

Electronic Supplementary Information (ESI) for

Optically Active Uniform Potassium and Lithium Rare Earth Fluoride Nanocrystals Derived from Metal Trifluoroacetate Precursors

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Table S1. Crystal Structure, Morphology, and Size of the As-Synthesized KREF₄ (RE = La to Gd, Y) and LiREF₄ (RE = Tb to Lu, Y) Nanocrystals *via* the Co-thermolysis of 1 mmol K(CF₃COO) or Li(CF₃COO) and 1 mmol RE(CF₃COO)₃ in Oleic Acid (OA)/Oleylamine (OM)/1-Octadecene (ODE) (40 mmol).

| | OA:OM:ODE | T [°C] | t [min] | structure | morphology | size [nm] ^[a] |
|--------------------|-----------|--------|---------|--------------|-------------------------------|--|
| KLaF ₄ | 1:1:2 | 280 | 60 | cubic | wormlike wire | (8.2±0.5) × (23–100) |
| | 1:1:2 | 300 | 60 | cubic | cube | (9.4±0.9) |
| | 1:1:2 | 300 | 60 | cubic | polygon | (9.5±0.5) |
| KCeF ₄ | 1:1:2 | 260 | 60 | cubic | wormlike wire | (7.8±0.4) × (30–120) |
| | 1:1:2 | 280 | 60 | cubic | cube | (10.4±1.1) |
| | 1:1:2 | 300 | 60 | cubic | cube (predominate) and rod | (15.4±1.3) (12.4±0.8) × (33.1±1.8) |
| | 1:1:2 | 320 | 60 | cubic | polygon | (13.5±0.5) |
| KPrF ₄ | 1:1:2 | 280 | 60 | cubic | polyhedron | (18.2±3.6) |
| KNdF ₄ | 1:1:2 | 280 | 60 | cubic | polyhedron | (16.4±4.2) |
| KSmF ₄ | 1:1:2 | 280 | 60 | cubic | polyhedron | (18.9±3.8) |
| KEuF ₄ | 1:1:2 | 280 | 60 | cubic | polyhedron | (19.5±4.1) |
| KGdF ₄ | 1:1:2 | 300 | 60 | cubic | polyhedron | (21.2±6.1) |
| KYF ₄ | 1:1:2 | 300 | 30 | cubic | polyhedron | (13.2–25.9) |
| LiTbF ₄ | 1:0:1 | 330 | 30 | tetragonal | rhombic plate | (27.1±2.4) × (25.8±4.3) |
| LiDyF ₄ | 1:0:1 | 330 | 30 | tetragonal | rhombic plate | (55.1±2.1) × (49.9±3.7) |
| LiHoF ₄ | 1:0:1 | 280 | 60 | tetragonal | rhombic plate | (53.1±3.4) × (49.8±2.3) |
| LiErF ₄ | 1:0:1 | 320 | 60 | tetragonal | rhombic plate | (51.1±2.3) × (50.9±3.0) |
| LiErF ₄ | 1:0:1 | 300 | 60 | cubic (ErOF) | polyhedron | (23.2±0.4) |
| LiTmF ₄ | 1:0:1 | 320 | 60 | tetragonal | rhombic plate | (56.1±2.3) × (54.9±3.0) |
| LiYbF ₄ | 1:0:1 | 320 | 60 | tetragonal | rhombic plate | (40.3±5.9) × (36.9±4.3) |
| LiLuF ₄ | 1:0:1 | 280 | 60 | tetragonal | rhombic plate | (91.5±2.3) × (89.3±3.2) |
| LiLuF ₄ | 1:0:1 | 300 | 60 | tetragonal | rhombic plate | (41.6±11.8) × (39.8±9.9) |
| LiYF ₄ | 1:0:1 | 330 | 8 | tetragonal | rhombic plate | (29.2±3.9) × (23.2±3.0) |

^[a] The statistic standard deviation from at least 50 particles.

