Amalgamated Titanium Oxide-Carbon Hollow Sphere/Nickel-Layered Double Hydroxide as an Efficient Photocatalyst for the Degradation of Methyl Orange

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Supplementary Materials

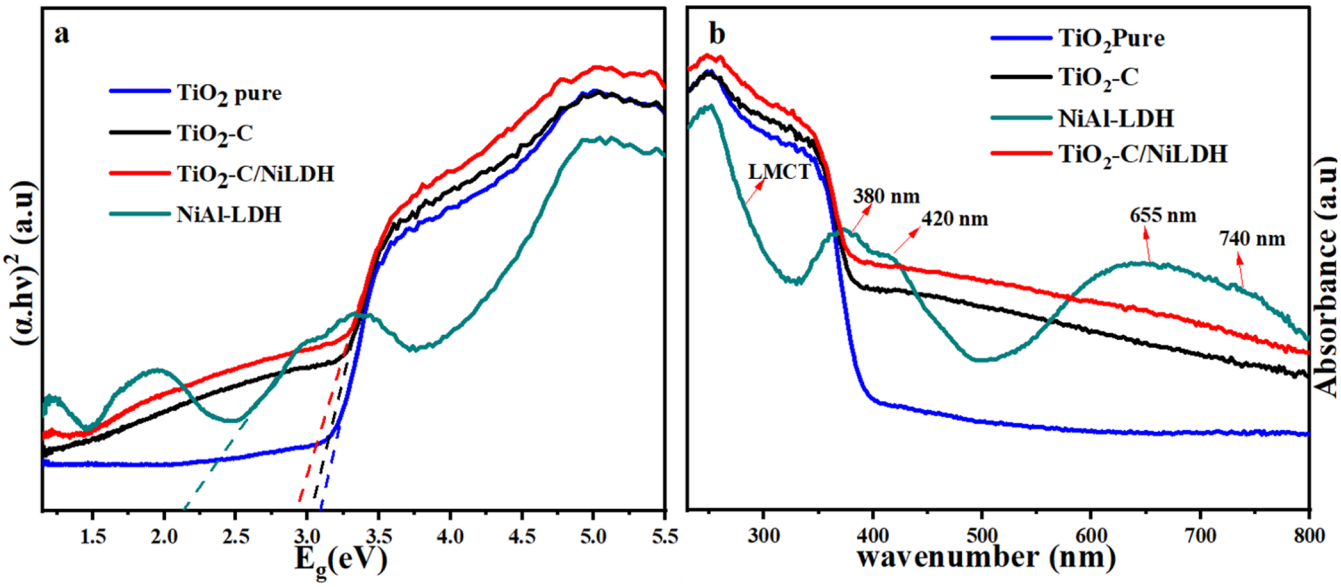

Figure S1. (a) Tauc plots to determine the optical band gaps and (b) UV-VIS DRS spectra of TiO_2, TiO_2-C, NiAl-LDH and TiO_2-C/NiLDH catalysts.

Calculation of Band Gap Using Tauc Plot

The band gap values for the catalysts were determined by using the Tauc plot is a method[1]. The Tauc method is based on the assumption that the energy-dependent absorption coefficient α can be expressed by the following Equation (S1):

$$(\alpha . h\nu)^{1/\gamma} = B(h\nu - E_g) \quad \text{(S1)}$$

where B is a constant, v is the frequency of the photon, E_g is the energy of the band gap, and h is the Planck constant. The factor γ is equal to 1/2 or 2 for the direct and indirect transition band gaps, depending on the type of electron transfer.[2].

The band gap energy is usually determined from diffuse reflectance spectra. According to the theory of P. Kubelka and F. Munk presented in 1931, the measured reflectance spectra can be transformed to the corresponding absorption spectra by applying the Kubelka–Munk function (F(R∞), **eq S2**).

$$F(R_\infty)=\frac{K}{S}=\frac{(1-R_\infty)^2}{2R_\infty} \qquad (S2)$$

Where $R_\infty=\frac{R_{sample}}{R_{standard}}$ is the reflectance of an infinitely thick specimen, while K and S are the absorption and scattering coefficients, respectively[3]. Putting $F(R_\infty)$ instead of α into **eq S1**

