Data Article

Experimental data of CaTiO₃ photocatalyst for degradation of organic pollutants (Brilliant green dye) – Green synthesis, characterization and kinetic study

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A B S T R A C T

The data presented here focuses on the physicochemical characterization of perovskite CaTiO₃ nanoparticles (orthorhombic) as photocatalysts and the kinetic study of their photodegradation performance toward organic pollutant, i.e. brilliant green (BG) which is azo derivatives dye. The CaTiO₃ nanoparticles was synthesized using chicken eggshell-derived CaCO₃ and anatase TiO₂ with molar ratio of (1:1), (1:3), (2:5), and (2:7). The physical and microstructural properties of CaTiO₃ were characterized by X-ray diffractometer (XRD), scanning electron microscope (SEM), Fourier Transform Infrared (FTIR) and UV/vis spectrometer. The effect of initial dye concentration, catalyst composition, and catalyst dosage on the adsorption mechanism of dye on CaTiO₃ was investigated in jacketed photoreactor under UV irradiation. The analysis reveals that BG molecules are efficiently chemisorbed, as indicated by pseudo first order kinetic, and degraded within 120 min. Considering the low-cost preparation process and high photocatalytic performance, the resul-
Specifications Table

| Subject | Materials Chemistry |
|---------|---------------------|
| Specific subject area | Photocatalysis |
| Type of data | Table, Image, Graph |
| How data were acquired | CaTiO₃ powder was prepared using wet chemical synthesis, in which chicken eggshells as precursor source were collected from the farm field in Samboja, Balikpapan, Indonesia. Physicochemical characterizations were carried out by scanning electron microscope (SEM), X-ray diffractometer (XRD), Fourier Transform Infrared (FTIR) spectrometer. The kinetic data was fitted using both pseudo first order and pseudo second order adsorption model. |
| Data format | X-ray diffractometer was operated at 40 kV, and 40 mA with Cu-Kα as a radiation source. Diffraction patterns were scanned between 10 and 100° (2θ) with resolutions of 0.05° FTIR spectra were collected in wavenumber range between 400 and 4000 cm⁻¹. SEM images were collected at 100 kV accelerating voltage with 500 × magnification. UV photoreactor was filled with 10 ppm of brilliant green solution and run under continuous stirring (500 rpm) at 28 °C. |
| Parameters for data collection | FTIR spectra were recorded using Thermo Nicolette 50 spectrometer at room temperature. Degradation of aqueous brilliant green (BG) dyes was probed under UV photoreactor using simulated UV irradiation (T5-UV7W, 254 nm). UV/vis absorption spectra to probe degradation of brilliant green dye were measured using UV/vis spectrometer (Rayleigh UV-9200). |
| Description of data collection | Morphology of CaTiO₃ was assessed using SEM (FEI Inspect 21). XRD patterns were collected using a diffractometer (PAN analytical type X'Pert Pro). FTIR spectra were recorded using Thermo Nicolo is50 spectrometer at room temperature. Degradation of aqueous brilliant green (BG) dyes was probed under UV photoreactor using simulated UV irradiation (T5-UV7W, 254 nm). UV/vis absorption spectra to probe degradation of brilliant green dye were measured using UV/vis spectrometer (Rayleigh UV-9200). |
| Data source location | Department of Chemical Engineering, Institut Teknologi Kalimantan, Balikpapan, East Kalimantan, Indonesia (−11.35330, 116.858093) |
| | Department of Engineering Physics, Institut Teknologi Sepuluh Nopember, Surabaya, East Java, Indonesia (−7.283395, 112.795727) |
| | Central Laboratory, State University Malang, East Java, Indonesia (−7.961229, 112.618759) |
| Data accessibility | Data are available within the article |

Value of the Data

The CaTiO₃ nanomaterial investigated here renders perovskite based photocatalyst which has been proven its functionality for photocatalytic degradation of azo dyes derivative, i.e. brilliant green (BG).

The current data, particularly the kinetic of degradation of aqueous BG solution, is useful for relevant studies of photocatalytic azo dye degradation using other catalysts, which is not limited to pristine CaTiO₃, CaCO₃, TiO₂ or composite materials. The photocatalytic degradation data suggest that the current prepared CaTiO₃ materials can be readily utilized as photocatalyst for wastewater treatment in textile industry, food processing industry, and for water treatment in water utility company.

The physicochemical data highlights the current synthesis route could not yield 100% CaTiO₃ and hence, optimization of precursor composition and mechanochemical as well as post heat treatment will be the focus of further research.
The preparation of CaTiO₃ nanomaterial investigated here is considered low cost and green since the wet chemical synthetic route didn’t require sophisticated apparatus while the precursor employed chicken eggshells (waste or by-product of farming activities).

