

Electronic Supplementary Information for

**Synergetic contribution of enriched selenium vacancies and out-of-plane ferroelectric polarization in AB-stacked MoSe<sub>2</sub> nanosheets as efficient piezocatalysts for TC degradation**

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Jinfen Niu<sup>a</sup>, Yan Yu<sup>a</sup>, Zheng Chang<sup>a</sup>, Yangqing He<sup>a</sup>

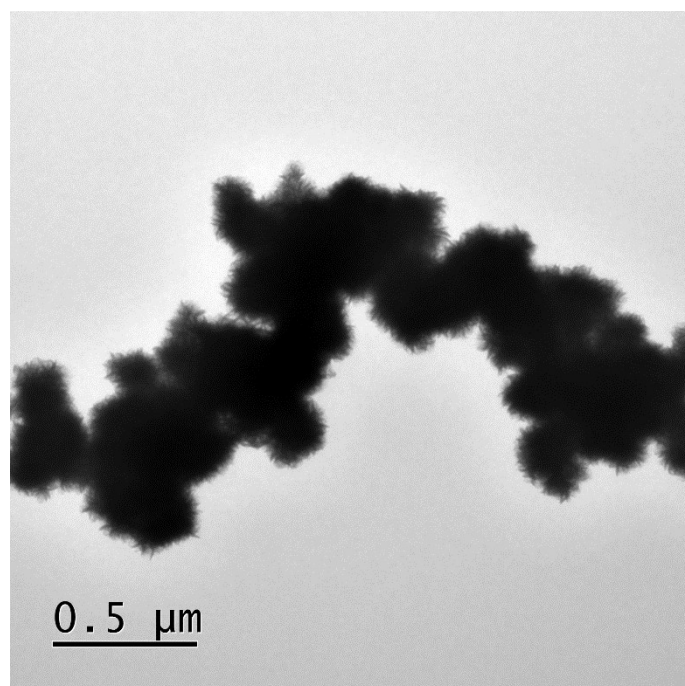
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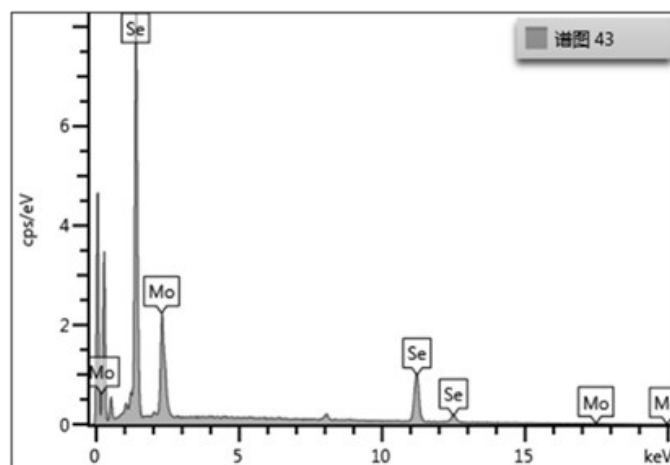
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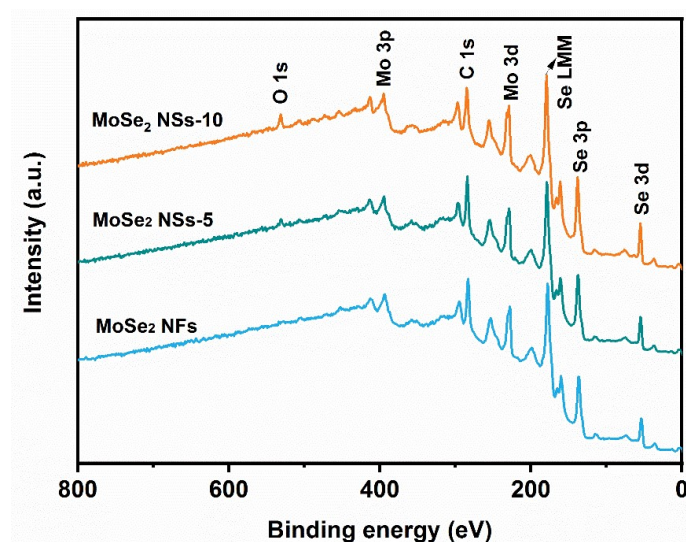


