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Electronic Supplementary Information

Structure and luminescence of a novel orange-yellow-emitting $Ca_{1.62}Eu_{0.38}Si_5O_3N_6$ phosphor for warm white LEDs, discovered by a single-particle-diagnosis approach

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Table S1. Anisotropic displacement parameters ($Å^2$) of $Ca_{1.62}Eu_{0.38}Si_5O_3N_6$.

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.007	0.0049	0.0065	0.0003	0.0041	0.0001
Ca2	0.0052	0.0057	0.0064	0.001	0.0023	-0.0008
Ca3	0.0058	0.006	0.0069	-0.0009	0.0025	0.0008
Ca4	0	0	0	0	0	0
Ca5	0	0	0	0	0	0
Ca6	0	0	0	0	0	0
Ca7	0.0181	0.0154	0.0175	0	0.0045	0
Ca8	0.0171	0.0123	0.0205	0	0.0064	0
Eu1	0.0181	0.0154	0.0175	0	0.0045	0
Eu2	0.0171	0.0123	0.0205	0	0.0064	0
Si1	0.0029	0.0036	0.0034	-0.0002	0.0008	-0.0004
Si2	0.003	0.0047	0.0029	-0.0001	0.0009	0
Si3	0.0027	0.0035	0.003	0	0.0006	-0.0003
Si4	0.0035	0.0045	0.0034	0.0006	0.0008	-0.0005
Si5	0.0026	0.0031	0.0046	-0.0001	0.0013	0.0004
Si6	0.0032	0.0029	0.0031	0	0.001	-0.0003
Si7	0.0028	0.0041	0.003	0	0.0008	0.0003
Si8	0.0015	0.0045	0.0033	0.0002	0.0002	0
Si9	0.0046	0.0036	0.0043	-0.0004	0.0021	0
Si10	0.0027	0.0035	0.0033	-0.0003	0.0008	0.0003
N1	0.008	0.004	0.008	0	0.001	0
N2	0.008	0.002	0.011	0	0.004	0
N3	0.0045	0.0052	0.0021	-0.0014	-0.0006	0.0008
N4	0.009	0.006	0.01	0	0.001	0
N5	0.0045	0.0062	0.0064	0.001	0.0046	0.0006
N6	0.0035	0.0064	0.0039	0.0016	0.0024	0.0015
N7	0.0058	0.0076	0.0051	-0.0025	0.0034	-0.0028
N8	0.005	0.0081	0.0033	-0.0018	0.0024	-0.0019
N9	0.0043	0.006	0.0043	-0.0005	0.0016	0.001
N10	0.0056	0.0087	0.0037	0.0052	0.0018	0.0005
N11	0.006	0.001	0.0009	0	0.0008	0
N12	0.0011	0.0084	0.0044	0.0007	0.0006	-0.0003
N13	0.0046	0.0059	0.0038	0.0007	0.0014	0.0002
N14	0.0057	0.0075	0.002	0.0014	0.0008	-0.0004
O1	0.0082	0.0051	0.0094	0.0026	0.0014	-0.0014
O2	0.0083	0.005	0.008	-0.0008	0.0024	-0.0019
O3	0.0097	0.0046	0.0101	0.002	0.0045	-0.0002
O4	0.0042	0.0035	0.0137	-0.0003	0.0026	-0.0011
O5	0.0069	0.0072	0.0094	-0.002	0.0007	-0.0018

O6	0.0079	0.0041	0.0082	-0.0008	0.0011	-0.0017