

Supporting Information

for

**Surface vs. core N/S/Se-heteroatom doping of carbon nanodots produces divergent yet consistent optical responses to reactive oxygen species**

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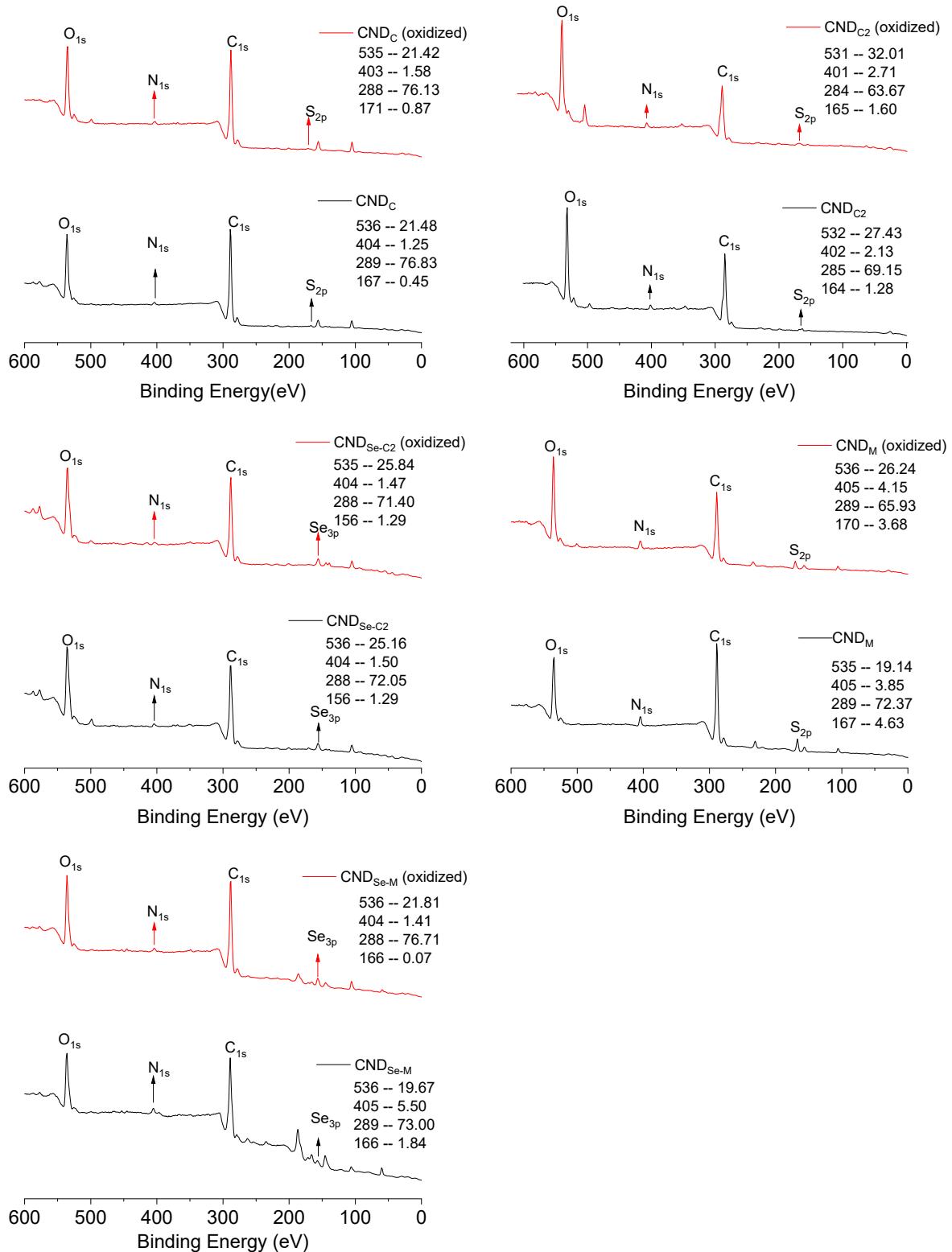


Figure S1 | Full Survey XPS spectra of as-prepared and oxidized CNDs.

