Supporting Information

Single-band red upconversion luminescence of Yb^{3+}-Er^{3+} via nonequivalent substitution in perovskite $KMgF_3$ nanocrystals

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Table S1. Initial lattice constants for an 8×2×1 supercell of $KMgF_3$.

Lattice Constants	Value
a **(Å)**	32.3287
b **(Å)**	8.0826
c **(Å)**	4.0413
α **(degree)**	90.0000
β **(degree)**	90.0000
γ **(degree)**	90.0000
V **(Å^3)**	1055.9807

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Table S2. Optimized cell parameters and forming energy (*E*) of four K-Mg substitution geometry modes (denoted as M1, M2, M3, M4) for an 8×2×1 supercell of $KMgF_3$: Er^{3+} with one K^+ ion and one Mg^{2+} ion substituted by two Er^{3+} ions.

Parameters	M1	M2	M3	M4
***a* (Å)**	33.2048	33.1347	34.4393	33.5208
***b* (Å)**	8.1560	8.1530	8.1771	8.2821
***c* (Å)**	4.0303	4.0357	4.0543	4.0275
α (degree)	90.0000	90.0000	90.0000	90.0000
β (degree)	90.0000	90.0000	90.0000	90.0000
γ (degree)	90.0000	90.0000	90.0000	90.0000
***V* (Å^3)**	1091.4763	1090.2268	1141.7644	1118.1154
***E* (eV)**	-397.8999	-397.8883	-396.9790	-396.0048
$\triangle E$(eV)	0.0000	0.0116	0.9209	1.8951
$R_{Er\text{-}Er}$ (Å)	3.5666	3.5723	8.4850	11.5542

$\triangle E_{(Mi)} = E_{(Mi)} - E_{(M1)}$ (i=1, 2, 3 and 4).

Table S3. Optimized cell parameters and forming energy (*E*) of four Mg-Mg substitution geometry modes (denoted as N1, N2, N3, N4) for an 8×2×1 supercell of $KMgF_3$: Er^{3+} with two Mg^{2+} ions substituted by two Er^{3+} ions.

Parameters	N1	N2	N3	N4
a **(Å)**	33.1527	33.1505	33.1308	32.9757
b **(Å)**	8.2187	8.2419	8.2436	8.2481
c **(Å)**	4.0803	4.0942	4.0959	4.1741
α **(degree)**	90.0000	90.0000	90.0000	90.0000
β **(degree)**	90.0000	90.0000	90.0000	90.0000
γ **(degree)**	90.0000	90.0000	90.0000	90.0000
V **(Å^3)**	1111.7563	1118.6249	1118.6714	1135.3048
E **(eV)**	-397.4641	-397.4463	-397.4555	-397.0425
△E (eV)	0.0000	0.0178	0.0086	0.4216
$R_{Er\text{-}Er}$ **((Å))**	4.4528	8.6241	12.6058	16.4878

$\triangle E_{(Ni)} = E_{(Ni)} - E_{(N1)}$ (i=1, 2, 3 and 4).