

## Experimental and Computational Study of Zn Doping in $\text{Li}_{5+x}\text{La}_3\text{Nb}_{2-x}\text{Zr}_x\text{O}_{12}$ Garnet Solid State Electrolytes

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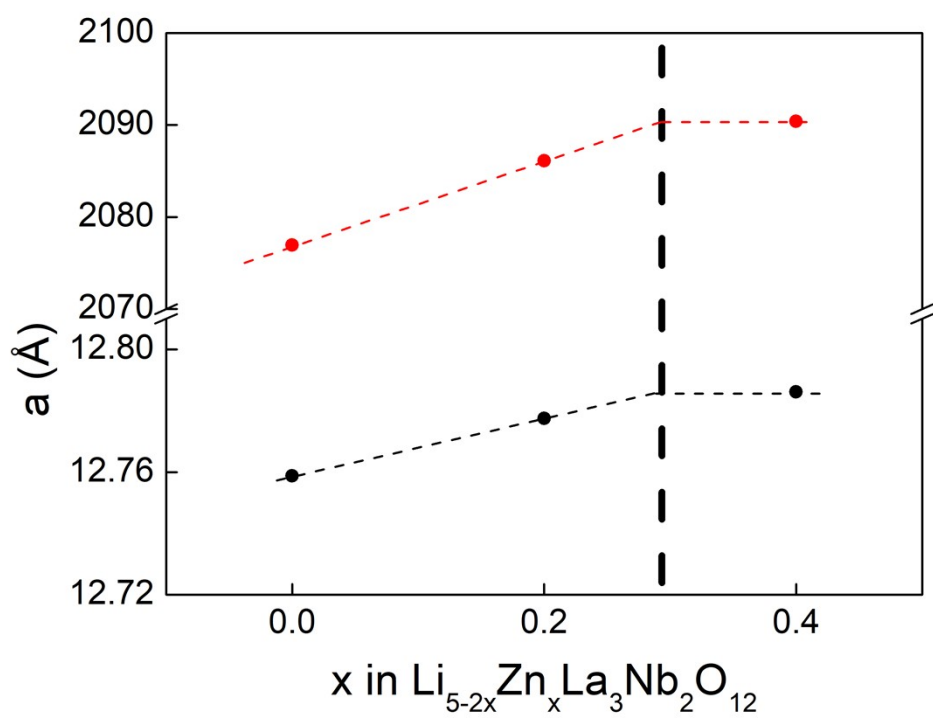


Figure S1 Variation of lattice parameter  $a$  and volume  $V$  for  $\text{Li}_{5-2y}\text{Zn}_y\text{La}_3\text{Nb}_2\text{O}_{12}$  with composition  $y$ .

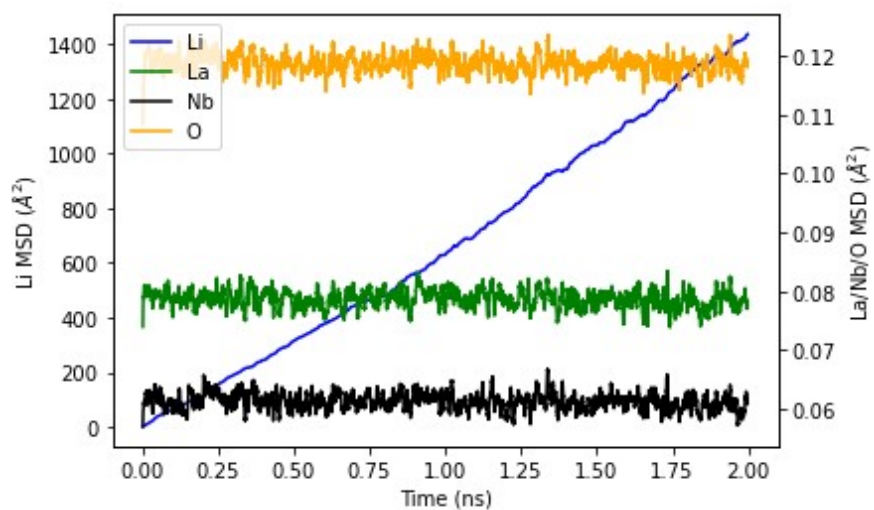


Figure S2: MSD against time for the pure LLNO system at 1100 K using an NVT ensemble for 2 ns.

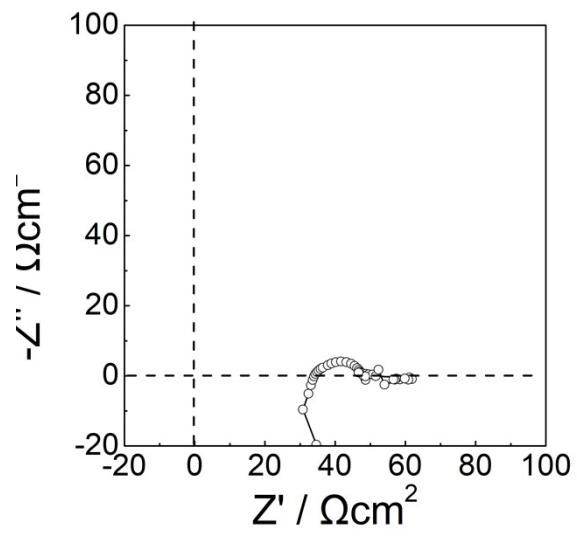


Figure S3 Electrochemical impedance spectra Li//LLZN//Li symmetric cell.

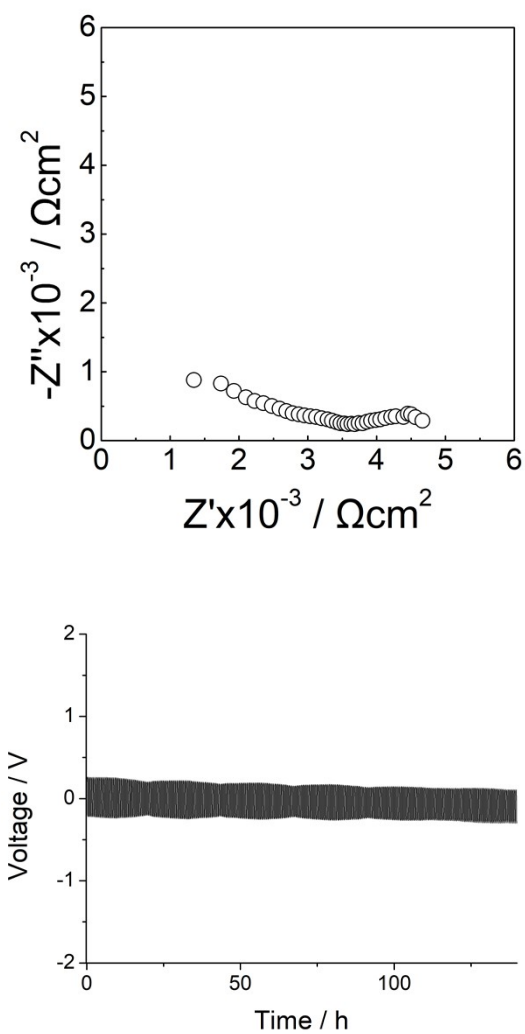


Figure S4 (a) Electrochemical impedance spectra of Li//LLZnZ-PTFE//Li symmetric cells. (b) Charge – discharge voltage profile of the Li//LLZnZ-PTFE//Li symmetry cell at room temperature with  $100 \mu\text{A cm}^{-2}$  current density.