Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary material: Oxygen diffusion in ceria doped with rare-earth elements

In this supplementary we provide the simulation cell, the possible oxygen ion transitions in the simulation cell and the corresponding barriers in a format so that the interested reader can set up and run their own KMC simulations for ceria doped with Pr, Nd, Pm, Sm, Eu, and Gd, in four different distributions. The doped CeO_2 simulation cell and the dopant distributions are given in Sec. S1, and the coordinates of the oxygen sites in the simulation cell are given in Sec. S2. In Sec. S3 are the barriers for the symmetrically unique transitions in the model system (see Fig. S1) for all the dopant elements tabulated for the different distribution (Tables S2, S3, S4, and S5). Notice that there are 384 possible transitions in the system in total, but many are symmetrically identical, i.e., although they are between different sites in the system, they are identical, and correspond to the same diffusion barrier. In the barrier tables in Sec. S3 are all the symmetrically identical transitions grouped together. The barriers were calculated with DFT at 0 K using the PBE functional and a lattice constant of $a = 5.47$ Å (see paper for more details). The supplementary also contains plots of calculated diffusion constant versus temperature for the different dopants grouped by dopant distribution (Sec. S4), and a table of the difference between the forward and backward barriers averaged over the studied system (Sec. S5).

S1. STRUCTURE

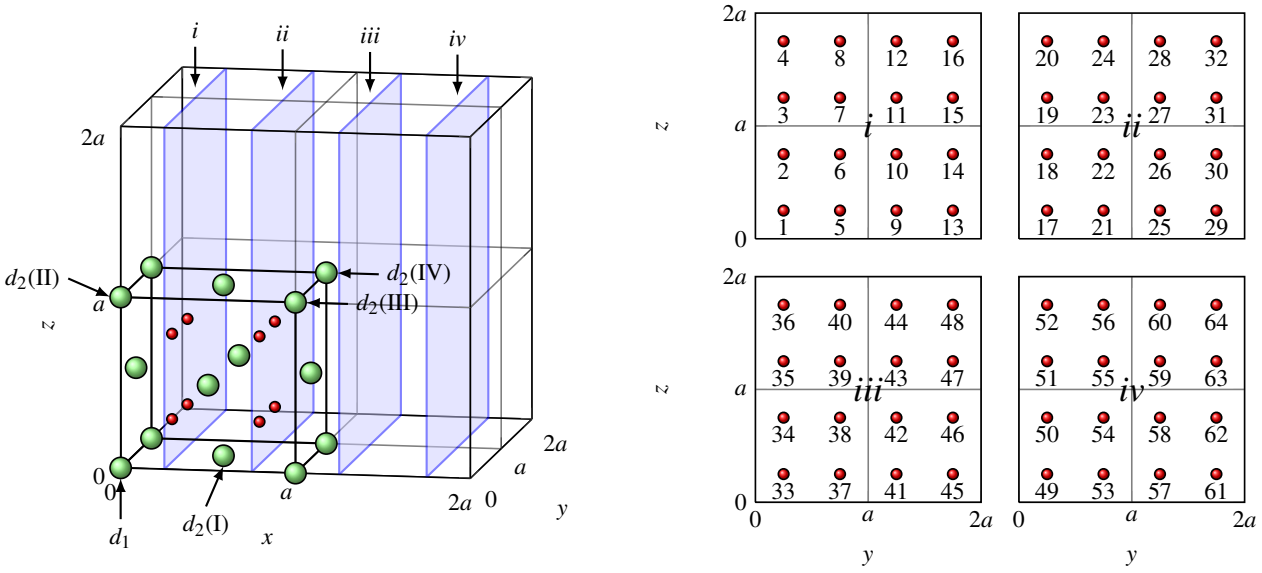

FIG. S1. (LEFT: The $2 \times 2 \times 2$ (96 sites) cerium oxide supercell structure is shown in thin lines and the cerium oxide unit cell in thick lines. Large green circles are Ce atoms and red small circles are O atoms. From the supercell one O atom is removed to create a vacancy, and two Ce atoms are replaced by dopant atoms (d_1, d_2) at positions: d_1=(0, 0, 0), and $d_2 \in \{(a/2, a/2, 0), (0, 0, a), (a, 0, a), (a, a, a)\}$, marked by small arrows in the figure. Roman numerals I–IV mark the different dopant distributions. a is the lattice constant. The four layers of oxygen atoms in the YZ-plane are shown in blue and marked *i*–*iv*. RIGHT: The four layers (*i*–*iv*) of the supercell with oxygen site indices 1–64. Upper right plane is layer *i*, the upper left is layer *ii*, lower left is layer *iii*, and the lower right is layer *iv*.

S2. OXYGEN SITE COORDINATES AND COORDINATION

TABLE S1: Oxygen ideal site fractional coordinates (x, y, z) in the simulation cell numbered 1–64 (Site idx), and the corresponding dopant coordination (n_1, n_2) of the oxygen site, for the different dopant distributions (I–IV) in Fig. S1.