**Fig. S1.** The TEM image of MoSe<sub>2</sub> NFs.

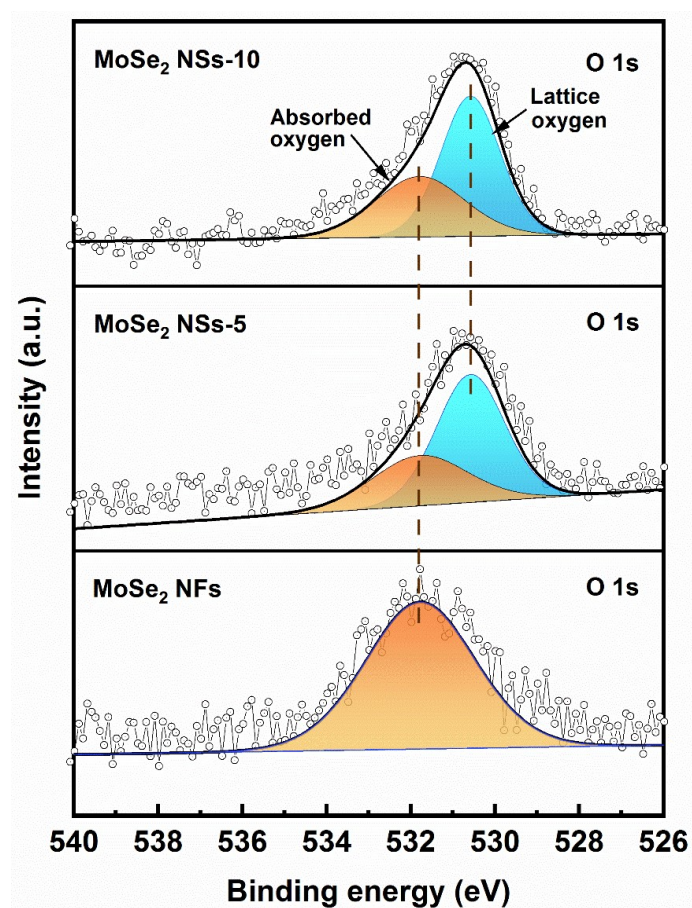


| Element | wt%    | wt% Sigma | Atomic ratio (%) |
|---------|--------|-----------|------------------|
| Se      | 58.28  | 0.53      | 62.93            |
| Mo      | 41.72  | 0.53      | 37.07            |
| Total:  | 100.00 |           | 100.00           |

