The data presented in this article are related to a research article entitled ‘Highly efficient solar-driven photocatalytic degradation on environmental pollutants over a novel C fibers@MoSe₂ nanoplates core–shell composite’ (Wang et al., 2018) [1]. In this article, we report original data on the synthesis processes optimization of the proposed composite together with its formation mechanism. The report includes the composition, microstructure and morphology of the corresponding samples, and the photocatalytic activity and stability of the optimal composite. Compared with commercially available MoSe₂ powder, the reaction rate constant of the optimal composite catalyst for the degradation of methylene blue (MB) and rhodamine B (RhB) under simulated sunlight irradiation (SSI) could be increased in a factor of about 14 and 8, respectively. The data are presented in this format to allow the comparison with those from other researchers in this field, and
understanding the synthesis and photocatalysis mechanism of similar catalysts.
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Specifications table

| Subject area                        | Environmental engineering, Environmental science, Chemical engineering, Materials science, Materials engineering |
|-------------------------------------|-------------------------------------------------------------------------------------------------------------|
| More specific subject area          | Photocatalytic degradation, New energy devices                                                             |
| Type of data                        | Tables, Figures                                                                                             |
| How data was acquired               | X-ray diffraction (XRD, Rigaku D/max-RB, Japan), Field emission scanning electron microscope (FE-SEM, Quanta FEG-650, America), Photocatalytic reaction system (PCX50A Discover, Beijing Perfectlight Technology Co., Beijing, China) |
| Data format                         | Raw and analyzed data                                                                                        |
| Experimental factors               | The amounts of the used reaction resources: absolute ethanol (constantly 5 mL), MoO3 powder (1.0–1.6 g), Se powder (0.5–3.0 g), pre-oxidized polyacrylonitrile (PAN) fiber (constantly 0.15 g). Temperature: 900–1100 °C for synthesizing the photocatalysts Reaction time: 1 h for synthesizing the photocatalysts |
| Experimental features              | The designed experiments included the optimization of synthesis processes and comparison on the photocatalytic degradation of MB, RhB, p-chlorophenol (4-CP) and K2Cr2O7 (Cr, VI) |
| Data source location                | The composite was grown in Beijing, China                                                                   |
| Data accessibility                  | The data are available with this article                                                                    |

Value of the data

- The data on the synthesis processes optimization of the C fibers@MoSe2 nanoplates core–shell composite (NPCSC) could give an insight into its formation and photocatalysis mechanisms to other researchers interested in the synthesis and application of photocatalysts.
- The data can be used by researchers interested in developing other composite photocatalysts and understanding their photocatalytic mechanism.
- The data can be used by researchers interested in developing new energy materials, and energy storage and conversion devices.

1. Data

The data presented in this paper are related to a research article entitled ‘Highly efficient solar-driven photocatalytic degradation on environmental pollutants over a novel C fibers@MoSe2 nanoplates core–shell composite’ [1].

It includes data on the synthesis processes optimization and formation mechanism of the present C fibers@MoSe2 NPCSC (Figs. 1–5), which reveal that numerous MoSe2 thin nanoplates are grown in-situ, densely and even vertically on the surface of the C fibers, forming the optimal core–shell composite. Data on the photocatalytic performance and stability of the optimal composite catalyst are also presented (Figs. 6–14). In addition, data on the activity for the photodegradation of 4-CP and Cr (VI) over the present C fibers@MoSe2 NPCSC and other photocatalysts are compared in Tables 1 and 2.
2. Experimental design, materials and methods

Novel highly efficient C fibers@MoSe₂ NPCSC photocatalyst for environmental remediation was described by Wang et al. [1]. In order to improve the photocatalytic performance of the composite, the synthesis processes were optimized by changing the reaction temperature from 900 to 1100 °C, and adjusting the applied amounts of MoO₃ powder from 1.0 to 1.6 g in 5 mL absolute ethanol and Se

Fig. 1. (a) Typical XRD patterns of the samples prepared at different temperatures, and their corresponding SEM images: (b) 900, (c) 950, (d) 1000, (e) 1050 and (f) 1100 °C. In this group of experiments, 2.0 g of MoO₃ powder and 0.5 g of Se powder were used.