	Coordinate			Coordination per distr.			
Site idx	x	y	z	I	II	III	IV
1	0.125	0.125	0.125	(1, 1)	(1, 2)	(1, 3)	(1, 4)
2	0.125	0.125	0.375	(2, 2)	(1, 2)	(2, 2)	(2, 3)
3	0.125	0.125	0.625	(2, 2)	(1, 2)	(2, 2)	(2, 3)
4	0.125	0.125	0.875	(1, 1)	(1, 2)	(1, 3)	(1, 4)
5	0.125	0.375	0.125	(1, 2)	(2, 3)	(2, 4)	(2, 3)
6	0.125	0.375	0.375	(2, 3)	(2, 3)	(3, 3)	(2, 3)
7	0.125	0.375	0.625	(2, 3)	(2, 3)	(3, 3)	(2, 3)
8	0.125	0.375	0.875	(1, 2)	(2, 3)	(2, 4)	(2, 3)
9	0.125	0.625	0.125	(2, 2)	(2, 3)	(2, 4)	(2, 3)
10	0.125	0.625	0.375	(3, 3)	(2, 3)	(3, 3)	(2, 3)
11	0.125	0.625	0.625	(3, 3)	(2, 3)	(3, 3)	(2, 3)
12	0.125	0.625	0.875	(2, 2)	(2, 3)	(2, 4)	(2, 3)
13	0.125	0.875	0.125	(1, 2)	(1, 2)	(1, 3)	(1, 4)
14	0.125	0.875	0.375	(2, 3)	(1, 2)	(2, 2)	(2, 3)
15	0.125	0.875	0.625	(2, 3)	(1, 2)	(2, 2)	(2, 3)
16	0.125	0.875	0.875	(1, 2)	(1, 2)	(1, 3)	(1, 4)
17	0.375	0.125	0.125	(1, 2)	(2, 3)	(2, 2)	(2, 3)
18	0.375	0.125	0.375	(2, 3)	(2, 3)	(1, 3)	(2, 3)
19	0.375	0.125	0.625	(2, 3)	(2, 3)	(1, 3)	(2, 3)
20	0.375	0.125	0.875	(1, 2)	(2, 3)	(2, 2)	(2, 3)
21	0.375	0.375	0.125	(1, 3)	(3, 4)	(3, 3)	(2, 3)
22	0.375	0.375	0.375	(2, 4)	(3, 4)	(2, 4)	(1, 4)
23	0.375	0.375	0.625	(2, 4)	(3, 4)	(2, 4)	(1, 4)
24	0.375	0.375	0.875	(1, 3)	(3, 4)	(3, 3)	(2, 3)
25	0.375	0.625	0.125	(2, 3)	(3, 4)	(3, 3)	(2, 3)
26	0.375	0.625	0.375	(3, 4)	(3, 4)	(2, 4)	(1, 4)
27	0.375	0.625	0.625	(3, 4)	(3, 4)	(2, 4)	(1, 4)
28	0.375	0.625	0.875	(2, 3)	(3, 4)	(3, 3)	(2, 3)
29	0.375	0.875	0.125	(2, 2)	(2, 3)	(2, 2)	(2, 3)
30	0.375	0.875	0.375	(3, 3)	(2, 3)	(1, 3)	(2, 3)
31	0.375	0.875	0.625	(3, 3)	(2, 3)	(1, 3)	(2, 3)
32	0.375	0.875	0.875	(2, 2)	(2, 3)	(2, 2)	(2, 3)
33	0.625	0.125	0.125	(2, 2)	(2, 3)	(2, 2)	(2, 3)
34	0.625	0.125	0.375	(3, 3)	(2, 3)	(1, 3)	(2, 3)
35	0.625	0.125	0.625	(3, 3)	(2, 3)	(1, 3)	(2, 3)
36	0.625	0.125	0.875	(2, 2)	(2, 3)	(2, 2)	(2, 3)
37	0.625	0.375	0.125	(2, 3)	(3, 4)	(3, 3)	(2, 3)
38	0.625	0.375	0.375	(3, 4)	(3, 4)	(2, 4)	(1, 4)
39	0.625	0.375	0.625	(3, 4)	(3, 4)	(2, 4)	(1, 4)
40	0.625	0.375	0.875	(2, 3)	(3, 4)	(3, 3)	(2, 3)
41	0.625	0.625	0.125	(3, 3)	(3, 4)	(3, 3)	(2, 3)
42	0.625	0.625	0.375	(4, 4)	(3, 4)	(2, 4)	(1, 4)
43	0.625	0.625	0.625	(4, 4)	(3, 4)	(2, 4)	(1, 4)
44	0.625	0.625	0.875	(3, 3)	(3, 4)	(3, 3)	(2, 3)
45	0.625	0.875	0.125	(2, 3)	(2, 3)	(2, 2)	(2, 3)
46	0.625	0.875	0.375	(3, 4)	(2, 3)	(1, 3)	(2, 3)
47	0.625	0.875	0.625	(3, 4)	(2, 3)	(1, 3)	(2, 3)
48	0.625	0.875	0.875	(2, 3)	(2, 3)	(2, 2)	(2, 3)
49	0.875	0.125	0.125	(1, 2)	(1, 2)	(1, 3)	(1, 4)
50	0.875	0.125	0.375	(2, 3)	(1, 2)	(2, 2)	(2, 3)
51	0.875	0.125	0.625	(2, 3)	(1, 2)	(2, 2)	(2, 3)
52	0.875	0.125	0.875	(1, 2)	(1, 2)	(1, 3)	(1, 4)
53	0.875	0.375	0.125	(2, 2)	(2, 3)	(2, 4)	(2, 3)
54	0.875	0.375	0.375	(3, 3)	(2, 3)	(3, 3)	(2, 3)

55	0.875	0.375	0.625	(3, 3)	(2, 3)	(3, 3)	(2, 3)
56	0.875	0.375	0.875	(2, 2)	(2, 3)	(2, 4)	(2, 3)
57	0.875	0.625	0.125	(2, 3)	(2, 3)	(2, 4)	(2, 3)
58	0.875	0.625	0.375	(3, 4)	(2, 3)	(3, 3)	(2, 3)
59	0.875	0.625	0.625	(3, 4)	(2, 3)	(3, 3)	(2, 3)
60	0.875	0.625	0.875	(2, 3)	(2, 3)	(2, 4)	(2, 3)
61	0.875	0.875	0.125	(1, 3)	(1, 2)	(1, 3)	(1, 4)
62	0.875	0.875	0.375	(2, 4)	(1, 2)	(2, 2)	(2, 3)
63	0.875	0.875	0.625	(2, 4)	(1, 2)	(2, 2)	(2, 3)
64	0.875	0.875	0.875	(1, 3)	(1, 2)	(1, 3)	(1, 4)

S3. BARRIERS

TABLE S2: Oxygen vacancy diffusion barriers for dopants in distribution I (see Fig. S1). Transitions are between oxygen sites with indices defined in Table. S1. The first barrier value is the forward barrier in direction of the arrow in the "Transition" column ($a \rightarrow b$), and the second value is the reverse barrier ($a \leftarrow b$).

