

Description of Additional Supplementary Files

Supplementary Data 1. Atomic coordinates for the optimized structure of EM calculated from DFT.

Supplementary Data 2. Atomic coordinates for the optimized structure of PM calculated from DFT.

Supplementary Data 3. Atomic coordinates for the optimized structure of BM calculated from DFT.

Supplementary Data 4. Atomic coordinates for the optimized structure of TFEM calculated from DFT.

Supplementary Data 5. Atomic coordinates for the optimized structure of TFPM calculated from DFT.

Supplementary Data 6. Atomic coordinates for the optimized structure of TFBM calculated from DFT.

Supplementary Data 7. Atomic coordinates for the optimized structure between one Li^+ and one PM molecule calculated from DFT.

Supplementary Data 8. Atomic coordinates for the optimized structure between one Li^+ and one BM molecule calculated from DFT.

Supplementary Data 9. Atomic coordinates for the optimized structure between one Li^+ and one TFPM molecule calculated from DFT.

Supplementary Data 10. Atomic coordinates for the optimized structure between one Li^+ and one TFBM molecule calculated from DFT.

Supplementary Data 11. Atomic coordinates for the optimized structure between one Li^+ and one EM molecule calculated from DFT.

Supplementary Data 12. Atomic coordinates for the optimized structure between one Li^+ and one TFEM molecule calculated from DFT.

Supplementary Data 13. Atomic coordinates for the 2 M LiFSI/PM electrolyte calculated from MD simulations.

Supplementary Data 14. Atomic coordinates for the 2 M LiFSI/BM electrolyte calculated from MD simulations.

Supplementary Data 15. Atomic coordinates for the 2 M LiFSI/TFPM electrolyte calculated from MD simulations.

Supplementary Data 16. Atomic coordinates for the 2 M LiFSI/TFBM electrolyte calculated from MD simulations.

Supplementary Data 17. Atomic coordinates for the most probable solvation structure of 2 M LiFSI/PM electrolyte from MD simulations.

Supplementary Data 18. Atomic coordinates for the most probable solvation structure of 2 M LiFSI/BM electrolyte from MD simulations.

Supplementary Data 19. Atomic coordinates for the most probable solvation structure of 2 M LiFSI/TFPM electrolyte from MD simulations.

Supplementary Data 20. Atomic coordinates for the most probable solvation structure of 2 M LiFSI/TFBM electrolyte from MD simulations.