Erratum: First-principles study of the luminescence of Eu^{2+} -doped phosphors **[Phys. Rev. B *96*, 125132 (2017)]**

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Although exploiting the data published in the original paper for another purpose, we noted several problems with the reported values: (1) for the analysis of the luminescence of Eu^{2+} -doped phosphors, a higher numerical accuracy for the one-dimensional-CCD parameters was needed (rounding errors were present); (2) the data for $\text{Ba}_3\text{Si}_6\text{O}_{12}\text{N}_2:\text{Eu}^{2+}$ in Table III were incorrectly reported; (3) the point corresponding to $\text{Sr}_5(\text{PO}_4)_3\text{Cl}:\text{Eu}$ in Fig. 5 was misplaced.

In this Erratum, we list the corrected data and compare them to the published values. Detailed results can be found in Tables I–VI. Based on these corrections, the comparison among calculated transition energy, Stokes shift, and FWHM and the corresponding experimental data are shown in Figs. 1 and 2.

In Table III, the revised $\text{KSrPO}_4:\text{Eu}^{2+}$ and $\text{CaAlSiN}_3:\text{Eu}$, M-II data yield appearance or disappearance of the crossing point x . See Eq. (9) in the original paper: Increasing/decreasing the value of ΔC can have such an effect. Anyhow, the value of E_{fd} , when it exists, is very high, so the conclusion about the possibility to have thermal quenching due to f - d crossing remains unchanged. All the acronyms have the same meaning as the definitions in the original paper: M -I and M -II in CaAlSiN_3 stand for two ordered structures considered in our calculations, and Eu1 and Eu2 stand for inequivalent Eu sites available in SrAl_2O_4 and $\text{Sr}[\text{LiAl}_3\text{N}_4]$ compounds.

All these corrections do not affect the discussions and conclusions in the original paper.

TABLE I. Comparison between the corrected and the published data of Table I from our paper. Large changes (>0.01 eV for absorption and emission energy, and $>10\text{ cm}^{-1}$ for ΔS) are underlined. Like in the original paper, the numbers in bold deviate by more than 1000 cm^{-1} from experiment.

Compounds	Corrected data			Data from the original paper		
	Abs (eV)	Em (eV)	ΔS (cm^{-1})	Abs (eV)	Em (eV)	ΔS (cm^{-1})
$\text{SrB}_4\text{O}_7:\text{Eu}$	3.845	3.633	1712	3.845	3.633	1710
$\text{KSrPO}_4:\text{Eu}$	3.611	2.999	4938	3.612	2.998	4920
$\text{CaMgSi}_2\text{O}_6:\text{Eu}$	2.969	2.446	4214	2.969	2.447	4218
$\text{SrAl}_2\text{O}_4:\text{Eu}2$	3.167	2.547	5004	3.167	2.547	4996
$\text{Sr}_5(\text{PO}_4)_3\text{Cl}:\text{Eu}$	3.238	2.925	2524	3.238	2.926	2516
$\text{CaF}_2:\text{Eu}$	3.257	3.045	<u>1712</u>	3.257	3.045	1774
$\text{SrI}_2:\text{Eu}$	3.350	3.137	<u>1712</u>	3.349	3.138	2339
$\text{Sr}_2\text{MgSi}_2\text{O}_7:\text{Eu}$	3.108	2.522	4719	3.107	2.523	4726
$\text{SrAl}_2\text{O}_4:\text{Eu}1$	2.969	<u>2.316</u>	<u>5267</u>	2.968	2.361	4839
$\text{BaSi}_2\text{O}_2\text{N}_2:\text{Eu}$	2.854	2.297	4499	2.855	2.297	4436
$\text{Ba}_3\text{Si}_6\text{O}_{12}\text{N}_2:\text{Eu}$	<u>2.955</u>	2.457	<u>4016</u>	2.940	2.461	3952
$\text{CaAlSiN}_3:\text{Eu}$, M-I	2.367	2.027	2743	2.367	2.028	2742
$\text{CaAlSiN}_3:\text{Eu}$, M-II	2.389	2.079	2502	2.387	2.079	2508
$\text{Sr}[\text{Mg}_3\text{SiN}_4]:\text{Eu}$	2.215	2.054	1295	2.216	2.055	1290
$\text{CaS}:\text{Eu}$	2.120	1.810	2502	2.120	1.810	2500
$\text{Sr}[\text{LiAl}_3\text{N}_4]:\text{Eu}1$	2.095	1.962	<u>1075</u>	2.095	1.962	1129
$\text{Sr}[\text{LiAl}_3\text{N}_4]:\text{Eu}2$	2.161	1.989	<u>1383</u>	2.160	1.989	1371
$\text{Ca}[\text{LiAl}_3\text{N}_4]:\text{Eu}$	1.992	1.823	1361	1.992	1.823	1371

TABLE II. Comparison between the corrected and published data for the transition energies and Frank-Condon shift, Table III in the original paper and Table I in the original paper for the E_{em} . Large changes (> 0.01 eV) are underlined.