No.	Transition of O vacancy	Barriers [eV]					
		Pr	Nd	Pm	Sm	Eu	Gd
1	1→2, 4→3	0.28, 0.45	0.33, 0.43	0.38, 0.40	0.42, 0.38	0.46, 0.35	0.50, 0.32
2	1→4, 4→1	1.33, 1.33	1.21, 1.21	1.10, 1.10	1.03, 1.03	0.95, 0.95	0.88, 0.88
3	1→5, 1→13, 1→17, 1→49, 4→8, 4→16, 4→20, 4→52	0.59, 0.66	0.59, 0.62	0.58, 0.58	0.57, 0.55	0.56, 0.50	0.55, 0.46
4	2→3, 3→2	0.34, 0.34	0.36, 0.36	0.37, 0.37	0.38, 0.38	0.40, 0.40	0.41, 0.41
5	2→1, 3→4	0.45, 0.28	0.43, 0.33	0.40, 0.38	0.38, 0.42	0.35, 0.46	0.32, 0.50
6	2→6, 2→14, 2→18, 2→50, 3→7, 3→15, 3→19, 3→51	0.56, 0.40	0.54, 0.41	0.52, 0.42	0.50, 0.43	0.49, 0.43	0.48, 0.44
7	5→6, 8→7, 13→14, 16→15, 17→18, 20→19, 49→50, 52→51	0.44, 0.40	0.46, 0.40	0.47, 0.39	0.48, 0.39	0.49, 0.38	0.50, 0.37
8	5→8, 8→5, 13→16, 16→13, 17→20, 20→17, 49→52, 52→49	0.73, 0.73	0.68, 0.68	0.63, 0.63	0.60, 0.60	0.57, 0.57	0.54, 0.54
9	5→9, 8→12, 13→9, 16→12, 17→33, 20→36, 49→33, 52→36	0.31, 0.39	0.35, 0.39	0.38, 0.39	0.41, 0.38	0.44, 0.37	0.46, 0.36
10	5→1, 8→4, 13→1, 16→4, 17→1, 20→4, 49→1, 52→4	0.66, 0.59	0.62, 0.59	0.58, 0.58	0.55, 0.57	0.50, 0.56	0.46, 0.55
11	5→21, 8→24, 13→61, 16→64, 17→21, 20→24, 49→61, 52→64	0.78, 0.67	0.73, 0.64	0.67, 0.60	0.63, 0.57	0.59, 0.55	0.56, 0.53
12	5→53, 8→56, 13→29, 16→32, 17→29, 20→32, 49→53, 52→56	0.36, 0.44	0.39, 0.43	0.42, 0.42	0.44, 0.41	0.47, 0.40	0.49, 0.38
13	6→7, 7→6, 14→15, 15→14, 18→19, 19→18, 50→51, 51→50	0.40, 0.40	0.40, 0.40	0.41, 0.41	0.41, 0.41	0.41, 0.41	0.41, 0.41
14	6→5, 7→8, 14→13, 15→16, 18→17, 19→20, 50→49, 51→52	0.40, 0.44	0.40, 0.46	0.39, 0.47	0.39, 0.48	0.38, 0.49	0.37, 0.50
15	6→10, 7→11, 14→10, 15→11, 18→34, 19→35, 50→34, 51→35	0.52, 0.40	0.50, 0.41	0.48, 0.41	0.47, 0.41	0.46, 0.42	0.45, 0.42
16	6→2, 7→3, 14→2, 15→3, 18→2, 19→3, 50→2, 51→3	0.40, 0.56	0.41, 0.54	0.42, 0.52	0.43, 0.50	0.43, 0.49	0.44, 0.48
17	6→22, 7→23, 14→62, 15→63, 18→22, 19→23, 50→62, 51→63	0.45, 0.45	0.45, 0.45	0.45, 0.44	0.45, 0.44	0.45, 0.43	0.45, 0.43
18	6→54, 7→55, 14→30, 15→31, 18→30, 19→31, 50→54, 51→55	0.54, 0.42	0.52, 0.42	0.50, 0.43	0.48, 0.43	0.47, 0.43	0.46, 0.44
19	9→10, 12→11, 33→34, 36→35	0.61, 0.37	0.58, 0.38	0.55, 0.40	0.53, 0.41	0.50, 0.42	0.49, 0.43
20	9→12, 12→9, 33→36, 36→33	0.46, 0.46	0.46, 0.46	0.46, 0.46	0.46, 0.46	0.46, 0.46	0.46, 0.46
21	9→13, 9→5, 12→16, 12→8, 33→49, 33→17, 36→52, 36→20	0.39, 0.31	0.39, 0.35	0.39, 0.38	0.38, 0.41	0.37, 0.44	0.36, 0.46
22	9→25, 9→57, 12→28, 12→60, 33→37, 33→45, 36→40, 36→48	0.53, 0.41	0.52, 0.42	0.50, 0.42	0.49, 0.43	0.48, 0.44	0.47, 0.44
23	10→11, 11→10, 34→35, 35→34	0.44, 0.44	0.44, 0.44	0.43, 0.43	0.42, 0.42	0.42, 0.42	0.41, 0.41
24	10→9, 11→12, 34→33, 35→36	0.37, 0.61	0.38, 0.58	0.40, 0.55	0.41, 0.53	0.42, 0.50	0.43, 0.49
25	10→14, 10→6, 11→15, 11→7, 34→50, 34→18, 35→51, 35→19	0.40, 0.52	0.41, 0.50	0.41, 0.48	0.41, 0.47	0.42, 0.46	0.42, 0.45
26	10→26, 10→58, 11→27, 11→59, 34→38, 34→46, 35→39, 35→47	0.45, 0.46	0.44, 0.45	0.44, 0.44	0.44, 0.43	0.44, 0.43	0.44, 0.42
27	21→22, 24→23, 61→62, 64→63	0.35, 0.42	0.38, 0.41	0.41, 0.40	0.43, 0.39	0.45, 0.37	0.47, 0.35
28	21→24, 24→21, 61→64, 64→61	0.71, 0.71	0.67, 0.67	0.62, 0.62	0.59, 0.59	0.56, 0.56	0.53, 0.53
29	21→25, 21→37, 24→28, 24→40, 61→57, 61→45, 64→60, 64→48	0.35, 0.42	0.38, 0.41	0.41, 0.40	0.42, 0.39	0.44, 0.38	0.46, 0.36
30	21→17, 21→5, 24→20, 24→8, 61→49, 61→13, 64→52, 64→16	0.67, 0.78	0.64, 0.73	0.60, 0.67	0.57, 0.63	0.55, 0.59	0.53, 0.56
31	22→23, 23→22, 62→63, 63→62	0.39, 0.39	0.40, 0.40	0.41, 0.41	0.41, 0.41	0.42, 0.42	0.42, 0.42
32	22→21, 23→24, 62→61, 63→64	0.42, 0.35	0.41, 0.38	0.40, 0.41	0.39, 0.43	0.37, 0.45	0.35, 0.47
33	22→26, 22→38, 23→27, 23→39, 62→58, 62→46, 63→59, 63→47	0.51, 0.39	0.50, 0.40	0.48, 0.41	0.48, 0.42	0.46, 0.42	0.46, 0.43
34	22→18, 22→6, 23→19, 23→7, 62→50, 62→14, 63→51, 63→15	0.45, 0.45	0.45, 0.45	0.44, 0.45	0.44, 0.45	0.43, 0.45	0.43, 0.45
35	25→26, 28→27, 37→38, 40→39, 45→46, 48→47, 57→58, 60→59	0.52, 0.40	0.50, 0.41	0.49, 0.41	0.48, 0.41	0.47, 0.42	0.46, 0.42
36	25→28, 28→25, 37→40, 40→37, 45→48, 48→45, 57→60, 60→57	0.46, 0.46	0.46, 0.46	0.46, 0.46	0.45, 0.45	0.45, 0.45	0.45, 0.45
37	25→29, 28→32, 37→53, 40→56, 45→29, 48→32, 57→53, 60→56	0.36, 0.47	0.37, 0.47	0.39, 0.46	0.40, 0.46	0.41, 0.45	0.42, 0.45

