

Description of Additional Supplementary Files

Supplementary Data 1: Unit cell of NCM811.

Supplementary Data 2: NCM811 cathode structure shown in Supplementary Fig. 3.

Supplementary Data 3: Initial structures for the OAc electrolyte simulations.

Supplementary Data 4: Final structures for the OAc electrolyte simulations.

Supplementary Data 5: Initial structures for the OTf electrolyte simulations.

Supplementary Data 6: Final structures for the OTf electrolyte simulations.

Supplementary Data 7: Initial structures for the SO₄ electrolyte simulations.

Supplementary Data 8: Final structures for the SO₄ electrolyte simulations.

Supplementary Data 9: Initial structures for the TFSI electrolyte simulations.

Supplementary Data 10: Final structures for the TFSI electrolyte simulations.

Supplementary Data 11: Initial structures for the water at the surface of NCM811 simulations.

Supplementary Data 12: Final structures for the water at the surface of NCM811 simulations.

Supplementary Data 13: Initial structures for the SO₄ at the surface of NCM811 simulations.

Supplementary Data 14: Final structures for the SO₄ at the surface of NCM811 simulations.

Supplementary Data 15: Initial structures for the TFSI at the surface of NCM811 simulations.

Supplementary Data 16: Final structures for the TFSI at the surface of NCM811 simulations.