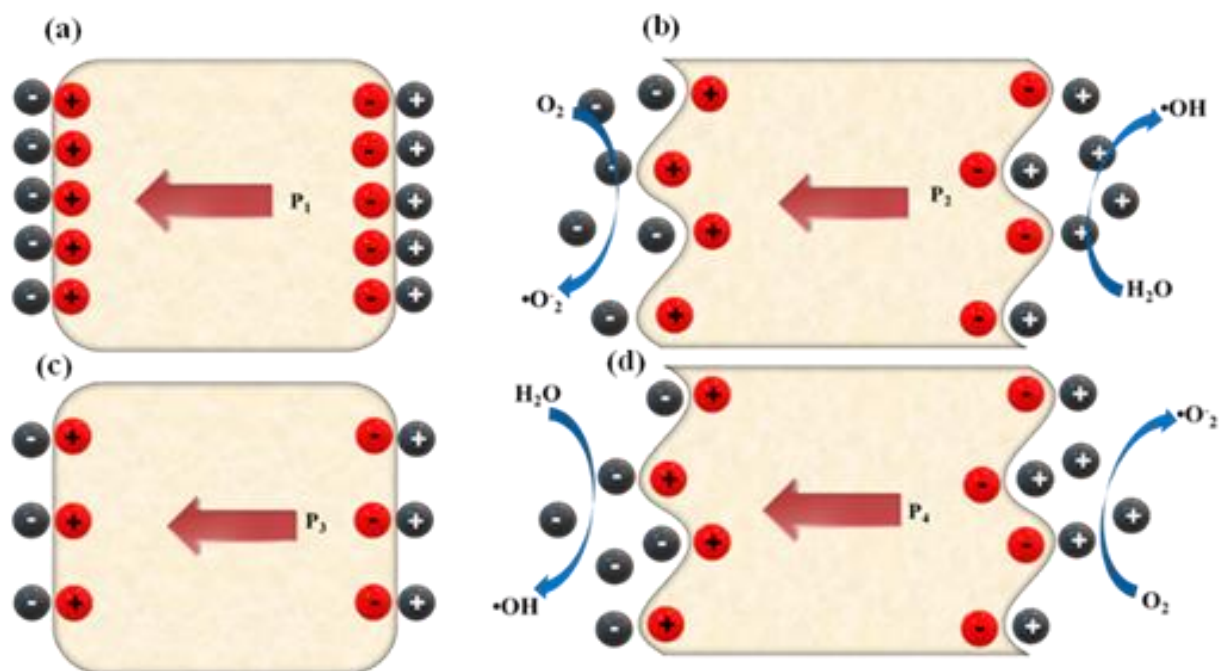
**Figure S6:** Piezocatalytic degradation of (a) Methylene blue, (b) Mixture of dyes, (c) Overall decomposition ratio of different pollutants



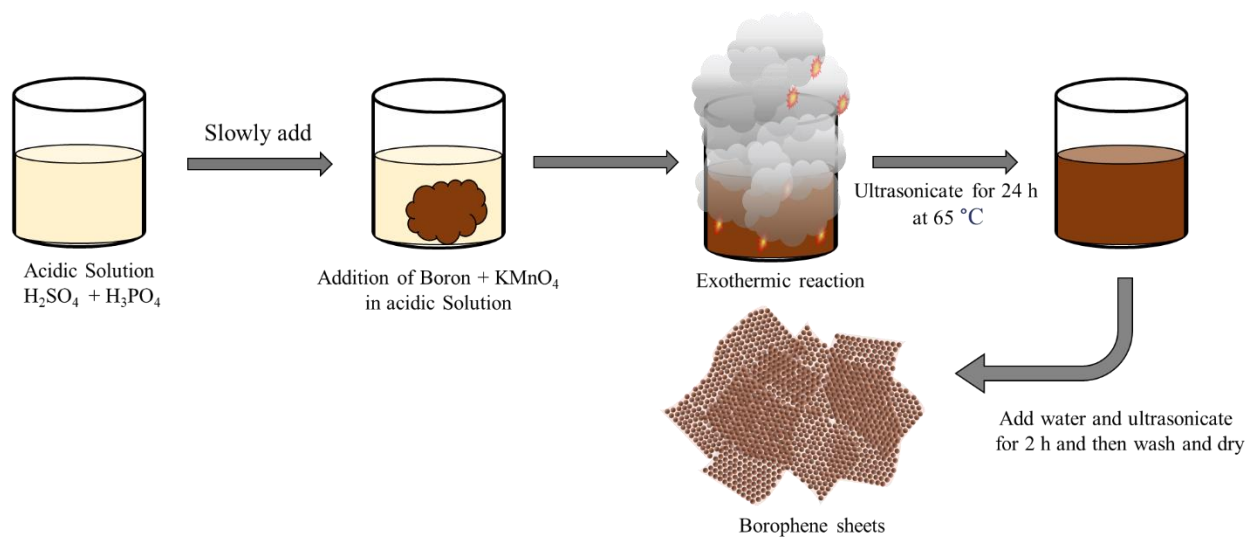
**Figure S7:** (a) Recyclability of borophene nanosheets for the degradation of methylene blue (10 mg/L, neutral pH), (b) XRD pattern of borophene before and after piezocatalysis (\* = B<sub>2</sub>O<sub>3</sub>) (c) High resolution spectra of used borophene



**Figure S8:** Comparative decomposition ratios with and without scavengers.



**Figure S9:** Schematic illustration of piezocatalysis.



**Figure S10:** Synthesis of Borophene sheets.



### Additional references

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