Compounds	Corrected data					Data from the original paper				
	E_{abs}	E_{em}	E_{ZPL}	$E_{FC,g}$	$E_{FC,e}$	E_{abs}	E_{em}	E_{ZPL}	$E_{FC,g}$	$E_{FC,e}$
SrB ₄ O ₇ :Eu	3.845	3.633	3.736	0.103	0.109	3.845	3.633	3.736	0.103	0.109
KSrPO ₄ :Eu	3.611	2.999	3.301	0.302	<u>0.310</u>	3.621	2.998	3.300	0.302	0.321
CaMgSi ₂ O ₆ :Eu	2.969	2.446	2.721	0.275	0.248	2.969	2.447	2.722	0.275	0.247
SrAl ₂ O ₄ :Eu2	3.167	2.547	2.893	0.346	0.275	3.167	2.547	2.892	0.345	0.275
Sr ₅ (PO ₄) ₃ Cl:Eu	3.238	2.925	3.094	0.169	0.144	3.238	2.925	3.094	0.169	0.144
CaF ₂ :Eu	3.257	3.045	3.159	0.114	0.098	3.257	3.045	3.159	0.114	0.098
SrI ₂ :Eu	3.350	3.137	3.227	0.090	0.122	3.349	3.138	3.227	0.089	0.122
Sr ₂ MgSi ₂ O ₇ :Eu	3.108	2.522	2.852	0.329	0.256	3.107	2.523	2.852	0.329	0.255
SrAl ₂ O ₄ :Eu1	2.969	<u>2.316</u>	2.678	0.362	0.291	2.968	2.361	2.677	0.361	0.291
BaSi ₂ O ₂ N ₂ :Eu	2.854	2.297	2.607	0.310	0.248	2.855	2.297	2.607	0.310	0.248
Ba ₃ Si ₆ O ₁₂ N ₂ :Eu	<u>2.955</u>	2.457	<u>2.724</u>	<u>0.267</u>	<u>0.231</u>	2.940	2.461	2.864	0.100	0.076
CaAlSiN ₃ :Eu, M-I	2.367	2.027	2.196	0.169	0.171	2.367	2.028	2.196	0.168	0.171
CaAlSiN ₃ :Eu, M-II	2.389	2.079	<u>2.220</u>	<u>0.141</u>	0.169	2.389	2.079	2.195	0.164	0.173
Sr[Mg ₃ SiN ₄]:Eu	2.215	2.054	2.139	0.084	0.076	2.216	2.055	2.140	0.085	0.076
CaS:Eu	2.120	1.810	1.976	0.166	0.144	2.120	1.810	1.976	0.166	0.144
Sr[LiAl ₃ N ₄]:Eu1	2.095	1.962	2.038	0.076	0.057	2.095	1.962	2.038	0.076	0.057
Sr[LiAl ₃ N ₄]:Eu2	2.161	1.989	2.049	0.060	0.112	2.160	1.989	2.049	0.060	0.111
Ca[LiAl ₃ N ₄]:Eu	1.992	1.823	1.910	0.087	0.082	1.992	1.823	1.910	0.087	0.082

TABLE III. Comparison between the corrected and published data for parameters yielding the E_{fd} (eV) barrier, Table III in our paper. Large changes (> 0.01) are underlined.