**Fig. S2.** The EDS of MoSe<sub>2</sub> NSs-10.



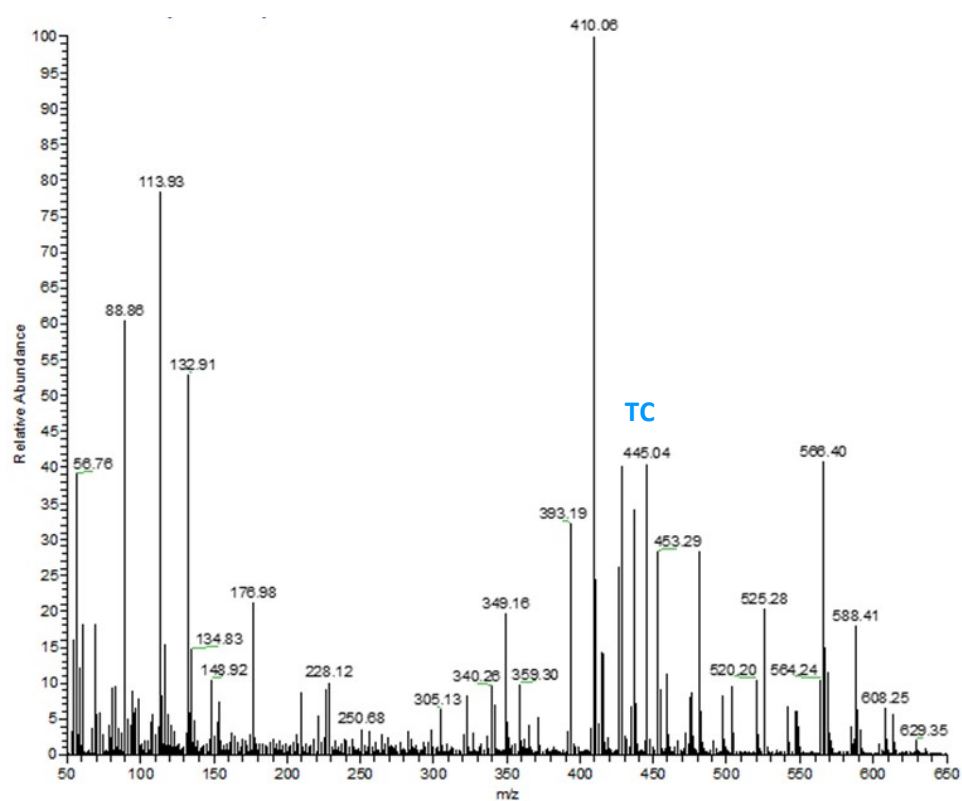
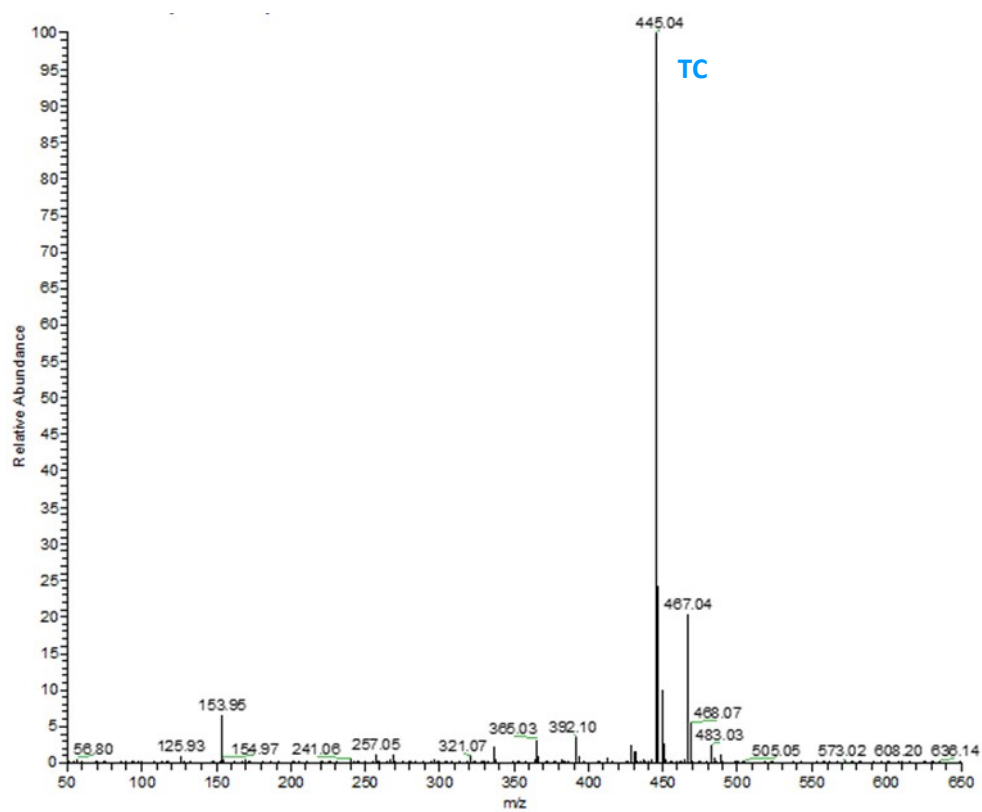
**Fig. S3.** The XPS survey spectra of MoSe<sub>2</sub> NFs, MoSe<sub>2</sub> NSs-5 and MoSe<sub>2</sub> NSs-10.

