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Supplemental Information of

"Treatment of dye wastewater nanofiltration concentrates containing high level anions by pH sensitive nano-size Fe(III)@silica microgel" for New Journal of Chemistry

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1. FT-IR Characterization

The FT-IR spectra of mSiO₂, Fe(III)@mSiO₂, Cys-Fe(III)@mSiO₂ and used Cys-Fe(III)@mSiO₂ after coagulation and Fenton-like degradation are shown in Fig. S1. The broad peak in the range of 3300-3600 cm⁻¹ could be associated with the stretching vibration of -OH. And the peaks at 1637-1641 cm⁻¹ correspond to the bending vibration of water adsorbed, polymerized and crystallized in the coagulant. Furthermore, the peaks at $2361 \sim 2365$ cm⁻¹ are due to carbon dioxide in air. The peaks at 1016-1018 cm⁻¹ and around 958 cm⁻¹ in Fe(III)@mSiO₂ and Cys-Fe(III)@mSiO₂ correspond to symmetrical stretching vibrations of Si-O-Fe respectively. In addition, the strong absorption peaks at 1098-1100 cm⁻¹ correspond to the stretching vibrations of Fe-OH-Fe, which indicates the polymer are formed in the Fe(III)@mSiO₂. But these peaks weakened at Cys-Fe(III)@mSiO₂. Fe-O-Fe and Fe-O are probably formed with the transformation of Fe-OH-Fe and Fe-OH bonds. The peaks at 603-605 and 459-460 cm⁻¹ correspond to the winding vibration of Si-O and Fe-O. Bending vibration of Fe-OH corresponds to the peaks at 667-668 cm⁻¹. The reason could be interpreted as the Fe-O-Fe and Fe-O bonds connect with Si in Cys-Fe(III)@mSiO₂, which forms the Si-O-Fe bonds after the addition of silicon to the solution. Overall, FT-IR analysis probably shows that Cys-Fe(III)@mSiO₂ is not a simple mixture of raw materials. New chemical compounds containing iron and silicon are formed during the synthesis of the samples.



Fig. S1. FT-IR spectra of mSiO₂, Fe(III)@mSiO₂, Cys-Fe(III)@mSiO₂ and used Cys-Fe(III)@mSiO₂ after the Fenton-like degradation and silica coagulation processes for nanofiltration concentrates

2. Effect of H_2O_2 concentration for the degradation of nanofiltration concentrates

The H₂O₂ consumption was related to color and COD removal in the nanofiltration concentrates. Fig. S2 shows the removal of color and COD at different H₂O₂ concentrations of Cys-Fe(III)@mSiO₂. When the mole ratio of Fe(III) ions to H₂O₂ increased from 1:10 to 1:20, the color and COD removal increased from 73.1 % and 52.6 % to 98.4 % and 83.3 %. However, the mole ratio of Fe(III) ions to H₂O₂ varied from 1:30 to 1:40, the color and COD removal decreased from 90.6 % and 69.8 % to 58.6 % and 27.4 %. The reduced efficiency of the color and COD might lie to the hydroperoxyl radical (HO₂•) was generated since the excess amount of H₂O₂ could attack the active hydroxyl radical (•OH). And HO₂• has little acceleration effect in the degradation processes. As well known in the references, the generation rates of Fe(III) with H₂O₂ to hydroxyl radicals is much lower than that of Fe(II) with H₂O₂. With the use of iron and cysteine in Cys-Fe(III)@mSiO₂, sulfur compounds could stimulate the

circulation valences of iron ions, thereby improve the Fenton-like catalytic activity of Fe(III) ions. And the similar enhancement of Fe(III) degradation was observed with the adding assistance of Cys in $Fe(III)/mSiO_2$ for the degradation of nanofiltration concentrates.



Fig. S2 Effect of H₂O₂ concentration for Cys-Fe(III)@mSiO₂ on color removal (A) and COD (B) during the degradation of nanofiltration concentrates (200 mg/L Fe(III),