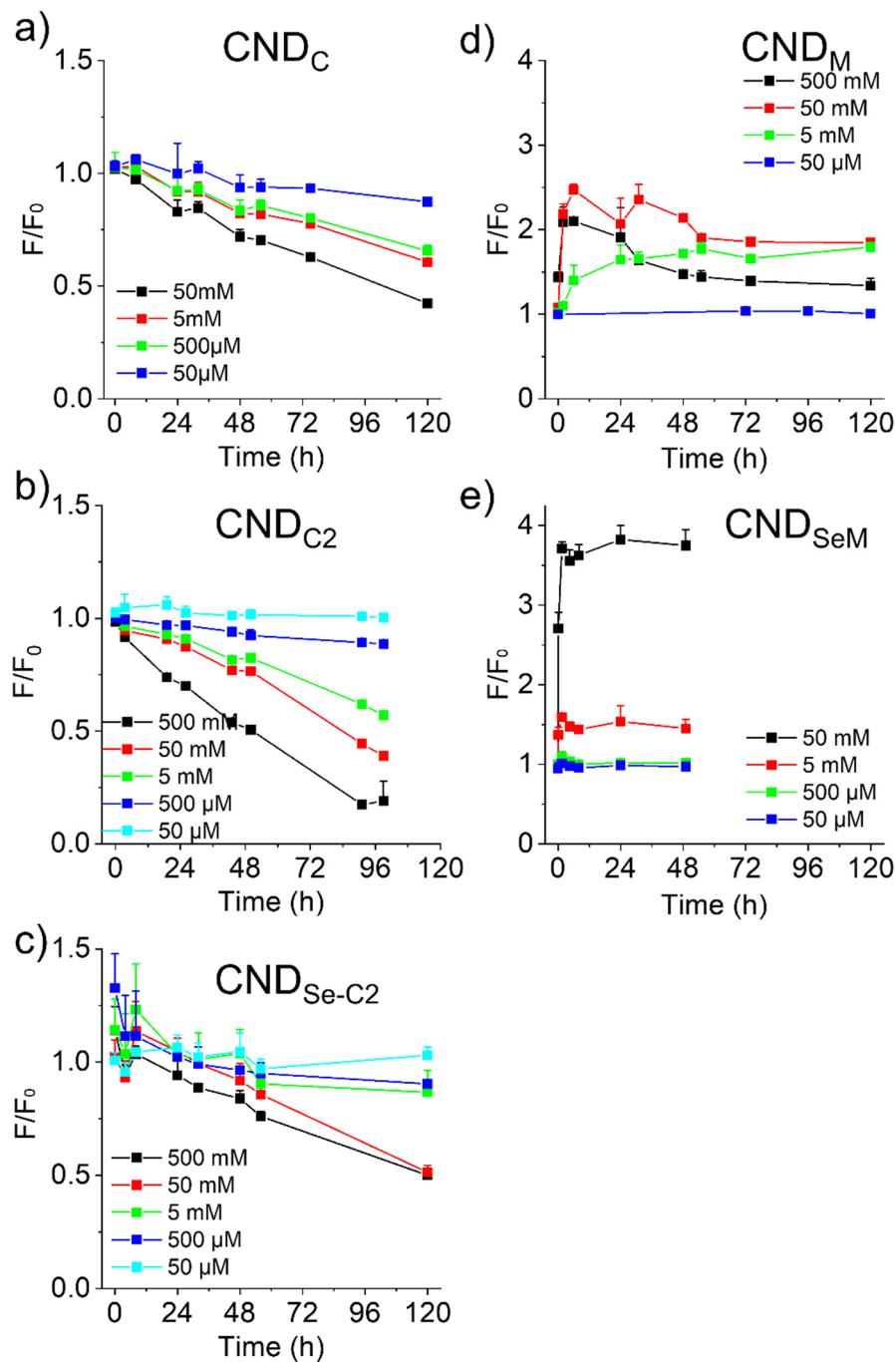


Figure S2 | Evolution of fluorescence emission of CNDs with time in the presence of different concentrations of H<sub>2</sub>O<sub>2</sub>. Data presented as Mean + SD, n = 3.

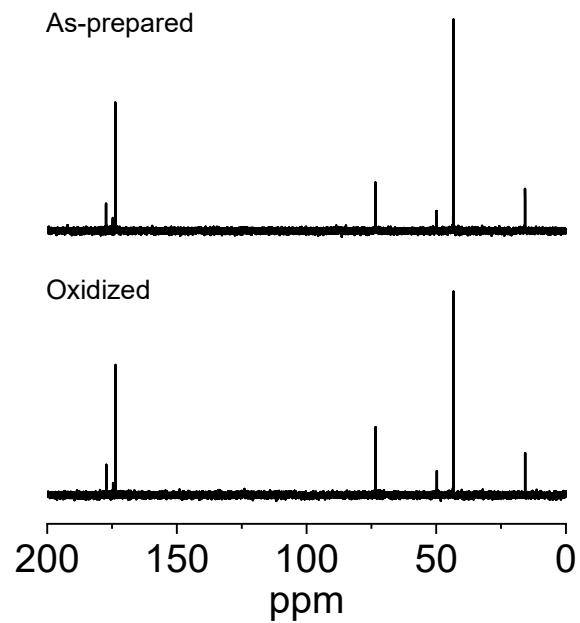


Figure S3 | <sup>13</sup>C NMR spectra of CND<sub>c</sub> before and after oxidation with H<sub>2</sub>O<sub>2</sub>.