Compounds	Corrected data				Data from the original paper			
	ΔC	x	Λ	E_{fd}	ΔC	x	Λ	E_{fd}
SrB ₄ O ₇ :Eu	0.006	—	0.028	∞	0.005	—	0.028	∞
KSrPO ₄ :Eu	<u>0.008</u>	<u>6.343</u>	0.086	<u>8.851</u>	0.068	—	0.089	∞
CaMgSi ₂ O ₆ :Eu	−0.027	4.762	0.083	3.488	−0.027	4.762	0.083	3.488
SrAl ₂ O ₄ -Eu2	−0.071	3.847	0.087	2.230	−0.071	3.846	0.087	2.236
Sr ₅ (PO ₄) ₃ Cl-Eu	−0.025	7.030	0.044	5.243	−0.025	7.030	0.044	5.243
CaF ₂ :Eu	−0.016	9.346	0.030	6.823	−0.016	9.346	0.030	6.823
SrI ₂ :Eu	0.032	—	0.036	∞	0.033	—	0.036	∞
Sr ₂ MgSi ₂ O ₇ :Eu	−0.073	3.876	0.082	2.144	−0.074	3.876	0.082	2.144
SrAl ₂ O ₄ -Eu1	−0.071	3.557	0.098	1.903	−0.071	3.559	0.098	1.907
BaSi ₂ O ₂ N ₂ -Eu	−0.063	3.876	0.087	2.040	−0.063	3.876	0.087	2.040
Ba ₃ Si ₆ O ₁₂ N ₂ -Eu	<u>−0.036</u>	<u>4.685</u>	<u>0.078</u>	<u>3.138</u>	−0.025	9.901	0.019	6.102
CaAlSiN ₃ :Eu, M-I	0.002	7.353	0.072	6.872	0.003	7.353	0.072	6.872
CaAlSiN ₃ :Eu, M-II	<u>0.028</u>	—	0.071	<u>∞</u>	0.003	7.353	0.074	6.872
Sr[Mg ₃ SiN ₄]:Eu	−0.008	9.615	0.034	5.634	−0.008	9.615	0.034	5.634
CaS:Eu	−0.022	5.253	0.065	2.601	−0.022	5.253	0.065	2.601
Sr[LiAl ₃ N ₄]:Eu1	−0.019	7.937	0.027	2.727	−0.019	7.937	0.027	2.727
Sr[LiAl ₃ N ₄]:Eu2	0.052	—	0.052	∞	0.052	—	0.051	∞
Ca[LiAl ₃ N ₄]:Eu	−0.005	9.346	0.041	5.638	−0.005	9.346	0.041	5.638

TABLE IV. Comparison between the corrected and the published data for the phonon frequencies (meV) and Huang-Rhys parameters, Table IV in the original paper. Large changes (> 0.2 for phonon frequency and > 0.1 for the Huang-Rhys parameter) are underlined.

Compounds	Corrected data				Data from the original paper			
	$\hbar\Omega_g$	$\hbar\Omega_e$	S_{abs}	S_{em}	$\hbar\Omega_g$	$\hbar\Omega_e$	S_{abs}	S_{em}
SrB ₄ O ₇ :Eu	28.1	28.8	3.78	3.69	28.0	28.8	3.78	3.69
KSrPO ₄ :Eu	8.8	<u>8.9</u>	<u>34.96</u>	34.50	8.8	9.7	38.18	34.51
CaMgSi ₂ O ₆ :Eu	36.2	34.4	7.20	7.59	36.3	34.4	7.20	7.57
SrAl ₂ O ₄ :Eu2	18.3	16.3	16.87	18.92	18.3	16.3	16.86	18.88
Sr ₅ (PO ₄) ₃ Cl:Eu	13.7	12.7	11.37	12.30	13.7	12.7	11.37	12.30
CaF ₂ :Eu	32.4	30.0	3.27	3.53	32.3	29.9	3.27	3.54
SrI ₂ :Eu	7.5	8.7	14.00	11.99	7.5	8.8	13.99	11.98
Sr ₂ MgSi ₂ O ₇ :Eu	23.7	20.9	12.25	13.90	23.7	20.8	12.26	13.89
SrAl ₂ O ₄ :Eu1	<u>24.2</u>	21.7	13.41	<u>14.96</u>	23.7	21.7	13.41	15.26
BaSi ₂ O ₂ N ₂ :Eu	14.8	13.2	18.76	21.00	14.8	13.2	18.77	21.00
Ba ₃ Si ₆ O ₁₂ N ₂ :Eu	24.5	22.8	10.15	10.90	24.5	22.8	10.16	10.88
CaAlSiN ₃ :Eu, M-I	10.4	10.5	<u>16.35</u>	<u>16.22</u>	10.4	10.5	16.49	16.08
CaAlSiN ₃ :Eu, M-II	13.1	14.3	11.84	10.84	13.1	14.2	11.84	10.84
Sr[Mg ₃ SiN ₄]:Eu	15.0	14.2	5.35	5.63	15.0	14.2	5.35	5.62
CaS:Eu	17.2	16.0	9.00	9.65	17.2	16.0	9.01	9.65
Sr[LiAl ₃ N ₄]:Eu1	33.4	28.9	<u>1.98</u>	<u>2.28</u>	33.4	29.0	1.71	2.63
Sr[LiAl ₃ N ₄]:Eu2	18.3	25.0	4.46	3.27	18.3	25.0	4.46	3.27
Ca[LiAl ₃ N ₄]:Eu	19.3	18.7	4.36	4.51	19.3	18.6	4.35	4.52