Fig. 2. (a) Typical XRD patterns of the samples prepared at a constant temperature of 1100 °C with different amounts of MoO₃ and a fixed amount (2.0 g) of Se powder, and their corresponding SEM images with (b) 1.0, (c) 1.2 and (d) 1.6 g of MoO₃ powder.
powder from 0.5 to 3.0 g. All the prepared samples were characterized by XRD and SEM. And all the experiments were conducted in duplicates.

From Fig. 1, it can be seen that the sample prepared at 900 °C almost consists of pure MoO₂ nanoparticles. As the temperature increased, MoO₂ nanoparticles were further, gradually reduced into

- **Fig. 3.** (a) Typical XRD patterns of the samples prepared with different amounts of Se powder but a fixed amount (1.0 g) of MoO₃ powder at a constant temperature of 1100 °C, and their corresponding SEM images with different amounts of Se powder: (b) 2.0 and (c) 3.0 g.

- **Fig. 4.** EDX spectra on the outer shell (a) and inner core (b) of typical fractured fiber after ultrasonic oscillation in ethyl alcohol (see the insets).

- **Fig. 5.** Formation mechanism of the C fibers@MoSe₂ NPCSC.

powder from 0.5 to 3.0 g. All the prepared samples were characterized by XRD and SEM. And all the experiments were conducted in duplicates.
Fig. 6. The decolourization of organic dyes MB and RhB during photodegradation under SSI without any catalyst.

Fig. 7. Composition and microstructure of the commercially available MoSe₂ powder. (a) Typical SEM image, indicating that the powder consists completely of MoSe₂ nanoplates. (b) Typical EDX spectrum on the imaging area of (a), revealing that the powder is composed of only Mo and Se. (c) Typical XRD pattern of the sample, in which the diffraction peaks are matching well with those of MoSe₂ phase (JCPDS card no. 29-0914). All these results reveal that the commercially available powder is composed of pure MoSe₂ nanoplates.
MoSe₂, resulting in nanoplates on the surfaces of the carbon fibers. When it increased up to 1100 °C, MoSe₂ nanoplates had completely replaced MoO₂ nanoparticles, although there was still a little amount of metallic Mo in the sample.

This figure reveals that when 1.0 g of MoO₃ powder was used, the desirable product had MoSe₂ nanoplates in a quite high density, and the by-products such as MoO₂ were in the least amount.

Based on the results presented in Figs. 1 and 2 in Ref. [1] and the corresponding discussion, in combination with the present Figs. 1–4, a possible formation mechanism called in-situ “symplastic growth” can be used to explain the growth of the present C fibers@MoSe₂ NPCSC. The whole process can be schematically shown in Fig. 5. In the first step, a composite of PAN fibers@MoO₃ particles was formed by soaking the PAN fibers in MoO₃ suspension, where the MoO₃ particles were uniformly distributed.
coating on the surface of the PAN fibers. In the second step, at 400–600 °C under the action of inert gas, the oxygen-containing functional groups of the pre-oxidized PAN fibers were dehydrated and cross-linked to form a more stable trapezoidal structure. The trapezoid molecules were connected into a graphene-like structure by the dehydrogenation reaction. When the temperature raised up to above 600 °C, in the third step, denitration reaction would occur, forming structured C fibers and releasing H2, NH3, HCN, H2O and so on [2]. Synchronously, the partially pyrolyzed C reacted with MoO3 to produce MoO2 and reducing gas CO. As the amounts of reducing H2 and CO gases increased, and more Se vapor was fed from the upstream, MoO2 nanocrystals were further selenized to form MoSe2 nanoplates, finally producing the C fibers@MoSe2 NPCSC.