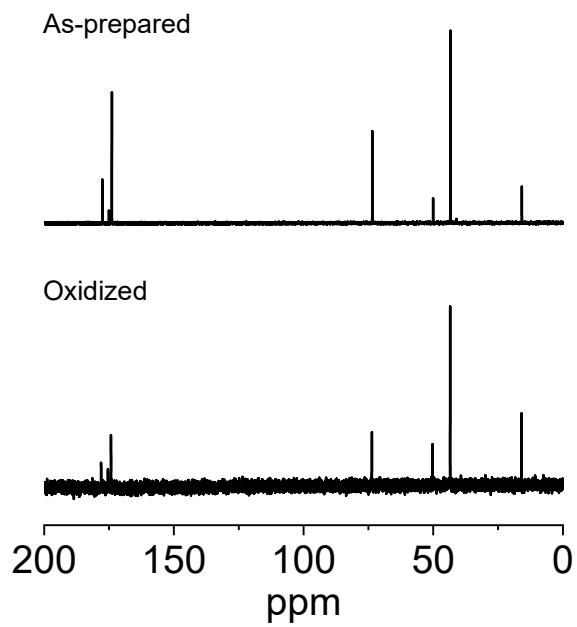
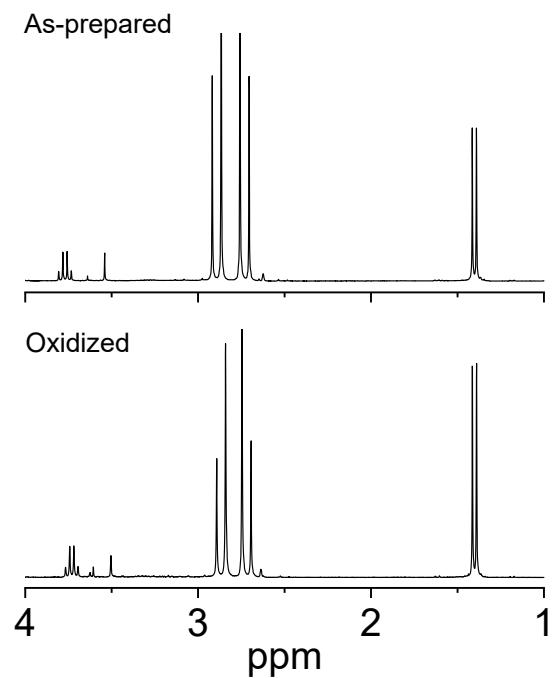


Figure S4 | <sup>1</sup>H (top) and <sup>13</sup>C NMR (bottom) spectra of CND<sub>C2</sub> in D<sub>2</sub>O before and after oxidation with H<sub>2</sub>O<sub>2</sub>.

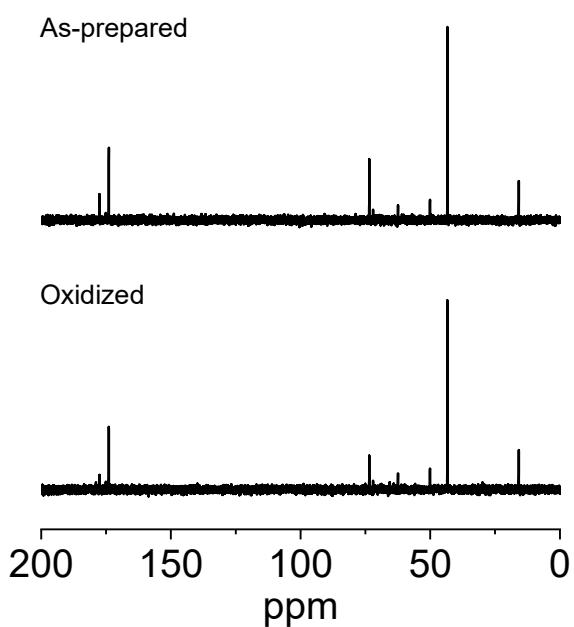
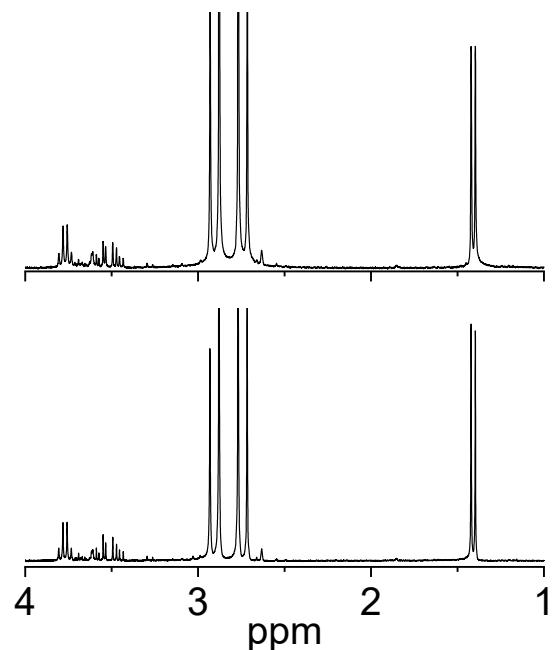


