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Supplementary Information

Preferential Proton Conduction along Three-Dimensional Dopant Network in Yttrium-Doped Barium Zirconate: A First-Principles Study

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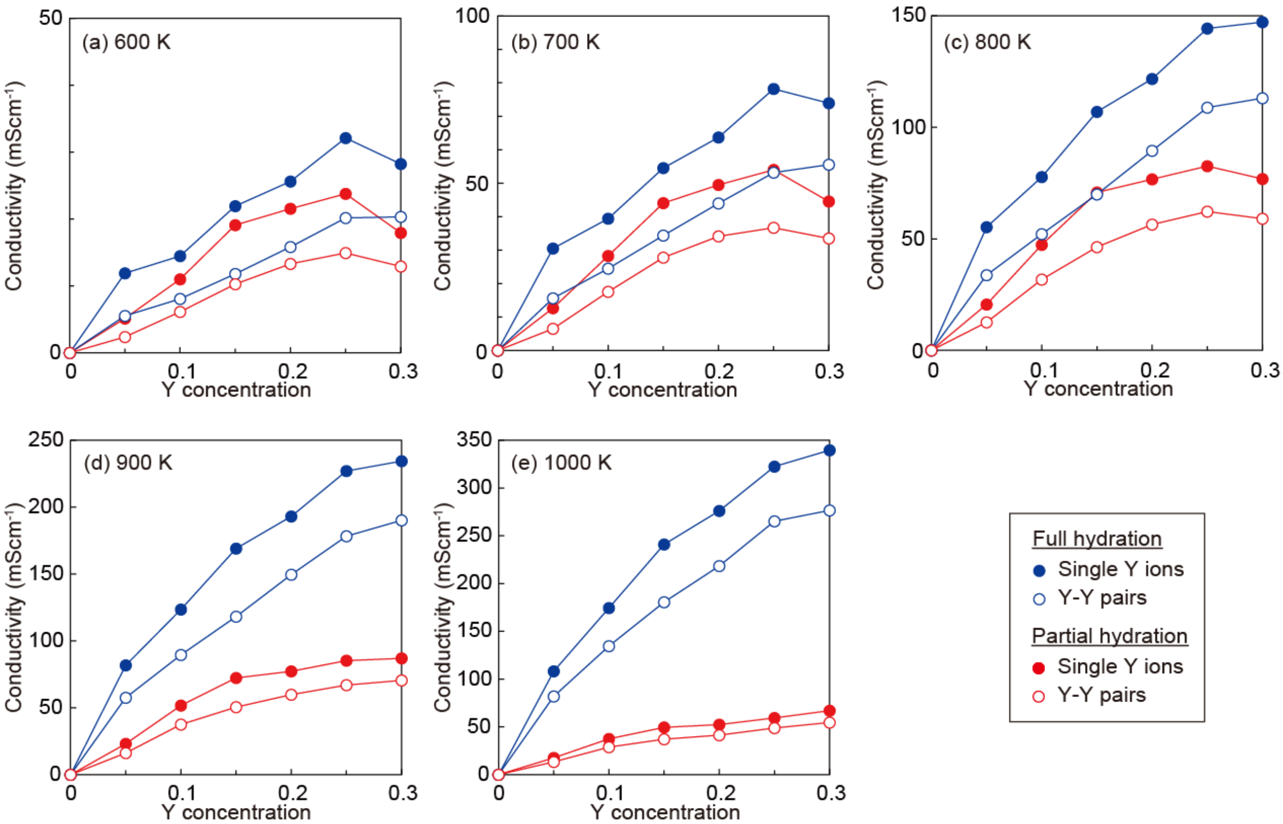

Fig. S1. The estimated proton conductivities in the range of 600 and 1000 K as a function of Y concentration. The blue and red lines correspond to the fully and partially hydrated crystals, respectively. In the partially-hydrated situation, the proton concentrations were estimated from the actual proton concentrations measured by the Karl Fischer titration method in the literature [16]. The solid and open circles correspond to the random and adjacent configuration of Y dopants, respectively.