1. Data description

Physicochemical characteristics of various CaTiO₃ are evaluated from the raw data, including scanning electron micrograph, X-ray diffraction pattern and FTIR spectra (available in the Supplementary Material). The surface morphology of different nanostructured CaTiO₃ prepared using different CaCO₃/TiO₂ molar ratio are depicted in Fig. 1. Higher TiO₂ fraction breaks the aggregation formed in CaTiO₃ prepared using large fraction of CaCO₃ due to higher surface energy of TiO₂ (1.4 × 10⁷ erg/cm²) than that of CaCO₃ (1.7 × 10⁴ erg/cm²) [1, 2]. Electronic vibrational characteristics and microstructural properties are indicated by FTIR spectra (Fig. 2) and X-ray diffraction pattern (Fig. 3), respectively. The decreasing IR bands at ~3630 cm⁻¹ and ~1440 cm⁻¹ are associated with the vibration characteristics of the hydroxy (OH) group and symmetric as well as asymmetric vibration between metal oxides, respectively [3]. In addition, the decreasing signal amplitude at ~1150 cm⁻¹ associated with C-O-Ti group vibration upon increasing TiO₂ mol fraction might indicate the more efficient interconversion into Ca-O-Ti reflected by higher absorption at ~660 cm⁻¹ [4]. XRD patterns indicate the formation orthorhombic CaTiO₃ with the presence of excess precursors, i.e. CaCO₃ and TiO₂. The diffraction peaks at 2θ of 23.2°, 33.1°, 47.5°, 58.8°, and 59.3° are assigned to the crystal planes of (101), (121), (202), (321), and (123), respectively [5]. Increasing the TiO₂ fraction from CaCO₃/TiO₂ molar ratio in the preparation of CaTiO₃ nanoparticles increases the crystallite size, i.e. 17.7, 22.9, 34.6, and 37.2 nm for (1:1), (1:3), (2:5), and (2:7), respectively. This implies that the specific surface area decreases upon increasing TiO₂ molar fraction.

Having characterized the physicochemical properties, the photocatalytic degradation of aqueous BG dyes using the resulting CaTiO₃ catalyst were investigated by probing the temporal change of UV/vis absorption spectra (Fig. 4, representative/selected raw data is available in the Supplementary Material). Kinetic of degradation mechanism to understand the adsorption process of dye molecules toward catalyst surface is evaluated using both pseudo first order and pseudo second order kinetic fit (Figs. 5–7). For pseudo first order fit, a plot of ln(Cₒ/Cₜ) vs t (Cₒ and Cₜ denote concentration at initial condition and time t, respectively) results in a linear curve, in which the slope equals to the observed rate constant (K₁) [6]. Meanwhile, pseudo second order fit, the off-set of the linear plot of t/qₑ vs t, where qₑ is the concentration at equilibrium condition, yield the rate constant (K₂) [6]. The rate constant of photocatalytic degradation upon varying the catalyst composition, catalysts dosage and pollutant concentration is summarized in Tables 1–3. The analysis indicates that increasing the fraction of TiO₂ in the precursor composition, i.e. CaCO₃/TiO₂ molar ratio, alters the adsorption behavior from physisorption (following second order reaction, R² > 0.9) to chemisorption (following first order reaction, R² > 0.9). In addition, increasing amount of CaTiO₃ catalyst implies on the increasing chemisorbed BG molecules and faster catalytic reaction. Even though the degradation rate is slower than the highest reported in literature using CaTiO₃ [7–9], the photodegradation rate of BG molecules using CaTiO₃ in this work (0.0185 ppm·min⁻¹) is found comparable to the photodegradation rate.

Table 1
Reaction rate constants (K) derived from both pseudo first order (K₁) and pseudo second order (K₂) as well as the corresponding coefficient of determination (R²) obtained for photodegradation of BG using different CaTiO₃ composition.

| CaCO₃/TiO₂ Molar Ratio | K₁ (min⁻¹) | R²  | K₂ (min⁻¹) | R²  |
|------------------------|------------|-----|------------|-----|
| (1:1)                  | 0.0014     | 0.5153 | 0.1301     | 0.9718 |
| (1:3)                  | 0.0023     | 0.6834 | 0.1403     | 0.9771 |
| (2:5)                  | 0.0176     | 0.9687 | 0.7022     | 0.9322 |
| (2:7)                  | 0.0183     | 0.9818 | 0.8185     | 0.9063 |
Fig. 1. Scanning electron micrographs of CaTiO$_3$ prepared using different CaCO$_3$/TiO$_2$ molar ratio, i.e. (a) (1:1), (b) (1:3), and (c) (2:5). All samples were annealed at 900 °C for 4 h.
Fig. 2. FTIR spectra of CaTiO₃ prepared with different CaCO₃/TiO₂ molar ratio.

