

Electronic Supplementary Information

Novel biomass-based support (Starbon) for TiO₂ hybrid photocatalysts: a versatile green tool for water purification

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Materials characterization and measurements

Nitrogen physisorption

The specific surface area and porosity of the catalysts were measured in a Tristar II apparatus from Micromeritics. The samples were initially degassed under vacuum (120 mTorr) at 100°C for 1h and then at 300°C for 3h before analysis. Analysis was performed using the static method at 77K with nitrogen as the adsorbant. The Brunauer–Emmett–Teller (BET) method¹ was applied to calculate the total surface area, which is used for comparative purposes. The pore size distribution was obtained by applying the Barret–Joyner–Halenda (BJH) model² to the adsorption branch of the isotherm.

X-Ray diffraction

Powder XRD measurements were performed using standard Bragg–Brentano configuration. This type of arrangement was provided using Siemens D5000 diffractometer (equipped with a horizontal goniometer) with θ –2 θ geometry and Ni filtered Cu K α radiation, powered at 40 kV and 40 mA. Data were collected in the range of $2\theta = 10$ –90° with step interval of 0.02° and counting time up to 5 s per step.

The average crystallite size (D in nm) was determined according to the Scherrer equation³:

$$D = \frac{k\lambda}{\beta \cos\theta} \quad (1)$$

where D is the average crystallite size of the catalyst (nm), λ is the wavelength of the Cu k λ X-ray radiation ($\lambda = 0.154056$ nm), k is a coefficient usually taken as 0.94, β is the full width at half maximum (FWHM) intensity of the peak observed at 2θ (radian), and θ is the diffraction angle. The phase contents of the samples can be estimated from the respective XRD peak intensities using the following equation⁴:

$$f_A = \frac{1}{1 + \frac{1}{K} \frac{I_R}{I_A}} \quad (2)$$

$$K = 0.79 f_A > 0.2$$

$$K = 0.68 f_A \leq 0.2$$

where:

f_A is the fraction of anatase phase in the powder, and I_A and I_R are the X-ray intensities of the anatase (101) and rutile (110) diffraction peaks, respectively.

EDXRF elemental analysis

The elemental compositions of the samples were determined using the energy dispersive X-ray fluorescence (EDXRF) spectrometer (MiniPal 4, PANalytical&Co) with Rh tube and silicon drift detector. The spectra were collected in air atmosphere, without using a filter, at a tube voltage of 30 kV. The time of acquisition was set to 30 s and the tube current up to 50 μ A.

SEM images

The surface morphology of the photocatalysts was explored by a Nova 450 NonoSEM scanning electron microscope (SEM) with energy resolution of 130 eV.

DRS UV-vis

Ultraviolet-visible Diffuse Reflectance spectroscopy was performed using a UV-2501PC Shimadzu spectrophotometer. Band-gaps values were calculated based on the Kubelka–Munk functions⁵ $f(R)$, which are proportional to the absorption of radiation, by plotting $[f(R)hv]^{1/2}$ against hv . The function $f(R)$ was calculated using Eq. (3):

$$f(R) = \frac{(1-R)^2}{2R} \quad (3)$$

Band gap values were obtained from the plot of the Kubelka–Munk function $[F(R_\infty)E]^{1/2}$ versus the energy of the absorbed light E. Regarding absorption threshold, it was determined according to the formula⁶:

$$\lambda = \frac{1240}{E_{gap}} \quad (4)$$

Calculations for photocatalytic activity

The degradation rate can be expressed as first-order with respect to the concentration of phenol:

$$r = \frac{-dC}{dt} = k_{app} * C \quad (5)$$

where k_{app} is the apparent rate constant of a pseudo first order reaction.⁷ Integral form of reaction rate can be described as:

$$\ln\left(\frac{C_0}{C}\right) = k_{app} * t \quad (6)$$

where C_0 is the initial phenol concentration and C is the concentration of phenol at time t.

By plotting $\ln(C_0/C)$ versus t, the apparent rate constant (k_{app}) can be determined from the slope of the curve obtained.

Extraction was performed in order to determine the amount of phenol adsorbed on composite photocatalysts surface after 240 minutes of illumination. For this purpose, the photocatalyst was filtered and phenol was extracted at 20% acetonitrile solution under ultrasound for 20 minutes.⁸

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