Supplementary E-File

Analysis of crystal-field effect on luminescence spectra of Mn^{4+} ($3d^3$) ion doped double perovskite La$_2$ZnTiO$_6$ phosphor by semiempirical computations: exchange charge model and superposition model

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Table S1 Structural parameters of pure La$_2$ZnTiO$_6$ and doped La$_2$ZnTiO$_6$:Mn^{4+} compounds.

System Ref.	La$_2$ZnTiO$_6$ [33]	La$_2$ZnTiO$_6$ [34]	La$_2$ZnTiO$_6$:Mn^{4+} [14]
a (Å)	7.89497	7.8975	7.89042
b (Å)	5.5964	5.6172	5.60145
c (Å)	5.58089	5.578	5.57979
β (°)	90.034	89.973	90.063
V (Å^3)	246.584	247.451	246.614

Table S2 Atomic coordinates, metal-ligand bond distances (Å) and bond angles (°) of pure La_2ZnTiO_6.

System Ref.	La_2ZnTiO_6 [33]	La_2ZnTiO_6 [34]
La (site 4*e*: C_1)		
x	0.25	0.2499
y	0.033	0.0361
z	0.9933	0.0076
Zn (2*c* : C_i)		
x	0	0
y	0.5	0.5
z	0	0
Ti (2*b* : C_i)		
x	0	0
y	0	0
z	0.5	0.5
O1 (site 4*e*: C_1)		
x	0.9605	0.043
y	0.2059	0.2832
z	0.2234	0.2995
O2 (site 4*e*: C_1)		
x	0.9593	0.0394
y	0.7211	0.7952
z	0.2971	0.223
O3 (site 4*e*: C_1)		
x	0.2415	0.2448
y	0.9837	0.9814
z	0.4244	0.5794
Bond lengths		
Ti−O(1)	1.9513	1.9512

Ti –O(2)	1.9548	1.9739
Ti –O(3)	1.9576	1.9863
O(3) –Ti–O(2)	90.3193	90.087
O(3) –Ti–O(2)	89.6807	89.9131
O(3) –Ti–O(1)	89.5574	90.5338
O(3) –Ti–O(1)	90.4426	89.4662
O(2) –Ti–O(1)	89.2616	90.0482
O(2) –Ti–O(1)	90.7384	89.9519
Zn–O(1)	2.0883	2.095
Zn –O(2)	2.0938	2.096
Zn –O(3)	2.088	2.066
La-O	2.4116	2.4087
	2.4403	2.4191
	2.4517	2.4568
	2.5662	2.5484
	2.6772	2.6734
	2.6919	2.6916
	2.782	2.7885
	2.795	2.781

Table S3 Comparative listing of the SPM intrinsic parameters, $\overline{B}_k$, and the respective exchange contributions (defined in text), calculated using the structural data [33,34] (all values are in cm^{-1}).

SPM	[33]	[34]
$\overline{B}_2$	20250	29550
$\overline{B}_2^S$	10805	21350
$\overline{B}_4$	13468	13394
$\overline{B}_4^S$	11870	11858
$\overline{B}_2 / \overline{B}_4$	1.5	2.21
$\overline{B}_2^S / \overline{B}_4^S$	0.91	1.8