Supporting Information

Fc-content dependence of composition, structure and degradation degree in supramolecular aggregates of polypropylene glycol, ferrocene and *β*-cyclodextrin

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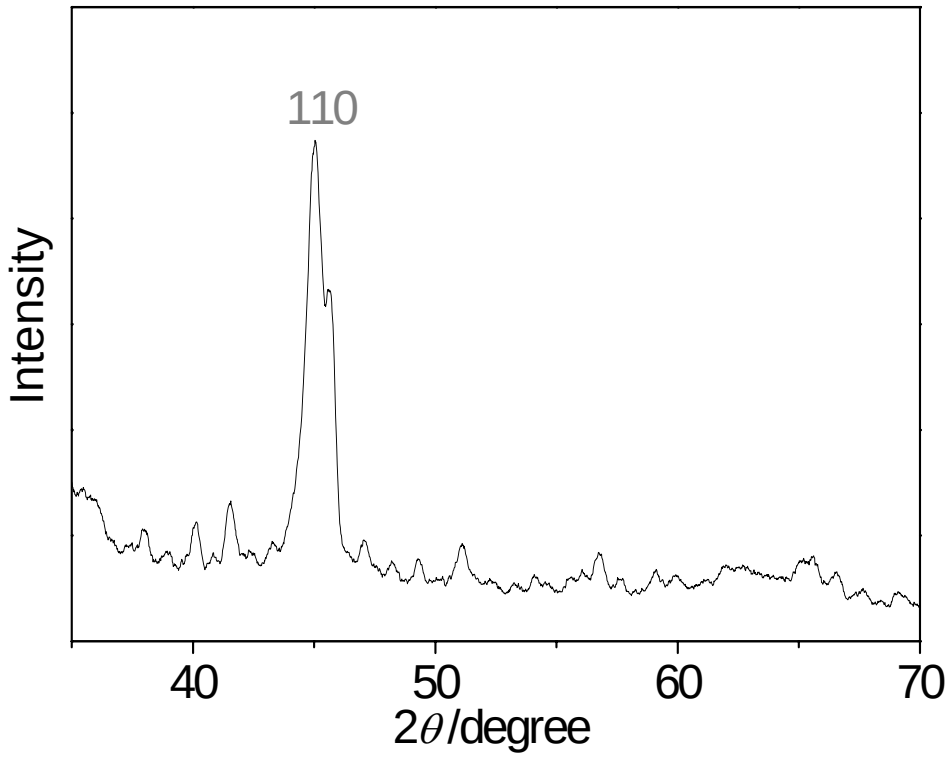
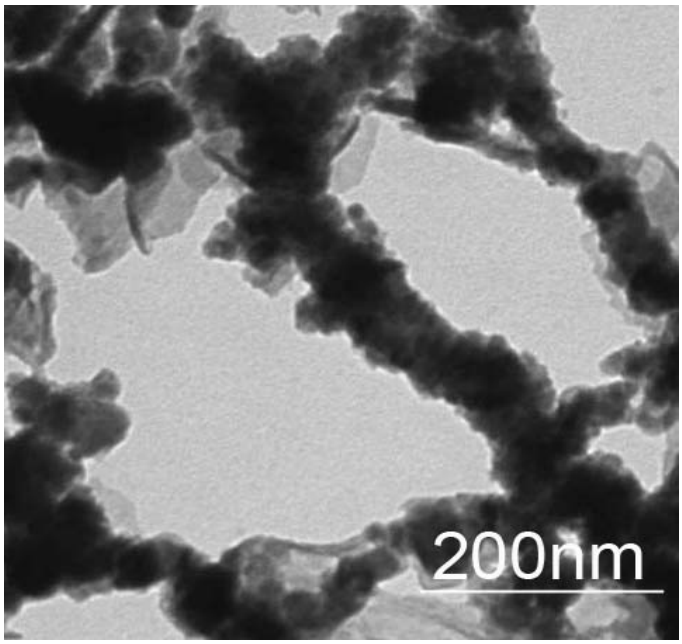
A list of the contents for all the Supporting Information

