

## Supplementary Material

### **Adsorption performance and mechanisms of ciprofloxacin onto microplastics: Effects of different texture and aging degree**

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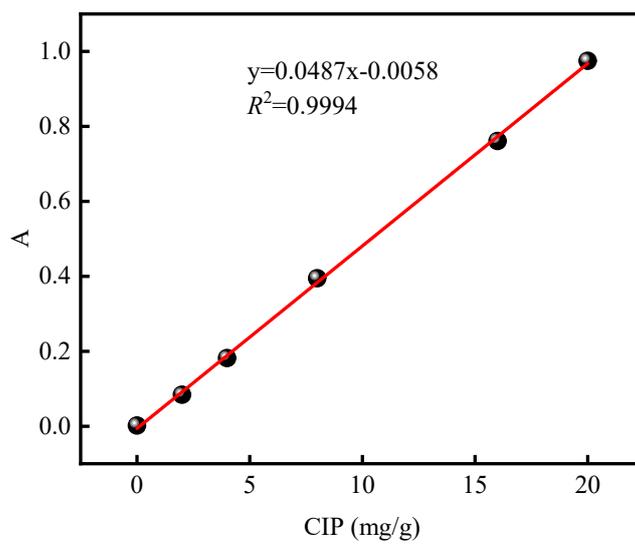