Fig. 6 reveals that without photocatalysts, MB is self-sensitized but RhB is stable under SSI. Under the present conditions, MB will be decolourized by SSI at about 10%, but without photocatalysts, no photodegradation under SSI could be observed on RhB.

Fig. 8 shows the decolourization effects on MB under SSI over the as-prepared C fibers@MoSe2 NPCSC and commercially available MoSe2 powder, respectively. As is seen from Fig. 8a, a dark adsorption for 60 min was performed prior to light irradiation so as to reach the adsorption–desorption equilibrium. In this stage, the decolourized MB over the C fibers@MoSe2 NPCSC was 25.9%, while that over the MoSe2 powder was only 7.3%. During the photocatalytic degradation, the degraded MB over the C fibers@MoSe2 NPCSC reached 19.2%, whereas that over the commercially bought MoSe2 powder was only 1.9%. This result reveals that the commercially bought MoSe2 powder has no usable photocatalytic activity on the degradation of MB; however, after compositing with C fiber, the photocatalytic performance of MoSe2 nanoplates can be greatly enhanced.
The photocatalytic degradation of MB follows the pseudo-first-order kinetics as described by the equation of $-\ln\left(C/C_0\right) = kt$ \cite{3,4}. Through this equation, straight lines can be fitted into Fig. 8b, in which the slope of the straight lines can be explained as the photocatalytic reaction rate constant $k$. The rate constants of the photodegradation reactions on MB over the as-prepared C fibers@MoSe2 NPCSC and commercially available MoSe2 powder, and (b) their corresponding $-\ln(C/C_0)$ vs. irradiation time plots. (c) Decolourization effects on RhB under SSI over fresh C fibers@MoSe2 NPCSC and that stored for 4 months. (d) Recycle experiment of photocatalytic degradation on RhB under SSI over the as-prepared C fibers@MoSe2 NPCSC.

![Figure 8b](image1)

![Figure 8c](image2)

![Figure 8d](image3)

**Fig. 8.** Photocatalytic degradation on RhB over the sample. (a) Decolourization effects on RhB under SSI over the as-prepared C fibers@MoSe2 NPCSC and commercially available MoSe2 powder, and (b) their corresponding $-\ln(C/C_0)$ vs. irradiation time plots. (c) Decolourization effects on RhB under SSI over fresh C fibers@MoSe2 NPCSC and that stored for 4 months. (d) Recycle experiment of photocatalytic degradation on RhB under SSI over the as-prepared C fibers@MoSe2 NPCSC.

The photocatalytic degradation of MB follows the pseudo-first-order kinetics as described by the equation of $-\ln(C/C_0) = kt$ \cite{3,4}. Through this equation, straight lines can be fitted into Fig. 8b, in which the slope of the straight lines can be explained as the photocatalytic reaction rate constant $k$. The rate constants of the photodegradation reactions on MB over the as-prepared C fibers@MoSe2 NPCSC and commercially bought MoSe2 powder are 0.0043 and 0.0003 min$^{-1}$, respectively. This result indicates that after compositing with C fibers in the form of the present C fibers@MoSe2 NPCSC, the rate constant of MB photodegradation over MoSe2 nanoplates under SSI was increased in a factor of about 14.

**Fig. 8c** illustrates the photocatalytic activity of the sample stored for 4 months on degrading MB under SSI. It is seen that the totally decolourized MB by the catalyst stored for 4 months was 57.3%, almost equaling to that by the fresh one (54.9%). This result reveals an excellent structural stability of the C fibers@MoSe2 NPCSC photocatalyst for a long period of storage.