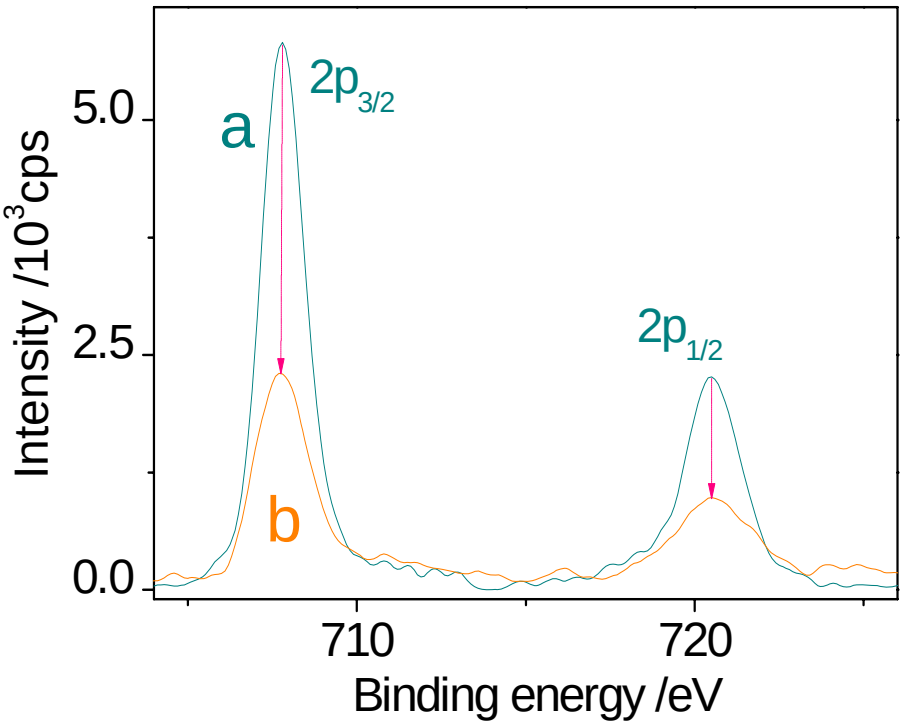
XRD pattern of Fe nanoparticles.



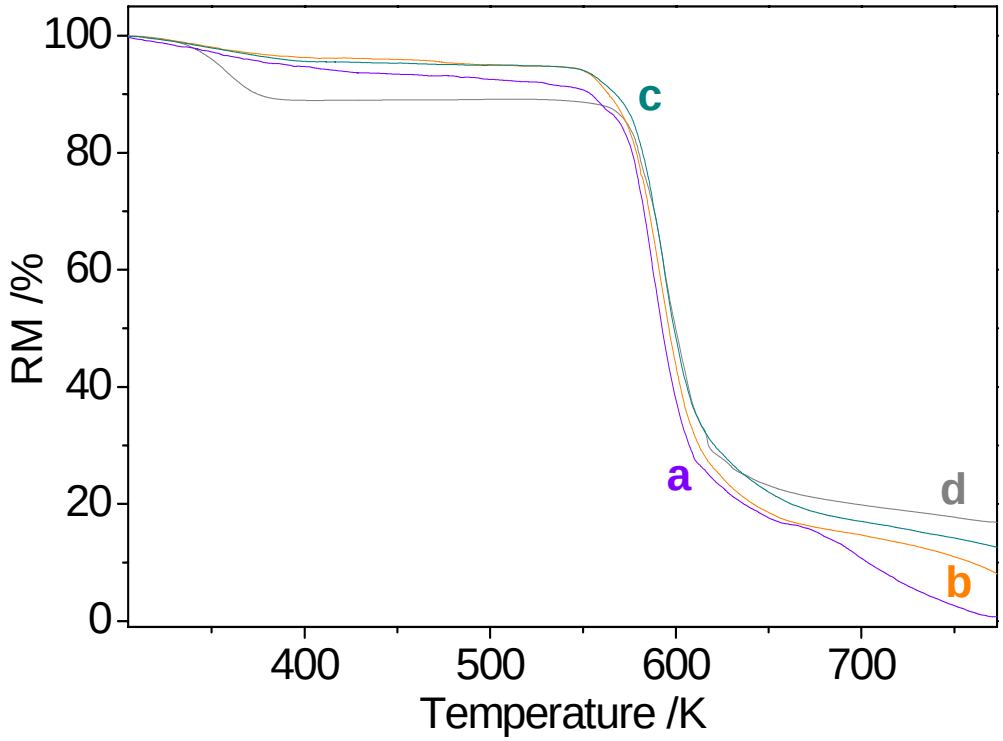
TEM image of Fe nanoparticles.