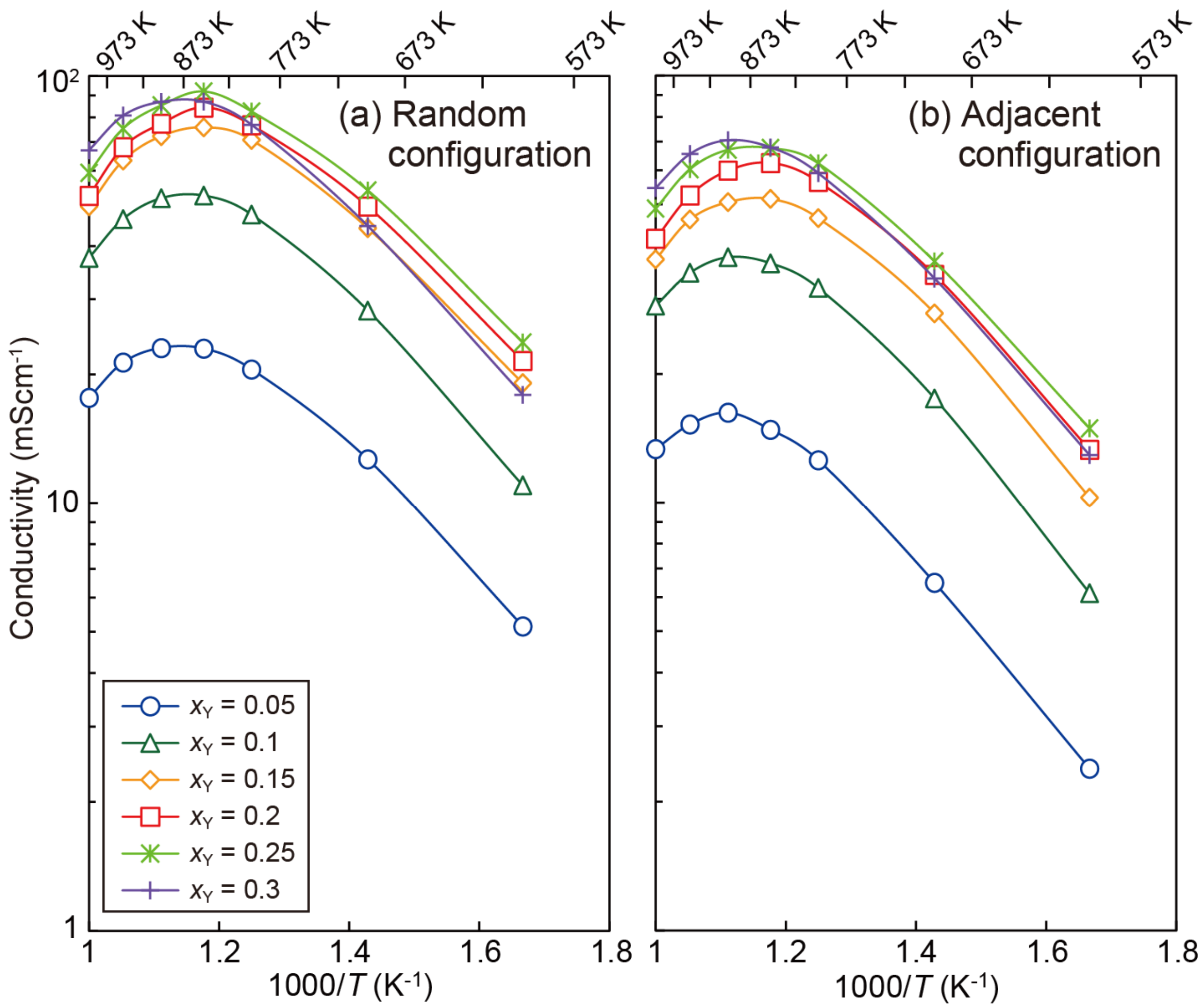

Fig. S2. The estimated proton conductivities as a function of inverse temperature in the range of $0 \leq x_Y \leq 0.3$ with the (a) random and (b) adjacent configurations of Y dopants. The proton concentrations were estimated from the actual proton concentrations measured by the Karl Fischer titration method in the literature [16].

Table S1. All proton sites in Y-doped $BaZrO_3$ classified by the types of proton rotation and hopping paths from the individual proton site. "a" and "b" in path ID mean the forward and backward migrations, respectively. #Y is the total number of Y dopants around the four paths.

