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## 2024 CTCI Foundation Science and Technology Scholarship

### 境外生研究獎學金

#### Research Scholarship for International Graduate Students



## Advancing Resource Recovery and Sustainable Energy Production using MXene/Biochar Composites within the Soil-Water-Energy Nexus

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### Abstract

The study explores the synthesis and utilization of biochar (BC) and multi-layer MXene to MXene/biochar (MB) composites for wastewater treatment. Simultaneously, it also investigates their energy generation potential through biomass and soil property assessments. The integrated column and batch treatments have shown significant results, elevating total dissolved solids from 63.7 to 125.5 mg L<sup>-1</sup> with column treatment, while reducing them to 6.37% and 1.35% with BC and MB treatment, respectively. BC with high carbon content, demonstrated increased hydrophobicity, which was amplified by the integration of MXene, thereby enhancing its potential for advanced wastewater treatment. Treated wastewater exhibited elevated nutrient concentrations (Ca, Cu, Fe, K, Na, and NH<sub>4</sub><sup>+</sup>), promoting the growth of *Pennisetum purpureum*. WW\_B shows promising energy potential, with a higher heating value of 25.03 MJ kg<sup>-1</sup> and a lower heating value of 23.57 MJ kg<sup>-1</sup>. They demonstrated high volatile matter exceeding 70.9 wt%, and a fixed carbon from 10.02 to 27.53 wt%, signifying their potential for efficient conversion and bio-oil yield during pyrolysis. The ultimate analysis emphasized significant carbon, with oxygen content ranging from 43.42 to 47.78 wt%, influencing combustion characteristics. MT\_B exhibited its suitability for energy production through thermochemical conversion, underlined by its high flammability and low volatile ignition values. In the absence of BC, the E<sub>a</sub> ranged from 24.77 to 77.88 kJ mol<sup>-1</sup> in wastewater and from 21.67 to 69.6 kJ mol<sup>-1</sup> in MB treated wastewater. Meanwhile, when soil contained BC was irrigated with wastewater, the E<sub>a</sub> varied from 24.66 to 80.91 kJ mol<sup>-1</sup>. In the case of MB treated wastewater, it ranged from 25.01 to 75.79 kJ mol<sup>-1</sup>. The research thereby affirms the potential of MB composites to advance water and energy sustainability setting us for broader nexus-based applications.

### Preparation of MB composites

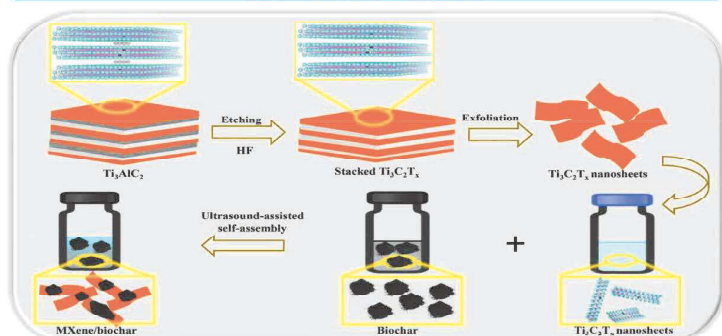


Figure 1: Schematic representation of the synthesis process for Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene/biochar composites.

### Results and Discussion

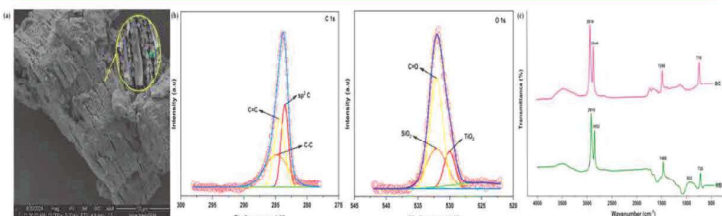


Figure 2: (a) SEM images of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene, (b) XPS survey spectra of MB composites, and (c) FTIR spectra of BC and MB at different wavenumbers.