$$F(R_\infty).\ h\nu)^{1/\gamma} = B(h\nu - Eg) \qquad (S3)$$

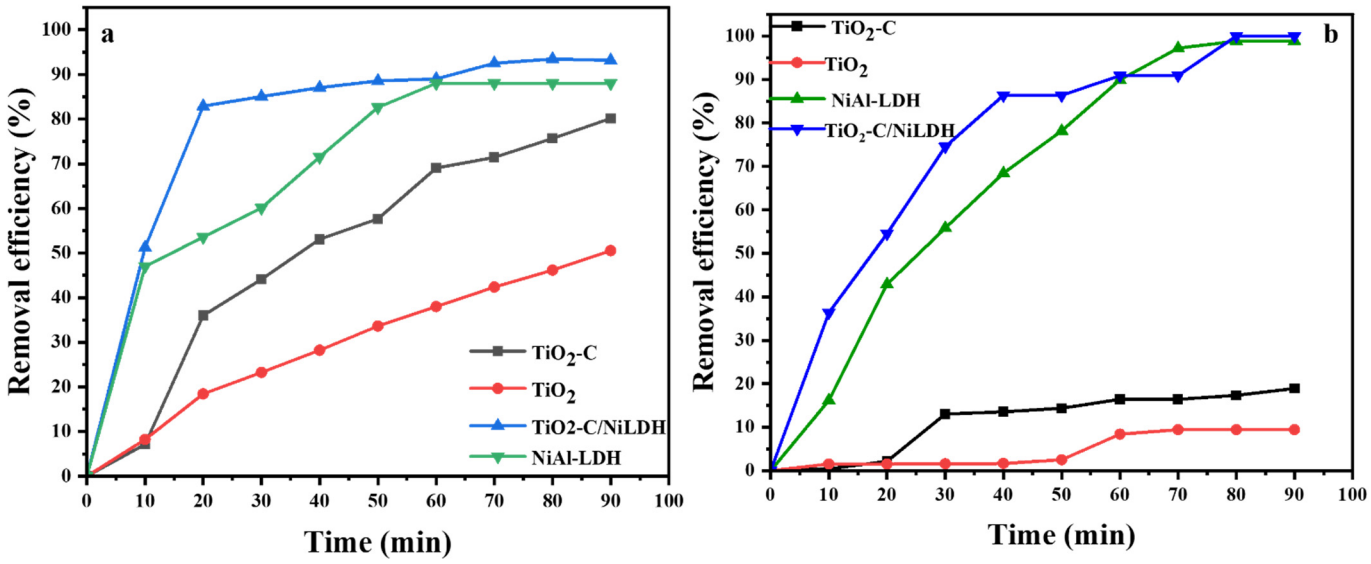

Figure S2. (a and b) removal efficiency of all the investigated catalysts under UV and VIS irradiation, respectively.