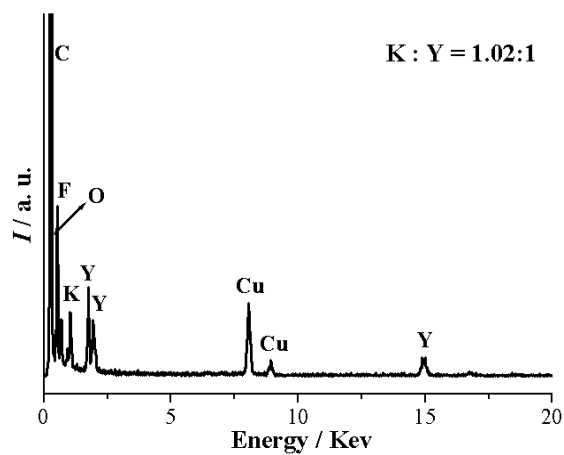


Fig. S1. Energy-dispersive X-ray analysis (EDAX) spectrum of KYF_4 nanopolyhedra, from which the atomic ratio of K:Y was determined as 1.02:1.

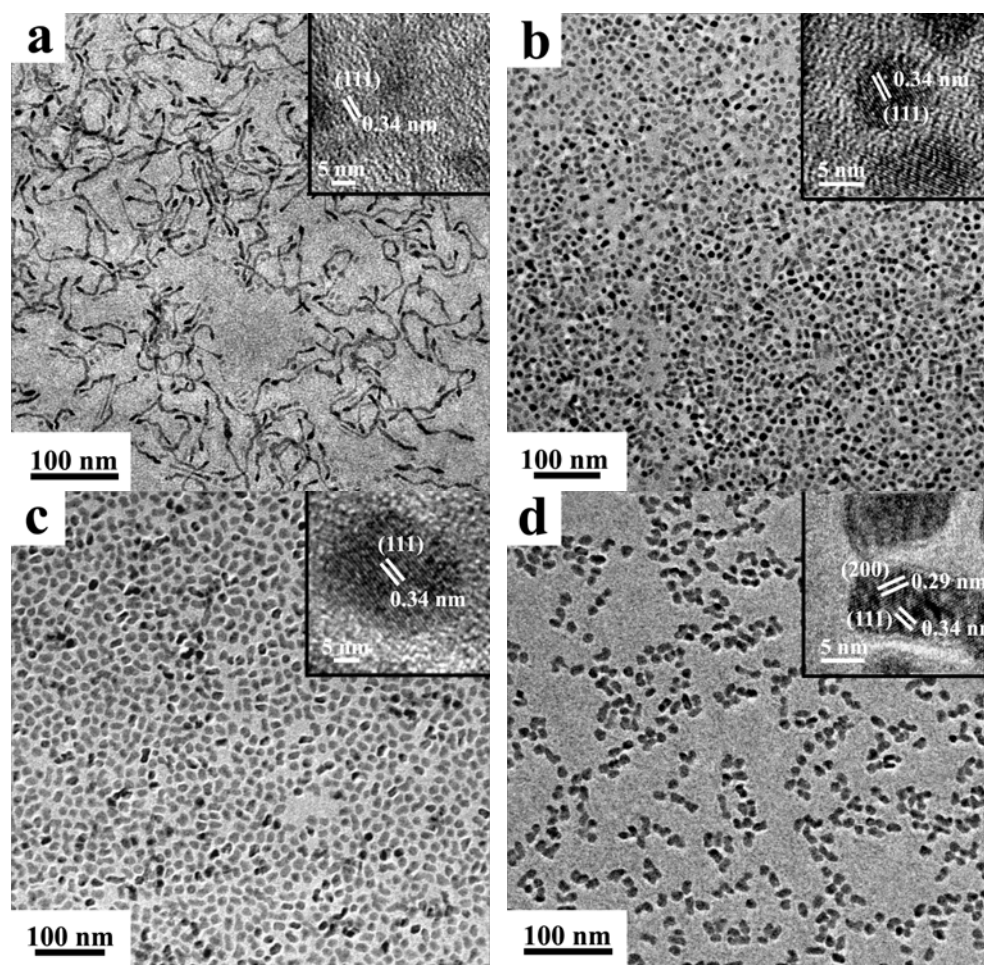


Fig. S2. TEM images of (a) KCeF_4 wormlike nanowires, (b) KNdF_4 (c) KSmF_4 , and (d) KGdF_4 nanopolyhedra.

