$BaTiO_2$@MXene Nanocomposites as Efficient Photocatalysts for Organic Dye Degradation

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Supporting Information

Experimental Design and Techniques

Synthesis of $BaTiO_2$@MXene nanocomposite material

$BaTiO_2$@MXene nanocomposites were synthesised via a hydrothermal route using $Ti_3C_2T_x$, $BaCl_2$, and titanium isopropoxide as precursors. A uniformly dispersed $Ti_3C_2T_x$ suspension was mixed with Ba–Ti precursor solution, adjusted to pH 10, and hydrothermally treated at 120 °C for 12 h. The obtained product was filtered, washed, dried, and calcined at 500 °C. Composites with different MXene contents (4 and 12 wt%) and corresponding control samples were prepared using the same procedure.

XRD Analysis

XRD patterns (Figure 2a) show that pristine $Ti_3C_2T_x$ exhibits diffraction peaks consistent with reported literature. The $BaTiO_2$@MXene composite displays additional reflections at 2θ = 25.42°, 33.79°, 39.59°, 58.48°, 70.38°, and 74.13°, corresponding to the (101), (103), (104), (110), (113), and (201) planes of spinel $BaTiO_2$, confirming composite formation.

FTIR Analysis

FTIR spectra (Figure 2b) reveal characteristic functional groups associated with $Ti_3C_2T_x$ and $BaTiO_2$@MXene. Changes in band intensity and the absence of the Ti–O–Ti vibration (~713 cm^{-1}) in the composite indicate structural modification following $BaTiO_2$ incorporation.

SEM Analysis

SEM images (Figure 3) show $BaTiO_2$ particles with a more uniform, rice-grain-like morphology distributed on multilayered $Ti_3C_2T_x$ sheets. This observation suggests that the MXene layers influence particle growth during the hydrothermal process.

Thermal Analysis (TGA–DSC)

TGA profiles (Figure 4a) display two-step weight loss associated with moisture removal and hydroxyl group decomposition, with similar behaviour observed for the composites. DSC curves (Figure 4b) show a shift in the Curie temperature of $BaTiO_2$ upon MXene addition, indicating an effect on thermal phase behaviour.

XPS Analysis

XPS spectra (Figure 5) confirm the presence of Ba, Ti, C, and O in the $BaTiO_2$@MXene composite. Small shifts in the Ba 3d and Ti 2p binding energies relative to the pristine materials suggest changes in the local chemical environment at the interface.

Photocatalytic method

The photocatalytic activity of $BaTiO_2$, 4 wt% $BaTiO_2$@MXene, and 12 wt% $BaTiO_2$@MXene was evaluated via UV-light-driven degradation of methylene blue (MB). Experiments were conducted using a 10 ppm MB solution (30 mL) with a catalyst loading of 0.5 g L^{-1}, and concentration changes were monitored by UV–visible spectroscopy at regular intervals. Control experiments for photolysis and dark adsorption were also performed. MB degradation efficiency was calculated using standard concentration–time relations.

Table:1 Reusability study of 12%$BaTiO_2$@MXene catalyst for Methylene blue degradation over two consecutive cycles.

Time (mins)	**Degradation studies of 12%BTM catalyst**	
	Cycle -1	**Cycle-2**
0 min	10.8135	7.0872
30 min	12.1524	33.0352
60 min	43.2131	53.5951
90 min	54.3460	69.8648
120 min	64.7785	75.8987