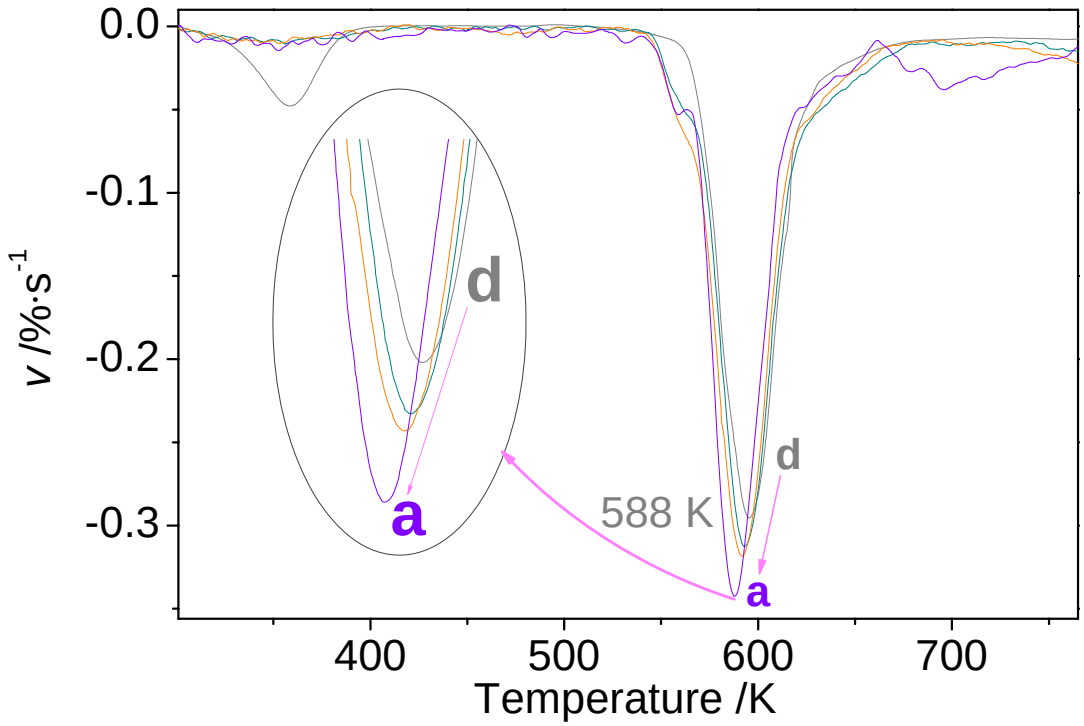
XPS-Fe_{2p} spectra of (a) PP–0.5 and (b) PP–0.1.