38	25→21, 28→24, 37→21, 40→24, 45→61, 48→64, 57→61, 60→64	0.42, 0.35	0.41, 0.38	0.40, 0.41	0.39, 0.42	0.38, 0.44	0.36, 0.46
39	25→41, 28→44, 37→41, 40→44, 45→41, 48→44, 57→41, 60→44	0.53, 0.40	0.51, 0.41	0.49, 0.41	0.48, 0.41	0.46, 0.42	0.45, 0.42
40	25→9, 28→12, 37→33, 40→36, 45→33, 48→36, 57→9, 60→12	0.41, 0.53	0.42, 0.52	0.42, 0.50	0.43, 0.49	0.44, 0.48	0.44, 0.47
41	26→27, 27→26, 38→39, 39→38, 46→47, 47→46, 58→59, 59→58	0.43, 0.43	0.43, 0.43	0.43, 0.43	0.43, 0.43	0.42, 0.42	0.42, 0.42
42	26→25, 27→28, 38→37, 39→40, 46→45, 47→48, 58→57, 59→60	0.40, 0.52	0.41, 0.50	0.41, 0.49	0.41, 0.48	0.42, 0.47	0.42, 0.46
43	26→30, 27→31, 38→54, 39→55, 46→30, 47→31, 58→54, 59→55	0.44, 0.43	0.43, 0.43	0.42, 0.43	0.42, 0.43	0.41, 0.43	0.40, 0.42
44	26→22, 27→23, 38→22, 39→23, 46→62, 47→63, 58→62, 59→63	0.39, 0.51	0.40, 0.50	0.41, 0.48	0.42, 0.48	0.42, 0.46	0.43, 0.46
45	26→42, 27→43, 38→42, 39→43, 46→42, 47→43, 58→42, 59→43	0.43, 0.44	0.44, 0.44	0.43, 0.43	0.43, 0.42	0.43, 0.42	0.43, 0.42
46	26→10, 27→11, 38→34, 39→35, 46→34, 47→35, 58→10, 59→11	0.46, 0.45	0.45, 0.44	0.44, 0.44	0.43, 0.44	0.43, 0.44	0.42, 0.44
47	29→30, 32→31, 53→54, 56→55	0.61, 0.37	0.57, 0.39	0.54, 0.40	0.52, 0.41	0.50, 0.42	0.48, 0.43
48	29→32, 32→29, 53→56, 56→53	0.46, 0.46	0.45, 0.45	0.45, 0.45	0.45, 0.45	0.45, 0.45	0.45, 0.45
49	29→17, 29→13, 32→20, 32→16, 53→49, 53→5, 56→52, 56→8	0.44, 0.36	0.43, 0.39	0.42, 0.42	0.41, 0.44	0.40, 0.47	0.38, 0.49
50	29→25, 29→45, 32→28, 32→48, 53→57, 53→37, 56→60, 56→40	0.47, 0.36	0.47, 0.37	0.46, 0.39	0.46, 0.40	0.45, 0.41	0.45, 0.42
51	30→31, 31→30, 54→55, 55→54	0.44, 0.44	0.43, 0.43	0.42, 0.42	0.42, 0.42	0.41, 0.41	0.41, 0.41
52	30→29, 31→32, 54→53, 55→56	0.37, 0.61	0.39, 0.57	0.40, 0.54	0.41, 0.52	0.42, 0.50	0.43, 0.48
53	30→18, 30→14, 31→19, 31→15, 54→50, 54→6, 55→51, 55→7	0.42, 0.54	0.42, 0.52	0.43, 0.50	0.43, 0.48	0.43, 0.47	0.44, 0.46
54	30→26, 30→46, 31→27, 31→47, 54→58, 54→38, 55→59, 55→39	0.43, 0.44	0.43, 0.43	0.43, 0.42	0.43, 0.42	0.43, 0.41	0.42, 0.40
55	41→42, 44→43	0.42, 0.45	0.43, 0.44	0.43, 0.43	0.43, 0.42	0.43, 0.41	0.43, 0.41
56	41→44, 44→41	0.47, 0.47	0.46, 0.46	0.45, 0.45	0.45, 0.45	0.44, 0.44	0.44, 0.44
57	41→45, 41→37, 41→57, 41→25, 44→48, 44→40, 44→60, 44→28	0.40, 0.53	0.41, 0.51	0.41, 0.49	0.41, 0.48	0.42, 0.46	0.42, 0.45
58	42→43, 43→42	0.42, 0.42	0.42, 0.42	0.43, 0.43	0.43, 0.43	0.43, 0.43	0.43, 0.43
59	42→41, 43→44	0.45, 0.42	0.44, 0.43	0.43, 0.43	0.42, 0.43	0.41, 0.43	0.41, 0.43
60	42→46, 42→38, 42→58, 42→26, 43→47, 43→39, 43→59, 43→27	0.51, 0.50	0.43, 0.43	0.43, 0.43	0.42, 0.43	0.42, 0.43	0.42, 0.43

TABLE S3: Oxygen vacancy diffusion barriers for dopants in distribution II (see Fig .S1). Transitions are between oxygen site with indices defined in Table. S1. The first barrier value is the forward barrier in direction of the arrow in the "Transition" column ($a \rightarrow b$), and the second value is the reverse barrier ($a \leftarrow b$).

