Electronic Supplementary Information

Bismuth Oxyhalide Quantum Dots Anchored Bismuth Molybdate Nanosheets as Z-Scheme Heterojunction for Photocatalytic Tetracycline Hydrochloride Degradation and Toxicity Analysis

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2. Experimental

2.6 Photoelectrochemical measurement.

Photoelectrochemical analysis was conducted using a Shanghai Chenhua CHI760E electrochemical workstation in a standard three-electrode configuration, with a 0.5 M Na_2SO_4 solution as the electrolyte. The FTO glass coated with the sample served as the working electrode. A mixture was prepared by grinding 5 mg of photocatalyst with 10 mL of Nafion solution to obtain a slurry, which was then spin-coated onto the FTO substrate. A platinum sheet and an Ag/AgCl electrode were used as the counter electrode and reference electrode, respectively. Transient photocurrent, electrochemical impedance spectroscopy, and Mott-Schottky analyses were performed under open-circuit voltage conditions.

2.7. Toxicity analysis.

The potential developmental toxicity of degradation products was evaluated utilizing the Toxicity Estimation Software Tool (T.E.S.T. 5.1.1), which is grounded in the principles of Quantitative Structure-Activity Relationship (QSAR) theory. This area of research is actively pursued both nationally and internationally, focusing on establishing qualitative and quantitative correlations between a compound's molecular structure and its physicochemical properties, biological activities, toxicological impacts, and environmental behavior using various molecular descriptors and model algorithms.

In this study, ninety uniform soybeans were systematically organized into three distinct groups, each soaked overnight in one of the following solutions: distilled water, a

degraded tetracycline (TC) solution, and a 10 mg/L TC solution. Following the soaking period, the soybeans were placed into separate containers and fully submerged in their respective solutions. The culture media were refreshed daily, and photographic documentation of the soybeans' growth was conducted throughout the experiment.

2.8. Computational methods

Spin-polarized density functional theory (DFT) calculations were performed using the CP2K software package. The computational approach implemented a mixed basis set comprising both Gaussian and plane wave functions. Core electrons were modeled utilizing norm-conserving Goedecker-Teter-Hutter pseudopotentials, while valence electron wavefunctions were expressed using a double-zeta basis set augmented with polarization functions, along with an auxiliary plane wave basis that had an energy cutoff of 400 eV. The generalized gradient approximation (GGA) exchange-correlation functional of Perdew, Burke, and Ernzerhof (PBE) was employed for the calculations. Each molecular configuration underwent optimization using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm, adhering to a self-consistent field (SCF) convergence criterion of 1.0×10^-6 atomic units. Additionally, corrections for van der Waals interactions were implemented using Grimme's DFT-D3 methodology.