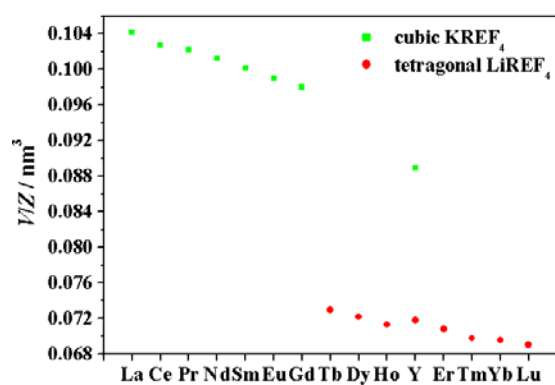


Fig. S3. Plots of the measured lattice volume over the number of KREF₄ and LiREF₄ molecules (Z) in one unit cell against the rare-earth series.

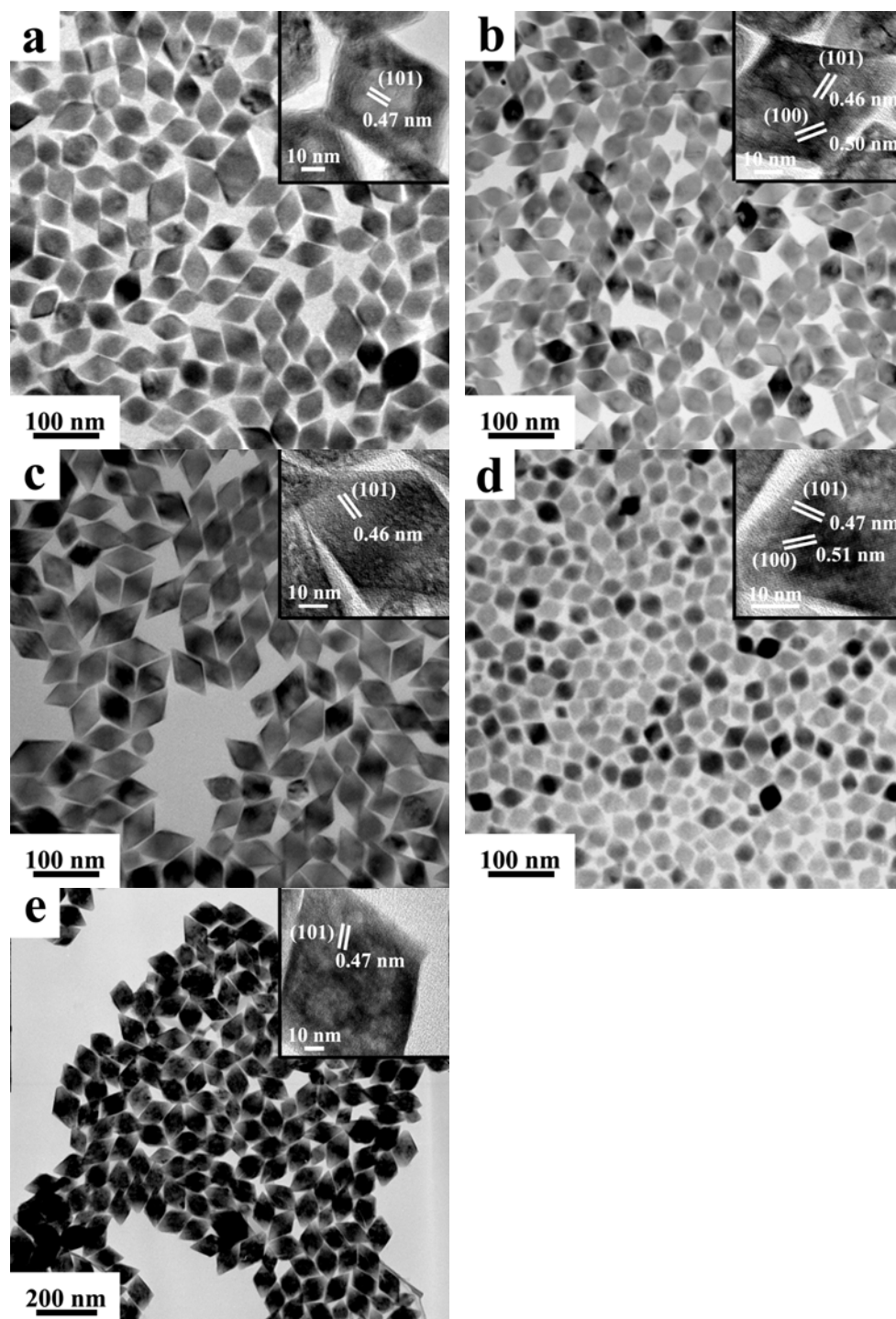


Fig. S4. TEM images of (a) LiDyF₄, (b) LiHoF₄, (c) LiTmF₄, (d) LiYbF₄, and (e) LiLuF₄ nanoplates.