Table 2
Reaction rate constants (K) derived from both pseudo first order (K₁) and pseudo second order (K₂) as well as the corresponding coefficient of determination (R²) obtained for photodegradation of BG using different amount of CaTiO₃ (2:7).

| CaTiO₃(2:7) Dosage (mg) | K₁ (min⁻¹) | R²  | K₂ (min⁻¹) | R²  |
|------------------------|------------|-----|------------|-----|
| 50                     | 0.0185     | 0.9502 | 0.8185     | 0.9061 |
| 100                    | 0.0183     | 0.9818 | 0.8032     | 0.9198 |
| 150                    | 0.0178     | 0.9518 | 0.8491     | 0.9247 |
| 200                    | 0.0176     | 0.9626 | 0.9802     | 0.95153 |

Table 3
Reaction rate constants (K) derived from both pseudo first order (K₁) and pseudo second order (K₂) as well as the corresponding coefficient of determination (R²) obtained for photodegradation of various BG concentration using 50 mg of CaTiO₃ (2:7).

| BG Concentration (ppm) | K₁ (min⁻¹) | R²  | K₂ (min⁻¹) | R²  |
|------------------------|------------|-----|------------|-----|
| 10                     | 0.0183     | 0.9818 | 0.8185     | 0.9061 |
| 20                     | 0.0113     | 0.9696 | 0.3971     | 0.8588 |
| 30                     | 0.0094     | 0.9664 | 0.2984     | 0.9185 |
| 40                     | 0.0076     | 0.9571 | 0.2363     | 0.9394 |

of other organic dye pollutants using solvothermal prepared CaTiO₃ (0.162 ppm•min⁻¹) [8] and hydrothermally prepared CaTiO₃ (0.05•ppm•min⁻¹) [9].

2. Experimental design, materials, and methods

Synthesis of CaTiO₃ nanoparticles employed a precursor mixture of commercial anatase TiO₂ (MTI, 99%) and CaCO₃ extracted from eggshells [9]. The collected chicken eggshells were washed thoroughly with ethanol-water mixture and dried at ambient atmosphere for 48 h. Afterwards, the dried eggshells were grounded for 30 min into fine particles. The fine powder was treated with 0.1 M HCl for 1 h and then washed with distilled water prior heat treatment at 100°C for 3 h. The heat-treated samples were then sieved (300 mesh) to yield fisted CaCO₃ nanoparticles.
Fig. 3. X-ray diffraction pattern of CaTiO$_3$ prepared using different CaCO$_3$/TiO$_2$ molar ratio. Triangle (▲), square (■) and circle (●) denote CaTiO$_3$, CaCO$_3$, and TiO$_2$, respectively.

(up to 86.6%). The initial step for CaTiO$_3$ synthesis was to prepare a mixture of CaCO$_3$ and TiO$_2$ in different CaCO$_3$/TiO$_2$ molar ratio of (1:1), (1:3), (2:5), and (2:7), which was dissolved in 100 ml of ethanol and homogenized by continuous stirring at 300 rpm for 2 h at room temperature. The suspension was filtered and washed with distilled water several times and dried in an oven at 100 °C for 2 h. The dried white powder was subsequently grounded into fine and homogeneous granules, and eventually annealed at 900 °C for 4 h. Characterization of CaTiO$_3$ nanoparticles follows the description in the specifications table (vide supra).

Initial investigation of 10 ppm brilliant green (BG) photodegradation was carried out employing different CaTiO$_3$ composition, i.e. different CaCO$_3$/TiO$_2$ molar ratio, in a custom-made photoreactor under UV irradiation [10,11]. Additionally, the dosage of CaTiO$_3$ and the initial concentration of BG solution were varied. It should be noted that the reactor was isolated from ambient light so that the photodegradation was driven only by UV irradiation. The solution in photoreactor was also continuously stirred to increase contact between CaTiO$_3$ photocatalyst and BG molecules and hence, driving a rapid photodegradation. Photodegradation of BG was monitored through the absorption change (300 nm < λ < 800 nm) measured using UV/vis spectrometer. The decrease of BG optical density was used to determine the decreasing BG concentration due to the catalytic activity of CaTiO$_3$, which was later used to evaluate the adsorption kinetics.
Fig. 4. The time dependent absorption spectra of BG (10 ppm) upon photodegradation using CaTiO₃ with CaCO₃/TiO₂ molar ratio of (a) (1:3) and (b) (2:7). The amount of catalyst was fixed at 50 mg.
Fig. 5. (a) Pseudo second order and (b) pseudo first order kinetic fit from photodegradation data of 10 ppm BG employing CaTiO$_3$ prepared from different CaCO$_3$/TiO$_2$ composition.
Fig. 6. (a) Pseudo second order and (b) pseudo first order kinetic fit from photodegradation data of 10 ppm BG employing CaTiO$_3$ (2:7) with different catalyst dosages.
Fig. 7. (a) Pseudo second order and (b) pseudo first order kinetic fit from photodegradation data of different BG concentration employing 50 mg CaTiO$_3$ (2:7).
Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found in the online version, at doi:10.1016/j.dib.2020.106099.

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