No.	Transition of O vacancy	Barriers [eV]					
		Pr	Nd	Pm	Sm	Eu	Gd
1	1→2, 2→1, 3→4, 4→3, 13→14, 14→13, 15→16, 16→15, 49→50, 50→49, 51→52, 52→51, 61→62, 62→61, 63→64, 64→63	0.32, 0.32	0.35, 0.35	0.38, 0.38	0.39, 0.39	0.40, 0.40	0.40, 0.40
2	1→4, 2→3, 3→2, 4→1, 13→16, 14→15, 15→14, 16→13, 49→52, 50→51, 51→50, 52→49, 61→64, 62→63, 63→62, 64→61	0.65, 0.65	0.61, 0.61	0.58, 0.58	0.56, 0.56	0.54, 0.54	0.51, 0.51
3	1→5, 1→17, 2→6, 2→18, 3→7, 3→19, 4→8, 4→20, 13→9, 13→29, 14→10, 14→30, 15→11, 15→31, 16→12, 16→32, 49→53, 49→33, 50→54, 50→34, 51→55, 51→35, 52→56, 52→36, 61→57, 61→45, 62→58, 62→46, 63→59, 63→47, 64→60, 64→48	0.42, 0.37	0.44, 0.38	0.46, 0.38	0.47, 0.38	0.49, 0.38	0.49, 0.36
4	1→13, 1→49, 2→14, 2→50, 3→15, 3→51, 4→16, 4→52, 13→1, 13→61, 14→2, 14→62, 15→3, 15→63, 16→4, 16→64, 49→61, 49→1, 50→62, 50→2, 51→63, 51→3, 52→64, 52→4, 61→49, 61→13, 62→50, 62→14, 63→51, 63→15, 64→52, 64→16	0.72, 0.72	0.68, 0.68	0.63, 0.63	0.60, 0.60	0.57, 0.57	0.54, 0.54
5	5→6, 6→5, 7→8, 8→7, 9→10, 10→9, 11→12, 12→11, 17→18, 18→17, 19→20, 20→19, 29→30, 30→29, 31→32, 32→31, 33→34, 34→33, 35→36, 36→35, 45→46, 46→45, 47→48, 48→47, 53→54, 54→53, 55→56, 56→55, 57→58, 58→57, 59→60, 60→59	0.48, 0.48	0.47, 0.47	0.47, 0.47	0.46, 0.46	0.46, 0.46	0.46, 0.46
6	5→8, 6→7, 7→6, 8→5, 9→12, 10→11, 11→10, 12→9, 17→20, 18→19, 19→18, 20→17, 29→32, 30→31, 31→30, 32→29, 33→36, 34→35, 35→34, 36→33, 45→48, 46→47, 47→46, 48→45, 53→56, 54→55, 55→54, 56→53, 57→60, 58→59, 59→58, 60→57	0.46, 0.46	0.45, 0.45	0.44, 0.44	0.44, 0.44	0.44, 0.44	0.44, 0.44
7	5→9, 6→10, 7→11, 8→12, 9→5, 10→6, 11→7, 12→8, 17→33, 18→34, 19→35, 20→36, 29→45, 30→46, 31→47, 32→48, 33→17, 34→18, 35→19, 36→20, 45→29, 46→30, 47→31, 48→32, 53→57, 54→58, 55→59, 56→60, 57→53, 58→54, 59→55, 60→56	0.39, 0.39	0.40, 0.40	0.40, 0.40	0.41, 0.41	0.41, 0.41	0.41, 0.41
8	5→1, 6→2, 7→3, 8→4, 9→13, 10→14, 11→15, 12→16, 17→1, 18→2, 19→3, 20→4, 29→13, 30→14, 31→15, 32→16, 33→49, 34→50, 35→51, 36→52, 45→61, 46→62, 47→63, 48→64, 53→49, 54→50, 55→51, 56→52, 57→61, 58→62, 59→63, 60→64	0.37, 0.42	0.38, 0.44	0.38, 0.46	0.38, 0.47	0.38, 0.49	0.36, 0.49
9	5→21, 6→22, 7→23, 8→24, 9→25, 10→26, 11→27, 12→28, 17→21, 18→22, 19→23, 20→24, 29→25, 30→26, 31→27, 32→28, 33→37, 34→38, 35→39, 36→40, 45→41, 46→42, 47→43, 48→44, 53→37, 54→38, 55→39, 56→40, 57→41, 58→42, 59→43, 60→44	0.52, 0.41	0.51, 0.41	0.49, 0.41	0.48, 0.41	0.47, 0.42	0.46, 0.42
10	5→53, 6→54, 7→55, 8→56, 9→57, 10→58, 11→59, 12→60, 17→29, 18→30, 19→31, 20→32, 29→17, 30→18, 31→19, 32→20, 33→45, 34→46, 35→47, 36→48, 45→33, 46→34, 47→35, 48→36, 53→5, 54→6, 55→7, 56→8, 57→9, 58→10, 59→11, 60→12	0.47, 0.47	0.46, 0.46	0.46, 0.46	0.45, 0.45	0.45, 0.45	0.45, 0.45
11	21→22, 22→21, 23→24, 24→23, 25→26, 26→25, 27→28, 28→27, 37→38, 38→37, 39→40, 40→39, 41→42, 42→41, 43→44, 44→43	0.44, 0.44	0.43, 0.43	0.43, 0.43	0.43, 0.43	0.42, 0.42	0.42, 0.42
12	21→24, 22→23, 23→22, 24→21, 25→28, 26→27, 27→26, 28→25, 37→40, 38→39, 39→38, 40→37, 41→44, 42→43, 43→42, 44→41	0.45, 0.45	0.44, 0.44	0.44, 0.44	0.44, 0.44	0.43, 0.43	0.43, 0.43

13	21→25, 21→37, 22→26, 22→38, 23→27, 23→39, 24→28, 24→40, 25→21, 25→41, 26→22, 26→42, 27→23, 27→43, 28→24, 28→44, 37→41, 37→21, 38→42, 38→22, 39→43, 39→23, 40→44, 40→24, 41→37, 41→25, 42→38, 42→26, 43→39, 43→27, 44→40, 44→28	0.43, 0.43	0.43, 0.43	0.43, 0.43	0.42, 0.42	0.42, 0.42	0.42, 0.42
14	21→17, 21→5, 22→18, 22→6, 23→19, 23→7, 24→20, 24→8, 25→29, 25→9, 26→30, 26→10, 27→31, 27→11, 28→32, 28→12, 37→33, 37→53, 38→34, 38→54, 39→35, 39→55, 40→36, 40→56, 41→45, 41→57, 42→46, 42→58, 43→47, 43→59, 44→48, 44→60	0.41, 0.52	0.41, 0.51	0.41, 0.49	0.41, 0.48	0.42, 0.47	0.42, 0.46

TABLE S4: Oxygen vacancy diffusion barriers for dopants in distribution III (see Fig. S1). Transitions are between oxygen sites with indices defined in Table. S1. The first barrier value is the forward barrier in direction of the arrow in the "Transition" column ($a \rightarrow b$), and the second value is the reverse barrier ($a \leftarrow b$).