3. Results and Discussion

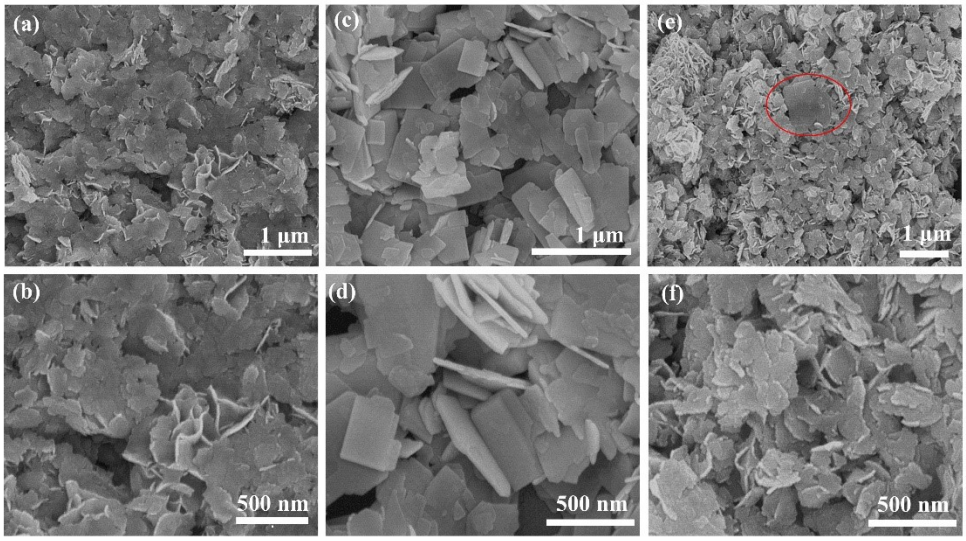

Fig.S1 SEM images of (a-b) BMO, (c-d) BOCI and (e-f) 8:2 BMO-BOCI

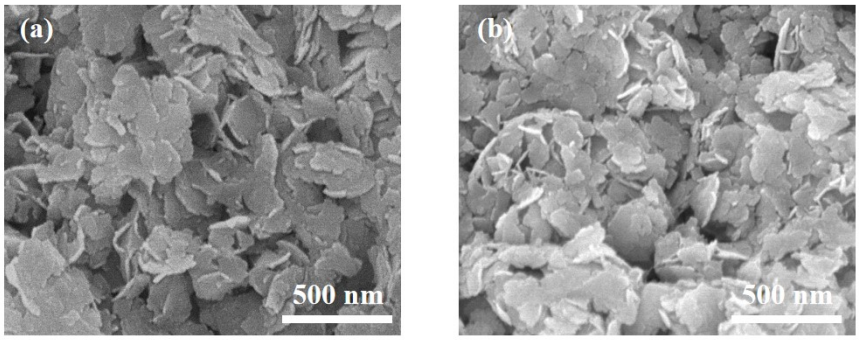

Fig.S2 SEM comparison before and after degradation

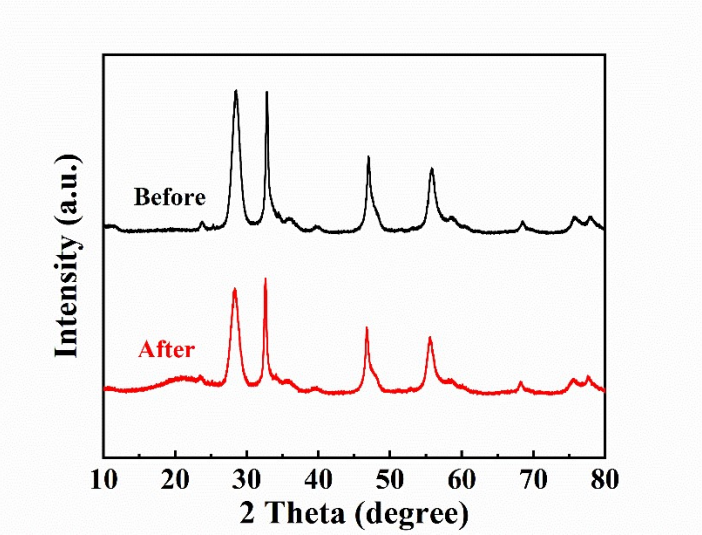

Fig. S3. XRD comparison before and after degradation

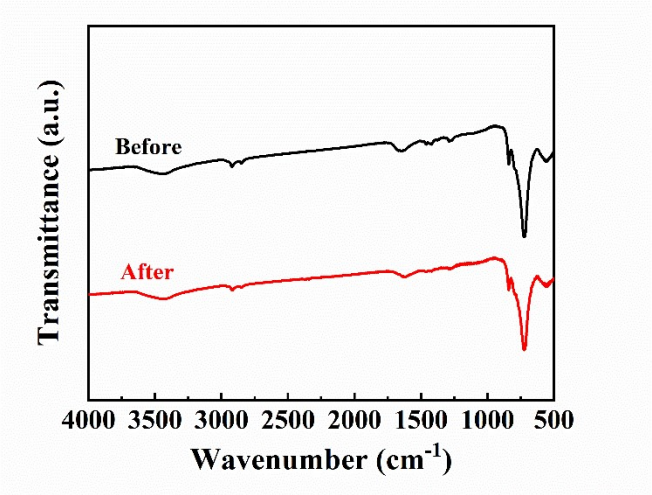

Fig. S4. FTIR comparison before and after degradation

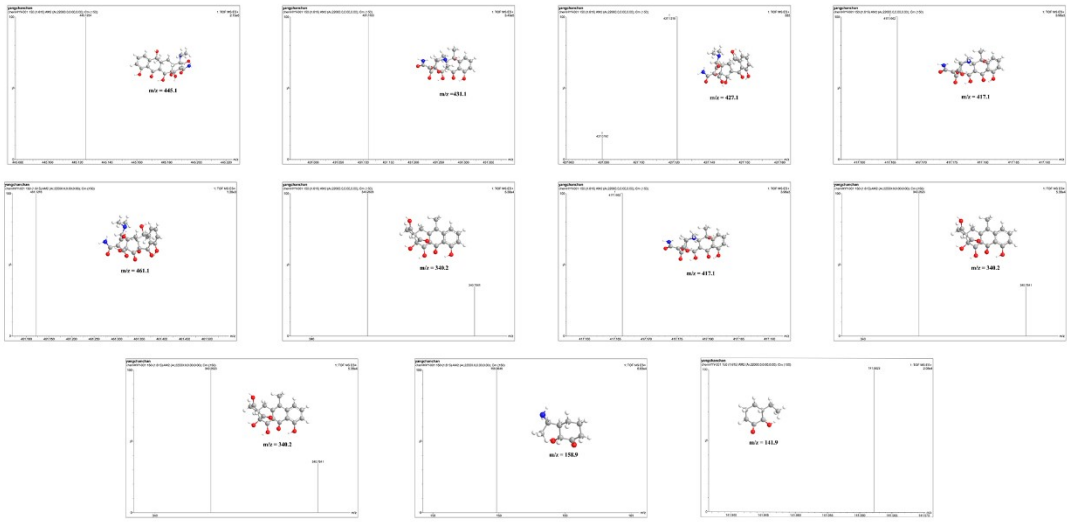

Fig. S5. Products spectra obtained by HPLC-MS for photocatalytic degradation of TCH in the presence of 7:3 BOCI-BMO catalysts under stimulated sunlight irradiation.