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Supporting Information

Defect clustering in an Eu-doped $NaMgF_3$ compound and its influence on luminescent properties

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(A) Cubic $NaMgF_3$

Table S1- Lattice parameters and interatomic distance for cubic $NaMgF_3$.

Lattice parameters	Ref. 1	This work	%
a(A)	3.876	3.885	0.22
V(A^3)	58.2306	58.6139	0.66
Interatomic distance	Ref.1	This work	%
Na-F (x12)	2.741	2.747	0.22
Mg-F (x6)	1.938	1.942	0.20
F-F (x8)	2.741	2.747	0.22

Table S2- Elastic constants for cubic $NaMgF_3$.

Elastic Constants	Ref. 2	This work
C_{11}	136.9082	151.4231
C_{12}	31.8473	41.7655
C_{44}	51.0104	41.7655

(B) Fluoride precursors (NaF and MgF_2)

Table S3- Lattice parameters for NaF.

Lattice parameters	Ref. 3	This work	%
a (A)	4.65	4.6599	0.2129
V (A^3)	100.5450	101.1895	0.6410

Table S4- Elastic constants for NaF.

Elastic constants	Ref. 4	This work	%
C_{11}	108.5	98.7431	-8.99
C_{12}	22.90	28.3125	23.64
C_{44}	28.99	28.325	-2.34

Table S5- Dielectric constants for NaF

Dielectric constants	Ref. 4	This work	%
e_0	4.73	4.83	2.1
e_∞	1.75	1.91	9.1

Table S6- Lattice parameters for MgF_2.

Lattice parameters	Ref. 5	This work	%
a(A)	4.6213	4.5447	-1.66
b(A)	3.0519	3.1540	3.35
V(A^3)	65.1776	65.1456	-0.05

Table S7- Elastic constants for MgF_2.

Elastic Constants	Ref. 6	Ref. 7	This work
C_{11}	140.80	142.70	120.89
C_{12}	90.00	92.20	94.50
C_{13}	63.50	64.10	68.90
C_{33}	205.30	204.00	213.66
C_{44}	56.70	56.70	52.02
C_{66}	95.70	93.50	95.14

(C) Defect calculations

Table S8- Lattice energy for orthorhombic $NaMgF_3$, fluorides precursors and dopants.

Materials	Lattice energies (eV)
$NaMgF_3$	-39.784
NaF	-9.573
MgF_2	-29.998
EuF_3	-51.717
EuF_2	-25.430

Table S9-Defect formation energy for selected defects.

Defect Energy (eV)				
$V_{Na}^{'}$	$V_{Mg}^{''}$	$V_{F}^{'}$	$Na_{Mg}^{'}$	$Mg_{Na}^{\bullet}$
6.209	24.445	5.821	17.264	-15.016

Interstitial Position	Na_i	Mg_i	F_i
(1/2,1/4,1/4)	-2.848	-16.860	-2.171
(1/2,1/8,1/4)	-2.847	-16.865	-2.472
(1/2,1/2,1/4)	-2.848	-16.851	-2.433
(1/4,1/4,1/4)	-2.848	-16.854	-2.228

Table S10- Defect formation energy of Eu^{3+} and Eu^{2+} isolated ions doped orthorhombic $NaMgF_3$.

Impurity (Eu^{3+})	Energy defects (eV)
$Eu_{Na}^{\bullet\bullet}$	-31.047
$Eu_{Mg}^{\bullet}$	-15.276
Impurity (Eu^{2+})	**Energy defects (eV)**
$Eu_{Na}^{\bullet}$	-10.460
$Eu_{Mg}^{\times}$	6.564

Table S11- Solution energies of Eu^{3+} doped $NaMgF_3$.

Schemes	Solution Energies (bound defects) (in eV)
Incorporating into Na site	
$Eu_{Na}^{\bullet\bullet} + 2F_i^{'}$	3.256
$Eu_{Na}^{\bullet\bullet} + V_{Mg}^{''}$	2.758
$Eu_{Na}^{\bullet\bullet} + 2V_{Na}^{'}$	2.914
$Eu_{Na}^{\bullet\bullet} + 2Na_{Mg}^{'}$	2.580
$2Eu_{Na}^{\bullet\bullet} + V_{Mg}^{''} + 2F_i^{'}$	6.105
Incorporating into Mg site	
$Eu_{Mg}^{\bullet} + F_i^{'}$	2.449
$Eu_{Mg}^{\bullet} + V_{Na}^{'}$	2.129
$2Eu_{Mg}^{\bullet} + V_{Mg}^{''}$	5.641
$Eu_{Mg}^{\bullet} + Na_{Mg}^{'}$	2.843
$2Eu_{Mg}^{\bullet} + Mg_{Na}^{\bullet} + 3F_i^{'}$	5.173
Incorporating into Na and Mg sites	
$Eu_{Mg}^{\bullet} + Eu_{Na}^{\bullet\bullet} + 2V_{Na}^{'} + F_i^{'}$	5.310
$Eu_{Mg}^{\bullet} + Eu_{Na}^{\bullet\bullet} + V_{Mg}^{''} + Na_{Mg}^{'}$	7.247

Table S12- Solution energies of Eu^{2+} doped $NaMgF_3$.

Schemes	Solution Energy (bound defects) (in eV)
Incorporating into Na site	
$Eu_{Na}^{\bullet} + F_i^{'}$	2.623
$2Eu_{Na}^{\bullet} + V_{Mg}^{''}$	2.952
$Eu_{Na}^{\bullet} + V_{Na}^{'}$	1.572
$2Eu_{Na}^{\bullet} + V_{Na}^{'} + F_i^{'}$	3.729
$Eu_{Na}^{\bullet} + V_F^{'} + 2F_i^{'}$	2.438
$Eu_{Na}^{\bullet} + Na_{Mg}^{'}$	1.523
$Eu_{Na}^{\bullet} + V_{Mg}^{''} + V_F^{'}$	3.224
$Eu_{Na}^{\bullet} + 2V_{Na}^{'} + V_F^{'}$	3.589
Incorporating into Na site	
$Eu_{Mg}^{\times}$	1.996

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