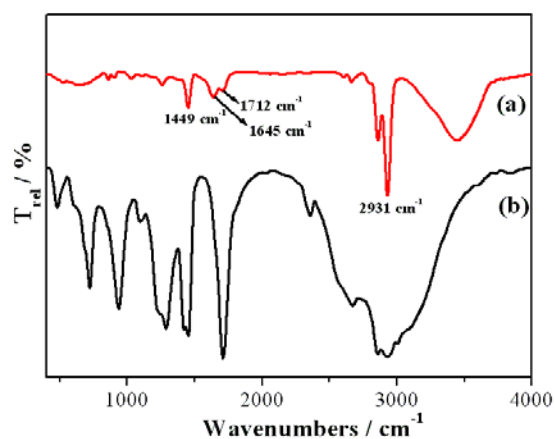


Fig. S5. FTIR spectra of (a) surfactants bound to LiYF₄ nanocrystals and (b) oleic acid.

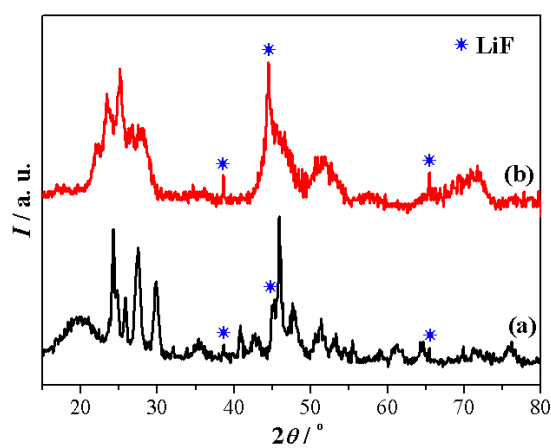


Fig. S6. XRD patterns of (a) LiLuF₄ and (b) LiYF₄ nanocrystals synthesized from co-thermolysis of 1 mmol Li(CF₃COO) and 1 mmol Lu(CF₃COO)₃ or Y(CF₃COO)₃ under OA/OM/ODE (4:1:5) at 280 °C for 60 min.

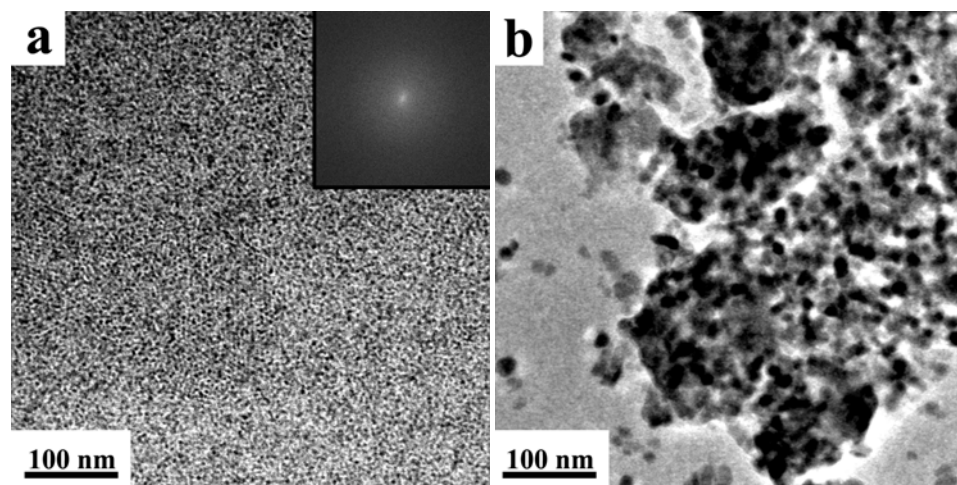


Fig. S7. TEM images of KYF_4 nanocrystals obtained from the co-thermolysis of 1 mmol $\text{K}(\text{CF}_3\text{COO})$ and 1 mmol $\text{Y}(\text{CF}_3\text{COO})_3$ in OA/OM/ODE (1:1:2) for 30 min at different reaction temperatures: (a) 300 °C and (b) 330 °C.