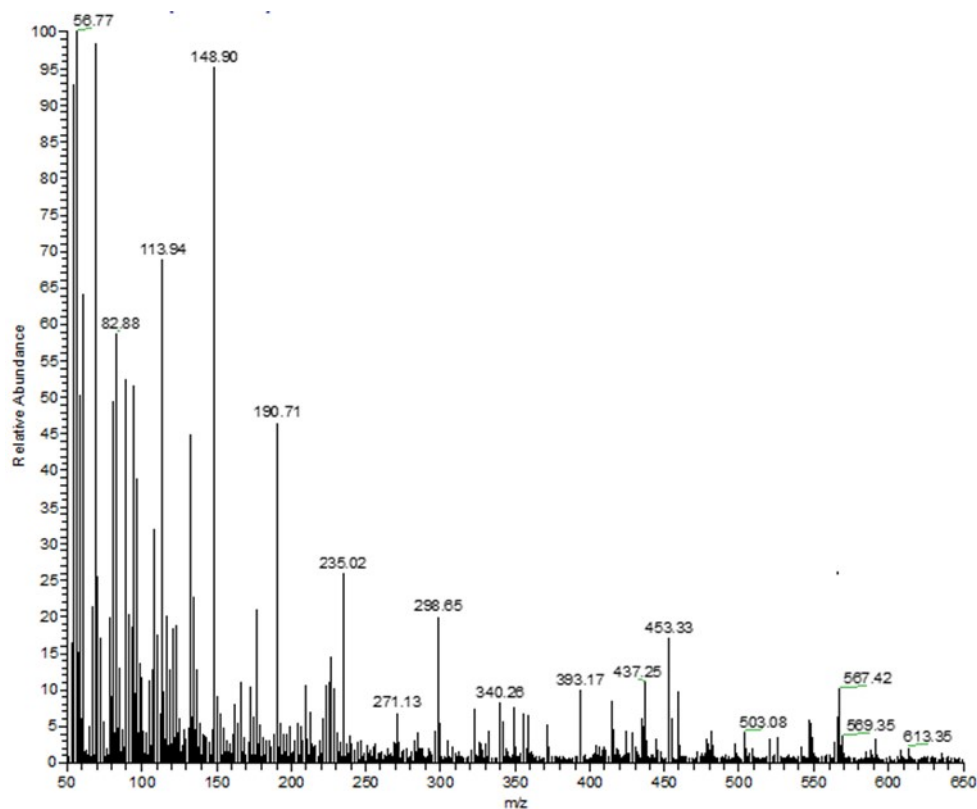
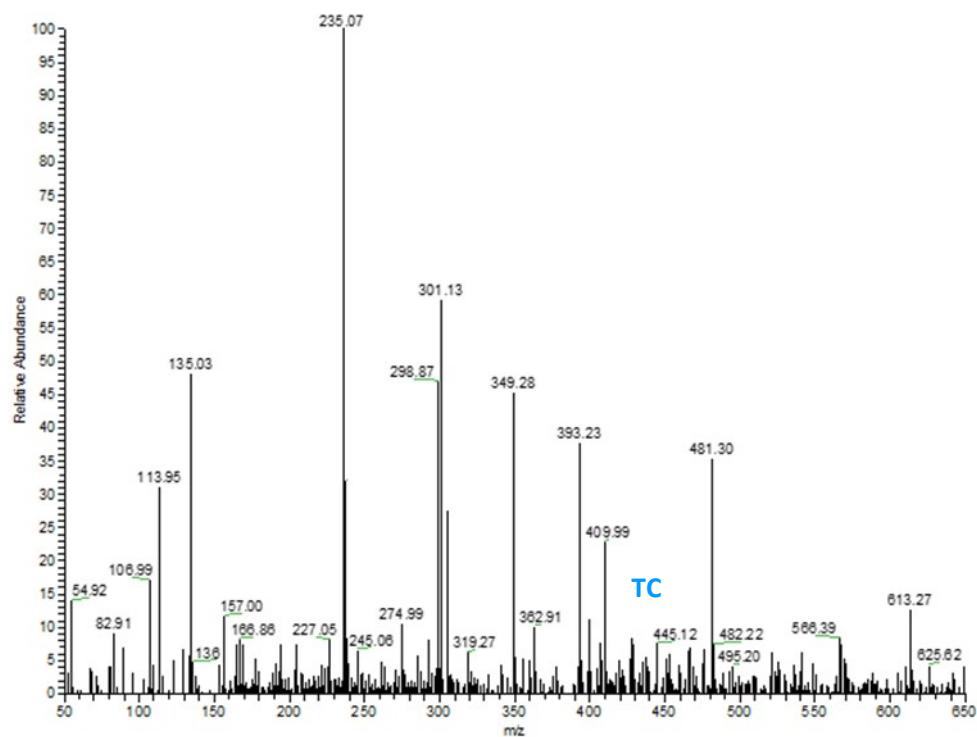