Fig. S1 the calibration curve

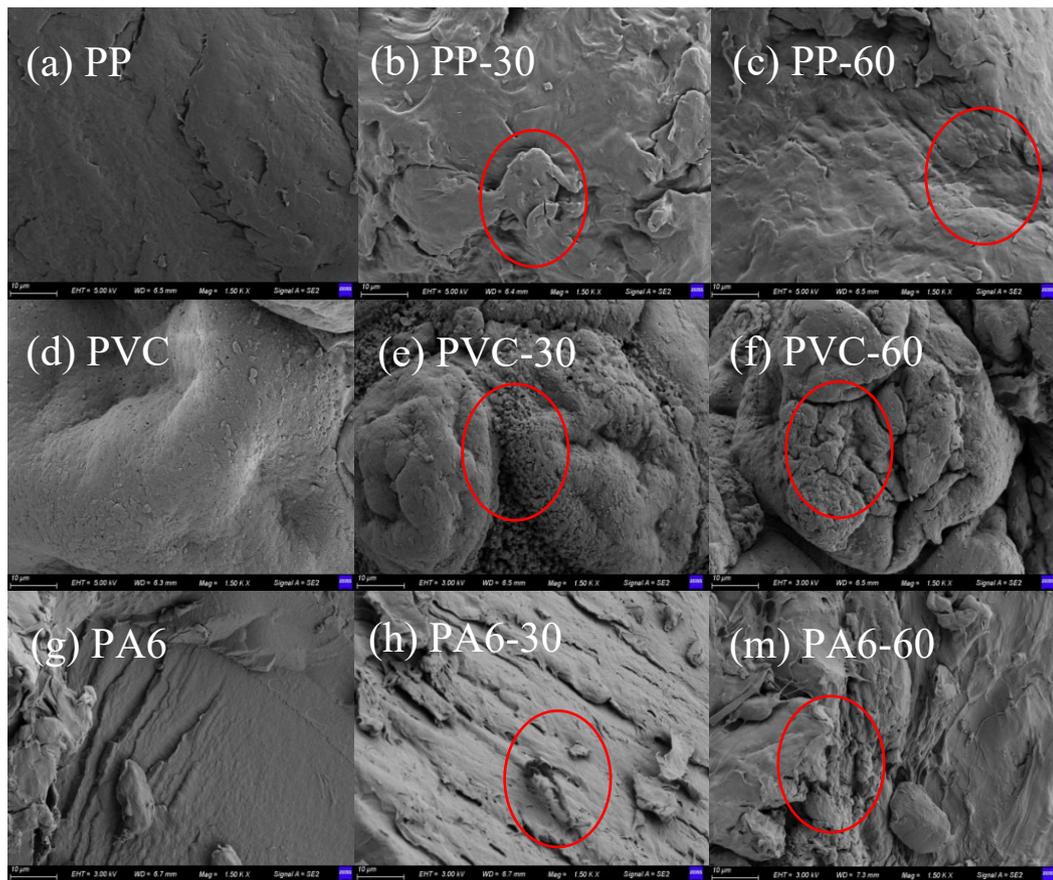


Fig S2 SEM images of MPs before and after aging

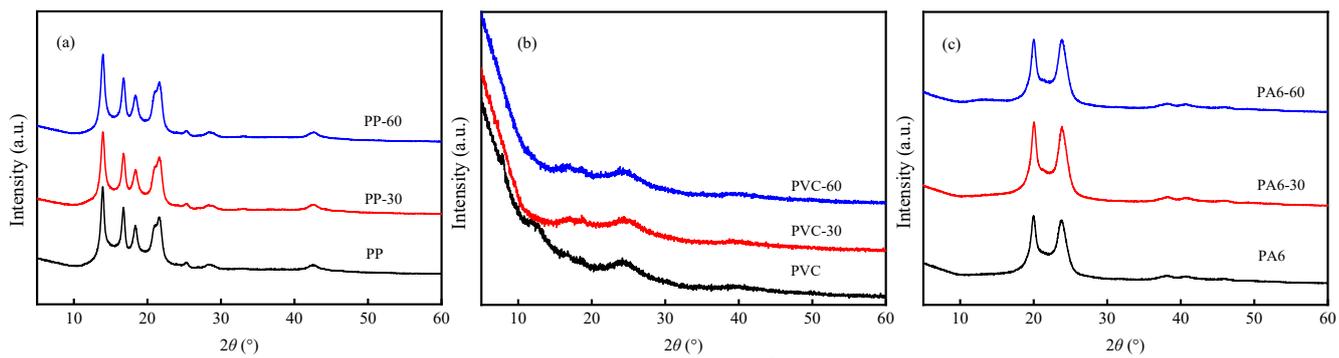


Fig. S3. XRD patterns of MPs

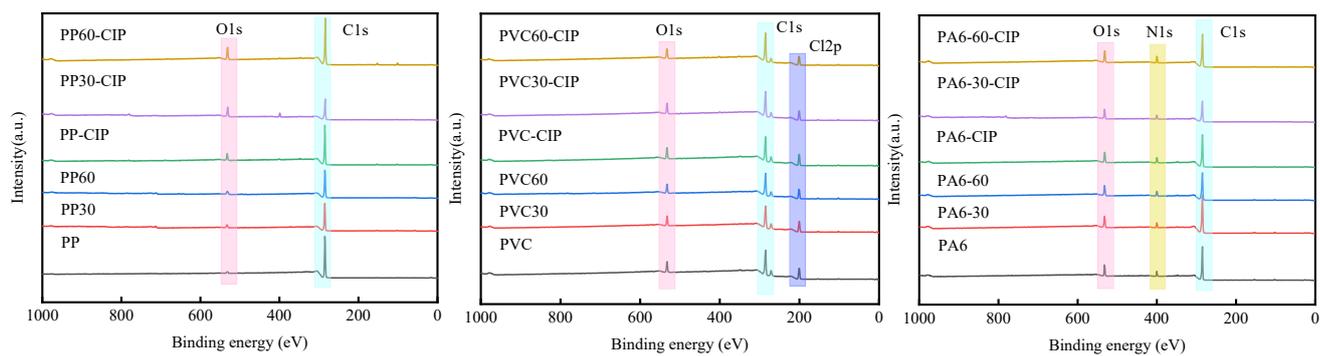


Fig. S4 XPS spectra of MPs before and after CIP adsorption

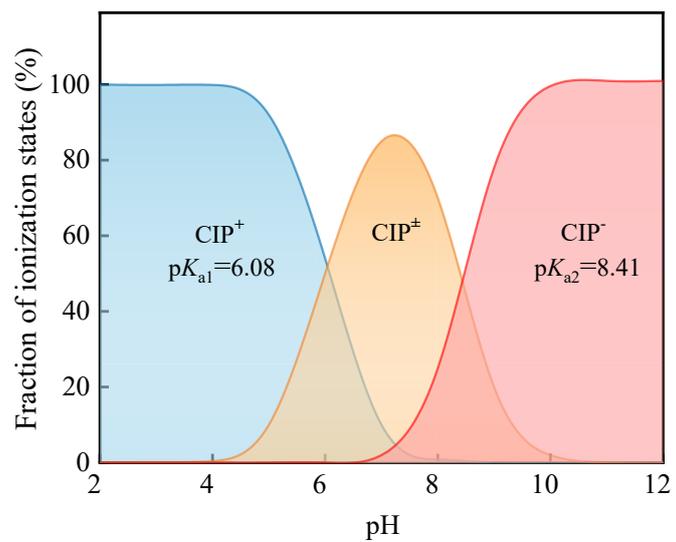


Fig. S5 The speciation diagram of the CIP

Table S1 Carbonyl index (CI) of pristine and aged microplastics

| MPs    | Carbonyl index (CI) |
|--------|---------------------|
| PP     | 0.19                |
| PP-30  | 0.31                |
| PP-60  | 0.74                |
| PVC    | 0.41                |
| PVC-30 | 0.88                |
| PVC-60 | 1.39                |
| PA6    | 1.06                |
| PA6-30 | 1.48                |
| PA6-60 | 1.75                |

