

Controlled size and morphology, phase transition of YF₃:Yb³⁺, Er³⁺ and YOF:Yb³⁺, Er³⁺ nanocrystals for fine color tuning

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Size, morphology and phase transformation of YF_3 and YOF UCNCs

The morphology and size of UCNCs prepared at different OA/OM ratios of 4:1, 8:3, 2:1, 1:1, 1:2, 3:8 were first studied by TEM, as shown in Fig. 1 (a-f) and (g-l). It can be seen that the NCs prepared at OA/OM ratios of 4:1, 8:3, 2:1 are uniform, monodisperse with rhombic shapes, as shown in Fig. 1(a-c). The average side lengths of these nanoparticles (NPs) are determined to be 10.7, 9.8 and 8.8 nm with a standard deviation of 1.0 nm (see Fig.1 (g-l)). As the OA/OM ratio increased to 1:1, some spherical NPs appeared and the size of NPs decreased to ~ 6.3 nm (see Fig.1d and Fig.1j). As the OA/OM ratio increased further to 1:2, 3:8 (see Fig. 1(e-f)), the rhombic shape NPs disappeared completely and transformed into small sphere NPs, the average sizes of the small NPs decreased to ~ 2.6 nm and 2.5 nm, with a standard deviation of 0.2 nm (Fig. 1(k-l)). These NPs still retained the uniformity and monodispersity after morphology transforming. The TEM results demonstrated that the changing the OA/OM ratio from low to high by increasing the OA content induced the morphology change of rhombic NPs to spherical NPs as well as the gradual decrease of the NPs size.

The crystal structure evolution was further monitored by tracking the changes in the XRD patterns of the respective UCNCs. Fig. 1 (s-x) shows the XRD patterns of the as-prepared UCNCs and the standard data of YF_3 (JCPDS 32-1431) and YOF (JCPDS 06-0347). All of the notable diffraction peaks in the XRD patterns can be perfectly assigned to orthorhombic YF_3 and tetragonal YOF, and we can observe clearly that, with the increasing ratio of OA/OM, the crystal structure evolved from orthorhombic YF_3 to tetragonal YOF. The lattice fringes confirmed the high crystallinity of the samples, as

shown in the HR-TEM images (Fig. 1 (m-r)). The distances between adjacent lattice fringes were determined to be ~ 0.201 , 0.195 and 0.20 nm in Fig. 1 (m-o), which can be well assigned as the d spacing value of the (201) plane of orthorhombic YF_3 . The distance of 0.233 , 0.226 and 0.224 nm in Fig. 1(p-r) can be well assigned as the d spacing value of the (202) plane of tetragonal YOF.

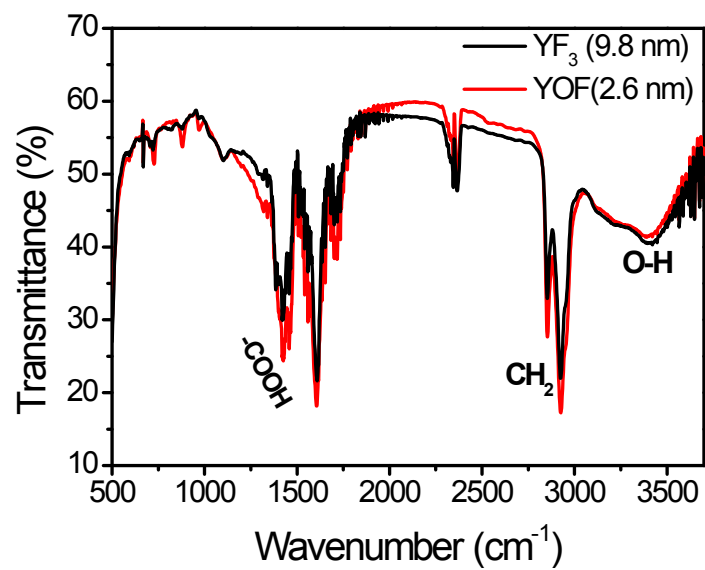


Fig. S1 FT-IR spectra of the obtained YF₃:Yb, Er and YOx: Yb, Er prepared at different OA/OM ratios of 8:3, 3:8, respectively.