Figure S5 | <sup>1</sup>H (top) <sup>13</sup>C (bottom) NMR spectra of CND<sub>Se-C2</sub> in D<sub>2</sub>O before and after oxidation with H<sub>2</sub>O<sub>2</sub>.

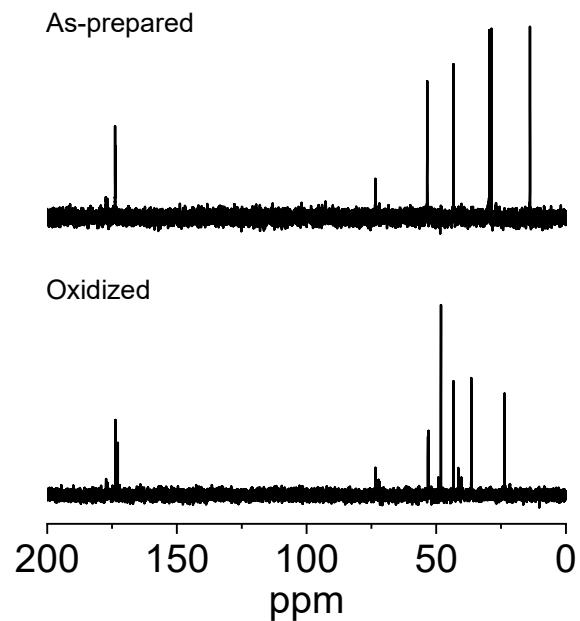


Figure S6 |  $^{13}\text{C}$  NMR spectra of CND<sub>M</sub> before and after oxidation with H<sub>2</sub>O<sub>2</sub>.

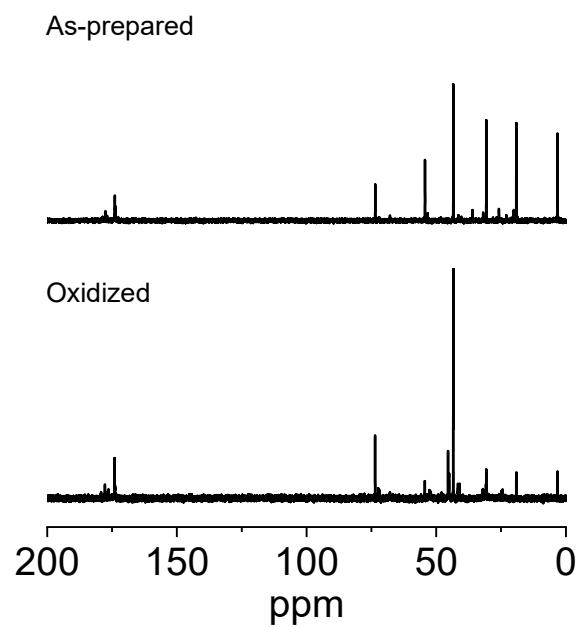


Figure S7 |  $^{13}\text{C}$  NMR spectra of CND<sub>Se-M</sub> before and after oxidation with H<sub>2</sub>O<sub>2</sub>.