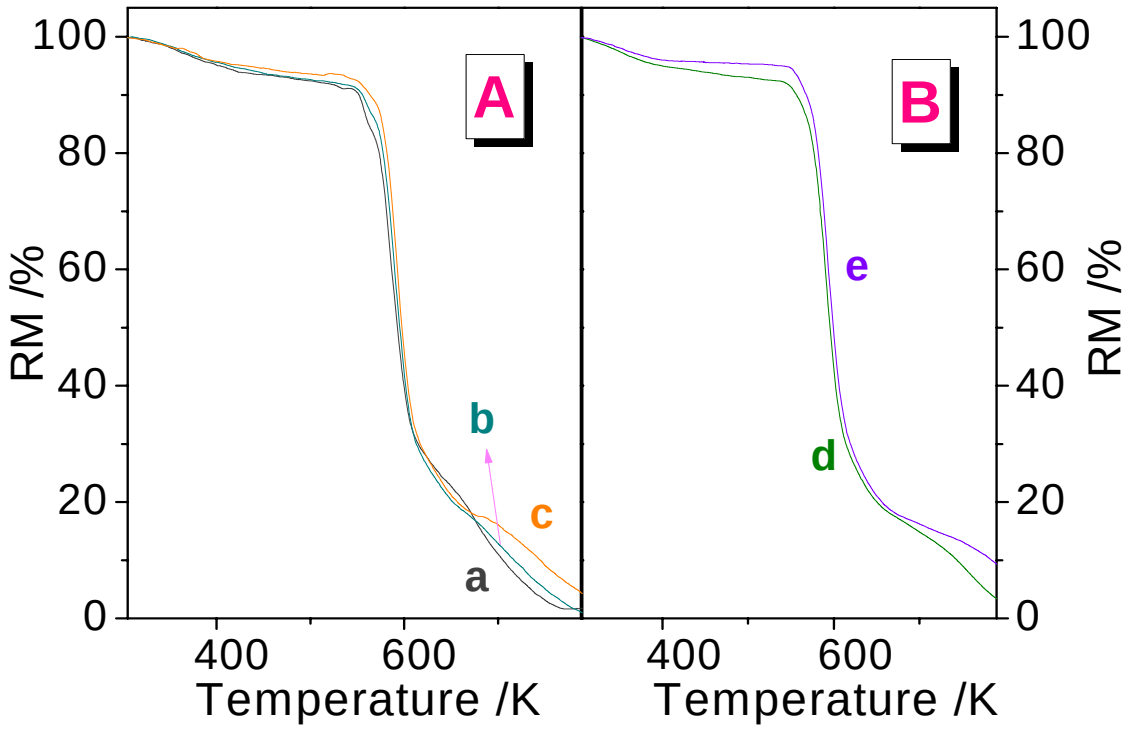
TG curves of (a) PP–0.3, (b) PP–0.03, (c) PP–0.01 and (d) *β*-CD.



DTG curves of (a) PP–0.3, (b) PP–0.03, (c) PP–0.01 and (d) *β*-CD.



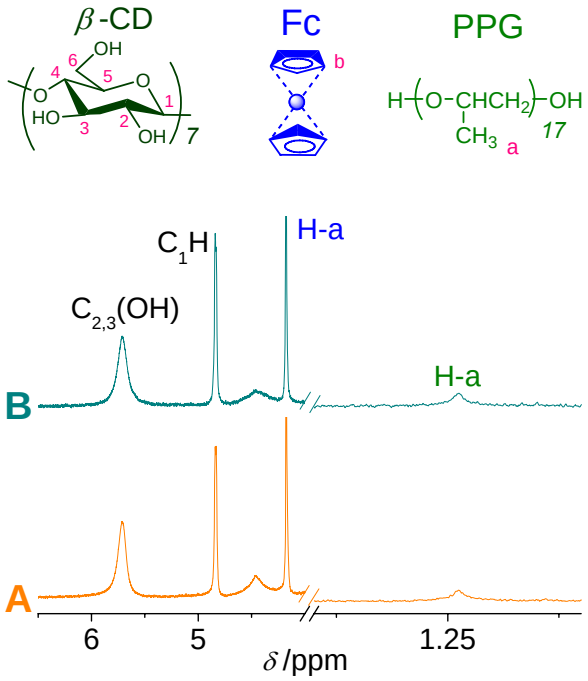
TG profiles of (a) PP–0.4, (b) PP–0.2, (c) PP–0.1, (d) PP–0.05 and (e) PP–0.01.



α values of the PP series samples as well as PPG·(β-CD)$_5$ and β-CD at 600, 660, 720 and 780 K.

