## **Understanding Ionic Transport in Perovskite Lithium-Ion Conductor**

## Li<sub>3/8</sub>Sr<sub>7/16</sub>Ta<sub>3/4</sub>Hf<sub>1/4</sub>O<sub>3</sub>:

A Neutron Diffraction and Ab Initio Molecular Dynamics Simulations Study

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Figure S1. Electrochemical impedance spectrum of the synthesized impurity-free LSTH made

by sol-gel method.

Table S1. Normalized elemental concentrations of LSTH ( $Li_{0.375}Sr_{0.4375}Ta_{0.75}Hf_{0.25}O_3$ ) measured by ICP.

Sample LSTH	X <sub>Li</sub>	X <sub>Sr</sub>	X <sub>Hf</sub>	X <sub>Ta</sub>
Target composition	0.375	0.4375	0.25	0.75
ICP results	0.34	0.42	0.24	0.75



Figure S2. MSD of all species in LSTH perovskite with Li@1a (ESGS).



Figure S3. MSD of all species in LSTH perovskite with Li@24k (ESGS).



Figure S4. MSD of all species in LSTH perovskite with Li@1a (SQS).



Figure S5. MSD of all species in LSTH perovskite with Li@24k (SQS).