Supplementary Information for

First Principles Assessment of Perovskite Dopants for Proton Conductors with Chemical Stability and High Conductivity

Sung Gu Kang and David S. Sholl*

School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, 311 Ferst Dr., Atlanta, GA 30332-0100, USA

Table S.1 shows determined energy barriers for all 10 proton hops using DFT for each of the 13 dopants we considered.

Table S.1 Energy barriers of the proton in the case where a dopant is a nearest neighbor of the initial or final proton, where M = Y, Er, Ho, Al, Ga, Dy, In, Sc, La, Nd, Pm, Sm, and Tl.

	Y	Er	Ho	Al	Ga	Dy	In	Sc	La	Nd	Pm	Sm	Tl
Transfer 1	0.98	0.74	0.84	0.64	0.41	0.95	0.56	0.28	2.18	1.94	1.72	1.58	1.46
Transfer 2	0.35	0.32	0.33	0.18	0.21	0.34	0.30	0.22	0.53	0.48	0.45	0.40	0.40
Transfer 3	0.55	0.44	0.48	0.45	0.08	0.53	0.34	0.13	1.57	1.31	1.13	0.77	0.89
Transfer 4	0.59	0.52	0.55	0.69	0.37	0.57	0.49	0.39	1.11	1.04	0.92	0.70	0.90
Transfer 5	0.40	0.40	0.40	0.80	0.72	0.40	0.45	0.57	0.61	0.54	0.46	0.45	0.49
Transfer 6	0.39	0.33	0.36	0.06	0.12	0.38	0.28	0.18	0.77	0.65	0.56	0.53	0.51
Transfer 7	0.29	0.29	0.29	0.29	0.29	0.29	0.29	0.29	0.29	0.29	0.29	0.29	0.29
Rotation 1	0.84	0.68	0.75	0.30	0.16	0.84	0.46	0.13	2.48	2.10	1.31	1.23	1.38
Rotation 2	0.11	0.12	0.11	0.17	0.17	0.47	0.14	0.17	0.08	0.07	0.07	0.07	0.61
Rotation 3	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15

* Corresponding author. Email: david.sholl@chbe.gatech.edu