

Supporting Information

Leaf-like Al₂O₃-based Quasi-Solid Electrolyte with a Fast Li⁺ Conductive Interface for Stable Lithium Metal Anodes

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Computational Analysis

All calculations were implemented using the Vienna Abinitio Simulation Package (VASP) code based on Density Functional Theory (DFT). All structural models were entirely relaxed until the ionic Hellmann–Feynman forces were smaller than 0.01 eV/Å and the energy tolerances were less than 10⁻⁶ eV/atom. The interaction between core electrons and valence electrons was described using the frozen-core projector-augmented wave (PAW) method. Wave functions were expanded in a plane wave basis with a high energy using plane-wave cutoff energy of 500 eV, and The corresponding K-point samplings were denser than 0.2 Å⁻¹. The bulk of Al₂O₃ was optimized for the

PBE functional with a $12 \times 12 \times 4$ k-point mesh. The (110) surface containing 150 atoms were cleaved for the surface energy study with a $4 \times 2 \times 1$ k-point mesh, respectively.

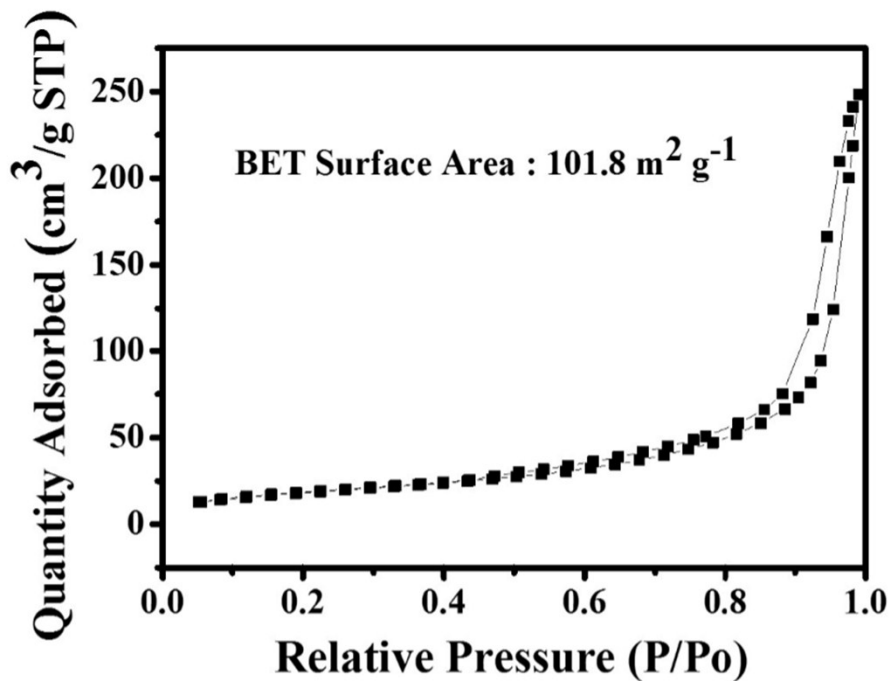


Figure S1 The Brunauer-Emmett-Teller specific surface area of Al₂O₃ skeleton.

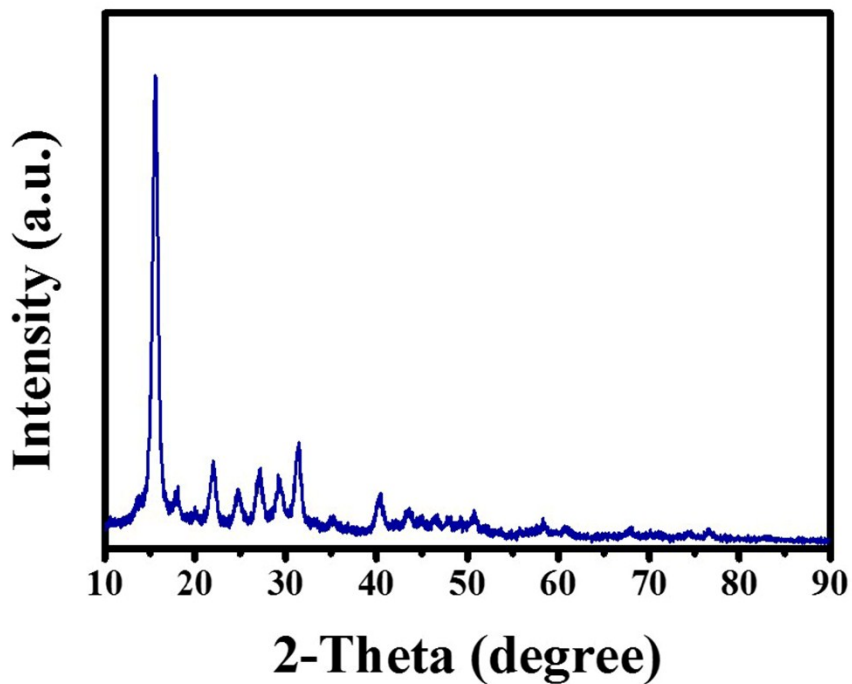


Figure S2 The XRD pattern of Al₂O₃ skeleton.

