Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Eu^{2+} doped halide perovskite $KCaCl_3$ with high-efficiency blue emission and the scintillation application

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Table S1 The total energy (E_0) of fifteen proposed substitution geometry models fora 2×2×2 supercell of $KCaCl_3$:0.13Eu^{2+} with two Ca^{2+} ions replaced by two Eu^{2+} ions.

Model	E_0 (eV)
M1	-632.448
M2	-632.448
M3	-632.447
M4	-632.452
M5	-632.448
M6	-632.452
M7	-632.451
M8	-632.45
M9	-632.448
M10	-632.452
M11	-632.446
M12	-632.448
M13	-632.449
M14	-632.453
M15	-632.453

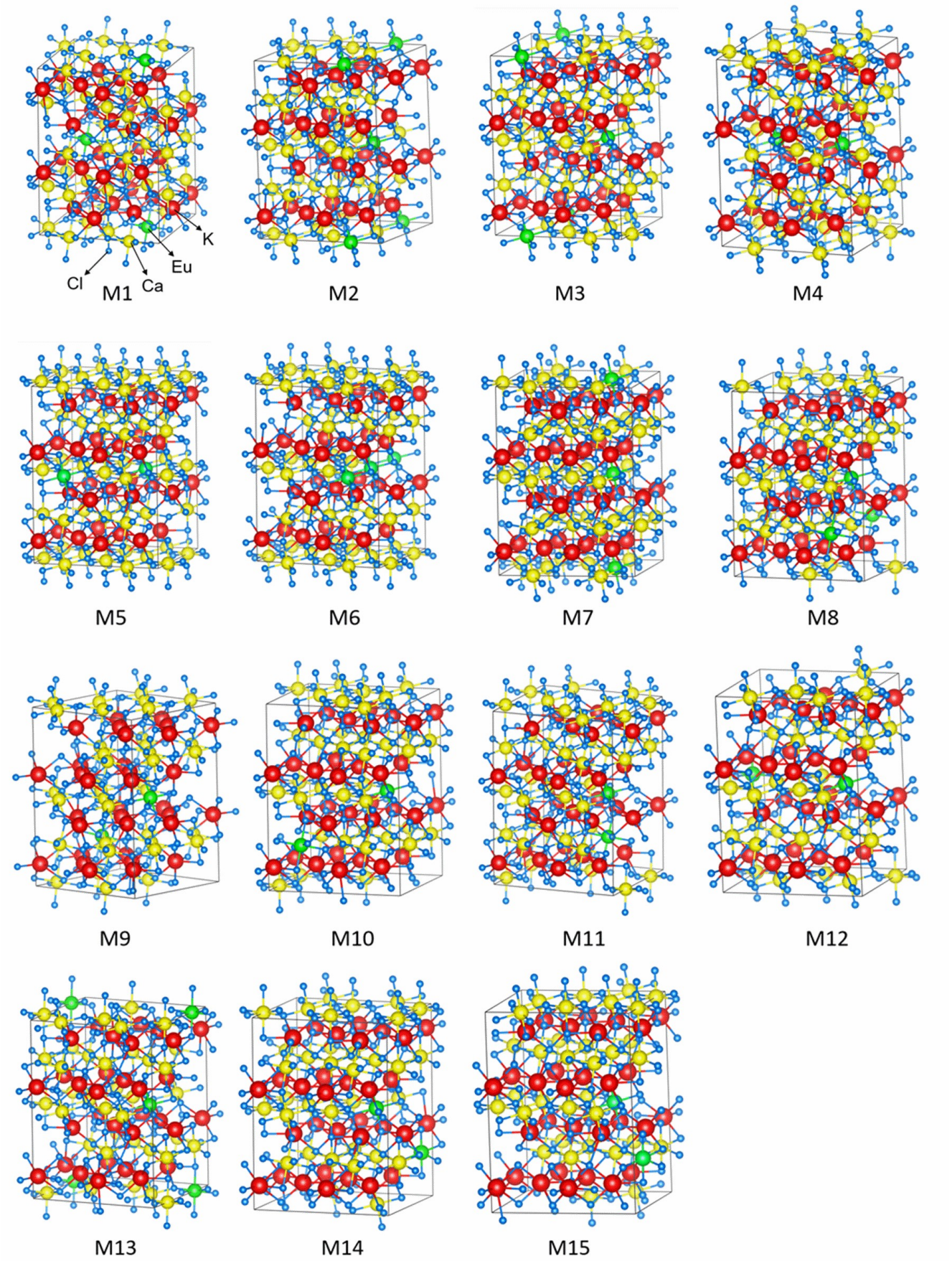

Figure S1. Possible substitution geometry models (denoted as M1-M15) for a 2×2×2 supercell of $KCaCl_3$:Eu^{2+} with two Ca^{2+} replaced by two Eu^{2+}.

