

Supporting Information

Ba₂ScHO₃: H⁻ Conductive Layered Oxyhydride with H⁻ Site Selectivity

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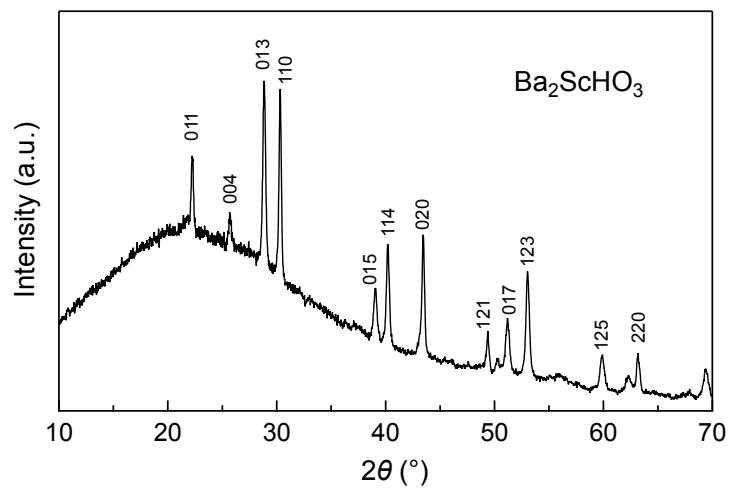


Figure S1. Laboratory XRD profile of BaScHO₃. The large background at lower angles was derived from the Kapton film attached to the sample holder for air-sensitive samples.