No.	Transition of O vacancy	Barriers [eV]					
		Pr	Nd	Pm	Sm	Eu	Gd
1	1→2, 1→17, 4→3, 4→20, 13→14, 13→29, 16→15, 16→32, 18→17, 18→2, 19→20, 19→3, 30→29, 30→14, 31→32, 31→15, 34→33, 34→50, 35→36, 35→51, 46→45, 46→62, 47→48, 47→63, 49→50, 49→33, 52→51, 52→36, 61→62, 61→45, 64→63, 64→48	0.31, 0.50	0.35, 0.48	0.38, 0.46	0.41, 0.44	0.44, 0.42	0.46, 0.39
2	1→4, 1→49, 4→1, 4→52, 13→16, 13→61, 16→13, 16→64, 18→19, 18→34, 19→18, 19→35, 30→31, 30→46, 31→30, 31→47, 34→35, 34→18, 35→34, 35→19, 46→47, 46→30, 47→46, 47→31, 49→52, 49→1, 52→49, 52→4, 61→64, 61→13, 64→61, 64→16	0.71, 0.71	0.66, 0.66	0.62, 0.62	0.59, 0.59	0.55, 0.55	0.52, 0.52
3	1→5, 4→8, 13→9, 16→12, 18→22, 19→23, 30→26, 31→27, 34→38, 35→39, 46→42, 47→43, 49→53, 52→56, 61→57, 64→60	0.35, 0.42	0.38, 0.42	0.41, 0.40	0.43, 0.39	0.45, 0.38	0.47, 0.35
4	1→13, 4→16, 13→1, 16→4, 18→30, 19→31, 30→18, 31→19, 34→46, 35→47, 46→34, 47→35, 49→61, 52→64, 61→49, 64→52	0.73, 0.73	0.69, 0.68	0.64, 0.64	0.61, 0.61	0.57, 0.57	0.54, 0.54
5	2→3, 2→50, 3→2, 3→51, 14→15, 14→62, 15→14, 15→63, 17→20, 17→33, 20→17, 20→36, 29→32, 29→45, 32→29, 32→48, 33→36, 33→17, 36→33, 36→20, 45→48, 45→29, 48→45, 48→32, 50→51, 50→2, 51→50, 51→3, 62→63, 62→14, 63→62, 63→15	0.41, 0.41	0.42, 0.42	0.42, 0.42	0.43, 0.43	0.43, 0.43	0.44, 0.44
6	2→1, 2→18, 3→4, 3→19, 14→13, 14→30, 15→16, 15→31, 17→18, 17→1, 20→19, 20→4, 29→30, 29→13, 32→31, 32→16, 33→34, 33→49, 36→35, 36→52, 45→46, 45→61, 48→47, 48→64, 50→49, 50→34, 51→52, 51→35, 62→61, 62→46, 63→64, 63→47	0.50, 0.31	0.48, 0.35	0.46, 0.38	0.44, 0.41	0.42, 0.44	0.39, 0.46
7	2→6, 3→7, 14→10, 15→11, 17→21, 20→24, 29→25, 32→28, 33→37, 36→40, 45→41, 48→44, 50→54, 51→55, 62→58, 63→59	0.60, 0.36	0.57, 0.38	0.54, 0.40	0.53, 0.41	0.50, 0.42	0.48, 0.43
8	2→14, 3→15, 14→2, 15→3, 17→29, 20→32, 29→17, 32→20, 33→45, 36→48, 45→33, 48→36, 50→62, 51→63, 62→50, 63→51	0.46, 0.46	0.46, 0.46	0.46, 0.46	0.46, 0.46	0.46, 0.46	0.46, 0.46
9	5→6, 5→21, 8→7, 8→24, 9→10, 9→25, 12→11, 12→28, 22→21, 22→6, 23→24, 23→7, 26→25, 26→10, 27→28, 27→11, 38→37, 38→54, 39→40, 39→55, 42→41, 42→58, 43→44, 43→59, 53→54, 53→37, 56→55, 56→40, 57→58, 57→41, 60→59, 60→44	0.53, 0.40	0.51, 0.40	0.49, 0.41	0.47, 0.42	0.46, 0.43	0.44, 0.43
10	5→8, 5→53, 8→5, 8→56, 9→12, 9→57, 12→9, 12→60, 22→23, 22→38, 23→22, 23→39, 26→27, 26→42, 27→26, 27→43, 38→39, 38→22, 39→38, 39→23, 42→43, 42→26, 43→42, 43→27, 53→56, 53→5, 56→53, 56→8, 57→60, 57→9, 60→57, 60→12	0.44, 0.45	0.44, 0.44	0.44, 0.44	0.44, 0.44	0.44, 0.44	0.44, 0.44
11	5→9, 8→12, 9→5, 12→8, 22→26, 23→27, 26→22, 27→23, 38→42, 39→43, 42→38, 43→39, 53→57, 56→60, 57→53, 60→56	0.39, 0.39	0.40, 0.40	0.40, 0.40	0.41, 0.41	0.42, 0.42	0.42, 0.42
12	5→1, 8→4, 9→13, 12→16, 22→18, 23→19, 26→30, 27→31, 38→34, 39→35, 42→46, 43→47, 53→49, 56→52, 57→61, 60→64	0.42, 0.35	0.42, 0.38	0.40, 0.41	0.39, 0.43	0.38, 0.45	0.35, 0.47
13	6→7, 6→54, 7→6, 7→55, 10→11, 10→58, 11→10, 11→59, 21→24, 21→37, 24→21, 24→40, 25→28, 25→41, 28→25, 28→44, 37→40, 37→21, 40→37, 40→24, 41→44, 41→25, 44→41, 44→28, 54→55, 54→6, 55→54, 55→7, 58→59, 58→10, 59→58, 59→11	0.45, 0.45	0.45, 0.45	0.44, 0.44	0.43, 0.43	0.43, 0.43	0.42, 0.42