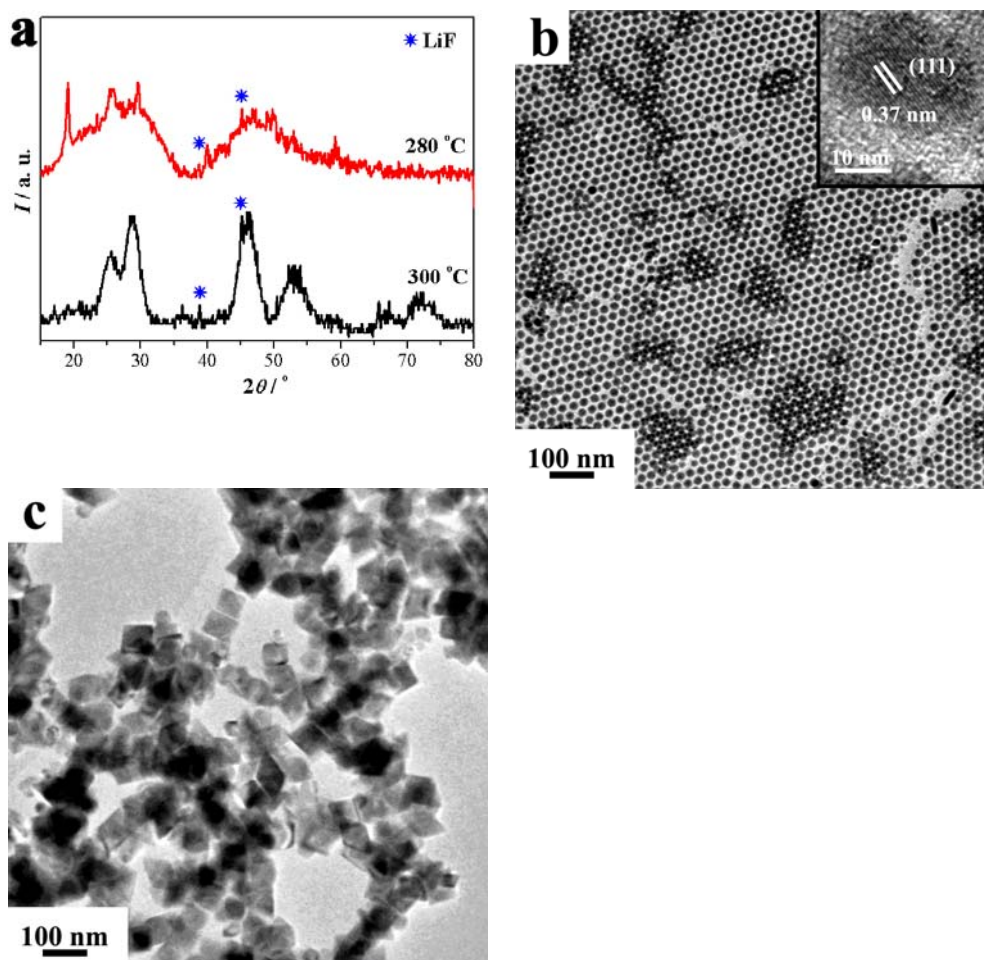


Fig. S8. XRD patterns of LiErF₄ nanocrystals obtained from the thermolysis of 1 mmol Li(CF₃COO) and 1 mmol Er(CF₃COO)₃ in OA/ODE (1:1) for 60 min at different reaction temperatures. TEM images of LiErF₄ nanocrystals obtained from the thermolysis of 1 mmol Li(CF₃COO) and 1 mmol Er(CF₃COO)₃ in OA/ODE (1:1) for 60 min at different reaction temperatures: (b) 300 °C and (c) 330 °C .

