Supplementary Material

Unraveling Anisotropic Li-Ion Transport in $Li_{3/8}Sr_{7/16}Ta_{3/4}Hf_{1/4}O_3$ via Machine Learning Molecular Dynamics and First-Principles Modeling

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Table S1 The computational details about *k*-points densities for CINEB calculations.

Migration direction	Lattice parameters	Expansion ratio	Atom number	*K*-points	*K*-points densities (/Å^{-1})
a	*a* = 11.35 Å *b* = 19.73 Å *c* = 13.95 Å $\alpha = \beta = \gamma = 90^{\circ}$	$1 \times \sqrt{3} \times \sqrt{3}$	231	3 2 3	34 39 42
b	*a* = *b* = 11.35 Å *c* = 16.05 Å $\alpha = \beta = \gamma = 90^{\circ}$	$1 \times 1 \times 2$	154	3 3 2	34 34 32
c	*a* = *b* = 16.05 Å *c* = 8.03 Å $\alpha = \beta = \gamma = 90^{\circ}$	$\sqrt{2} \times \sqrt{2} \times 1$	154	2 2 4	32 32 32

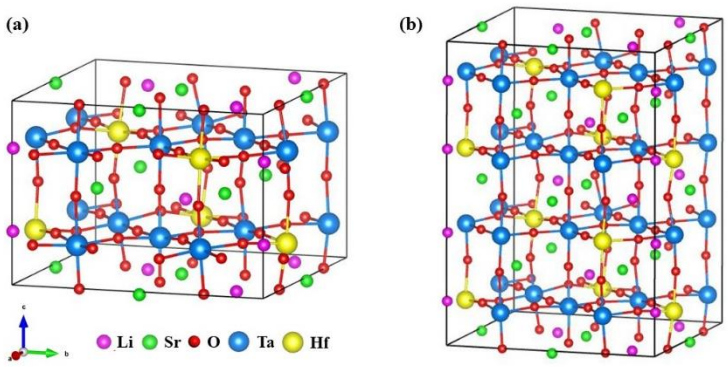

Figure S1 (a) LSTH unit cell structure, (b) LSTH supercell (1×1×2) structure.

Table S2 The Li^+ ions diffusion coefficients and conductivity at 300-700 K.

T (K)	300	400	500	600	700
D (cm^2/S)	9.4×10^{-9}	1.2×10^{-7}	9.6×10^{-7}	3.1×10^{-6}	5.7×10^{-6}
σ (mS/cm)	0.492	3.0	20.5	54.1	86.0

Table S3 The estimated diffusion coefficients along *a*-direction, *b*-direction, and *c*-direction under room temperature.

Migration path	d (Å)	ΔE (eV)	D (cm^2/S)
a-direction	3.68	0.92	$\sim 10^{-19}$
b-direction	3.61	0.83	$\sim 10^{-17}$
c-direction	3.16	0.30	$\sim 10^{-9}$

Table S4 The estimated diffusion coefficients along *c*-direction under the temperature range of 300 K-700 K.

T (K)	300	400	500	600	700
D (cm^2/S)	9.1×10^{-9}	1.7×10^{-7}	9.5×10^{-7}	3.0×10^{-6}	6.9×10^{-6}