Moreover, the sample was also repeatedly used for the photodegradation of MB to further evaluate its chemical stability. The result is displayed in **Fig. 8d**. It was revealed that during the repeated use, the photocatalytic activity of the catalyst for the degradation of MB under SSI decreased very little after 3 times of experiments were carried out. This result in combination of their well-kept morphology and composition as shown in the SEM images in **Fig. 9** after being used indicates that such catalyst has a relatively high stability during photocatalytic application. As for the very little reduction in photocatalytic activity during recycling use, it might be resulted from the exfoliation and loss of a
**Fig. 11.** Typical low- and high-magnification SEM image (a, b) with the corresponding XRD pattern (c) of the C fibers@MoSe$_2$ NPCSC catalyst after being applied in the photodegradation of RhB under SSI for 70 min.

**Fig. 12.** UV–vis absorption spectra of 4-CP at the beginning (blue line) and end (red line) of the photocatalytic reaction. As can be seen from Fig. 12, after a long period of SSI, the intensity of UV absorption peak of 4-CP (225 nm and 280 nm) decreased significantly. This result illustrates that the applied 4-CP has been substantially photocatalytically degraded.
few MoSe2 nanoplates from the sample during the repeated washing and drying after each cycle of photocatalytic test.

In combination with its original morphology and composition, Fig. 9 reveals that the morphology and composition of the catalyst can be well maintained during the photocatalytic degradation of MB, indicating that the catalyst has good stability during such reactions.

It can be seen from Fig. 10a that in the dark adsorption stage, the decolourized RhB by the C fibers@MoSe2 NPCSC was 11.2%, while that by the commercially available MoSe2 powder was only 1.4%. In the photocatalytic stage, the degraded RhB over the C fibers@MoSe2 NPCSC reached 18.9%, but that over the commercially bought MoSe2 powder was only 2.8%. This result reveals that the commercially available MoSe2 powder has no photocatalytic activity for the degradation of RhB. However, the photocatalytic activity of MoSe2 nanoplates can be greatly enhanced after compositing with C fiber in the form of the reported C fibers@MoSe2 NPCSC. On the basis of the recorded data on the photocatalytic degradation reactions, straight lines can be fitted for the plots of -ln(C/C0) versus irradiation time, and the results are shown in Fig. 10b. From the fitted graph, the rate constants of the photodegradation reaction on Rhb over the as-prepared C fibers@MoSe2 NPCSC and commercially available MoSe2 powder were calculated as 0.00347 and 0.00043 min⁻¹, respectively. It is seen that after composting with C fibers, the photodegradation rate of RhB over the present C fibers@MoSe2 NPCSC was 8 times higher than that over the commercially available MoSe2 powder.

Fig. 10c reveals the stability of the C fibers@MoSe2 NPCSC on degrading RhB under SSI. While the other conditions were fixed, the decolourized RhB by the C fibers@MoSe2 NPCSC catalyst stored for 4 months reached 72.6%, which is very close to that over the fresh C fibers@MoSe2 NPCSC (69.9%). This result indicates that after being stored for a long time, the fibers@MoSe2 NPCSC still had good
photocatalytic performance on the photodegradation of RhB. Fig. 10d displays the photocatalytic repeatability of the C fibers@MoSe\textsubscript{2} NPCSC on degrading MB under SSI. Three repeated tests were performed on the photodegradation of RhB over the same catalyst sample. It is seen from this graph that, the photocatalytic activity of the C fibers@MoSe\textsubscript{2} NPCSC on the degradation of RhB decreased very little after each test. In combination with their good morphology and well-kept composition after photodegradation test as shown in Fig. 11, it was revealed that the present C fibers@MoSe\textsubscript{2} NPCSC had excellent photocatalytic stability.

In combination with its original morphology and composition, Fig. 11 reveals that the catalyst could maintain its morphology and composition during the photocatalytic degradation of RhB, indicating that the C fibers@MoSe\textsubscript{2} NPCSC catalyst has good stability during such reactions.

In combination with its original morphology and composition, Fig. 13 reveals that the catalyst could maintain its morphology and composition during the photocatalytic degradation of 4-CP, indicating that the C fibers@MoSe\textsubscript{2} NPCSC catalyst has good stability during such photocatalytic reactions.