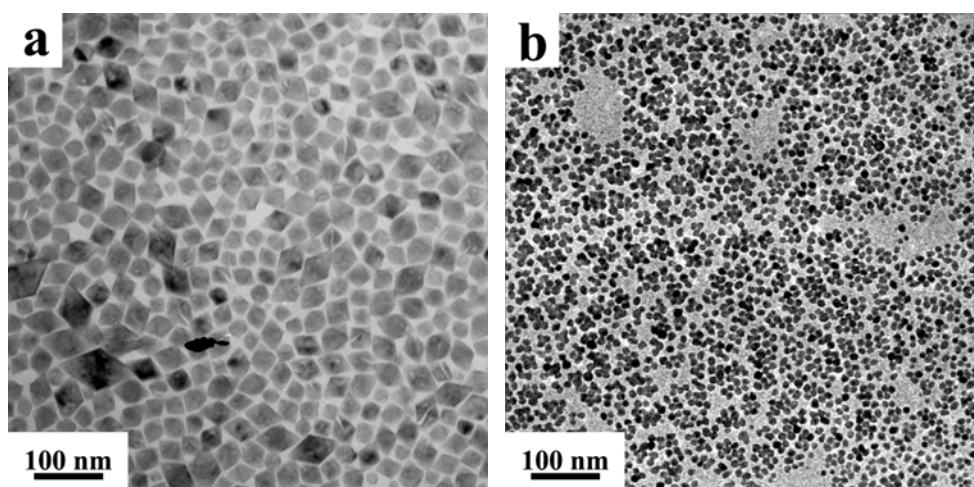


Fig. S9. TEM images of LiLuF_4 nanocrystals obtained from the co-thermolysis of 1 mmol $\text{Li}(\text{CF}_3\text{COO})$ and 1 mmol $\text{Lu}(\text{CF}_3\text{COO})_3$ in OA/ODE (1:1) for 60 min at different reaction temperatures: (a) 300 °C and (b) 320 °C.