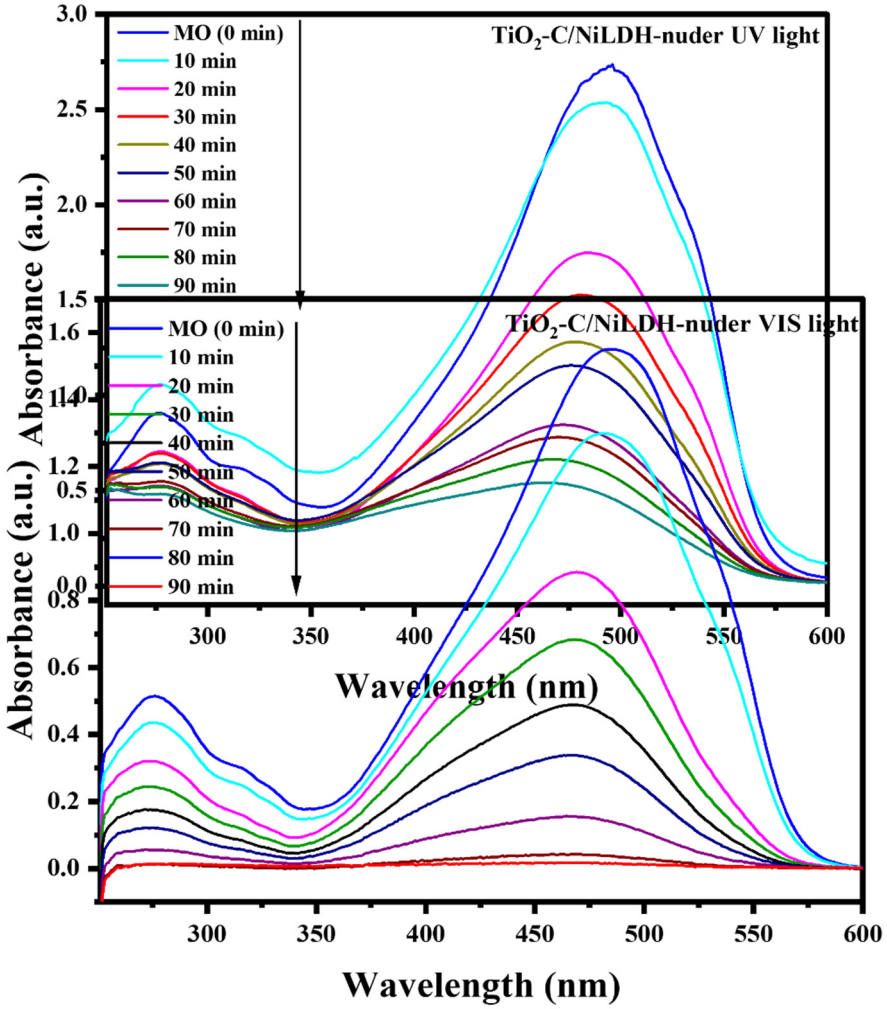

Figure S3. UV-visible absorption changes of methyl orange aqueous solution at 25°C in the presence of the TiO_2-C/NiLDH amalgam samples.

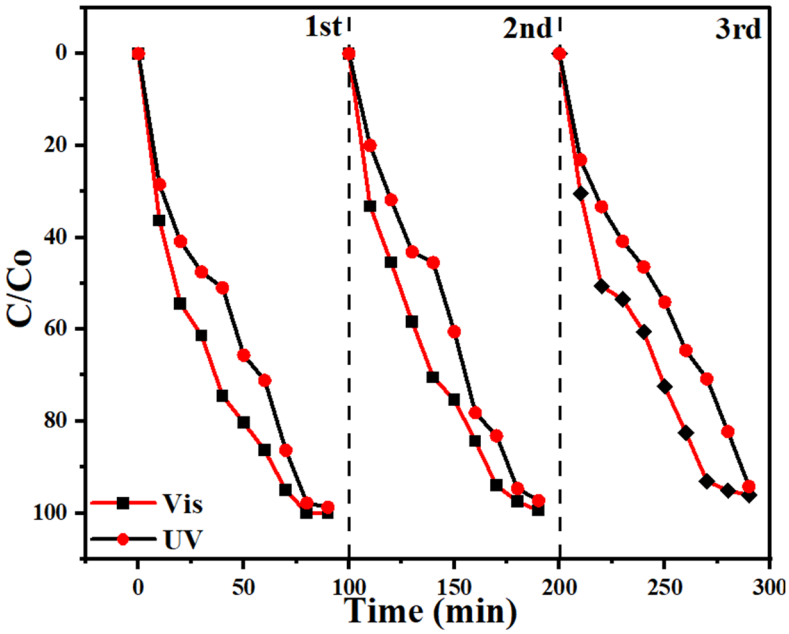

Figure S4. Recycling tests of the photocatalytic degradation of MO over TiO_2-C/NiLDH nanohybrid.

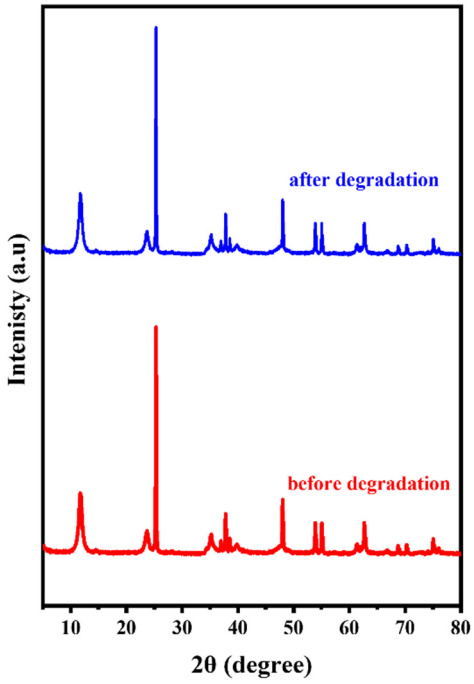

Figure S5. XRD of TiO_2-C/Ni-LDH core–shell amalgam before and after the degradation.

References

[1] P. Makuła, M. Pacia, and W. Macyk, "How To Correctly Determine the Band Gap Energy of Modified Semiconductor Photocatalysts Based on UV-Vis Spectra," J. Phys. Chem. Lett., vol. 9, no. 23, pp. 6814–6817, 2018, doi: 10.1021/acs.jpclett.8b02892.

[2] P. K. Basu, "Theory of Optical Processes in Semiconductors," Theory Opt. Process. Semicond., 2010, doi: 10.1093/acprof:oso/9780198526209.001.0001.

[3] R. López and R. Gómez, "Band-gap energy estimation from diffuse reflectance measurements on sol-gel and commercial TiO 2: A comparative

study," J. Sol-Gel Sci. Technol., vol. 61, no. 1, pp. 1–7, 2012, doi: 10.1007/s10971-011-2582-9.