14	6→5, 6→22, 7→8, 7→23, 10→9, 10→26, 11→12, 11→27, 21→22, 21→5, 24→23, 24→8, 25→26, 25→9, 28→27, 28→12, 37→38, 37→53, 40→39, 40→56, 41→42, 41→57, 44→43, 44→60, 54→53, 54→38, 55→56, 55→39, 58→57, 58→42, 59→60, 59→43	0.40, 0.53	0.40, 0.51	0.41, 0.49	0.42, 0.47	0.43, 0.46	0.43, 0.44
15	6→10, 7→11, 10→6, 11→7, 21→25, 24→28, 25→21, 28→24, 37→41, 40→44, 41→37, 44→40, 54→58, 55→59, 58→54, 59→55	0.44, 0.44	0.43, 0.43	0.43, 0.43	0.42, 0.42	0.42, 0.42	0.41, 0.41
16	6→2, 7→3, 10→14, 11→15, 21→17, 24→20, 25→29, 28→32, 37→33, 40→36, 41→45, 44→48, 54→50, 55→51, 58→62, 59→63	0.36, 0.60	0.38, 0.57	0.40, 0.54	0.41, 0.53	0.42, 0.50	0.43, 0.48

TABLE S5: Oxygen vacancy diffusion barriers for dopants in distribution IV (see Fig. S1). Transitions are between oxygen sites with indices defined in Table. S1. The first barrier value is the forward barrier in direction of the arrow in the "Transition" column ($a \rightarrow b$), and the second value is the reverse barrier ($a \leftarrow b$).

No.	Transition of O vacancy	Barriers [eV]					
		Pr	Nd	Pm	Sm	Eu	Gd
1	1→2, 1→5, 1→17, 4→3, 4→8, 4→20, 13→14, 13→9, 13→29, 16→15, 16→12, 16→32, 22→21, 22→18, 22→6, 23→24, 23→19, 23→7, 26→25, 26→30, 26→10, 27→28, 27→31, 27→11, 38→37, 38→34, 38→54, 39→40, 39→35, 39→55, 42→41, 42→46, 42→58, 43→44, 43→47, 43→59, 49→50, 49→53, 49→33, 52→51, 52→56, 52→36, 61→62, 61→57, 61→45, 64→63, 64→60, 64→48	0.35, 0.42	0.38, 0.42	0.40, 0.41	0.42, 0.40	0.44, 0.39	0.45, 0.37
2	1→4, 1→13, 1→49, 4→1, 4→16, 4→52, 13→16, 13→1, 13→61, 16→13, 16→4, 16→64, 22→23, 22→26, 22→38, 23→22, 23→27, 23→39, 26→27, 26→22, 26→42, 27→26, 27→23, 27→43, 38→39, 38→42, 38→22, 39→38, 39→43, 39→23, 42→43, 42→38, 42→26, 43→42, 43→39, 43→27, 49→52, 49→61, 49→1, 52→49, 52→64, 52→4, 61→64, 61→49, 61→13, 64→61, 64→52, 64→16	0.70, 0.70	0.66, 0.66	0.62, 0.62	0.59, 0.59	0.56, 0.56	0.53, 0.53
3	2→3, 3→2, 5→9, 6→54, 7→55, 8→12, 9→5, 10→58, 11→59, 12→8, 14→15, 15→14, 17→33, 18→30, 19→31, 20→36, 21→24, 24→21, 25→28, 28→25, 29→45, 30→18, 31→19, 32→48, 33→17, 34→46, 35→47, 36→20, 37→40, 40→37, 41→44, 44→41, 45→29, 46→34, 47→35, 48→32, 50→51, 51→50, 53→57, 54→6, 55→7, 56→60, 57→53, 58→10, 59→11, 60→56, 62→63, 63→62	0.41, 0.41	0.41, 0.41	0.42, 0.42	0.42, 0.42	0.42, 0.42	0.42, 0.42
4	2→1, 3→4, 5→1, 6→22, 7→23, 8→4, 9→13, 10→26, 11→27, 12→16, 14→13, 15→16, 17→1, 18→22, 19→23, 20→4, 21→22, 24→23, 25→26, 28→27, 29→13, 30→26, 31→27, 32→16, 33→49, 34→38, 35→39, 36→52, 37→38, 40→39, 41→42, 44→43, 45→61, 46→42, 47→43, 48→64, 50→49, 51→52, 53→49, 54→38, 55→39, 56→52, 57→61, 58→42, 59→43, 60→64, 62→61, 63→64	0.42, 0.35	0.42, 0.38	0.41, 0.40	0.40, 0.42	0.39, 0.44	0.37, 0.45
5	2→6, 2→18, 3→7, 3→19, 5→6, 5→21, 6→5, 6→2, 7→8, 7→3, 8→7, 8→24, 9→10, 9→25, 10→9, 10→14, 11→12, 11→15, 12→11, 12→28, 14→10, 14→30, 15→11, 15→31, 17→18, 17→21, 18→17, 18→2, 19→20, 19→3, 20→19, 20→24, 21→17, 21→5, 24→20, 24→8, 25→29, 25→9, 28→32, 28→12, 29→30, 29→25, 30→29, 30→14, 31→32, 31→15, 32→31, 32→28, 33→34, 33→37, 34→33, 34→50, 35→36, 35→51, 36→35, 36→40, 37→33, 37→53, 40→36, 40→56, 41→45, 41→57, 44→48, 44→60, 45→46, 45→41, 46→45, 46→62, 47→48, 47→63, 48→47, 48→44, 50→54, 50→34, 51→55, 51→35, 53→54, 53→37, 54→53, 54→50, 55→56, 55→51, 56→55, 56→40, 57→58, 57→41, 58→57, 58→62, 59→60, 59→63, 60→59, 60→44, 62→58, 62→46, 63→59, 63→47	0.48, 0.48	0.47, 0.47	0.47, 0.47	0.46, 0.46	0.46, 0.46	0.46, 0.46