In combination with its original morphology and composition, Fig. 14 indicates that the morphology and composition of the catalyst can be well maintained during the photocatalytic degradation of Cr(VI), indicating that the catalyst has good stability during such photocatalytic reactions.
Table 1
Comparison on the photocatalytic degradation of 4-CP over the C fibers@MoSe$_2$ NPCSC with those over TiO$_2$-based catalysts reported in literature.

| Catalysts                                | Light source                  | Light intensity (mW/cm$^2$) | Catalyst concentration (g/L) | Stirring | Decolourization rate | k (min$^{-1}$) | Recycling times | Refs. |
|------------------------------------------|-------------------------------|-----------------------------|-----------------------------|----------|----------------------|----------------|----------------|-------|
| C fiber@MoSe$_2$ NPCSC                   | 5 W LED lamp                  | 36                          | 1                           | no       | 19.4% in 70 min      | 0.00289        | 3              | [1]   |
| MoS$_2$ and WS$_2$ nanocluster sensitized TiO$_2$ nanoparticles | 300 W tungsten halogen lamp $\lambda \geq 400$ nm | -                           | 1                           | no       | 63% in 300 min       | -              | -              | [5]   |
| C-modified TiO$_2$ nanoparticles        | 250 W Xe lamp $\lambda \geq 420$ nm | 30                          | 1                           | yes      | 77.5% in 240 min     | 0.0061         | -              | [6]   |
| N-F-codoped TiO$_2$ nanoparticles       | 500 W Xe lamp $\lambda \geq 400$ nm | -                           | 2                           | yes      | 72.48% in 300 min    | -              | 5              | [7]   |
| N-doped TiO$_2$ nanoparticles           | 500 W Xe lamp $\lambda \geq 400$ nm | -                           | 0.5                          | yes      | 63.5% in 300 min     | -              | -              | [8]   |
### Table 2
Comparison on the photocatalytic reduction of Cr (VI) over the present C fibers@MoSe$_2$ NPCSC catalyst with those over other semiconductor-based catalysts reported in literature.

| Catalysts                        | Light source                  | Light intensity (mW/cm$^2$) | Catalyst concentration (g/L) | Stirring | Decolourization rate | $k$ (min$^{-1}$) | Recycling times |
|----------------------------------|-------------------------------|-------------------------------|-------------------------------|----------|----------------------|------------------|-----------------|
| C fiber@MoSe$_2$ NPCSC           | 5 W LED lamp                  | 36                            | 1                             | no       | 34.7% in 120 min     | 0.0034           | 3               |
| C quantum dots decorated MoSe$_2$| 300 W Xe lamp $\lambda \geq$ 400 nm | 741                           | 1                             | yes      | 99% in 180 min       | 0.026            | 3               |
| Hexagonal 2H-MoSe$_2$ nanoparticles | 300 W Xe lamp $\lambda \geq$ 400 nm | 741                           | 1                             | yes      | 94% in 180 min       | 0.027            | 3               |
| MoSe$_2$ nanosheets/TiO$_2$ nanoparticles composite | 400 W metal halogen lamp $\lambda \geq$ 400 nm | $-$                            | 1                             | yes      | 91% in 120 min       | 0.0141           | $-$              |
| MoSe$_2$ nanoparticles          | 400 W metal halogen lamp $\lambda \geq$ 400 nm | $-$                            | 1                             | yes      | 95% in 250 min       | $-$              | 5               |
| 3D MoS$_2$/r-GO aerogel          | 300 W Xe lamp                 | 545                           | 0.67                          | yes      | 92% in 120 min       | $-$              | $-$             |
| 2D MoS$_2$ nanosheet coated Bi$_2$S$_3$ discoids | 300 W Xe lamp $\lambda \geq$ 400 nm | 700                           | 0.25                          | yes      | 97% in 30 min        | $-$              | 3               |
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Transparency document. Supporting information

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2018.01.103.

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