Electronic Supporting Information(ESI for)

In Situ Synthesis of n-n Bi₂MoO₆&Bi₂S₃ Heterojunctions for Highly Efficient Photocatalytic Removal of Cr(VI)

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Experimental Section

Adsorption experiments

The selective adsorption experiments for various pollutants including RhB, MO, AF, MB, CIP, SF and Cr(VI) solution were performed on the as-prepared materials. In briefly, 20 mg of sample was added to 50 mL of various model pollutant solutions with different concentrations (10-30 mg L⁻¹). The solutions were stirred for 80 min under the dark condition to reach adsorption–desorption equilibrium. The pollutant concentrations were determined by colorimetrically at the maximum wavelength using the UV-vis spectroscopy. The adsorption kinetics and equilibrium studies were studied according to the previously reported method ¹. All experiments were conducted at 25°C.

For Cr(VI) adsorption, 20 mg of the BMO-S1 heterojunctions sample was added to 50 mL of Cr(VI) aqueous solution with a fixed concentration under stirring in dark condition. The concentration of Cr(VI) left in supernatant solutions at different time intervals were determined using a UV-vis spectrophotometer at λ_{max}^2 . The amount of Cr(VI) adsorbed per unit mass of Bi₂MoO₆/Bi₂S₃ (q_t) at equilibrium was calculated by the Eq. 1³:

$$q_t = \frac{(C_0 - C_t)V}{m} \tag{Eq. 1}$$

where $q_t (mg/g)$ is the adsorbed Cr(VI) at time t (min); C₀ is the initial concentration of Cr(VI) in the solution (mg/L), C_t is the Cr(VI) concentration at time t (mg/L); m is the total amount of the Bi₂MoO₆/Bi₂S₃ (g); and V is the volume of solution (L). The removal percentage of Cr(VI) is given by Eq. 2⁴:

% removal =
$$\frac{(C_0 - C_e)}{C_0} \times 100$$
 (Eq. 2)

where C_0 , C_e are the initial and equilibrium concentration (mg/L) of Cr(VI), respectively.



Figure S1. (a) SEM image. (b) EDS spectrum and the corresponding elemental mapping of (c) S, (d) Mo, (e) Bi, (d) O of BMO-S1.



Figure S2. TEM image of BMO-S1 and the coresponding EDX analysis.

Samples	BET surface area (m^2/g)	Mean pore diameter(nm)	Total pore volume (m ³ /g)
Bi ₂ MoO ₆	7.2	22.8	0.04
BMO - S0.5	17.9	38.3	0.19
BMO-S1	26.9	43.1	0.26
BMO- S2	19.5	41.3	0.2
BMO- S4	12.1	32.9	0.10
BMO- S6	9.0	40.7	0.09

Table S1. The BET specific surface areas, mean pore diameters and total pore volumes of all the samples



Figure S3. Adsorption behavior of BMO-S1 for various pollutants (a) Methylene blue. (b) Methyl orange. (c) Acid fuchsin. (d) Rhodamine B. (e) Ciprofloxacin. (f) Sodium fluorescein and (g) Cr(VI).



Figure S 4. (a) Adsorption rate of Cr(VI) by BMO-S1. (b) The effect of contact time on the adsorption capacity of Cr(VI) onto BMO-S1 at different initial concentrations. (c) Pseudo-first-order kinetic plots and d) Pseudo-second-order kinetic plots for the adsorption of Cr(VI) by BMO-S1.

As shown in Figure S4a, b, the amount of Cr(VI) adsorbed on the BMO-S1 increases rapidly during the first contact time, then increases slowly till the adsorption equilibrium state with the extension of contact time. Adsorption kinetic studies are thoroughly studied due to their importance in ascertaining the adsorption rate and mechanism. The adsorption kinetic was fitted by the pseudo-first order and pseudo-second order models. The differential and integral forms of the pseudo-first order model can be written as ⁵:

$$\frac{dq_t}{dt} = k_1(q_e - q_t) \tag{Eq. 3}$$

$$ln(q_e - q_t) = lnq_e - k_1 \tag{Eq. 4}$$

The pseudo-second-order model can be expressed as:

$$\frac{dq_t}{dt} = k_2 (q_e - q_t)^2 \tag{Eq. 5}$$

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e}$$
(Eq. 6)

where $q_t (mg/g)$ is the amount of Cr(VI) adsorbed on the BMO-S1 at time t (h); $q_e (mg/g)$ is the amount of Cr(VI) adsorbed at adsorption equilibrium state; k_1 and k_2 are the rate constants of the pseudo-first order and the pseudo-second order rate model, respectively. The kinetics plots feature is achieved and the relevant parameters were presented in Fig. S4c, d. Obviously, the correlation coefficient values (R_2) of pseudo-second order model is much higher than that of pseudo-first order model, which illustrates that the kinetics adsorption can be well described by the pseudo-second model. The results of pseudo- second-order kinetics found in this study are supported by the findings of many earlier works ^{6, 7}.



Figure S5. Time-dependent UV-vis absorption spectra of Cr(VI) for all the samples. (a) Bi₂MoO₆. (b) BMO-S0.5. (c) BMO-S1. (d) BMO-S2. (e) BMO-S4 and (f) BMO-S6(Bi₂S₃).



Figure S6. XRD patterns of the BMO-S1 and after five successive catalytic runs.



Figure S7. The plots of transformed Kubelka–Munk function versus the energy of light for (a) Bi_2MoO_6 and (b) BMO-S6(Bi_2S_3).

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