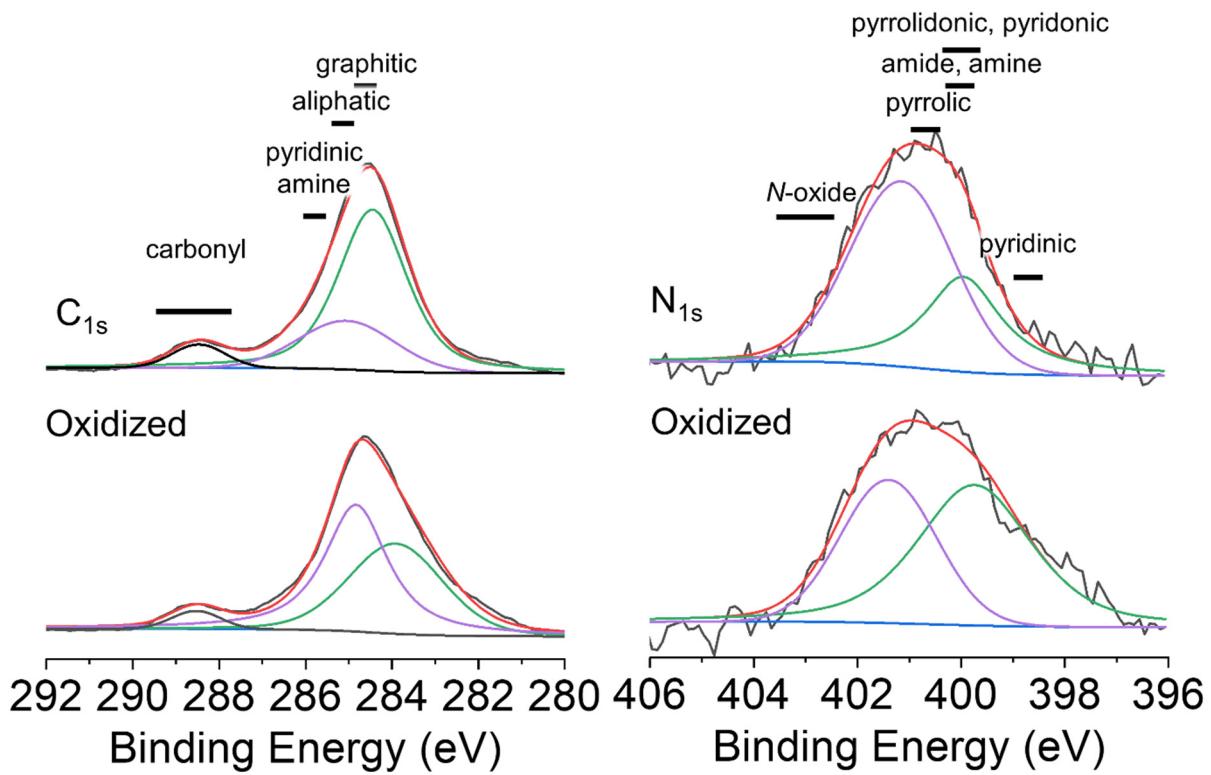


Figure S8 | High-resolution XPS spectra (C<sub>1s</sub>, N<sub>1s</sub>) of CND<sub>c</sub> before and after oxidation with H<sub>2</sub>O<sub>2</sub>. Spectral decomposition used to guide the eye.

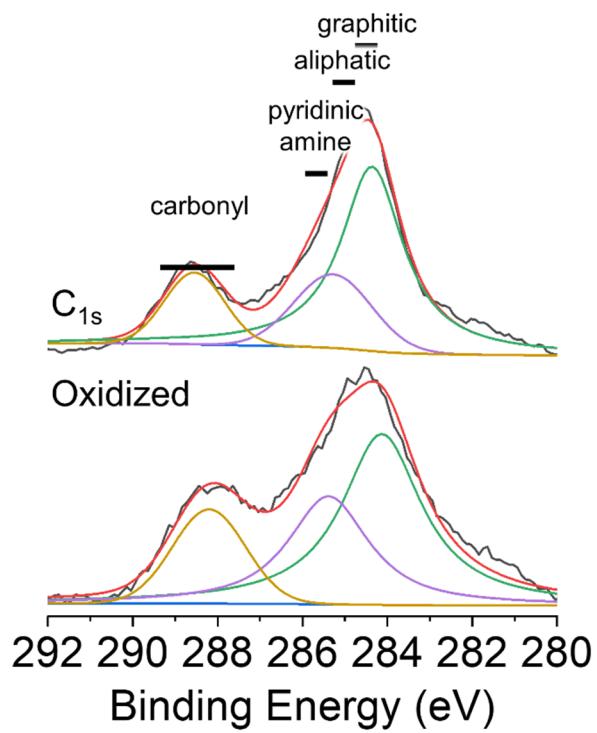


Figure S9 | High-resolution XPS spectra ( $C_{1s}$ ) of CND<sub>C2</sub> before and after oxidation with  $H_2O_2$ . Spectral decomposition used to guide the eye.