TABLE V. Comparison between the corrected and the published data of emission linewidth, Table IV in our paper. Large changes (> 0.01 eV) are underlined. In the corrected data column $W(298\text{ K})$, numbers in bold indicate deviation of theoretical values with respect to experimental ones by more than 30%. No consistent threshold had been used in the original publication.

Compound	Corrected data		Data from the original paper	
	$W(0\text{ K})$	$W(298\text{ K})$	$W(0\text{ K})$	$W(298\text{ K})$
SrB ₄ O ₇ :Eu	0.125	<u>0.176</u>	0.125	0.201
KSrPO ₄ :Eu	0.120	<u>0.291</u>	0.115	0.266
CaMgSi ₂ O ₆ :Eu	0.241	0.315	0.241	0.315
SrAl ₂ O ₄ -Eu2	0.198	0.358	0.198	0.358
Sr ₅ (PO ₄) ₃ Cl:Eu	0.118	0.239	0.118	0.240
CaF ₂ :Eu	0.149	0.205	0.149	0.206
SrI ₂ :Eu	0.057	0.138	0.057	0.139
Sr ₂ MgSi ₂ O ₇ :Eu	0.222	<u>0.357</u>	0.221	0.310
SrAl ₂ O ₄ :Eu1	0.233	0.368	0.233	0.369
BaSi ₂ O ₂ N ₂ :Eu	0.169	0.336	0.169	0.337
Ba ₃ Si ₆ O ₁₂ N ₂ :Eu	0.197	0.305	0.197	0.305
CaAlSiN ₃ :Eu, M-I	0.098	0.219	0.097	0.216
CaAlSiN ₃ :Eu, M-II	0.097	0.186	0.097	0.187
Sr[Mg ₃ SiN ₄]	0.086	0.165	0.081	0.156
CaS:Eu	0.130	0.237	0.130	0.237
Sr[LiAl ₃ N ₄]:Eu1	<u>0.128</u>	<u>0.179</u>	0.158	0.221
Sr[LiAl ₃ N ₄]:Eu2	0.067	0.099	0.067	0.099
Ca[LiAl ₃ N ₄]:Eu	0.098	0.166	0.099	0.168

TABLE VI. Comparison between the corrected and the published data for the statistical analysis of the data, Table II from the original paper. Large changes (affecting more than the last digit) are underlined.

	Corrected data				Data from the original paper			
	Absorption	Emission	Stokes shift	FWHM	Absorption	Emission	Stokes shift	FWHM
ME	0.110	<u>0.024</u>	<u>683</u>	0.023	0.111	0.058	651	0.023
MAE	0.143	<u>0.121</u>	<u>1146</u>	0.053	0.144	0.159	1118	0.052
MRE (%)	<u>3.79</u>	<u>1.00</u>	<u>40.77</u>	16.1	3.83	2.27	40.06	16.7
MARE (%)	<u>4.88</u>	<u>4.87</u>	<u>55.56</u>	<u>29.42</u>	5.03	6.36	54.85	30.03
Slope	1.123	1.037	<u>0.759</u>	<u>0.673</u>	1.127	1.040	0.723	0.584
Intercept	-0.223	-0.066	<u>1229</u>	<u>0.091</u>	-0.233	-0.069	1279	0.111
R^2 (%)	95.0	88.3	<u>27.7</u>	<u>25.7</u>	95.0	88.6	26.1	21.9

FIG. 1. Comparison between experimental results and first-principles calculations: (a) absorption energy, (b) emission energy, and (c) Stokes shift. The solid black line is the least-squares fit of the data. This figure supersedes Fig. 1 of the original paper.

FIG. 2. Comparison between the full width at half maximum (FWHM) computed by first-principles calculations and experimental values at room temperature. The solid black line is the least-squares fit of the data. This figure supersedes Fig. 2 of the original paper.