**Fig. S4.** The high-resolution O 1s spectra of MoSe<sub>2</sub> NFs, MoSe<sub>2</sub> NSs-5 and MoSe<sub>2</sub> NSs-10.

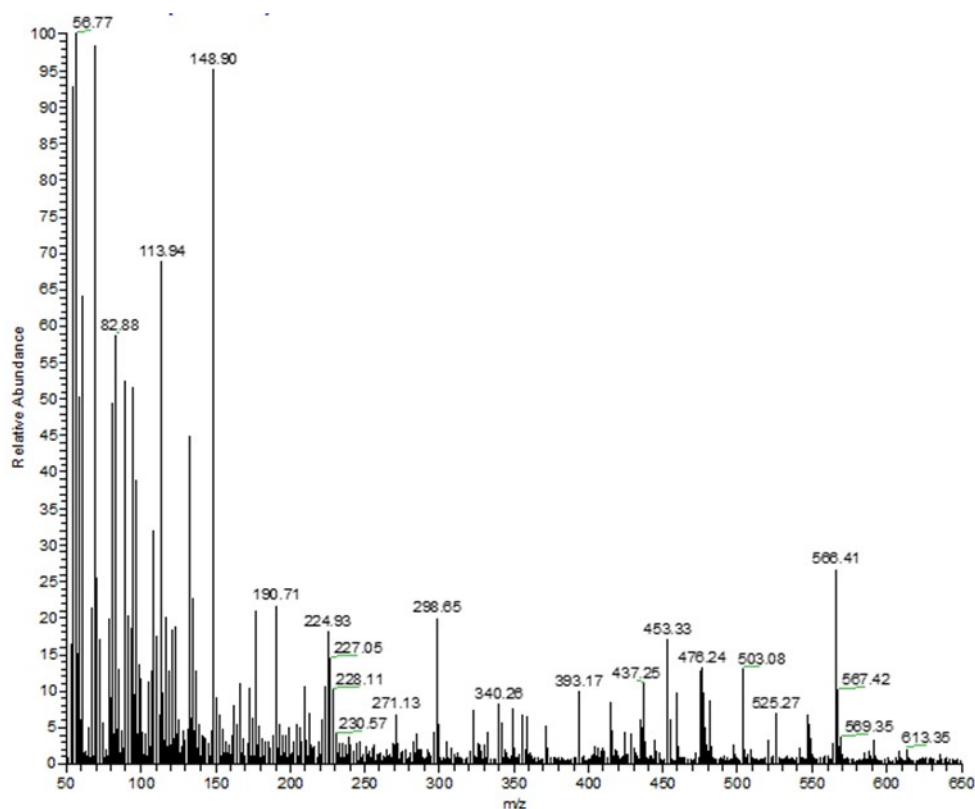
**Table S1.** A summarized Mo and Se ratio of MoSe<sub>2</sub> samples analyzed by X-ray photoelectron spectroscopy.

