

Description of Additional Supplementary Files

Supplementary Data 1 shows the optimized final configuration of Gaussian software for the binding energy of PTS4(N⁺)-TFSI⁻.

Supplementary Data 2 shows the optimized final configuration of Gaussian software for the binding energy of PTS4(N⁺)-TFSI⁻-Li⁺.

Supplementary Data 3 shows the optimized final configuration of Gaussian software for the binding energy of DBSA-TFSI⁻.

Supplementary Data 4 shows the optimized final configuration of Gaussian software for the binding energy of DBSA-TFSI⁻-Li⁺.

Supplementary Data 5 shows the optimized final configuration of Gaussian software for the binding energy of PTS1(N⁺)-TFSI⁻.

Supplementary Data 6 shows the optimized final configuration of Gaussian software for the binding energy of PTS1(N⁺)-TFSI⁻-Li⁺.

Supplementary Data 7 shows the optimized final configuration of Gaussian software for the binding energy of PTS8(N⁺)-TFSI⁻.

Supplementary Data 8 shows the optimized final configuration of Gaussian software for the binding energy of PTS8(N⁺)-TFSI⁻-Li⁺.

Supplementary Data 9 shows the initial configuration of Gaussian software for Li⁺ migration on the PTS4 (N⁺) chain.

Supplementary Data 10 shows the final configuration of Gaussian software for Li⁺ migration on the PTS4 (N⁺) chain.

Supplementary Data 11 shows the initial configuration of Gaussian software for Li⁺ migration on the PTS1 (N⁺) chain.

Supplementary Data 12 shows the optimized final configuration of Gaussian software for the solvation structure of PTS1(N⁺).

Supplementary Data 13 shows the optimized final configuration of Gaussian software for the solvation structure of PTS8(N⁺).

Supplementary Data 14 shows the optimized final configuration of Gaussian software for the solvation structure of PTS4(N⁺).

Supplementary Data 15 shows the optimized final configuration of Materials Studio software

for the solvation structure of $\text{Li}[(\text{TFSI})-(\text{PC})(\text{FEC})(\text{PTS4}(\text{N}+))]-$.

Supplementary Data 16 shows the optimized final configuration of Materials Studio software for the solvation structure of $\text{Li}[(\text{TFSI})-(\text{PC})(\text{FEC})]-$.

Supplementary Data 17 shows the optimized final configuration of PTS@LLZTO by Materials Studio-DMol3.

Supplementary Data 18 shows the optimized final configuration of $\text{Li}_2\text{CO}_3\text{@LLZTO}$ by Materials Studio-DMol3.

Supplementary Data 19 shows the optimized final configuration of PTS-PVHL by Materials Studio.

Supplementary Data 20 shows the optimized final configuration of PVHL by Materials Studio.

Supplementary Data 21 shows the final configuration of Gaussian software for Li^+ migration on the $\text{PTS1}(\text{N}^+)$ chain.

Supplementary Data 22 shows the initial configuration of Gaussian software for Li^+ migration on the $\text{PTS8}(\text{N}^+)$ chain.

Supplementary Data 23 shows the final configuration of Gaussian software for Li^+ migration on the $\text{PTS8}(\text{N}^+)$ chain.

Supplementary Data 24 shows the initial configuration of PVHL by Materials Studio.

Supplementary Data 25 shows the initial configuration of PTS-PVHL by Materials Studio.