

Description of Additional Supplementary Files

Supplementary Data 1: The initial structure of PVEC for molecular dynamics.

Supplementary Data 2: The simulated equilibrium structure of PVEC.

Supplementary Data 3: The initial structure of IWSWN-SPE for molecular dynamics.

Supplementary Data 4: The simulated equilibrium structure of IWSWN-SPE.

Supplementary Data 5: The optimized structure of VEC.

Supplementary Data 6: The optimized structure of HFBMA.

Supplementary Data 7: The optimized structure of TAP.

Supplementary Data 8: The optimized structure of PVEC-Li⁺ system.

Supplementary Data 9: The optimized structure of IWSWN-SPE-Li⁺ system.

Supplementary Data 10: The optimized structure of PVEC-TFSI⁻ system.

Supplementary Data 11: The optimized structure of IWSWN-SPE-TFSI⁻ system.