| Samples                  | Element | Atomic ratio (%) |        |
|--------------------------|---------|------------------|--------|
| MoSe <sub>2</sub> NFs    | Mo      | 34.64            | 1:1.83 |
|                          | Se      | 63.55            |        |
| MoSe <sub>2</sub> NSs-5  | Mo      | 36.25            | 1:1.64 |
|                          | Se      | 59.31            |        |
| MoSe <sub>2</sub> NSs-10 | Mo      | 39.45            | 1:1.41 |
|                          | Se      | 55.79            |        |





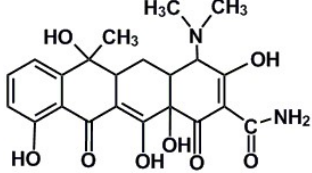
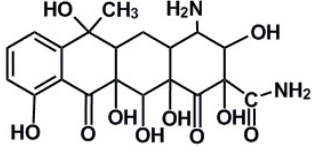
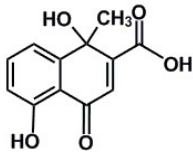
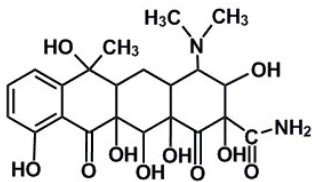
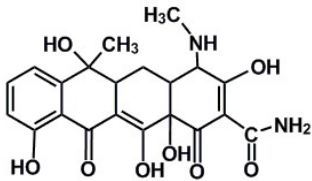
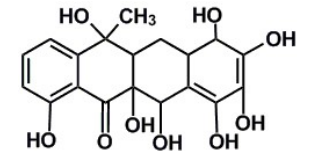
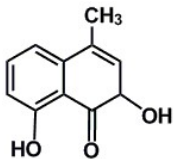
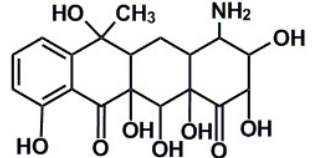


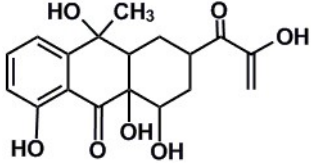
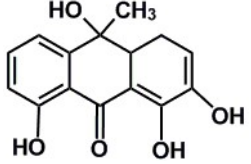
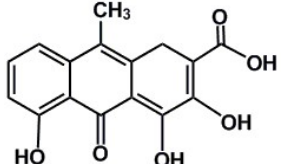
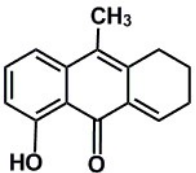