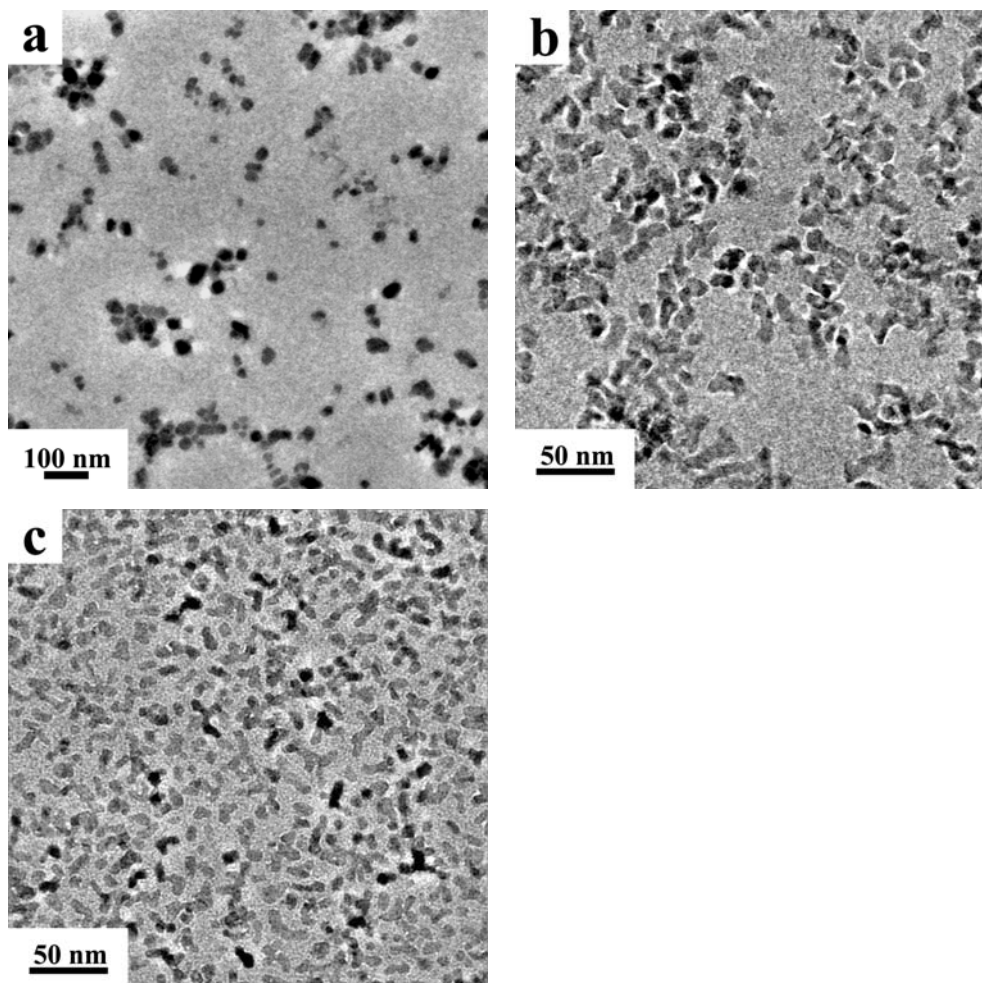


Fig. S10. TEM images of KYF_4 nanocrystals obtained from the thermolysis of 1 mmol $\text{K}(\text{CF}_3\text{COO})$ and 1 mmol $\text{Y}(\text{CF}_3\text{COO})_3$ in OA/OM/ODE (1:1:2) at 300°C for different reaction times: (a) 15 min, (b) 45 min, and (c) 60 min.

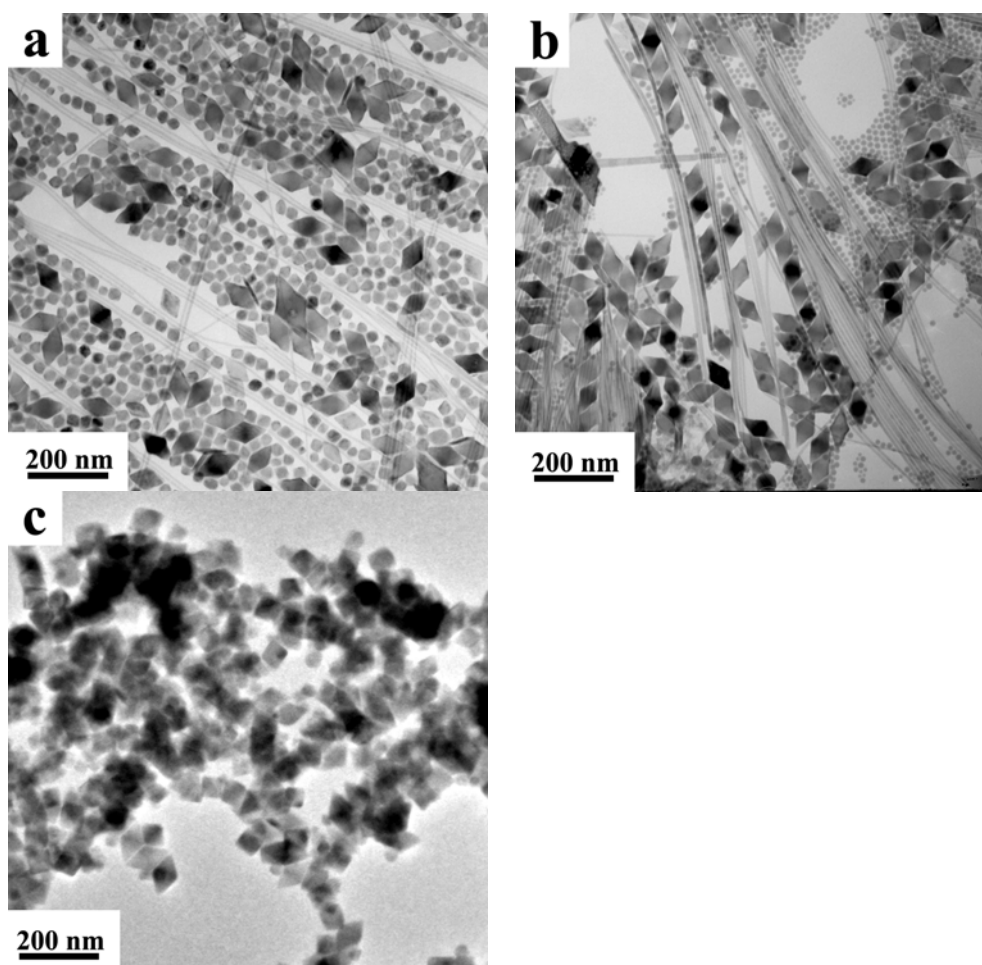


Fig. S11. TEM images of LiErF_4 nanocrystals obtained from the thermolysis of 1 mmol $\text{Li}(\text{CF}_3\text{COO})$ and 1 mmol $\text{Er}(\text{CF}_3\text{COO})_3$ in OA/ODE (1:1) at 330 °C for different reaction times: (a) 15 min, (b) 30 min, and (c) 120 min.