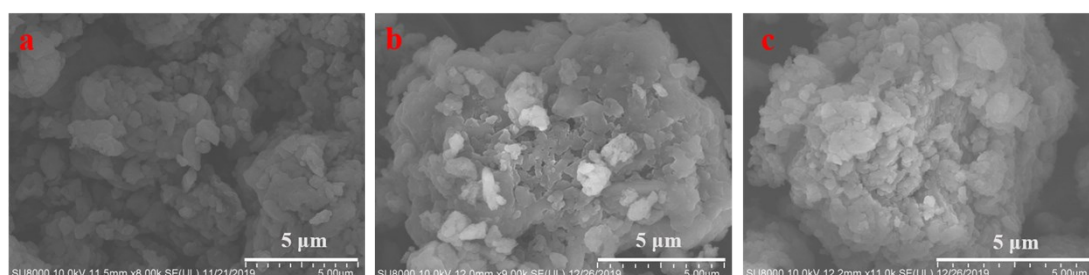


## Supporting Information

### Microwave-initiated recombination of hydrogen bonds of perylene diimide supramolecule for PPCPs photodegradation



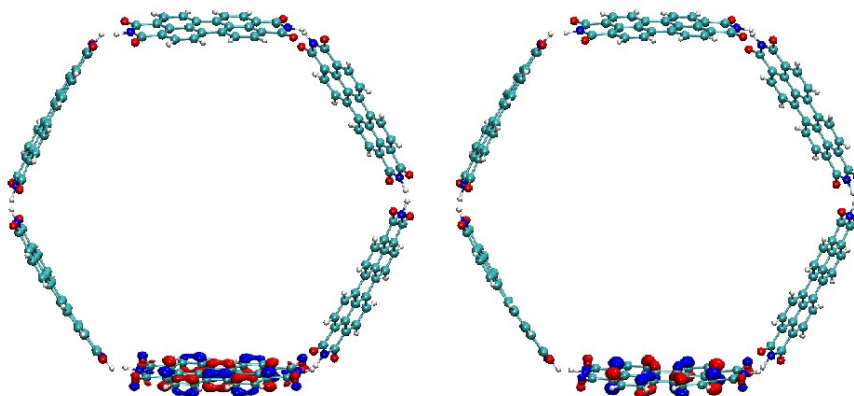
**Fig. S1** SEM images of cPDI (a), Rec-PDI-H<sub>2</sub>O (b) and Rec-PDI-HCl (c) on the scale of 5  $\mu$ m.

**Table. S1** The detail table of binding energy for two molecules.

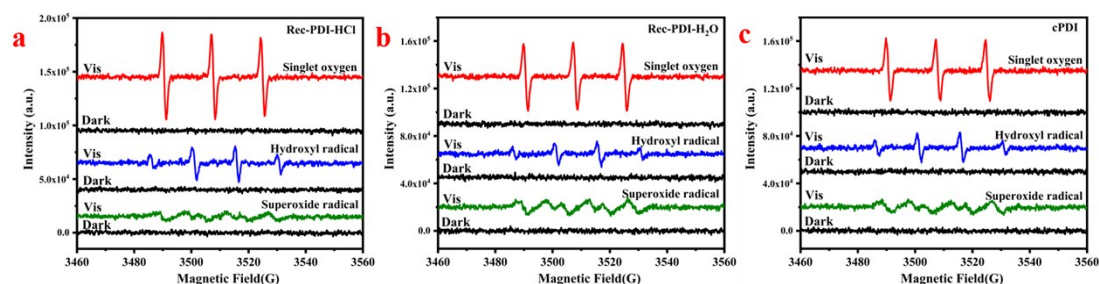
| Energy (Ha)               | Model 1    | Model 2    |
|---------------------------|------------|------------|
| Total Energy (Ha)         | -7986.6873 | -5324.4414 |
| Monocase 1 (Ha)           | 1331.0957  | 1331.0951  |
| Monocase 2 (Ha)           | 1331.0962  | 1331.0951  |
| Monocase 3 (Ha)           | 1331.0963  | 1331.0951  |
| Monocase 4 (Ha)           | 1331.0956  | 1331.0951  |
| Monocase 5 (Ha)           | 1331.0962  | -          |
| Monocase 6 (Ha)           | 1331.0963  | -          |
| Binding Energy (Ha)       | -0.1112    | -0.0610    |
| Binding Energy (kcal/mol) | -69.7645   | -38.2535   |

**Table. S2** The HOMO energy and LUMO energy for two molecules.

| Samples | HOMO (eV) | LUMO (eV) |
|---------|-----------|-----------|
| Model 1 | -6.051    | -3.545    |
| cPDI    | -6.114    | -3.582    |



**Fig. S2** The LUMO (left) and HOMO (right) orbital of model 1.



**Fig. S3** EPR spectra of singlet oxygen ( $^1\text{O}_2$ ), hydroxyl ( $\cdot\text{OH}$ ) and superoxide radical ( $\cdot\text{O}_2^-$ ) under visible light and dark for different samples.