**Fig. S5.** Mass spectra of tetracycline (TC) and possible intermediates.

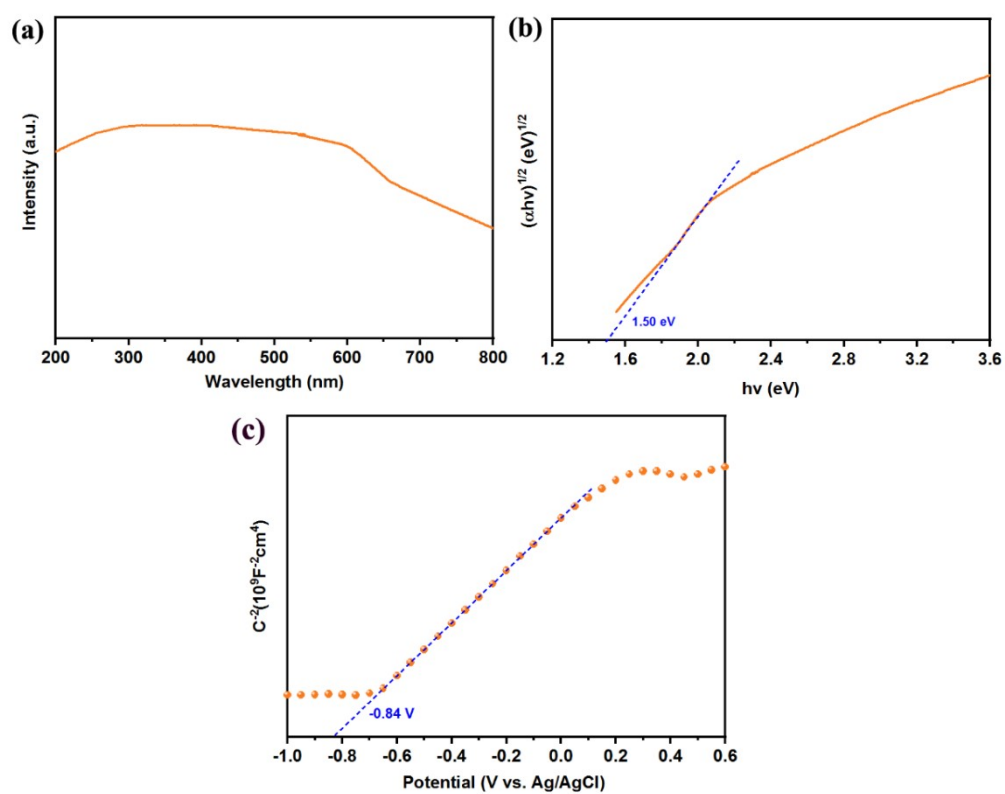
It could be found that the peak at 445 (the tetracycline peak) became smaller and smaller, which illustrated that TC molecules had been decomposed gradually. Meanwhile, intermediate products were generated and then decomposed by  $\cdot\text{OH}/\cdot\text{O}_2^-$  radicals, eventually these compounds were decomposed to  $\text{CO}_2$ ,  $\text{H}_2\text{O}$  and other small molecules.

**Table S2.** The intermediates identified by HPLC/MS during the degradation of tetracycline.

| Product No. | Molecular ion (m/z) | R.T. (min) | Molecular Formula  | Proposed Structure  |
|-------------|---------------------|------------|--|---|
| TC          | 445                 | 5.03       | C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub>  |    |
| A           | 453                 | 3.53       | C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>10</sub> |    |
| B           | 235                 | 3.86       | C <sub>12</sub> H <sub>10</sub> O <sub>5</sub>                 |    |
| C           | 481                 | 4.31       | C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>10</sub> |   |
| D           | 431                 | 4.65       | C <sub>21</sub> H <sub>22</sub> N <sub>2</sub> O <sub>8</sub>  |  |
| E           | 393                 | 4.86       | C <sub>19</sub> H <sub>20</sub> O <sub>9</sub>                 |  |
| F           | 190                 | 5.62       | C <sub>11</sub> H <sub>10</sub> O <sub>3</sub>                 |  |
| G           | 410                 | 6.33       | C <sub>19</sub> H <sub>23</sub> NO <sub>9</sub>                |  |

|   |     |       |  |   |
|---|-----|-------|--|---|
| H | 349 | 7.55  | C <sub>18</sub> H <sub>20</sub> O <sub>7</sub> |  |
| I | 274 | 8.37  | C <sub>15</sub> H <sub>14</sub> O <sub>5</sub> |  |
| J | 301 | 8.81  | C <sub>16</sub> H <sub>12</sub> O <sub>6</sub> |  |
| K | 227 | 10.57 | C <sub>15</sub> H <sub>14</sub> O <sub>2</sub> |  |

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**Fig. S6.** (a) UV-vis diffuse reflectance spectra of MoSe<sub>2</sub> NSs-10; (b) Tauc plot of MoSe<sub>2</sub> NSs-10 derived from the absorption spectra; (c) The Mott-Schottky plot of MoSe<sub>2</sub> NSs-10.