Electronic Supplementary Material (ESI) for Dalton Transactions.

Unlocking the effect of Li and Ce ions on the Thermoluminescence and Optically Stimulated Luminescence signals of the MgB_4O_7 compound

João V. B. Batista,[a] Henrique Trombini,[a] André Otsuka,[b] Iury S. Silveira,[c] Linda V. E. Caldas,[c] Antonio O. de Souza,[d] Adelmo S. Souza,[d] Jorge L. O. Santos,[d] Vinicius Coelho[d] and Heveson Lima[e*]

[a]Departamento de Ciências Exatas e Sociais Aplicadas, Universidade Federal de Ciências da Saúde de Porto Alegre, 90050-170, Porto Alegre, RS, Brazil

[b]Departamento de Física, Universidade Federal de Sergipe, 49100-000, São Cristóvão, SE, Brazil

[c]Instituto de Pesquisas Energéticas e Nucleares, Comissão Nacional de Energia Nuclear, 05508-000, São Paulo, SP, Brazil

[d]Centro Multidisciplinar de Bom Jesus da Lapa, Universidade Federal do Oeste da Bahia, 47600-000, Bom Jesus da Lapa, BA, Brazil

[e]Centro Multidisciplinar de Luís Eduardo Magalhães, Universidade Federal do Oeste da Bahia, 47850-000, Luís Eduardo Magalhães, BA, Brazil

(A) Defect calculations

Table S1 – Lattice energy for orthorhombic MgB_4O_7 and oxide precursors.

Materials	Lattice energies (eV)
MgB_4O_7	-466.399
MgO	-38.785
B_2O_3	-209.248
Ce_2O_3	-128.752
Li_2O	-30.512

Table S2 – Intrinsic defect formation energy for isolated defects.

Defect Energy (eV)				
V_B'''	V_{Mg}''	$V_O^{\bullet\bullet}$	Mg_B'	$B_{Mg}^{\bullet}$
82.455	24.051	31.586	52.730	-35.965

Interstitial Position	**B_i**	**Mg_i**	**O_i**
(4/5,3/5,9/10)	-60.716	-15.641	-
(3/10,3/10,1/10)	-	-15.641	-
(4/5,3/10,1/3)	-	-14.804	-23.314
(1/5,7/10,3/5)	-49.031	-15.641	-10.434

Table S3 – Extrinsic defect formation energy for isolated defects.

Defect Energy (eV)		
$\boldsymbol{Ce_{Mg}^{\bullet}}$	Ce_B^x	Li_{Mg}'
-10.513	42.857	14.950

Interstitial Position	**Ce_i**
(1/3,1/3,1/10)	-23.498
(1/10,6/7,1/3)	-23.501
(2/7,2/7,4/7)	-21.753
(2/3,8/10,4/10)	-23.539

There wasn't convergence for Li inserting at B site.