Controllable synthesis of $Sc_2Mo_3O_{12}$ microcrystals with exposed {001} facets and their remarkable tunable luminescence properties by doping lanthanides

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Fig. S1 The simulated shape of the single scandium molybdate precursor sample. (AB = 7.4 μ m, CD = 10 μ m, BE = 1.4 μ m)

$$S_{001} = 2AB^2 = 2 \times 7.4^2 = 109.52\mu m^2$$
$$S_{101} = 8 \times \frac{(AB + CD) \times BE}{2} = 8 \times \frac{(10 + 7.4) \times 1.4}{2} = 97.44\mu m^2$$

$$S_{001}\% = \frac{S_{001}}{S_{001} + S_{101}} = \frac{109.52}{109.52 + 97.44} = 53\%$$



Fig. S2 XRD patterns of the scandium molybdate precursors produced with different molar ratios of Mo/Sc.



Fig. S3 XRD patterns (A) and SEM images of the samples synthesized with different molar ratios of Mo/Sc: (B) 4.5, (C) 5 and (D) 7.

Fig. S3 shows XRD patterns and SEM images of the samples obtained with different molar ratios of Mo/Sc. When the molar ratio is 4.5, well defined uniform compressed decahedron microcrystals are observed (Fig. S3B) and pure orthorhombic phase of $Sc_2Mo_3O_{12}$ without impurity phases are obtained (Fig. S3A). When the molar ratio is adjusted to 5, the SEM image shows that the products exhibit compressed decahedral and belt-like microcrystals (Fig. S3C). Meanwhile, the XRD pattern shows impurity peaks of NaScMo₃O₁₂. When the molar ratio is then adjusted to 7, it is worth noting that the morphology of products all become belt-like microcrystals and all the characteristic diffraction peaks in Fig.S3A match well with the phase of NaScMo₃O₁₂ (JCPDS file no. 28-1128). With the increase of the molar ratio of Mo/Sc (from 4.5 to 7), the concentration of Na⁺ ions increase, which lead to the formation of NaScMo₃O₁₂ phase.



Fig. S4 The thickness of scandium molybdate precursors prepared at different pH values (A: 2.5, B: 4.5)



Fig.S5 Schematic illustration for the conversion process from nanosheets to final chocolate-like precursor crystals



Fig.S6 The emission spectra of MoO_4^{2-} in $Sc_2Mo_3O_{12}$:5%Tb³⁺ samples (A), and $Sc_2Mo_3O_{12}$:2%Eu³⁺ samples (B).



Fig.S7 The PL excitation and emission spectra of Sc2Mo3O12:2%Eu3+ samples (red line) and scandium molybdate precursor:2%Eu3+ samples (black line).