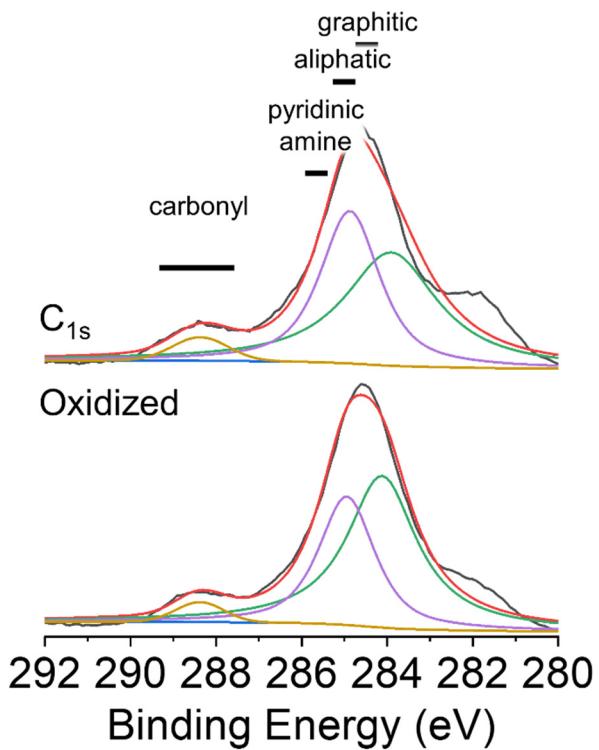


Figure S10| High-resolution XPS spectra ( $C_{1s}$ ) of  $CND_{5e-C2}$  before and after oxidation with  $H_2O_2$ . Spectral decomposition used to guide the eye.

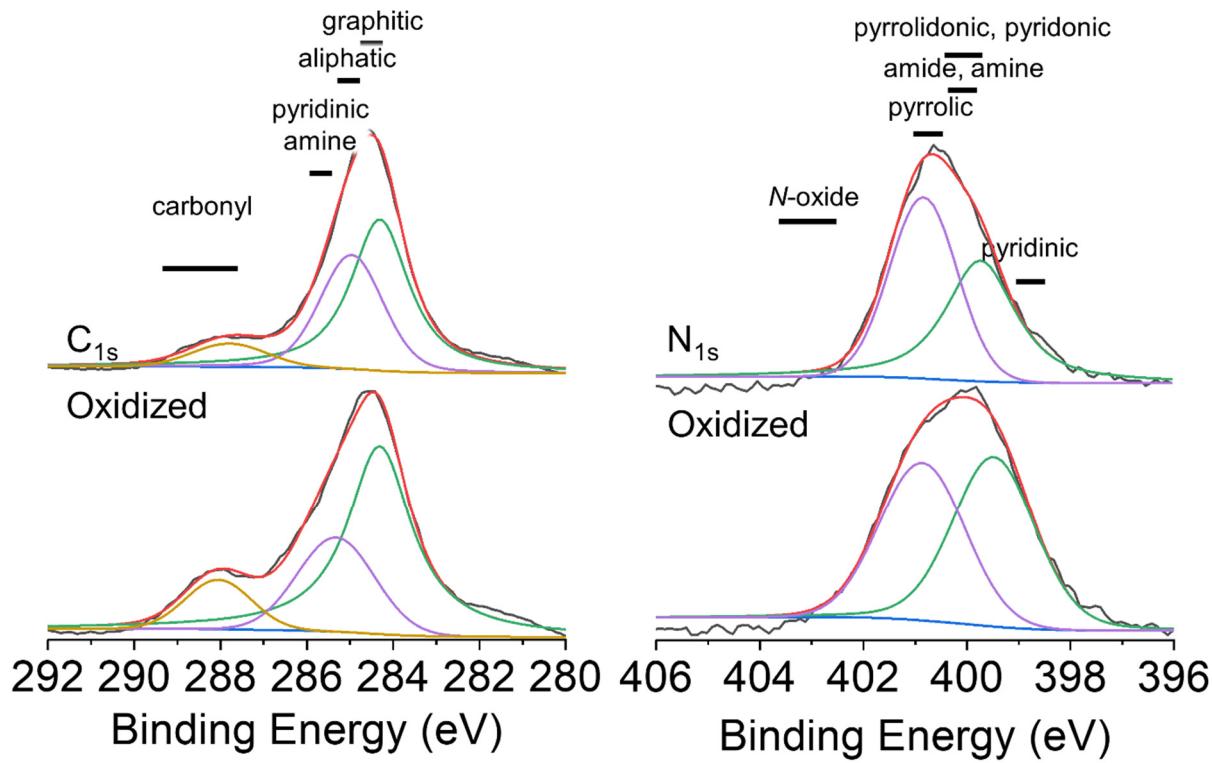


Figure S11 | High-resolution XPS spectra ( $C_{1s}$ ,  $N_{1s}$ ) of  $CND_M$  before and after oxidation with  $H_2O_2$ . Spectral decomposition used to guide the eye.