		Path ID						Path ID			
Site	# Y	Rotation		Hopping		Site	#Y	Rotation		Hopping	
1	0	R0-1a	R0-1a	H0-1a	H0-1a	43	10	R2-2b	R4-1a	H2-3a	H2-3a
2	1	R1-2a	R0-1a	H0-1a	H0-1a	44	10	R3-6a	R3-6a	H2-1b	H2-1b
3	2	R0-1a	R2-2a	H0-1a	H0-1a	45	10	R3-3a	R3-3a	H2-2a	H2-4a
4	2	R1-2a	R1-2a	H0-1a	H0-1a	46	10	R3-2a	R3-2a	H2-1a	H2-3b
5	3	R1-2a	R2-2a	H0-1a	H0-1a	47	10	R2-1a	R4-2b	H2-1b	H2-1b
6	4	R1-2b	R1-2b	H1-2a	H1-3a	48	10	R2-5b	R4-5b	H2-1a	H2-3b
7	4	R1-1a	R1-1a	H1-1a	H1-2b	49	11	R3-6a	R4-2b	H2-1b	H2-1b
8	4	R2-2a	R2-2a	H0-1a	H0-1a	50	11	R3-2a	R4-5b	H2-1a	H2-3b
9	5	R1-1a	R2-5a	H1-1a	H1-2b	51	11	R3-5b	R4-5b	H2-1a	H2-3b
10	5	R1-2b	R2-4a	H1-2a	H1-3a	52	11	R3-3a	R4-6b	H2-2a	H2-4a
11	5	R1-2b	R2-3a	H1-2a	H1-3a	53	11	R3-5a	R4-6b	H2-2a	H2-4a
12	5	R1-1a	R2-6a	H1-1a	H1-2b	54	11	R4-1a	R3-1b	H2-3a	H2-3a
13	6	R2-6a	R2-6a	H1-1a	H1-2b	55	12	R4-1a	R4-1a	H2-3a	H2-3a
14	6	R1-2b	R3-1a	H1-2a	H1-3a	56	12	R4-6b	R4-6b	H2-2a	H2-4a
15	6	R1-1a	R3-4a	H1-1a	H1-2b	57	12	R4-2b	R4-2b	H2-1b	H2-1b
16	6	R2-4a	R2-4a	H1-2a	H1-3a	58	12	R3-4b	R3-4b	H3-1a	H3-3a
17	6	R2-5a	R2-6a	H1-1a	H1-2b	59	12	R4-5b	R4-5b	H2-1a	H2-3b
18	6	R2-3a	R2-4a	H1-2a	H1-3a	60	12	R3-6b	R3-6b	H3-1b	H3-2a
19	6	R2-5a	R2-5a	H1-1a	H1-2b	61	13	R3-6b	R4-3a	H3-1b	H3-2a
20	6	R2-3a	R2-3a	H1-2a	H1-3a	62	13	R3-4b	R4-5a	H3-1a	H3-3a
21	7	R2-3a	R3-1a	H1-2a	H1-3a	63	13	R4-4a	R3-6b	H3-1b	H3-2a
22	7	R2-5a	R3-4a	H1-1a	H1-2b	64	13	R3-4b	R4-6a	H3-1a	H3-3a
23	7	R2-6a	R3-4a	H1-1a	H1-2b	65	14	R4-4a	R4-4a	H3-1b	H3-2a
24	7	R2-4a	R3-1a	H1-2a	H1-3a	66	14	R4-5a	R4-5a	H3-1a	H3-3a
25	8	R2-5b	R2-5b	H2-1a	H2-3b	67	14	R4-3a	R4-3a	H3-1b	H3-2a
26	8	R2-6b	R2-6b	H2-2a	H2-4a	68	14	R3-6b	R5-2b	H3-1b	H3-2a
27	8	R2-2b	R2-2b	H2-3a	H2-3a	69	14	R3-4b	R5-1a	H3-1a	H3-3a
28	8	R3-1a	R3-1a	H1-2a	H1-3a	70	14	R4-5a	R4-6a	H3-1a	H3-3a
29	8	R3-4a	R3-4a	H1-1a	H1-2b	71	14	R4-4a	R4-3a	H3-1b	H3-2a
30	8	R2-1a	R2-1a	H2-1b	H2-1b	72	14	R4-6a	R4-6a	H3-1a	H3-3a
31	9	R2-6b	R3-3a	H2-2a	H2-4a	73	15	R4-6a	R5-1a	H3-1a	H3-3a
32	9	R2-5b	R3-2a	H2-1a	H2-3b	74	15	R4-3a	R5-2b	H3-1b	H3-2a
33	9	R2-2b	R3-1b	H2-3a	H2-3a	75	15	R4-4a	R5-2b	H3-1b	H3-2a
34	9	R2-1a	R3-6a	H2-1b	H2-1b	76	15	R4-5a	R5-1a	H3-1a	H3-3a
35	9	R2-5b	R3-5b	H2-1a	H2-3b	77	16	R5-1a	R5-1a	H3-1a	H3-3a
36	9	R2-6b	R3-5a	H2-2a	H2-4a	78	16	R4-2a	R4-2a	H4-1a	H4-1a
37	10	R3-5a	R3-5a	H2-2a	H2-4a	79	16	R5-2b	R5-2b	H3-1b	H3-2a
38	10	R3-1a	R3-5a	H2-2a	H2-4a	80	17	R4-2a	R5-2a	H4-1a	H4-1a
39	10	R2-6b	R4-6b	H2-2a	H2-4a	81	18	R4-2a	R6-1a	H4-1a	H4-1a
40	10	R3-2a	R3-5b	H2-1a	H2-3b	82	18	R5-2a	R5-2a	H4-1a	H4-1a
41	10	R3-1b	R3-1b	H2-3a	H2-3a	83	19	R5-2a	R6-1a	H4-1a	H4-1a
42	10	R3-5b	R3-5b	H2-1a	H2-3b	84	20	R6-1a	R6-1a	H4-1a	H4-1a