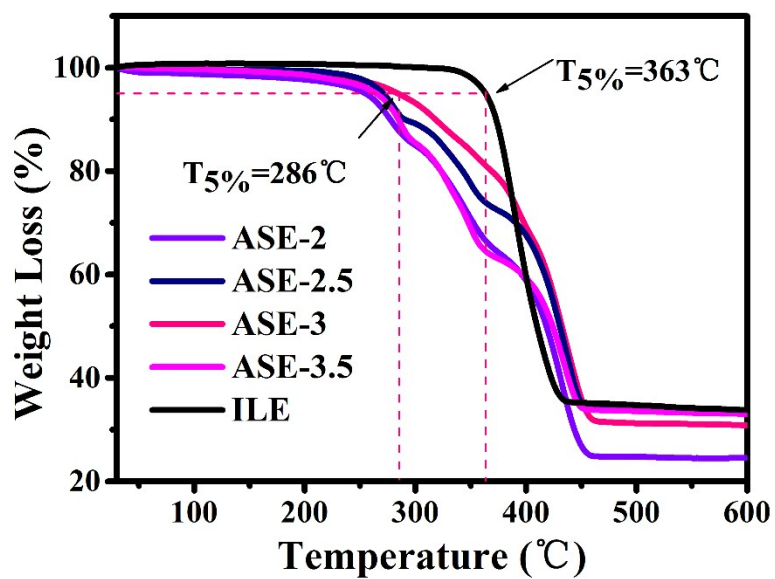


Figure S3 The thermogravimetric analysis thermograms of ASEs and ILE.

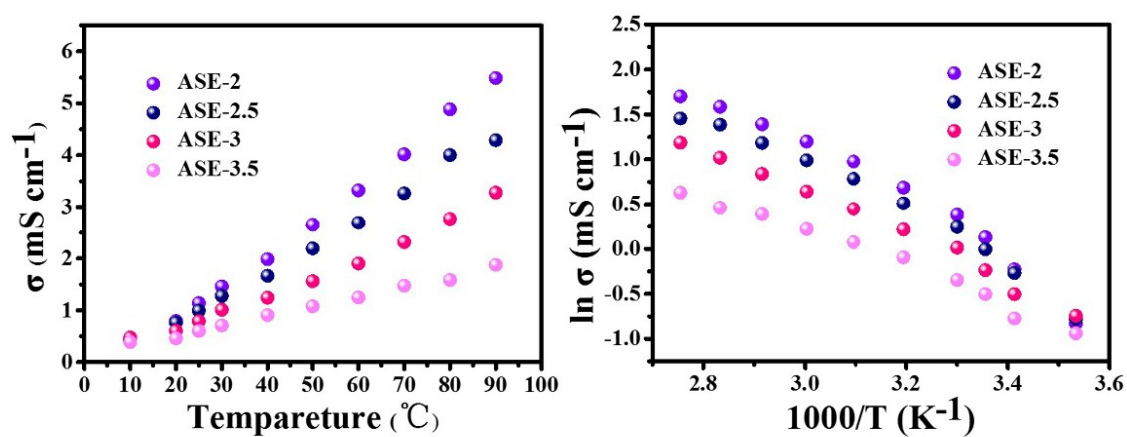


Figure S4 The ionic conductivities and Arrhenius curves of ASE electrolytes measured at different temperatures.

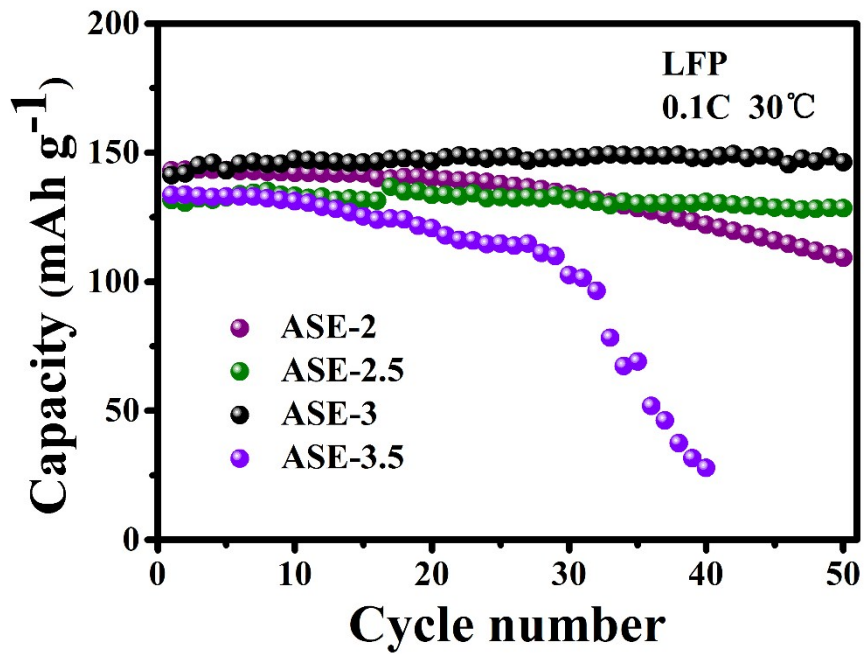


Figure S5 The cycling performance of four different ratio samples.

