Supplemental Material for "A DFT+U Study of Defect Association and Oxygen Migration in Samarium-Doped Ceria"

Table S1. Relative energies and relevant structural information of 6.6 % SDC structures recovered from DFT+U GA

Structure[a]	ΔE_{DFT+U} *(eV/cell)*[b,c]	*Vac-vac distance*[d] *(Å)*	*Sm-vac1 distance*[e]	*Sm-vac2 distance*[e]
U1/D1[f]	0.000	6.0	3 NNN, 1 NN	3 NNN, 1 NN
U2*	0.000	6.0	1 NNNN, 1 NNN, 2 NN	1 NNNN, 1 NNN, 2 NN
U3	0.027	6.0	1 NNNN, 1 NNN, 2 NN	3 NNN, 1 NN
U4*	0.039	6.0	2 NNN, 2 NN	1 NNNN, 2 NNN, 1 NN
U5	0.043	6.0	3 NNN, 1 NN	2 NNN, 2 NN
U6*	0.046	6.0	1 NNNN, 3 NN	1 NNNN, 2 NNN, 1 NN
U7*	0.056	6.0	1 NNNN, 3 NN	2 NNNN, 1 NNN, 1 NN
U8*	0.058	6.0	1 NNNN, 2 NNN, 1 NN	1 NNNN, 1 NNN, 2 NN
U9*	0.062	6.0	3 NNN, 1 NN	1 NNNN, 1 NNN, 2 NN
U10	0.066	6.0	3 NNN, 1 NN	3 NNN, 1 NN

[a]Structures with asterisks were newly found with DFT+U GA that were not a member of initial population. [b]Energy relative to the lowest-energy structure, which is assigned a value of zero. [c]Relative total electronic energies from DFT+U calculations. [d]The vac-vac distance reported is taken from the ideal lattice before geometry relaxation. [e]The column shows the number of Sm with that particular distance followed by a letter code for the distance value (NN is on average 2.4 Å, NNN is 4.5 Å, and NNNN is 5.9 Å). [f]Structure **U1** is identical to structure **D1** located from the DFT GA reported in Table 4.

Poscar file of structure U1 before relaxation.

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Sm Ce O
1.000000
10.8 0 0
0 10.8 0
0 0 10.8
4 28 62
Direct
0.0 0.25 0.25
0.5 0.25 0.75
0.5 0.5 0.5
0.0 0.5 0.5
0.0 0.0 0.0
0.25 0.25 0.0
0.25 0.0 0.25
0.0 0.25 0.75
0.75 0.75 0.0
0.25 0.5 0.25
0.25 0.0 0.75
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0.5 0.0 0.0
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Poscar file of structure U2 before relaxation.

Sm Ce O
1.000000
10.8 0 0
0 10.8 0
0 0 10.8
4 28 62
Direct
0.0 0.25 0.25
0.5 0.25 0.75
0.5 0.5 0.5
0.0 0.5 0.5
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