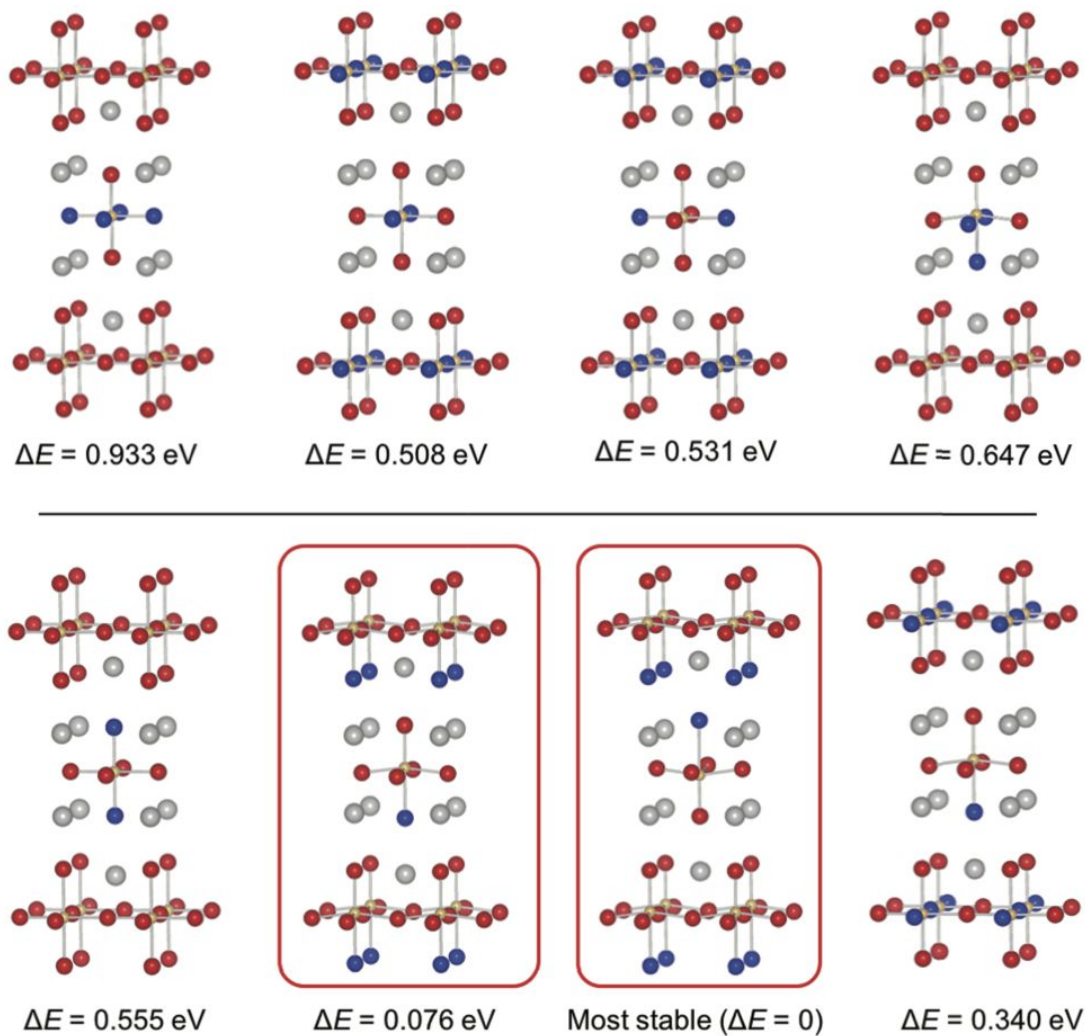


Figure S2. All symmetrically independent H/O configurations in the conventional unit cell of Ba_2ScHO_3 calculated in this study. The values of relative energies compared with the most stable configuration are shown.

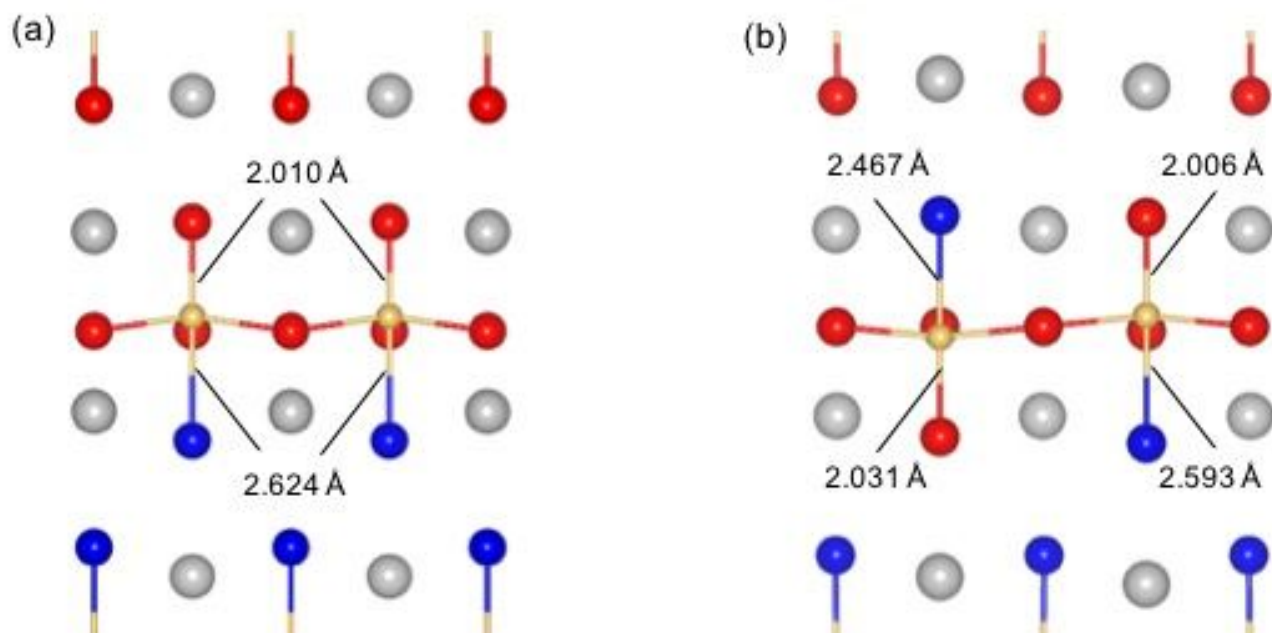


Figure S3. Optimized coordination environment of ScO₅H in the supercells of Ba₂ScO₃H. Left and right images correspond to the supercells of Figures 3(a) and (b), respectively.