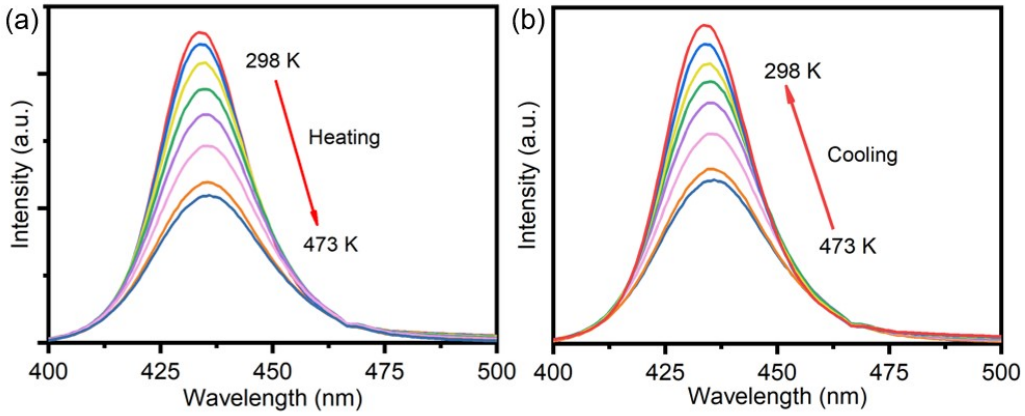

Figure S2. Temperature dependent emission spectrum of $KCaCl_3:0.13Eu^{2+}$ particles through heating (a) and cooling (b) processes.

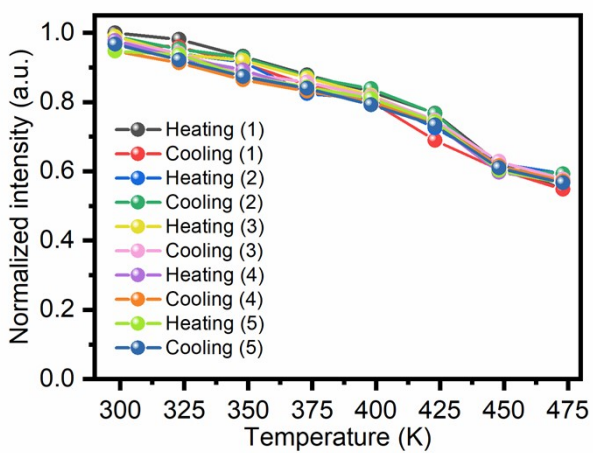

Figure S3. T-cycles of $KCaCl_3:0.13Eu^{2+}$ powders.

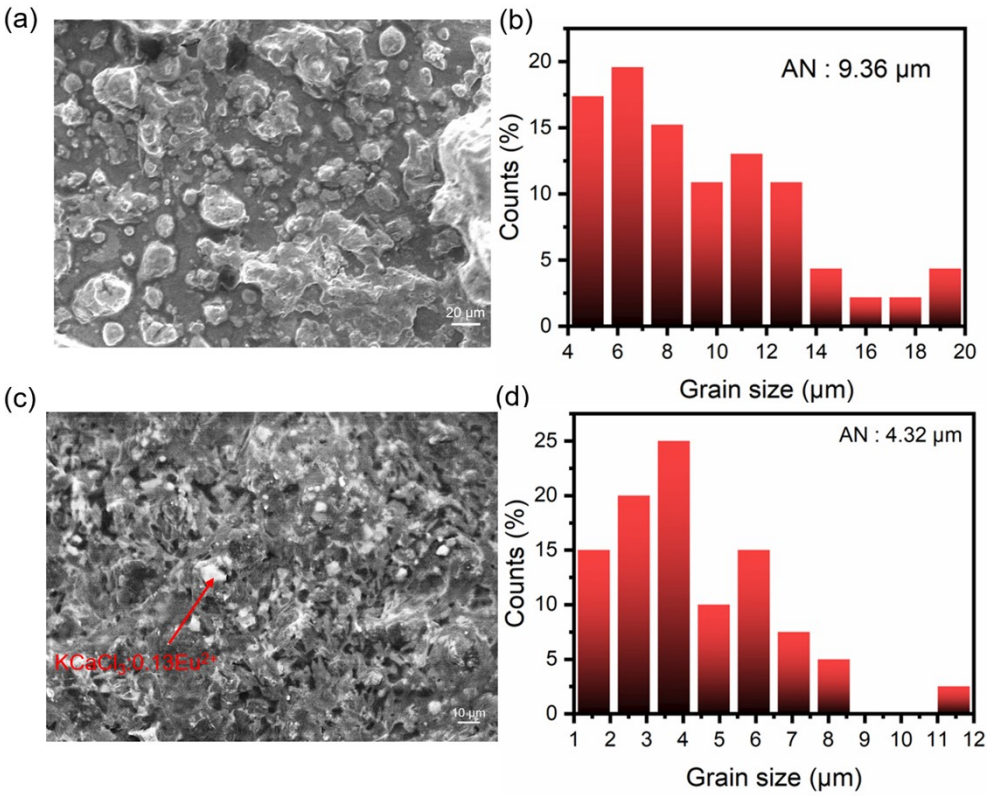

Figure S4. SEM image and size distribution of the $KCaCl_3$:0.13Eu^{2+} powders (a), (b); and $KCaCl_3$:0.13Eu^{2+} film (c), (d).