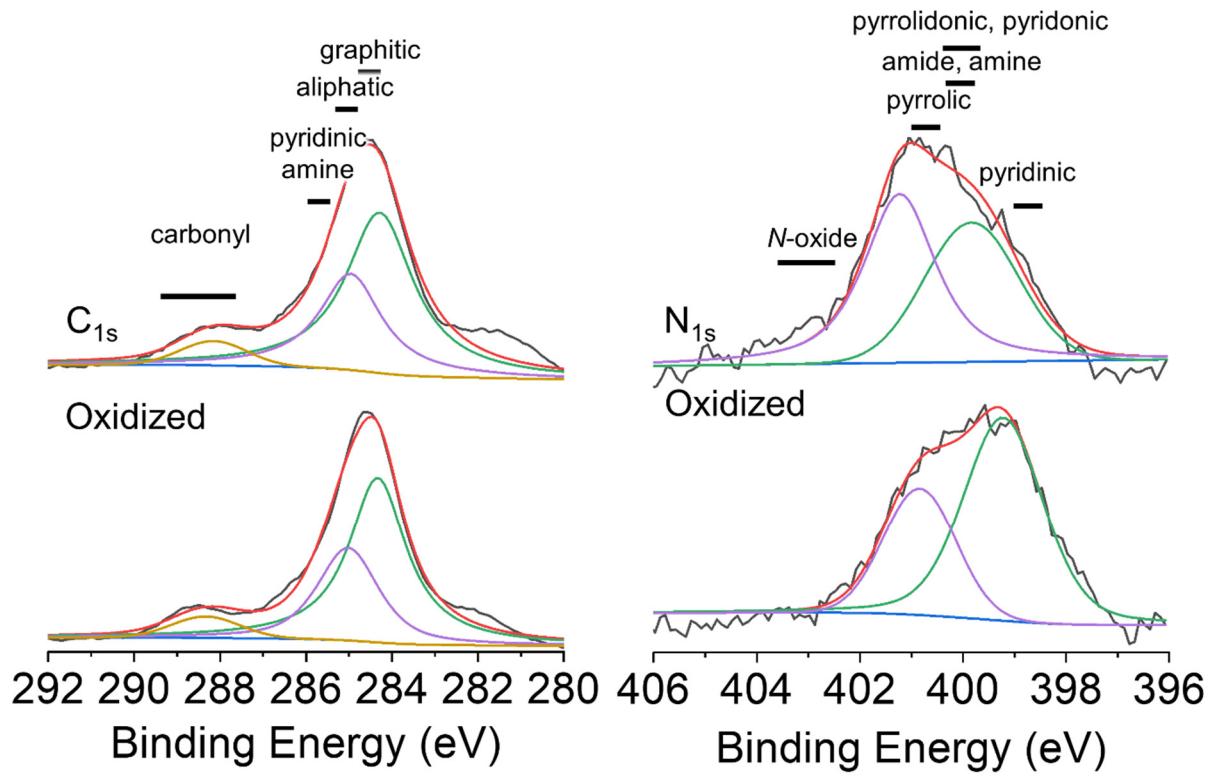


Figure S12 | High-resolution XPS spectra ( $C_{1s}$ ,  $N_{1s}$ ) of CND<sub>Se-M</sub> before and after oxidation with  $H_2O_2$ . Spectral decomposition used to guide the eye.