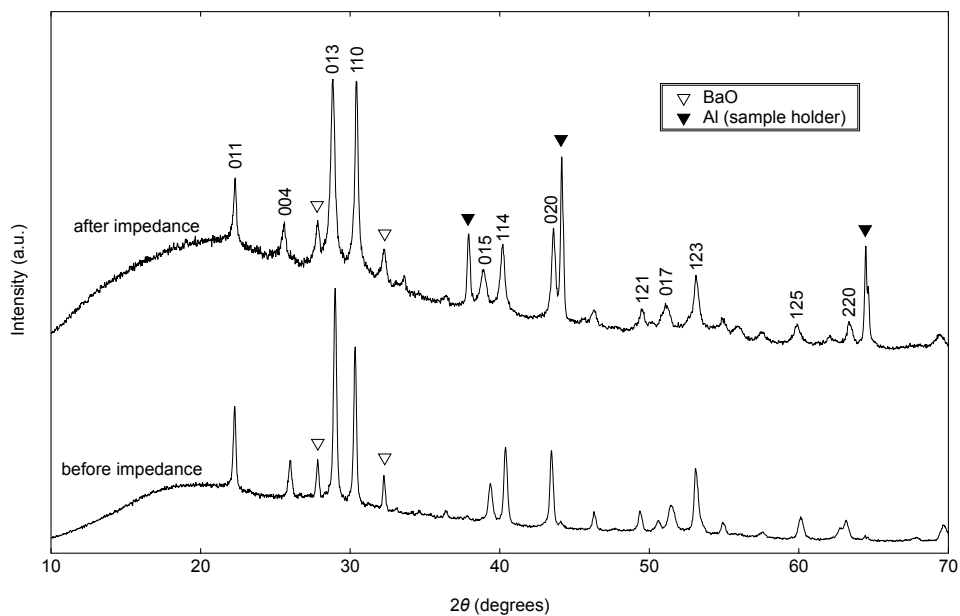


Figure S4. XRD profile of Ba_2ScHO_3 before and after impedance measurement. The peaks with the open and closed triangle represent those of BaO and Al (sample holder), respectively. The sample lot is different from one for Figure S1.

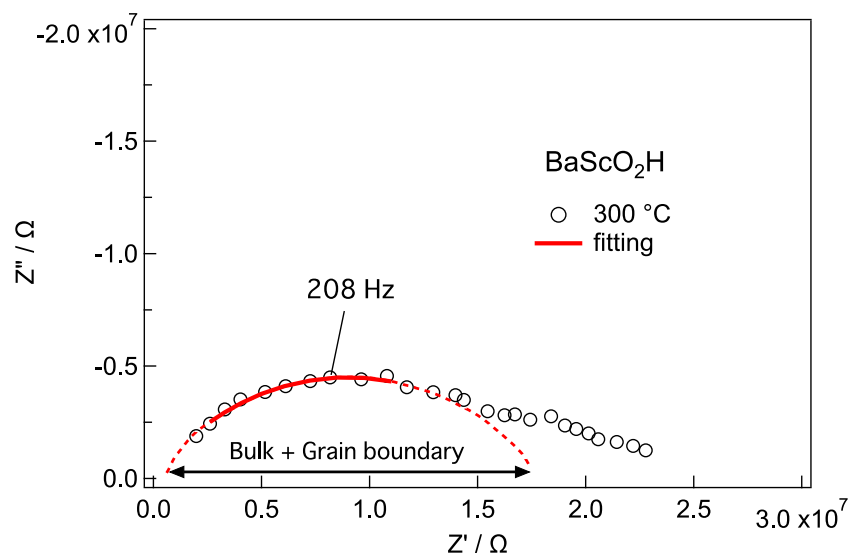


Figure S5. Impedance plot of BaScO₂H at 300 °C.

Table S1. Structural parameters of BaO and Sc₂O₃ from SXRD data.

BaO

Atom	Site	<i>g</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> / Å ²
Ba	4 <i>a</i>	1	0	0	0	0.4
O1	4 <i>b</i>	1	0.5	0.5	0.5	1.0

Fm-3*m*, *a* = 5.53599(7) Å.Sc₂O₃

Atom	Site	<i>g</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> / Å ²
Sc1	8 <i>b</i>	1	0.25	0.25	0.25	0.5
Sc2	24 <i>d</i>	1	0.4649	0	0.25	0.5
O	48 <i>e</i>	1	0.3928	0.1528	0.3802	1.0

Ia-3, *a* = 9.8484(11) Å.**Table S2.** Structural parameters of BaScO₂H from ND data.

Atom	Site	<i>g</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> / Å ²
Ba	1 <i>b</i>	1	0.5	0.5	0.5	0.4
Sc	1 <i>a</i>	1	0	0	0	0.70(3)
O	3 <i>d</i>	0.667	0.5	0	0	0.83(2)
H	3 <i>d</i>	0.333	0.5	0	0	= <i>B</i> (O)

Pm-3*m*, *a* = 4.15254(3) Å.