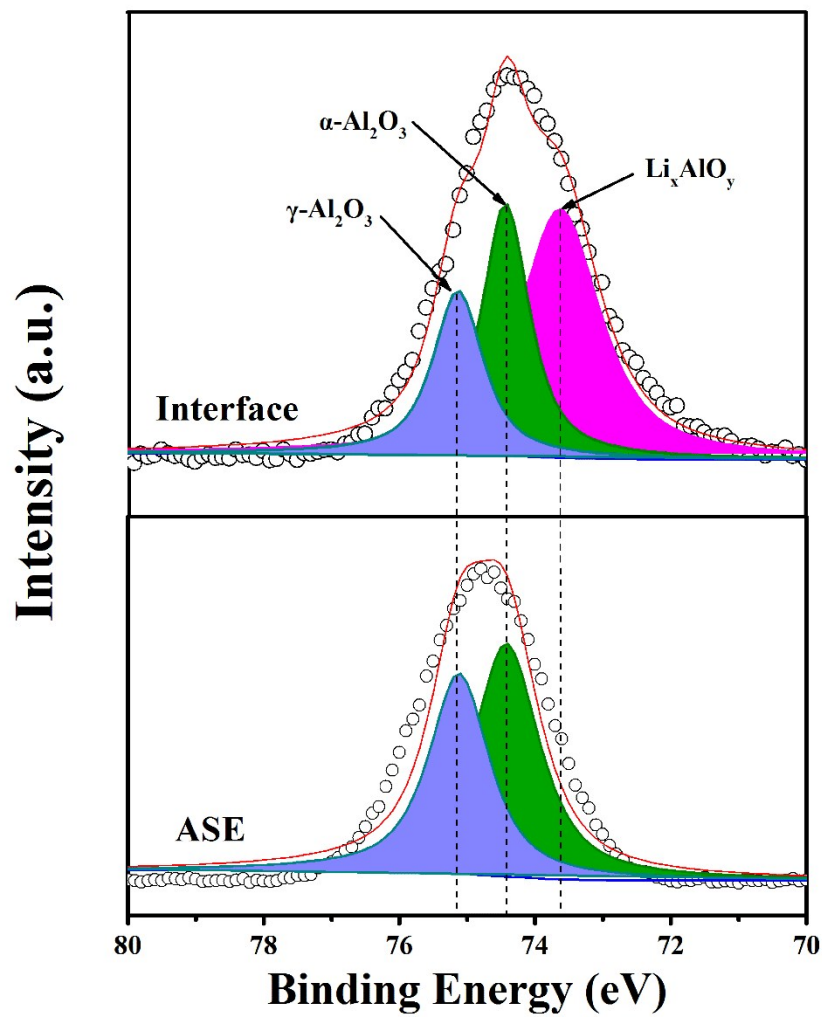


Figure S6 X-ray photoelectron spectrometer analysis of the Li metal surface and ASE.

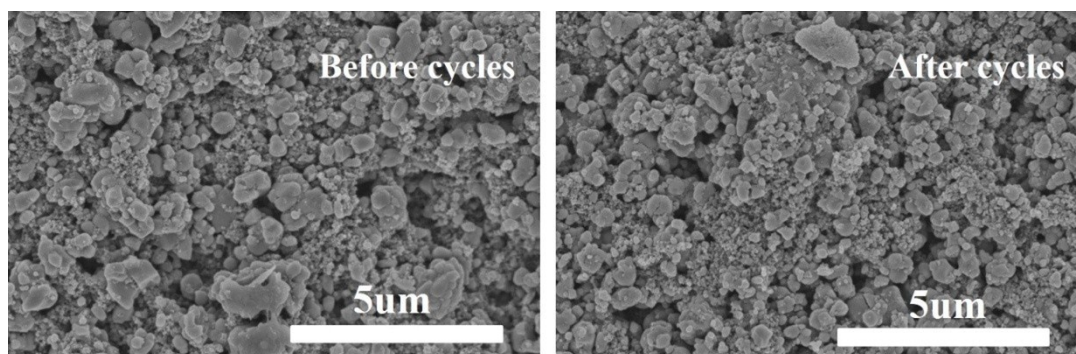


Figure S7 The surface morphology of the LiFePO_4 cathode before and after cycling.