α /%	Temperature /K			
	600	660	720	780
PP–0.5	58.28	78.61	90.96	99.05
PP–0.4	53.24	75.55	91.4	98.10
PP–0.3	56.73	80.99	92.24	99.32
PP–0.2	52.21	78.71	89.21	98.07
PP–0.1	49.53	78.58	85.08	94.05
PP–0.05	53.49	79.80	86.00	95.07
PP–0.03	53.74	81.74	85.75	92.75
PP–0.02	47.91	79.34	84.09	88.82
PP–0.01	48.59	78.37	83.05	87.16
PPG•(β-CD)$_5$	39.78	73.42	79.57	81.90
β-CD	43.86	75.14	78.68	81.02

300 MHz ^{1}H NMR spectra of (A) PP–351 and (B) PP–151 in DMSO-d_6.

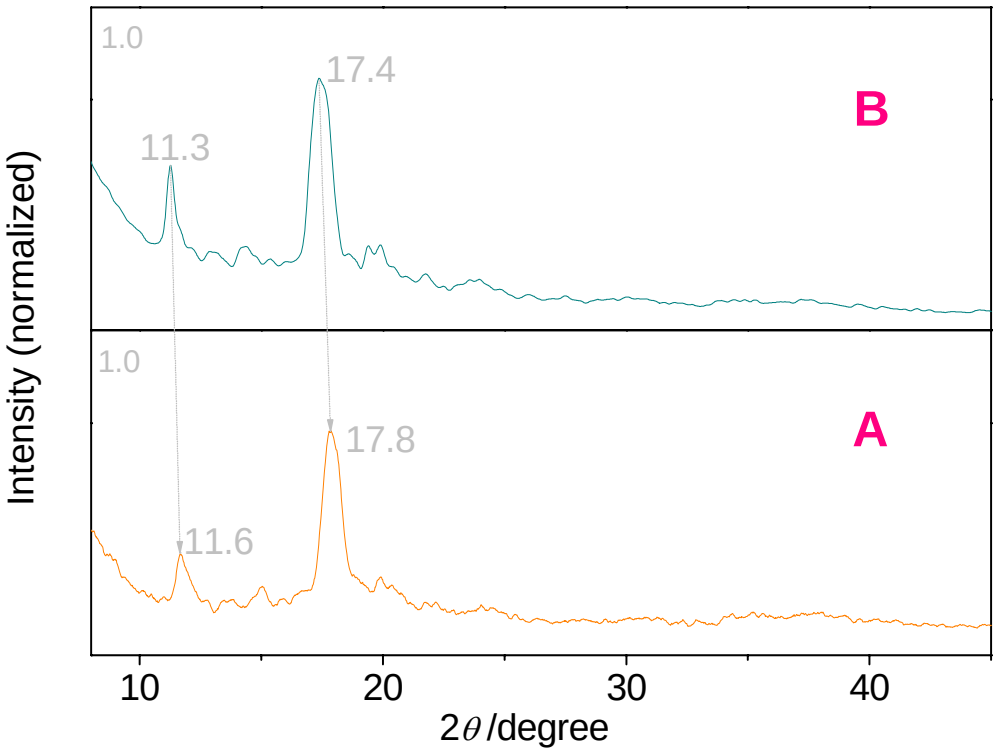


First, we performed a control study in which the initial ratio between Fc and PPG was fixed in 5:1, corresponding to 0.093 g (0.5 mmol) Fc and 0.100 g (0.1 mmol) PPG, then applied different initial concentrations (0.341 g, 0.3 mmol; 0.114 g, 0.1 mmol) of *β*-CD. In this method, two samples with the initial ratios: 3:5:1 (PP–351) and 1:5:1 (PP–151) of *β*-CD, Fc to PPG were obtained.

^{1}H NMR spectra of the two samples were shown in the above figure. We found that both the positions and the integrated area ratios of the typical proton signals of PPG (H-a), Fc (H-b) to *β*-CD (C_1-H) were almost the same in the two cases.