Table S2 Specific surface area of pristine and aged microplastics

| MPs    | surface area (m <sup>2</sup> /g) |
|--------|----------------------------------|
| PP     | 0.144                            |
| PP-30  | 0.198                            |
| PP-60  | 0.268                            |
| PVC    | 0.485                            |
| PVC-30 | 0.523                            |
| PVC-60 | 0.577                            |
| PA6    | 0.841                            |
| PA6-30 | 1.157                            |
| PA6-60 | 1.488                            |

Table S3 Fitting parameters with Intra-particle diffusion model

| MPs    | Stage1   |       |       | Stage2   |       |       |
|--------|--|-------|-------|--|-------|-------|
|        | $K_{d1}[\text{mg}/(\text{g}\times\text{h}^{1/2})]$ | $C_1$ | $R^2$ | $K_{d2}[\text{mg}/(\text{g}\times\text{h}^{1/2})]$ | $C_1$ | $R^2$ |
| PP     | 0.099  | 0.021 | 0.999 | 0.001  | 0.388 | 0.998 |
| PP-30  | 0.100  | 0.090 | 0.933 | 0.0002   | 0.474 | 0.004 |
| PP-60  | 0.121  | 0.125 | 0.997 | -0.004   | 0.618 | 0.668 |
| PVC    | 0.068  | 0.031 | 0.988 | 0.020  | 0.265 | 0.965 |
| PVC-30 | 0.080  | 0.239 | 0.882 | 0.014  | 0.423 | 0.999 |
| PVC-60 | 0.076  | 0.300 | 0.938 | 0.005  | 0.597 | 0.683 |
| PA6    | 0.093  | 0.333 | 0.993 | 0.015  | 0.651 | 0.972 |
| PA6-30 | 0.112  | 0.380 | 0.972 | 0.005  | 0.802 | 0.996 |
| PA6-60 | 0.135  | 0.420 | 0.979 | 0.003  | 0.964 | 0.993 |

Table S4 Fitting parameters of isothermal model

| MPs    | Langmuir     |              |       | Freundlich   |       |       |
|--------|--------------|--------------|-------|--------------|-------|-------|
|        | $K_L/(L/mg)$ | $q_m/(mg/g)$ | $R^2$ | $K_F/(L/mg)$ | $n$   | $R^2$ |
| PP     | 0.033        | 0.993        | 0.996 | 0.106        | 2.276 | 0.958 |
| PP-30  | 0.020        | 1.705        | 0.996 | 0.101        | 1.862 | 0.986 |
| PP-60  | 0.021        | 2.138        | 0.992 | 0.136        | 1.900 | 0.987 |
| PVC    | 0.032        | 1.210        | 0.995 | 0.126        | 2.254 | 0.976 |
| PVC-30 | 0.021        | 1.861        | 0.990 | 0.117        | 1.905 | 0.994 |
| PVC-60 | 0.022        | 2.215        | 0.992 | 0.143        | 1.911 | 0.993 |
| PA6    | 0.016        | 3.115        | 0.994 | 0.137        | 1.703 | 0.983 |
| PA6-30 | 0.015        | 3.892        | 0.993 | 0.153        | 1.657 | 0.993 |
| PA6-60 | 0.016        | 4.327        | 0.992 | 0.182        | 1.686 | 0.995 |

Table S5  $|\Delta pK_a|$  values

| MPs    | Zeta | CIP (pKa) | $ \Delta pK_a $ |
|--------|------|-----------|-----------------|
| PP     | 4.06 | 6.08      | 2.02            |
| PP-30  | 4.77 | 6.08      | 1.31            |
| PP-60  | 5.20 | 6.08      | 0.88            |
| PVC    | 4.12 | 6.08      | 1.96            |
| PVC-30 | 4.51 | 6.08      | 1.57            |
| PVC-60 | 5.07 | 6.08      | 1.01            |
| PA6    | 4.40 | 6.08      | 1.68            |
| PA6-30 | 5.33 | 6.08      | 0.75            |
| PA6-60 | 6.37 | 6.08      | 0.29            |

Table S6 Interaction energies between microplastics and CIP

| MPs    | $E_{\text{ads}}$ (kcal/mol) |
|--------|-----------------------------|
| PP     | -1.77                       |
| PP=O   | -2.02                       |
| PP-OH  | -2.56                       |
| PVC    | -3.24                       |
| PVC=O  | -6.75                       |
| PVC-OH | -8.42                       |
| PA6    | -8.39                       |
| PA6=O  | -21.21                      |
| PA6-OH | -11.97                      |