6	2→14, 2→50, 3→15, 3→51, 5→8, 5→53, 6→7, 6→10, 7→6, 7→11, 8→5, 8→56, 9→12, 9→57, 10→11, 10→6, 11→10, 11→7, 12→9, 12→60, 14→2, 14→62, 15→3, 15→63, 17→20, 17→29, 18→19, 18→34, 19→18, 19→35, 20→17, 20→32, 21→25, 21→37, 24→28, 24→40, 25→21, 25→41, 28→24, 28→44, 29→32, 29→17, 30→31, 30→46, 31→30, 31→47, 32→29, 32→20, 33→36, 33→45, 34→35, 34→18, 35→34, 35→19, 36→33, 36→48, 37→41, 37→21, 40→44, 40→24, 41→37, 41→25, 44→40, 44→28, 45→48, 45→33, 46→47, 46→30, 47→46, 47→31, 48→45, 48→36, 50→62, 50→2, 51→63, 51→3, 53→56, 53→5, 54→55, 54→58, 55→54, 55→59, 56→53, 56→8, 57→60, 57→9, 58→59, 58→54, 59→58, 59→55, 60→57, 60→12, 62→50, 62→14, 63→51, 63→15	0.45, 0.45	0.45, 0.45	0.44, 0.44	0.44, 0.44	0.44, 0.44	0.43, 0.43

S4. DIFFUSION CONSTANT FOR DIFFERENT DISTRIBUTIONS

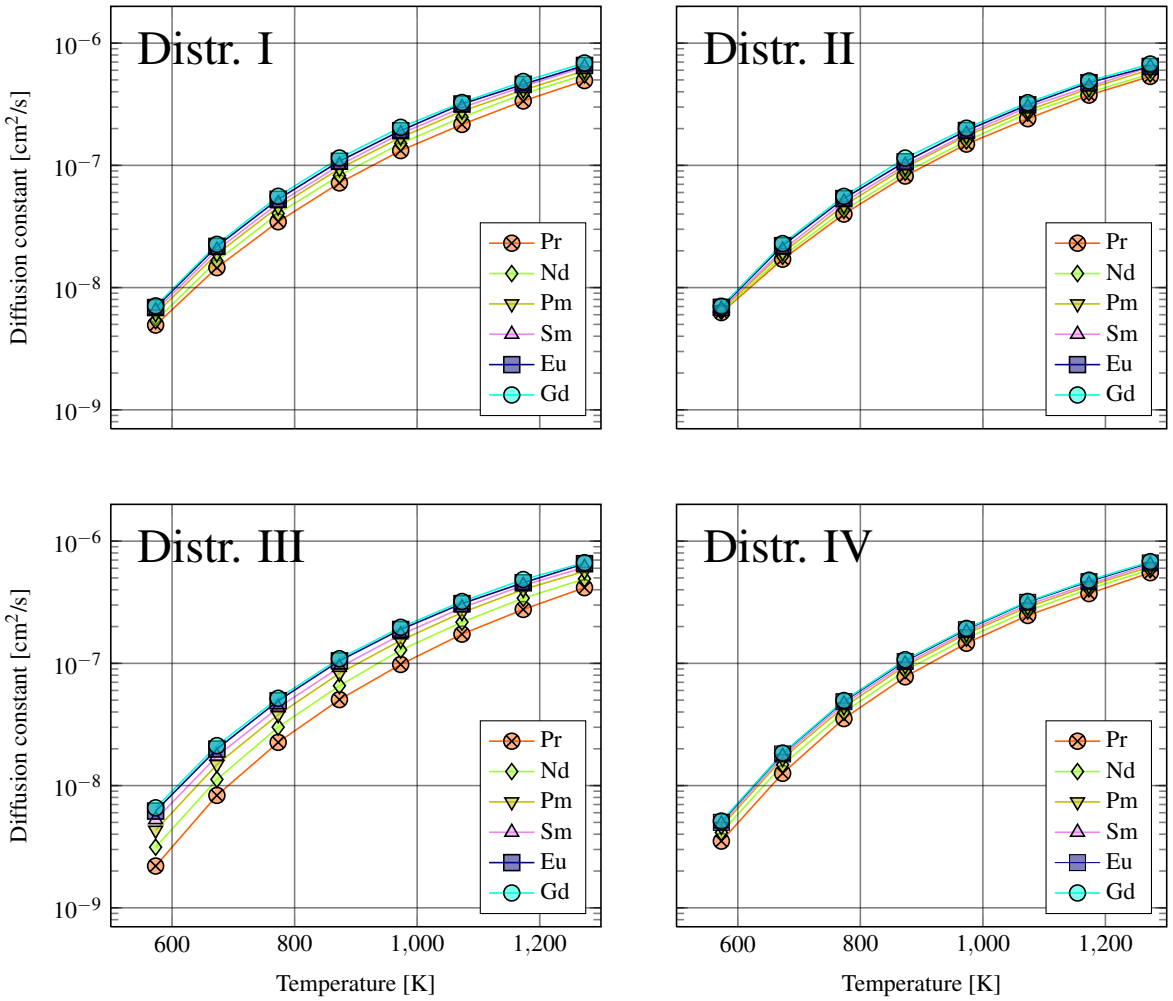

FIG. S2. Diffusion constant versus temperature for dopant distributions I–IV (see Fig. S1).

S5. SYMMETRY OF BARRIERS

TABLE S6. Average ion diffusion barriers symmetry $\langle dE\rangle^n = \frac{1}{N^n}\sum_i^{N^n} dE_i$, where N^n is the total number of barriers in the system for distribution $n \in \{I, II, III, IV\}$. $dE_i = |\Delta E_i^{fwd} - \Delta E_i^{bwd}|$) is the difference between the forward and backward barrier for barrier number i. The diffusion barrier averaged over the distributions (I–IV) is $\langle dE\rangle^{Avg} = \frac{1}{4}(\langle dE\rangle^I + \langle dE\rangle^{II} + \langle dE\rangle^{III} + \langle dE\rangle^{IV})$. Bold face numbers indicate the lowest average barrier in each column.

	Average barrier symmetry [eV]				
Dopant	$\langle dE\rangle^I$	$\langle dE\rangle^{II}$	$\langle dE\rangle^{III}$	$\langle dE\rangle^{IV}$	$\langle dE\rangle^{Avg.}$
Pr	0.0746	0.0287	0.0795	0.0165	0.0498
Nd	0.0563	0.0271	0.0583	0.0094	0.0378
Pm	**0.0401**	**0.0265**	0.0371	**0.0015**	0.0263
Sm	0.0402	0.0268	0.0267	0.0051	**0.0247**
Eu	0.0407	0.0271	**0.0214**	0.0125	0.0254
Gd	0.0432	0.0287	0.0272	0.0205	0.0299