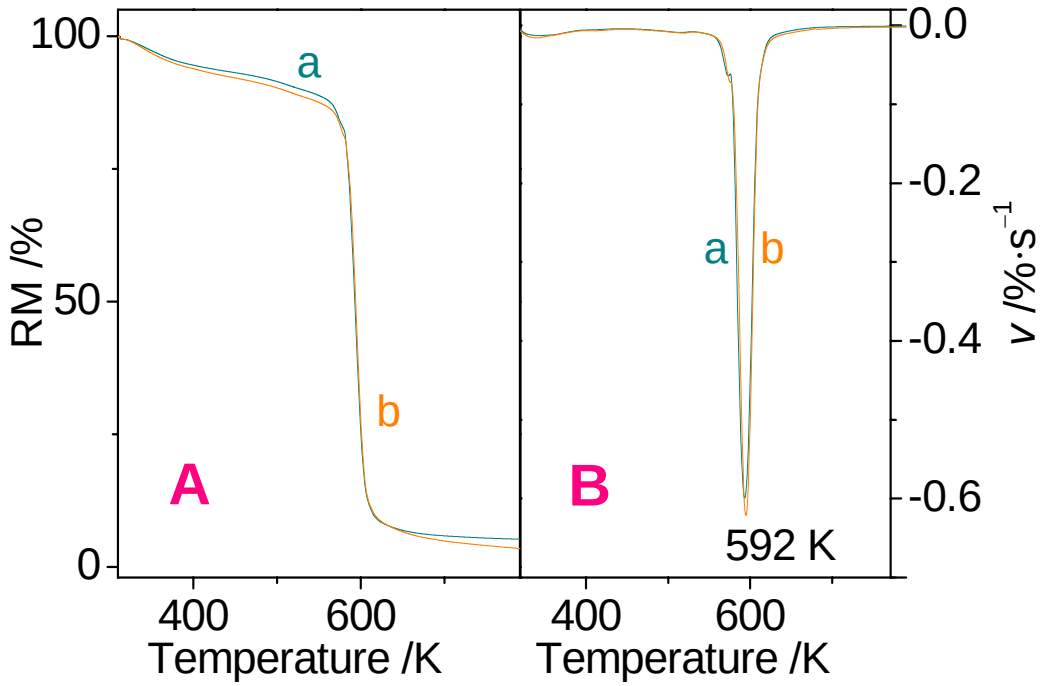
Further, the results of element analyses of the two samples were also highly similar in form: for PP–351, Anal. Calcd for (PPG)·18(Fc)·23(*β*-CD·5H_2O)·30H_2O: C, 43.43; H, 6.60; Fe, 3.05. Found: C, 43.13; H, 6.23; Fe, 3.20, and for PP–151, Anal. Calcd for (PPG)·18(Fc)·23(*β*-CD·5H_2O)·35H_2O: C, 43.32; H, 6.62; Fe, 3.04. Found: C, 43.13; H, 6.23; Fe, 3.28. Although no precipitates formed in the absence of *β*-CD, the change in the initial concentration of *β*-CD can cause the formation of aggregates with the same and different compositions. For example, the chemical stoichiometric ratio (CSR) of *β*-CD, Fc to PPG in PP–351 is 23:18:1, which is the same as that in PP–151, but different from that (32:28:1) in PP–0.5. This indicated the initial concentration of *β*-CD did not play a critical role in mediating the composition of the tri-component aggregates, even if it has a contribution to the generation of the aggregates.

XRD patterns of (A) PP–351 and (B) PP–151.



The above figure indicated the XRD patterns of PP–351 and PP–151. In general, the configurations of the two patterns are high similar, including some details (the number and the relative intensity of peaks) in local peaks and valleys. This result suggested that they had the same stacking structure, which indicated that the change in the initial concentration of β-CD did not make a significant difference in the stacking behaviour of PP–351 and PP–151.

(A) TG and DTG (B) spectra of (a) PP–351 and (b) PP–151 at a heating rate of 10.0 K·min^{-1}.



This figure depicted the TG/DTG profiles of PP–351 and PP–151. It was clear that the TG/DTG curves of two samples were almost completely overlapped, which indicated that they had the same thermal stability and the same degradation process.