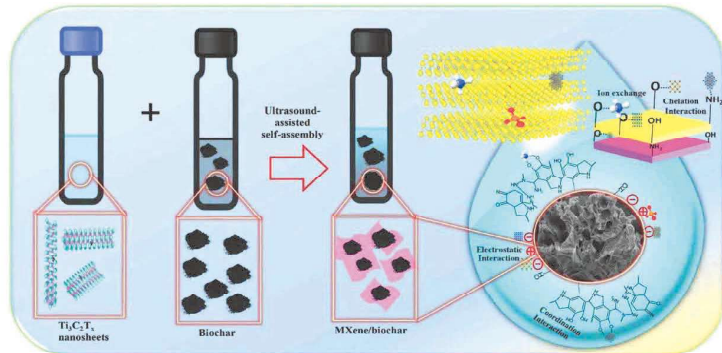


Figure 3: Schematic representation of the elimination mechanisms for inorganic and metallic pollutants by Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene/biochar composites.

### Conclusion

The study demonstrated that MXene combined with biochar effectively treats domestic wastewater, decreasing pH and EC by adsorbing alkaline compounds and dissolved salts. This treated wastewater supports the cultivation of *Pennisetum purpureum*, an efficient bioenergy crop with high volatile matter content, suitable for pyrolysis. Thermochemical analysis revealed that wastewater-treated biomass requires more energy for degradation, indicating higher activation energy under polluted conditions. These findings highlight the potential of MXene-biochar composites in the water-energy nexus, promoting sustainable wastewater treatment and bioenergy generation. Future research should focus on enhancing these composites and exploring their long-term effectiveness in various applications.

### Publications

(1) Kumar, A., Singh, E. and Lo, S.L., 2024. MXene/biochar composites for enhanced wastewater reclamation and bioenergy production: A kinetics and thermodynamics study. *Chemosphere*, 359, 142268. (2) Kumar, A., Singh, E. and Lo, S.L., 2025. Tunable 2D porous Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene@biochar composites synthesized via ultrasound-assisted self-assembly for simultaneous removal of co-existing wastewater contaminants. *Separation and Purification Technology*, 355, 129648.

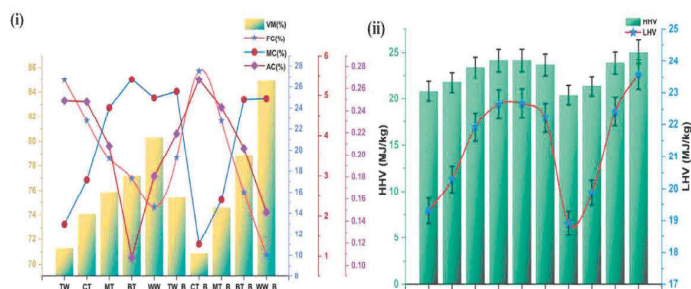


Figure 4: Proximate analysis and (ii) HHV and LHV of *Pennisetum purpureum* under various soil treatment and irrigation conditions.

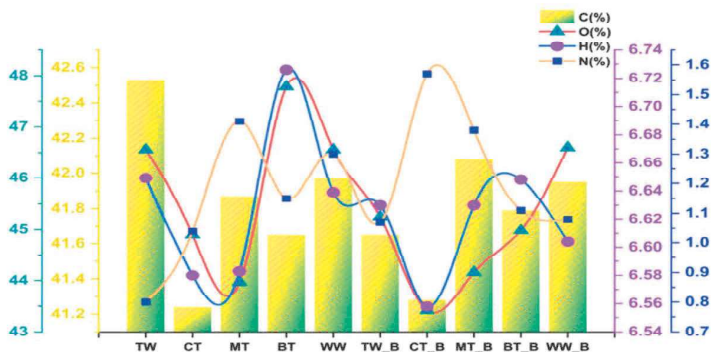


Figure 5: Elemental composition of *Pennisetum purpureum* under varied soil treatment and irrigation conditions.

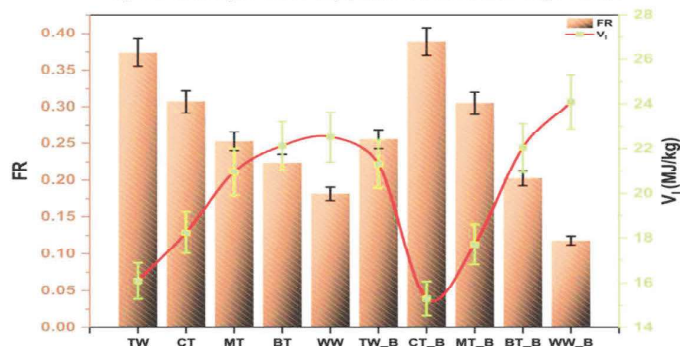


Figure 6: FR and V<sub>1</sub> in *Pennisetum purpureum* under varying soil treatment and irrigation conditions.