Lanthanide-doped Sr₂ScF₇ nanocrystals: controllable hydrothermal synthesis, growing mechanism and tunable up/down conversion luminescence properties

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| Formula | Sr_2ScF_7 | | |
|------------------------------------|-------------|--|--|
| Formula weight | 353.18 | | |
| Crystal system | monoclinic | | |
| Space group | P21/c (#14) | | |
| a/Å | 5.450 | | |
| b/Å | 12.190 | | |
| c/Å | 8.236 | | |
| a/° | 90 | | |
| β/° | 89.53 | | |
| $\gamma/^{\circ}$ | 90 | | |
| $V/Å^3$ | 547.1 | | |
| Ζ | 4 | | |
| ρ_{calc}/gcm^{-3} | 4.287 | | |
| µ/cm ⁻¹ | 201.32 | | |
| Sinθmax/λ | 0.8071 | | |
| Rint | 0.051 | | |
| $Rw(F_0)$ | 0.048 | | |
| $R(F_0)$ for $F_{02} > 3a(F_{02})$ | 0.045 | | |

Table S1 Crystallographic data for Sr₂ScF₇.

| P | | | | | |
|---|-------------|------------|--|--|--|
| doped $Ln^{3+}(30\%)$ | Length (nm) | Width (nm) | | | |
| no | 120 | 50 | | | |
| Lu | 80 | 40 | | | |
| Yb | 50 | 38 | | | |
| Tm | 35 | 30 | | | |
| Dy | 33 | 29 | | | |
| Tb | 31 | 26 | | | |
| Eu | 24 | 23 | | | |
| Sm | 20 | 20 | | | |
| La | 15 | 15 | | | |

Table S2 Length and diameter of the obtained products from the SEM images in Fig. 2.

| | Excitation | Emission | | Excitation | Emission |
|--|--|---|---|---|--|
| | peaks(nm)/transition | peaks(nm)/transition | | peaks(nm)/transition | peaks(nm)/transition |
| Sr ₂ ScF ₇ :6%Ce ³⁺ | 259,294/4f-5d | 354/5d-4f | Sr ₂ ScF ₇ :12%Tb ³⁺ | 222,265,284,351, | 489/ ⁵ D ₄ - ⁷ F ₆ |
| | | | | $367/4f_8-4f_75d^1$ | $546/{}^{5}D_{4}-{}^{7}F_{5}$ |
| | | | | | $586/^{5}D_{4}-^{7}F_{4}$ |
| | | | | | $624/{}^{5}D_{4}$ - ${}^{7}F_{3}$ |
| Sr ₂ ScF ₇ :9%Eu ³⁺ | 328/ ⁷ F ₀ - ⁵ H ₆ | $594/^{5}D_{0}-^{7}F_{1}$ | Sr ₂ ScF ₇ :1%Sm ³⁺ | $359/^{6}H_{5/2}-^{4}K_{17/2}$ | $562/^4G_{5/2}$ - $^6H_{5/2}$ |
| | $362/{}^{7}F_{0}-{}^{5}D_{4}$ | $619/{}^{5}D_{0}-{}^{7}F_{2}$ | | $372/^{6}H_{5/2}-^{4}D_{15/2}$ | $603/^4G_{5/2}$ - $^6H_{7/2}$ |
| | $381/{}^{7}F_{0}-{}^{5}G_{2}$ | | | $399/^{6}H_{5/2}-^{4}K_{11/2}$ | $651/^4G_{5/2}$ - $^6H_{9/2}$ |
| | $394/{}^{7}F_{0}-{}^{5}L_{6}$ | | | | |
| | $465/{}^{7}F_{0}-{}^{5}D_{2}$ | | | | |
| $Sr_2ScF_7:1\% Dy^{3+}$ | $294/^6H_{5/2}\text{-}{}^4D_{7/2}$ | $482,492/{}^4F_{9/2}\text{-}{}^6H_{15/2}$ | $Sr_2ScF_7:1\%Er^{3+}$ | $364/^4 I_{15/2} \textbf{-} {}^4 G_{7/2}$ | $524/^2H_{11/2}\text{-}{}^4I_{15/2}$ |
| | $324^{/6}H_{5/2}\text{-}{}^6P_{3/2}$ | $577/{}^4F_{9/2}\text{-}{}^6H_{13/2}$ | | $378/^4I_{15/2}\text{-}{}^4G_{11/2}$ | $547,558/^4S_{3/2}\text{-}^4I_{15/2}$ |
| | $348/^6H_{5/2}\text{-}{}^6P_{7/2}$ | | | $405/^4 I_{15/2} \text{-}{}^2 H_{9/2}$ | |
| | $364/^6H_{5/2}\text{-}{}^6P_{7/2}$ | | | | |
| | $384/^6H_{5/2}\text{-}{}^4M_{21/2}$ | | | | |
| $Sr_2ScF_7{:}2\%Ho^{3+}$ | $361/{}^{5}I_{8}$ - ${}^{5}G_{2}$ | $540,548/{}^{5}F_{4},{}^{5}S_{2}-{}^{5}I_{8}$ | $Sr_2ScF_7{:}2\% Er^{3+}$ | $357/^{3}H_{6}-^{1}D_{2}$ | $451/^{1}D_{2}-^{3}F_{4}$ |
| | $384/{}^{5}I_{8}$ - ${}^{5}G_{4}$ | | | | |
| | $417/{}^{5}I_{8}-{}^{5}G_{5}$ | | | | |
| | $452/{}^{5}I_{8}$ - ${}^{5}F_{1}$, ${}^{5}G_{6}$ | | | | |
| | 485/ ⁵ I ₈ - ⁵ G ₂ | | | | |

| Table S3 Summary of the photoluminescence properties of Sr_2ScF_7 :Ln ³⁺ (Ln = Ce, Tb, Eu, Sm |
|--|
| Dy, Er, Ho, and Tm) nanocrystals. |



Fig. S1 The photoluminescence emission intensity of Ln^{3+} ions as a function of their doping concentrations in Sr_2ScF_7 nanocrystals, respectively. The optimum concentrations of Ln^{3+} are determined to be as 6% (Ce³⁺), 12% (Tb³⁺), 9% (Eu³⁺), 1% (Sm³⁺), 1% (Dy³⁺), 1.0 (Er³⁺), 2% (Ho³⁺), 2% (Tm³⁺), respectively.



Fig. S2 The CIE chromaticity coordinates of Sr₂ScF₇: (A) 6% Ce³⁺, (B)12% Tb³⁺, (C) 9% Eu³⁺, (D) 1% Sm³⁺, (E) 1% Dy³⁺, (F) 1% Er³⁺, (G) 2% Ho³⁺, (H) 2% Tm³⁺, respectively.



Fig. S3 The CIE chromaticity coordinates of (a) $Sr_2ScF_7:10\%Yb^{3+}$, $2\%Tm^{3+}$, (b) $Sr_2ScF_7:1\%Er^{3+}$, (c) $Sr_2ScF_7:10\%Yb^{3+}$, $1\%Er^{3+}$ nanocrystals.



Fig. S4 The decay curves of ${}^{3}H_{4} \rightarrow {}^{3}H_{6}$ of Tm^{3+} in the $Sr_2ScF_7:10\%Yb^{3+},1\%Tm^{3+}$ and $S_{r2}ScF_7:10\%Yb^{3+},1\%Er^{3+},1\%Tm^{3+}$ nanocrystals.