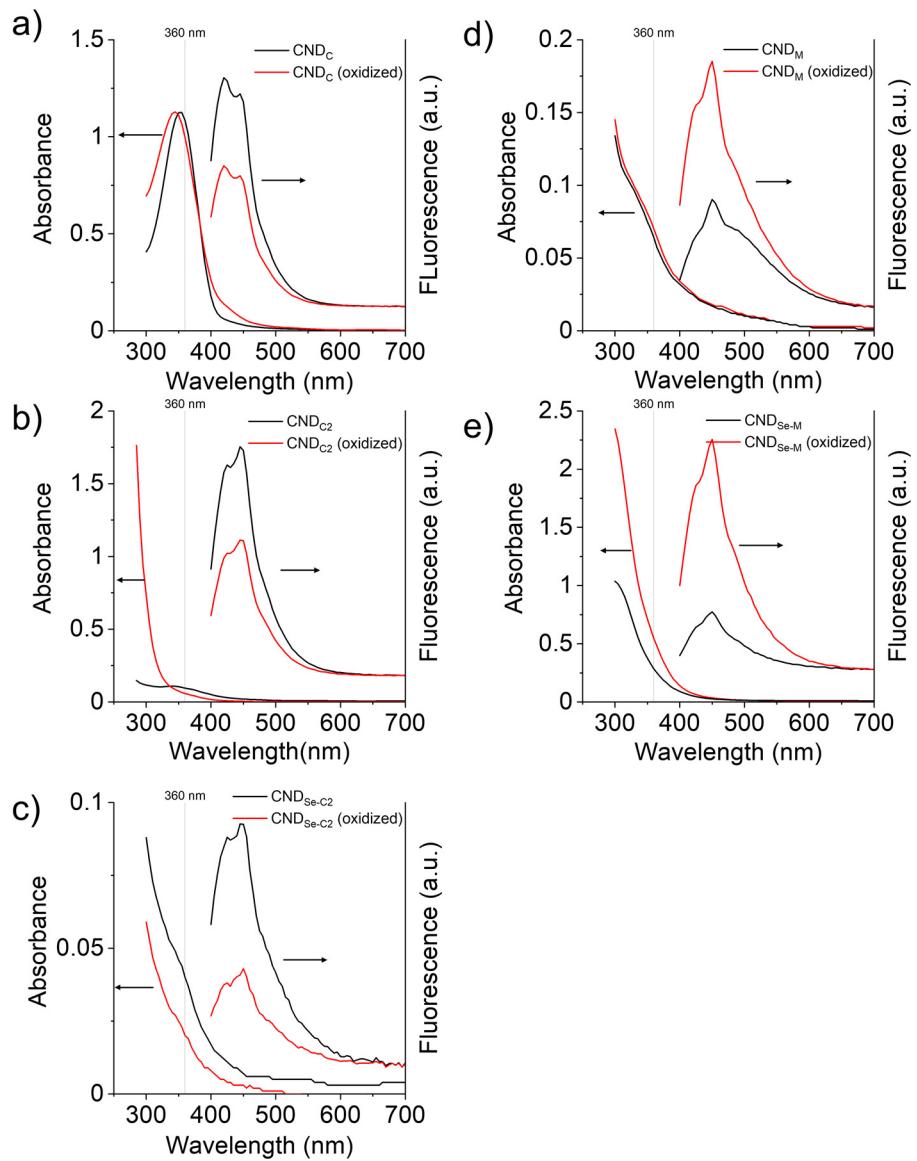


Figure S13 | Absorbance and fluorescence spectra ( $\lambda_{\text{ex}} 360 \text{ nm}$ ) of CNDs before and after oxidation.

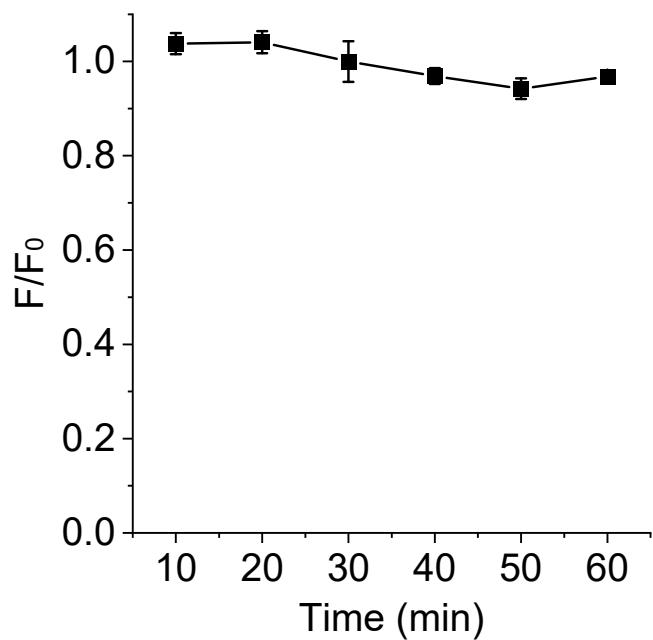


Figure S14 | Evolution of fluorescence emission of CND<sub>c</sub> with time in 200 mM phosphate buffer pH 7.4 under UV irradiation (256 nm, 4 W). Data presented as Mean  $\pm$  SD, n = 3.