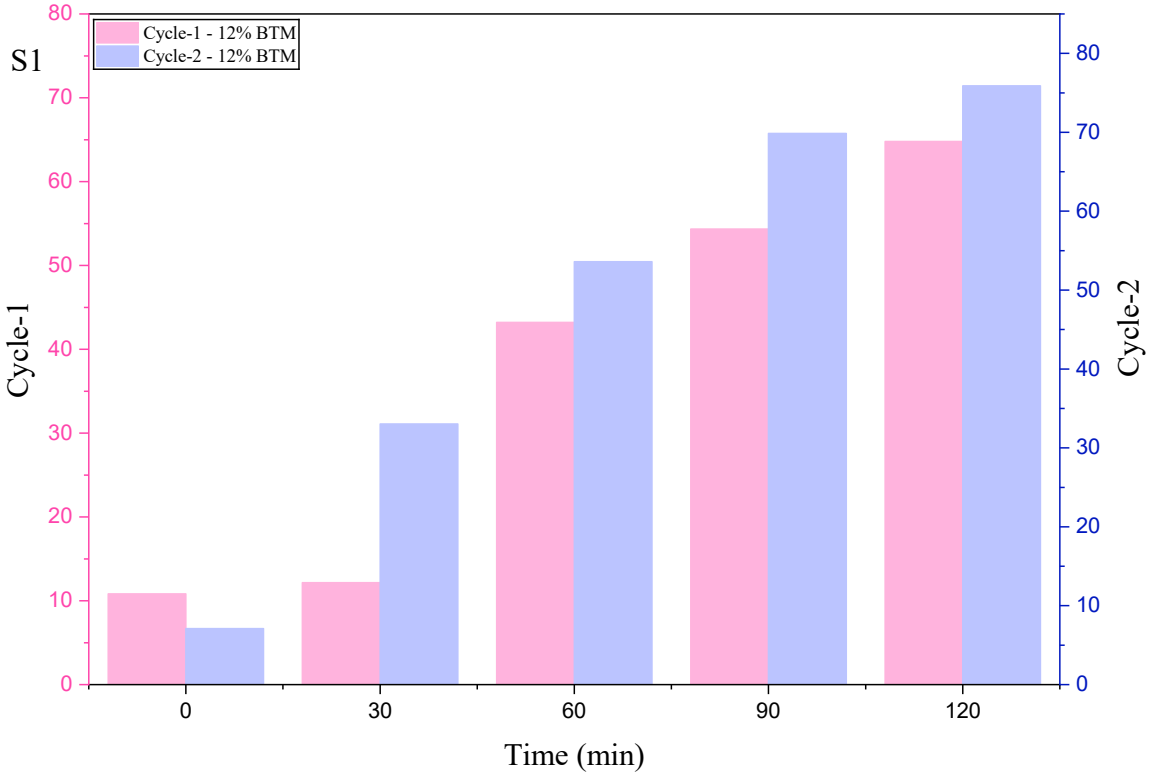

Figure: S1 Degradation efficiency (%) of 12% $BaTiO_2$@MXene catalyst for methylene blue degradation over two consecutive cycles.

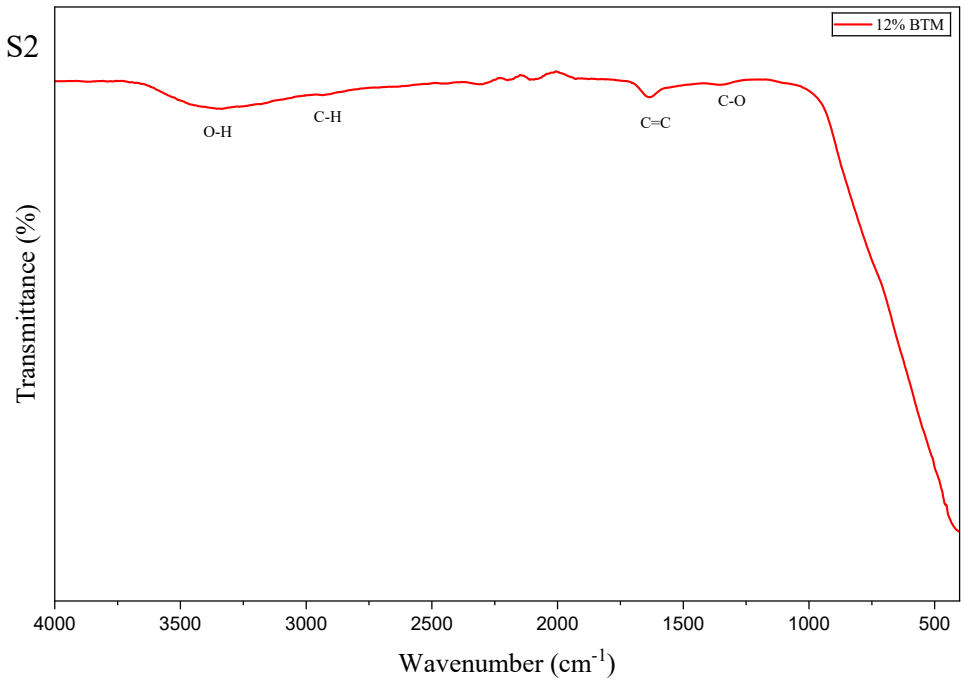

Figure: S2 shows the ATR-FTIR spectrum of the recovered $BaTiO_2$@MXene catalyst after methylene blue photo-degradation.

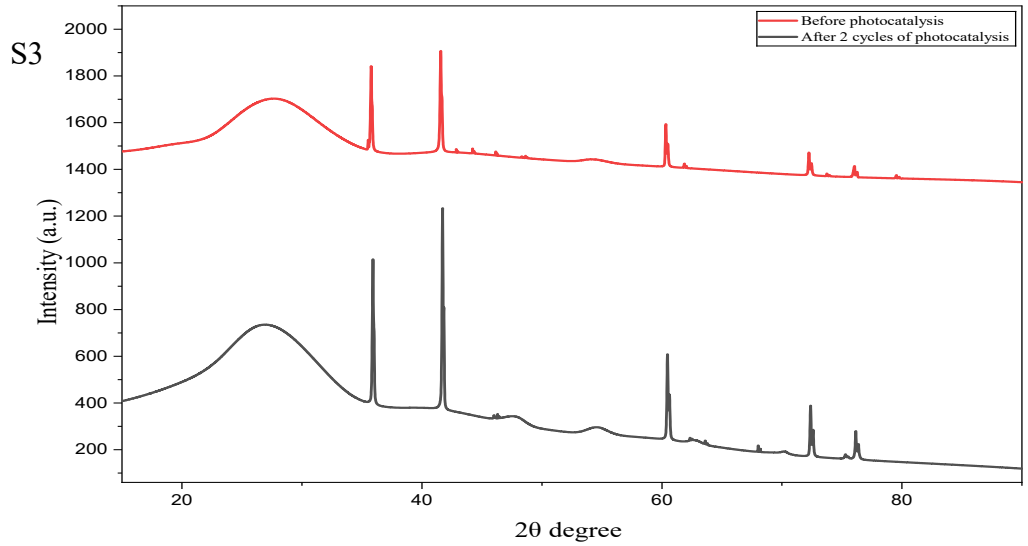

Figure: S3 XRD pattern of 12%BTM before and after photo-degradation.